Hyperparameter Tuning Cookbook

A guide for scikit-learn, PyTorch, river, and spotPython

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Preface

The goal of hyperparameter tuning (or hyperparameter optimization) is to optimize the hyperparameters to improve the performance of the machine or deep learning model.

spotPython ("Sequential Parameter Optimization Toolbox in Python") is the Python version of the well-known hyperparameter tuner SPOT, which has been developed in the R programming environment for statistical analysis for over a decade. The related open-access book is available here: Hyperparameter Tuning for Machine and Deep Learning with R—A Practical Guide.

scikit-learn is a Python module for machine learning built on top of SciPy and is distributed under the 3-Clause BSD license. The project was started in 2007 by David Cournapeau as a Google Summer of Code project, and since then many volunteers have contributed.

PyTorch is an optimized tensor library for deep learning using GPUs and CPUs.

River is a Python library for online machine learning. It is designed to be used in real-world environments, where not all data is available at once, but streaming in.

> ! Important: This book is still under development.

Citation

If this document has been useful to you and you wish to cite it in a scientific publication, please refer to the following paper, which can be found on arXiv: https://arxiv.org/abs/2305.11930.

```
@ARTICLE{bart23earxiv,
       author = {{Bartz-Beielstein}, Thomas},
        title = "{PyTorch Hyperparameter Tuning -- A Tutorial for spotPython}",
      journal = {arXiv e-prints},
     keywords = {Computer Science - Machine Learning, Computer Science - Artificial Intell
         year = 2023,
        month = may,
          eid = {arXiv:2305.11930},
```

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        pages = {arXiv:2305.11930},
          doi = {10.48550/arXiv.2305.11930},
archivePrefix = {arXiv},
       eprint = {2305.11930},
 primaryClass = {cs.LG},
       adsurl = {https://ui.adsabs.harvard.edu/abs/2023arXiv230511930B},
      adsnote = {Provided by the SAO/NASA Astrophysics Data System}
}
```

1 Introduction: Hyperparameter Tuning

Hyperparameter tuning is an important, but often difficult and computationally intensive task. Changing the architecture of a neural network or the learning rate of an optimizer can have a significant impact on the performance.

The goal of hyperparameter tuning is to optimize the hyperparameters in a way that improves the performance of the machine learning or deep learning model. The simplest, but also most computationally expensive, approach uses manual search (or trial-and-error (Meignan et al. 2015)). Commonly encountered is simple random search, i.e., random and repeated selection of hyperparameters for evaluation, and lattice search ("grid search"). In addition, methods that perform directed search and other model-free algorithms, i.e., algorithms that do not explicitly rely on a model, e.g., evolution strategies (Bartz-Beielstein et al. 2014) or pattern search (Lewis, Torczon, and Trosset 2000) play an important role. Also, "hyperband", i.e., a multi-armed bandit strategy that dynamically allocates resources to a set of random configurations and uses successive bisections to stop configurations with poor performance (Li et al. 2016), is very common in hyperparameter tuning. The most sophisticated and efficient approaches are the Bayesian optimization and surrogate model based optimization methods, which are based on the optimization of cost functions determined by simulations or experiments.

We consider below a surrogate model based optimization-based hyperparameter tuning approach based on the Python version of the SPOT ("Sequential Parameter Optimization Toolbox") (Bartz-Beielstein, Lasarczyk, and Preuss 2005), which is suitable for situations where only limited resources are available. This may be due to limited availability and cost of hardware, or due to the fact that confidential data may only be processed locally, e.g., due to legal requirements. Furthermore, in our approach, the understanding of algorithms is seen as a key tool for enabling transparency and explainability. This can be enabled, for example, by quantifying the contribution of machine learning and deep learning components (nodes, layers, split decisions, activation functions, etc.). Understanding the importance of hyperparameters and the interactions between multiple hyperparameters plays a major role in the interpretability and explainability of machine learning models. SPOT provides statistical tools for understanding hyperparameters and their interactions. Last but not least, it should be noted that the SPOT software code is available in the open source `spotPython` package on github[1], allowing replicability of the results. This tutorial descries the Python variant of SPOT, which is called

[1] https://github.com/sequential-parameter-optimization

`spotPython`. The R implementation is described in Bartz et al. (2022). SPOT is an established open source software that has been maintained for more than 15 years (Bartz-Beielstein, Lasarczyk, and Preuss 2005) (Bartz et al. 2022).

This tutorial is structured as follows. The concept of the hyperparameter tuning software `spotPython` is described in Section 1.1. Chapter 14 describes the execution of the example from the tutorial "Hyperparameter Tuning with Ray Tune" (PyTorch 2023a). The integration of `spotPython` into the `PyTorch` training workflow is described in detail in the following sections. Section 14.1 describes the setup of the tuners. Section 14.3 describes the data loading. Section 14.5 describes the model to be tuned. The search space is introduced in Section 14.5.3. Optimizers are presented in Section 14.6.1. How to split the data in train, validation, and test sets is described in Section 14.7.1. The selection of the loss function and metrics is described in Section 14.7.5. Section 14.8.1 describes the preparation of the `spotPython` call. The objective function is described in Section 14.8.2. How to use results from previous runs and default hyperparameter configurations is described in Section 14.8.3. Starting the tuner is shown in Section 14.8.4. TensorBoard can be used to visualize the results as shown in Section 14.9. Results are discussed and explained in Section 14.10. Finally, Section 14.11 presents a summary and an outlook.

> **Note**
>
> The corresponding `.ipynb` notebook (Bartz-Beielstein 2023) is updated regularly and reflects updates and changes in the `spotPython` package. It can be downloaded from https://github.com/sequential-parameter-optimization/spotPython/blob/main/notebooks/14_spot_ray_hpt_torch_cifar10.ipynb.

1.1 The Hyperparameter Tuning Software SPOT

Surrogate model based optimization methods are common approaches in simulation and optimization. SPOT was developed because there is a great need for sound statistical analysis of simulation and optimization algorithms. SPOT includes methods for tuning based on classical regression and analysis of variance techniques. It presents tree-based models such as classification and regression trees and random forests as well as Bayesian optimization (Gaussian process models, also known as Kriging). Combinations of different meta-modeling approaches are possible. SPOT comes with a sophisticated surrogate model based optimization method, that can handle discrete and continuous inputs. Furthermore, any model implemented in `scikit-learn` can be used out-of-the-box as a surrogate in `spotPython`.

SPOT implements key techniques such as exploratory fitness landscape analysis and sensitivity analysis. It can be used to understand the performance of various algorithms, while simultaneously giving insights into their algorithmic behavior. In addition, SPOT can be used as an

optimizer and for automatic and interactive tuning. Details on SPOT and its use in practice are given by Bartz et al. (2022).

A typical hyperparameter tuning process with `spotPython` consists of the following steps:

1. Loading the data (training and test datasets), see Section 14.3.
2. Specification of the preprocessing model, see Section 14.4. This model is called `prep_model` ("preparation" or pre-processing). The information required for the hyperparameter tuning is stored in the dictionary `fun_control`. Thus, the information needed for the execution of the hyperparameter tuning is available in a readable form.
3. Selection of the machine learning or deep learning model to be tuned, see Section 14.5. This is called the `core_model`. Once the `core_model` is defined, then the associated hyperparameters are stored in the `fun_control` dictionary. First, the hyperparameters of the `core_model` are initialized with the default values of the `core_model`. As default values we use the default values contained in the `spotPython` package for the algorithms of the `torch` package.
4. Modification of the default values for the hyperparameters used in `core_model`, see Section 14.6.0.1. This step is optional.
    1. numeric parameters are modified by changing the bounds.
    2. categorical parameters are modified by changing the categories ("levels").
5. Selection of target function (loss function) for the optimizer, see Section 14.7.5.
6. Calling SPOT with the corresponding parameters, see Section 14.8.4. The results are stored in a dictionary and are available for further analysis.
7. Presentation, visualization and interpretation of the results, see Section 14.10.

1.2 Spot as an Optimizer

The `spot` loop consists of the following steps:

1. Init: Build initial design X
2. Evaluate initial design on real objective f: $y = f(X)$
3. Build surrogate: $S = S(X, y)$
4. Optimize on surrogate: $X_0 = \text{optimize}(S)$
5. Evaluate on real objective: $y_0 = f(X_0)$
6. Impute (Infill) new points: $X = X \cup X_0$, $y = y \cup y_0$.
7. Got 3.

Central Idea: Evaluation of the surrogate model `S` is much cheaper (or / and much faster) than running the real-world experiment f. We start with a small example.

1.3 Example: `Spot` and the Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

1.3.1 The Objective Function: Sphere

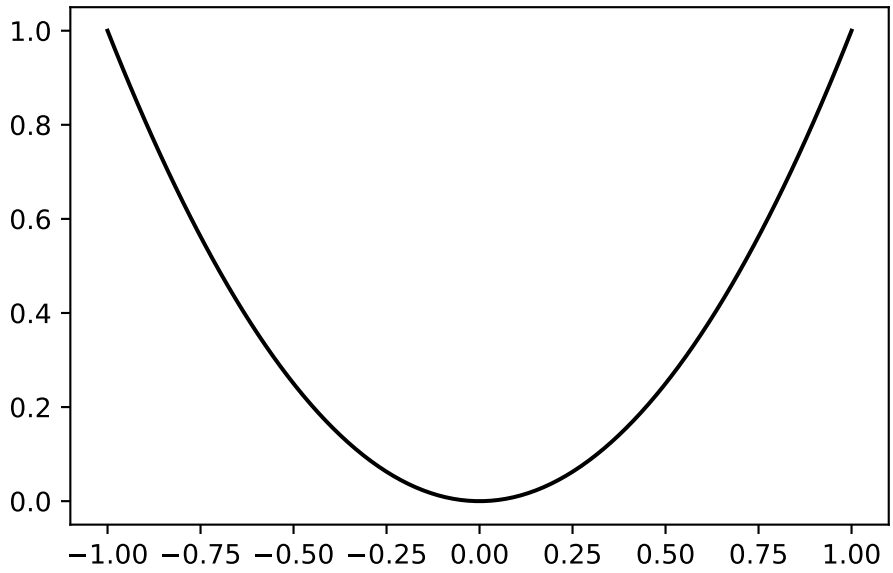
The `spotPython` package provides several classes of objective functions. We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = x^2$$

```
fun = analytical().fun_sphere
```

We can apply the function `fun` to input values and plot the result:

```
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x)
plt.figure()
plt.plot(x, y, "k")
plt.show()
```




```
spot_0 = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([1]))
```

```
spot_0.run()
```

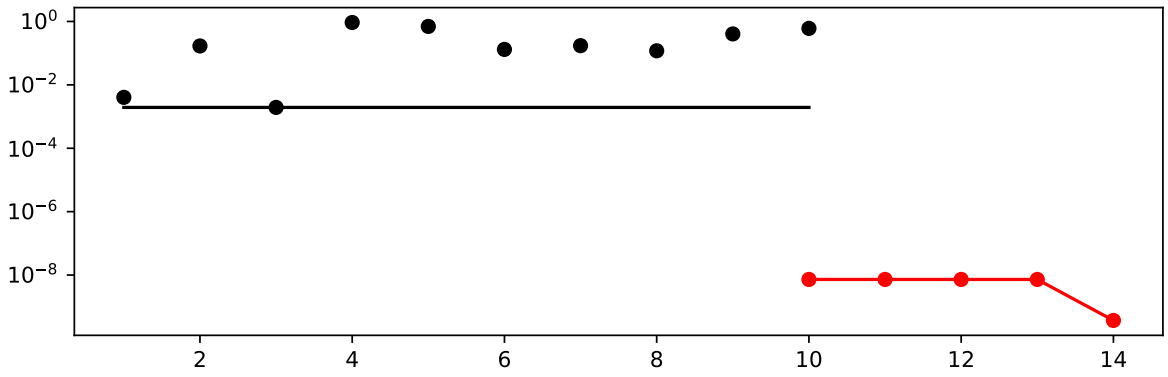
```
<spotPython.spot.spot.Spot at 0x107a5dc00>
```

```
spot_0.print_results()
```

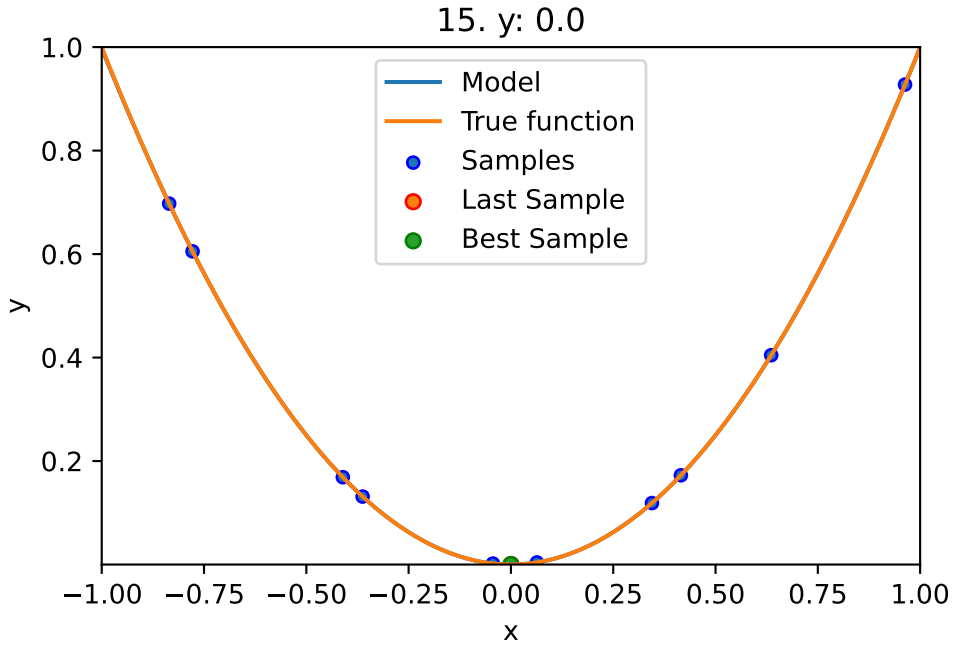
```
min y: 3.696886711914087e-10
x0: 1.922728975158508e-05

[['x0', 1.922728975158508e-05]]
```

```
spot_0.plot_progress(log_y=True)
```




```
spot_0.plot_model()
```



1.4 Spot Parameters: fun_evals, init_size and show_models

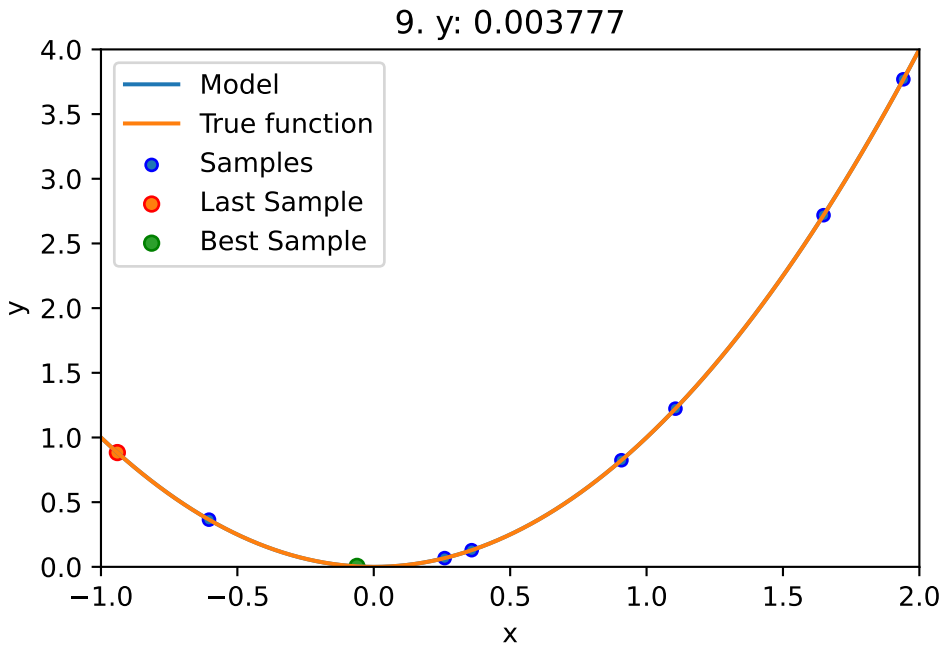
We will modify three parameters:

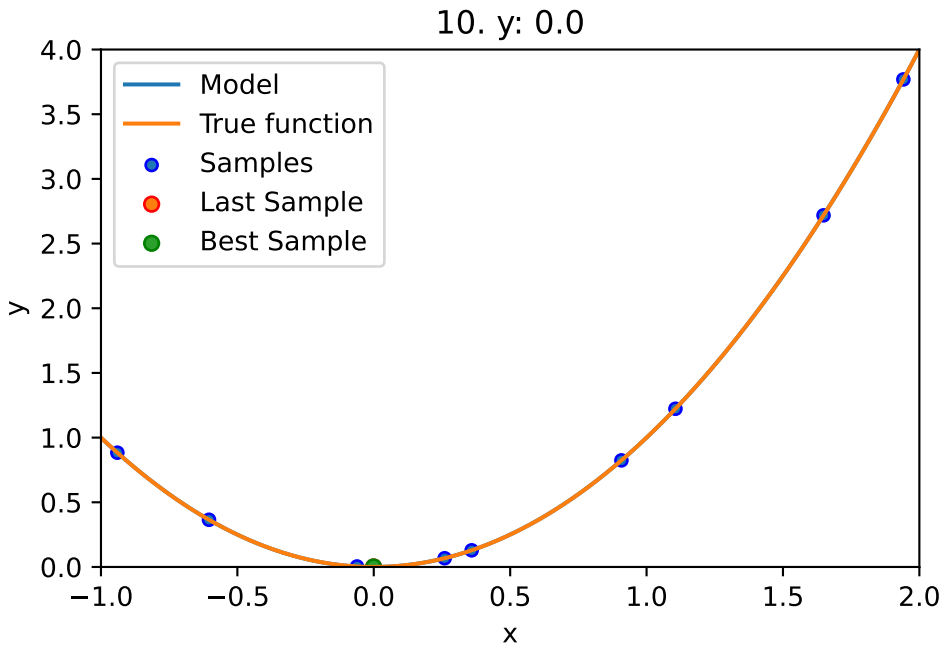
1. The number of function evaluations (`fun_evals`)
2. The size of the initial design (`init_size`)

3. The parameter `show_models`, which visualizes the search process for 1-dim functions.

The full list of the `Spot` parameters is shown in the Help System and in the notebook `spot_doc.ipynb`.

```
spot_1 = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([2]),
                   fun_evals= 10,
                   seed=123,
                   show_models=True,
                   design_control={"init_size": 9})
spot_1.run()
```






```
<spotPython.spot.spot.Spot at 0x2b00a39d0>
```

1.5 Print the Results

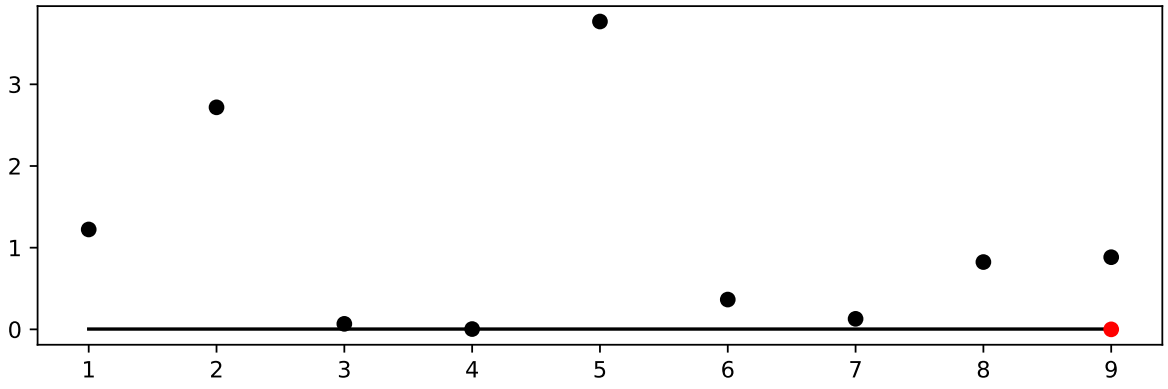
```
spot_1.print_results()
```

```
min y: 3.6779240309761575e-07
x0: -0.0006064589047063418

[['x0', -0.0006064589047063418]]
```

1.6 Show the Progress

```
spot_1.plot_progress()
```


3
2
1
0
1
2
3
4
5
6
7
8
9

2 Multi-dimensional Functions

This notebook illustrates how high-dimensional functions can be analyzed.

2.1 Example: `Spot` and the 3-dim Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
import pylab
from numpy import append, ndarray, multiply, isinf, linspace, meshgrid, ravel
from numpy import array
```

2.1.1 The Objective Function: 3-dim Sphere

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = \sum_{i}^{n} x_i^2$$

- Here we will use $n = 3$.

```
fun = analytical().fun_sphere
```

- The size of the `lower` bound vector determines the problem dimension.
- Here we will use `np.array([-1, -1, -1])`, i.e., a three-dim function.

- We will use three different `theta` values (one for each dimension), i.e., we set `surrogate_control={"n_theta": 3}`.

```
spot_3 = spot.Spot(fun=fun,
                   lower = -1.0*np.ones(3),
                   upper = np.ones(3),
                   var_name=["Pressure", "Temp", "Lambda"],
                   show_progress=True,
                   surrogate_control={"n_theta": 3})

spot_3.run()
```

```
spotPython tuning: 0.03443344056467332 [#######---] 73.33%

spotPython tuning: 0.03134865993507926 [########--] 80.00%

spotPython tuning: 0.0009629342967936851 [#########-] 86.67%

spotPython tuning: 8.541951463966474e-05 [#########-] 93.33%

spotPython tuning: 6.285135731399678e-05 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x10875d9f0>
```

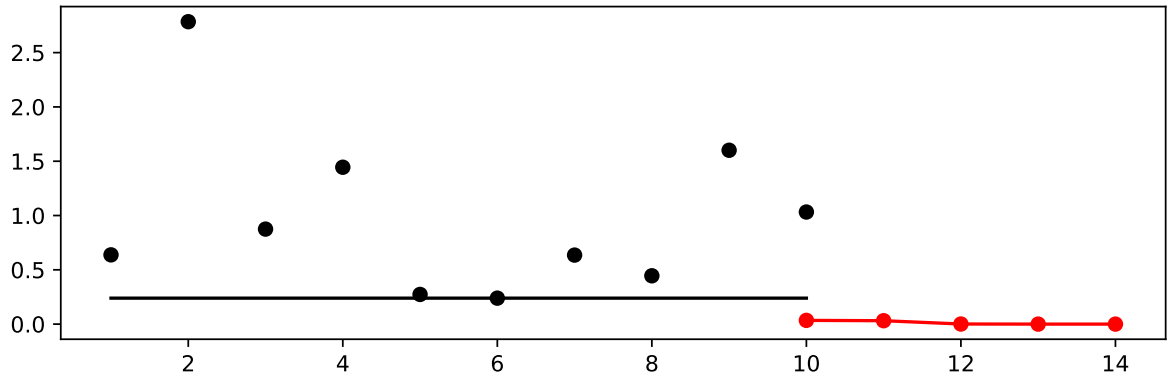
2.1.2 Results

```
spot_3.print_results()
```

```
min y: 6.285135731399678e-05
Pressure: 0.005236109709736696
Temp: 0.0019572552655686714
Lambda: 0.005621713639718905

[['Pressure', 0.005236109709736696],
 ['Temp', 0.0019572552655686714],
 ['Lambda', 0.005621713639718905]]
```

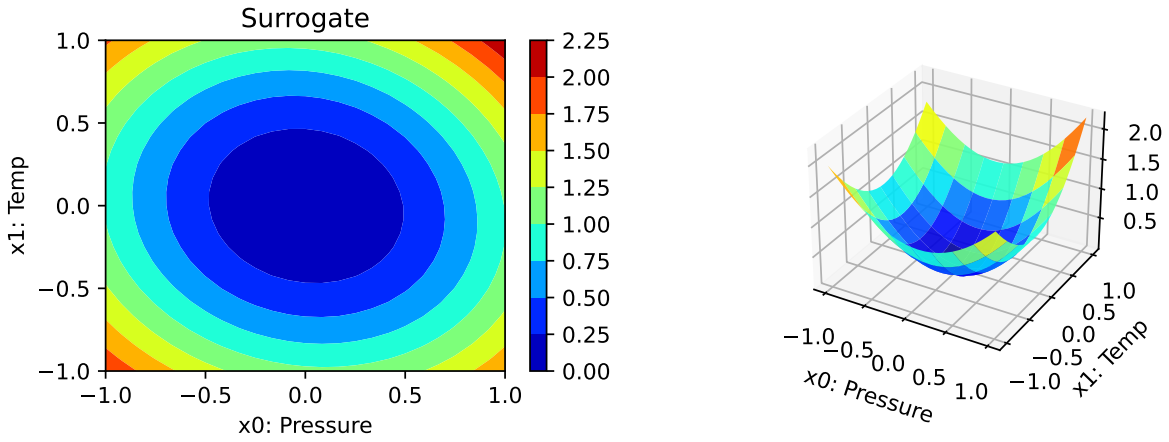
```
spot_3.plot_progress()
```



2.1.3 A Contour Plot

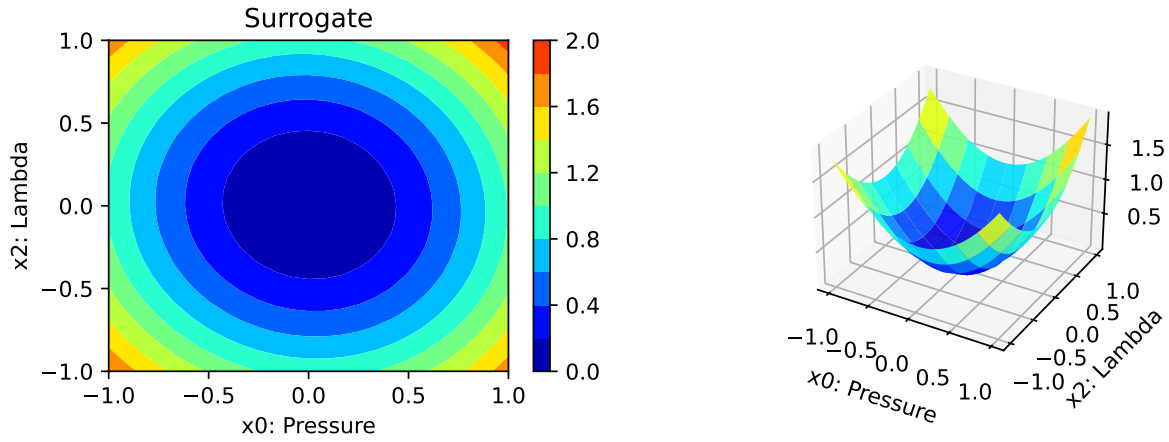
- We can select two dimensions, say $i = 0$ and $j = 1$, and generate a contour plot as follows.
  - Note: We have specified identical `min_z` and `max_z` values to generate comparable plots!

```
spot_3.plot_contour(i=0, j=1, min_z=0, max_z=2.25)
```



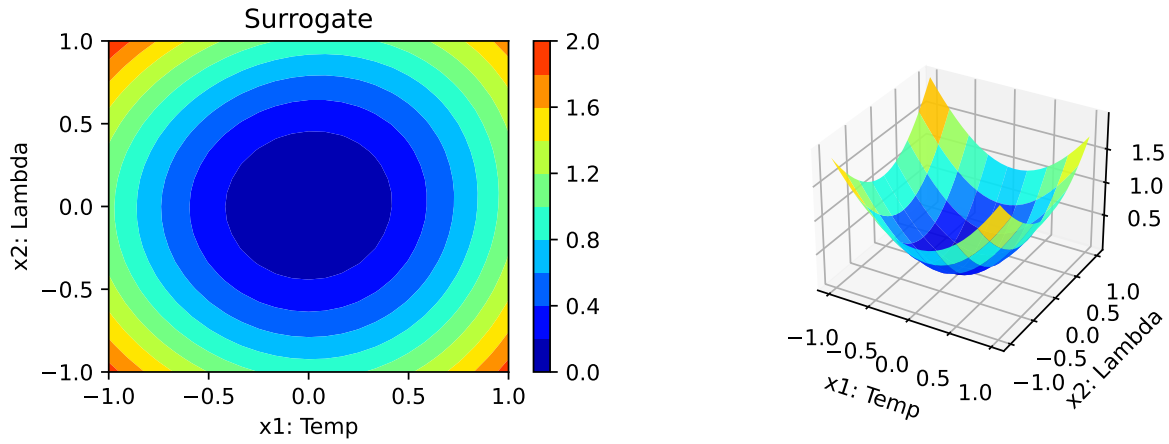
- In a similar manner, we can plot dimension $i = 0$ and $j = 2$:

```
spot_3.plot_contour(i=0, j=2, min_z=0, max_z=2.25)
```



- The final combination is $i = 1$ and $j = 2$:

```
spot_3.plot_contour(i=1, j=2, min_z=0, max_z=2.25)
```



- The three plots look very similar, because the `fun_sphere` is symmetric.
- This can also be seen from the variable importance:

```
spot_3.print_importance()
```

```
Pressure:  99.35185545837122
Temp:  99.99999999999999
```

```
Lambda:  94.31627052007231
```

```
[['Pressure', 99.35185545837122],
 ['Temp', 99.99999999999999],
 ['Lambda', 94.31627052007231]]
```

2.2 Conclusion

Based on this quick analysis, we can conclude that all three dimensions are equally important (as expected, because the analytical function is known).

2.3 Exercises

- Important:
  - Results from these exercises should be added to this document, i.e., you should submit an updated version of this notebook.
  - Please combine your results using this notebook.
  - Only one notebook from each group!
  - Presentation is based on this notebook. No addtional slides are required!
  - spotPython version `0.16.11` (or greater) is required

2.3.1 The Three Dimensional `fun_cubed`

- The input dimension is `3`. The search range is $-1 \leq x \leq 1$ for all dimensions.
- Generate contour plots
- Calculate the variable importance.
- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?

2.3.2 The Ten Dimensional `fun_wing_wt`

- The input dimension is `10`. The search range is $0 \leq x \leq 1$ for all dimensions.
- Calculate the variable importance.
- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?
  - Generate contour plots for the three most important variables. Do they confirm your selection?

2.3.3 The Three Dimensional `fun_runge`

- The input dimension is `3`. The search range is $-5 \leq x \leq 5$ for all dimensions.
- Generate contour plots
- Calculate the variable importance.
- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?

2.3.4 The Three Dimensional `fun_linear`

- The input dimension is `3`. The search range is $-5 \leq x \leq 5$ for all dimensions.
- Generate contour plots
- Calculate the variable importance.
- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?

3 Isotropic and Anisotropic Kriging

3.1 Example: Isotropic `Spot` Surrogate and the 2-dim Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

3.1.1 The Objective Function: 2-dim Sphere

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x, y) = x^2 + y^2$$

```
fun = analytical().fun_sphere
fun_control = {"sigma": 0,
               "seed": 123}
```

- The size of the `lower` bound vector determines the problem dimension.
- Here we will use `np.array([-1, -1])`, i.e., a two-dim function.

```
spot_2 = spot.Spot(fun=fun,
                   lower = np.array([-1, -1]),
                   upper = np.array([1, 1]))

spot_2.run()
```

```
<spotPython.spot.spot.Spot at 0x148c23880>
```

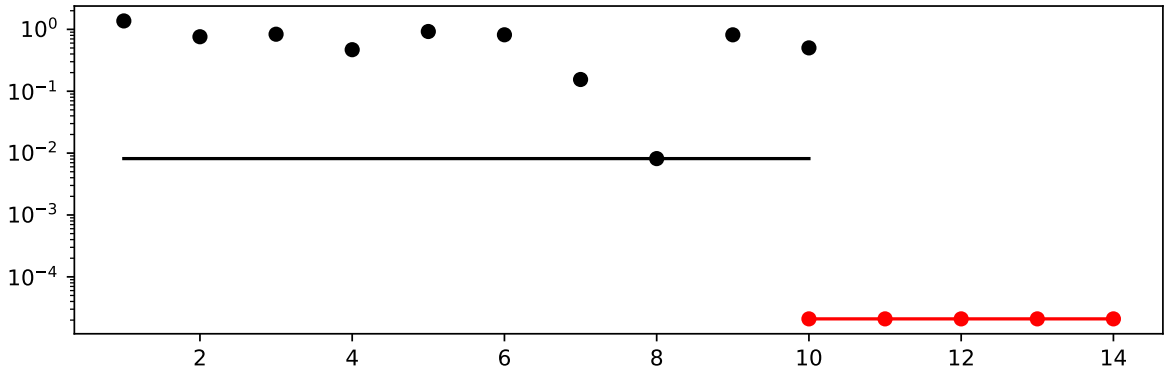
3.1.2 Results

```
spot_2.print_results()
```

```
min y: 2.093282610941807e-05
x0: 0.0016055267473267492
x1: 0.00428428640184529

[['x0', 0.0016055267473267492], ['x1', 0.00428428640184529]]
```

```
spot_2.plot_progress(log_y=True)
```



3.2 Example With Anisotropic Kriging

- The default parameter setting of `spotPython`'s Kriging surrogate uses the same `theta` value for every dimension.
- This is referred to as "using an isotropic kernel".
- If different `theta` values are used for each dimension, then an anisotropic kernel is used
- To enable anisotropic models in `spotPython`, the number of `theta` values should be larger than one.
- We can use `surrogate_control={"n_theta": 2}` to enable this behavior (2 is the problem dimension).

```
spot_2_anisotropic = spot.Spot(fun=fun,
                    lower = np.array([-1, -1]),
                    upper = np.array([1, 1]),
                    surrogate_control={"n_theta": 2})
spot_2_anisotropic.run()
```

```
<spotPython.spot.spot.Spot at 0x14ffaf6d0>
```

3.2.1 Taking a Look at the `theta` Values

- We can check, whether one or several `theta` values were used.
- The `theta` values from the surrogate can be printed as follows:

```
spot_2_anisotropic.surrogate.theta
```

```
array([0.19447342, 0.30813872])
```

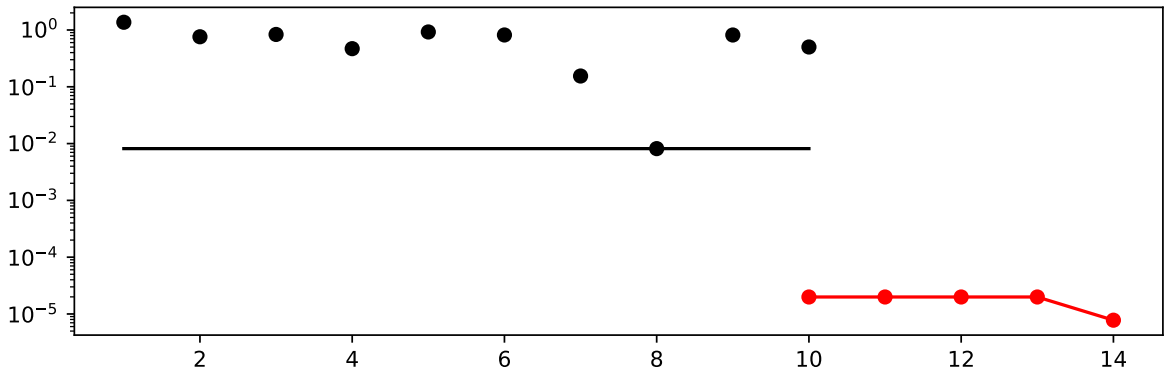
- Since the surrogate from the isotropic setting was stored as `spot_2`, we can also take a look at the `theta` value from this model:

```
spot_2.surrogate.theta
```

```
array([0.26287447])
```

- Next, the search progress of the optimization with the anisotropic model can be visualized:

```
spot_2_anisotropic.plot_progress(log_y=True)
```

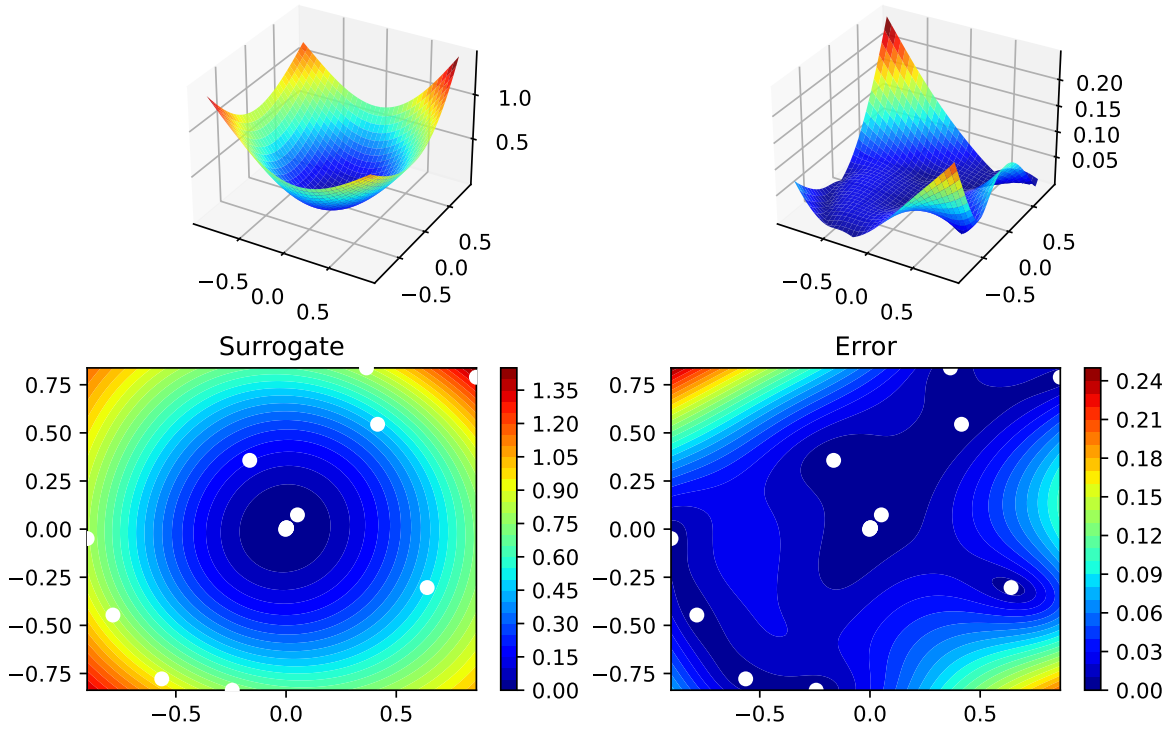


```
spot_2_anisotropic.print_results()
```

```
min y: 7.77061191821505e-06
x0: -0.0024488252797500764
x1: -0.0013318658594137815
```

```
[['x0', -0.0024488252797500764], ['x1', -0.0013318658594137815]]
```

```
spot_2_anisotropic.surrogate.plot()
```



3.3 Exercises

3.3.1 `fun_branin`

- Describe the function.
  - The input dimension is 2. The search range is $-5 \leq x_1 \leq 10$ and $0 \leq x_2 \leq 15$.

- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion: instead of the number of evaluations (which is specified via `fun_evals`), the time should be used as the termination criterion. This can be done as follows (`max_time=1` specifies a run time of one minute):

```
fun_evals=inf,
max_time=1,
```

3.3.2 `fun_sin_cos`

- Describe the function.
  - The input dimension is 2. The search range is $-2\pi \leq x_1 \leq 2\pi$ and $-2\pi \leq x_2 \leq 2\pi$.
- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion (`max_time` instead of `fun_evals`) as described for `fun_branin`.

3.3.3 `fun_runge`

- Describe the function.
  - The input dimension is 2. The search range is $-5 \leq x_1 \leq 5$ and $-5 \leq x_2 \leq 5$.
- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion (`max_time` instead of `fun_evals`) as described for `fun_branin`.

3.3.4 `fun_wingwt`

- Describe the function.
  - The input dimension is 10. The search ranges are between 0 and 1 (values are mapped internally to their natural bounds).
- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion (`max_time` instead of `fun_evals`) as described for `fun_branin`.

4 Using sklearn Surrogates in spotPython

This notebook explains how different surrogate models from `scikit-learn` can be used as surrogates in `spotPython` optimization runs.

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

4.1 Example: Branin Function with spotPython's Internal Kriging Surrogate

4.1.1 The Objective Function Branin

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula.
- Here we will use the Branin function:

  ```
  y = a * (x2 - b * x1**2 + c * x1 - r) ** 2 + s * (1 - t) * np.cos(x1) + s,
  where values of a, b, c, r, s and t are: a = 1, b = 5.1 / (4*pi**2),
  c = 5 / pi, r = 6, s = 10 and t = 1 / (8*pi).
  ```

- It has three global minima:

  ```
  f(x) = 0.397887 at (-pi, 12.275), (pi, 2.275), and (9.42478, 2.475).
  ```

```
from spotPython.fun.objectivefunctions import analytical
lower = np.array([-5,-0])
```

```
upper = np.array([10,15])
```

```
fun = analytical().fun_branin
```

4.1.2 Running the surrogate model based optimizer `Spot`:

```
spot_2 = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = 20,
                   max_time = inf,
                   seed=123,
                   design_control={"init_size": 10})
```

```
spot_2.run()
```

```
<spotPython.spot.spot.Spot at 0x104c72050>
```

4.1.3 Print the Results

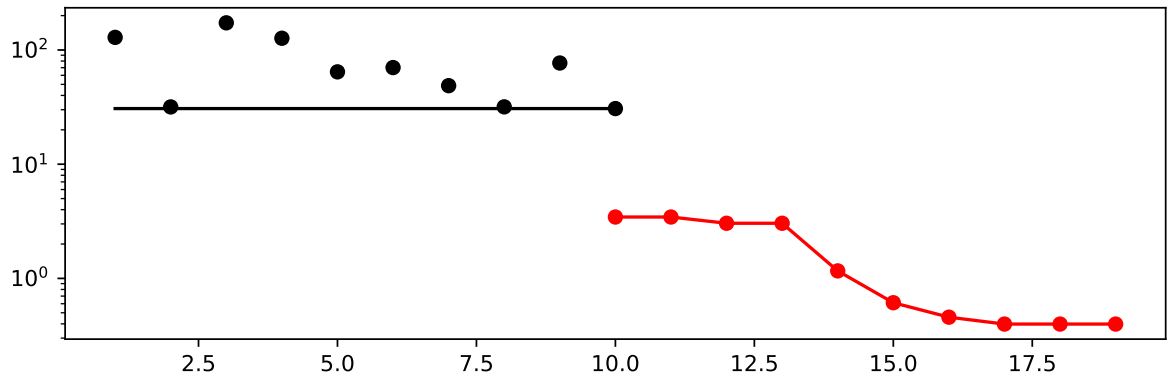
```
spot_2.print_results()
```

```
min y: 0.3982295132785083
x0: 3.135528626303215
x1: 2.2926027772585886

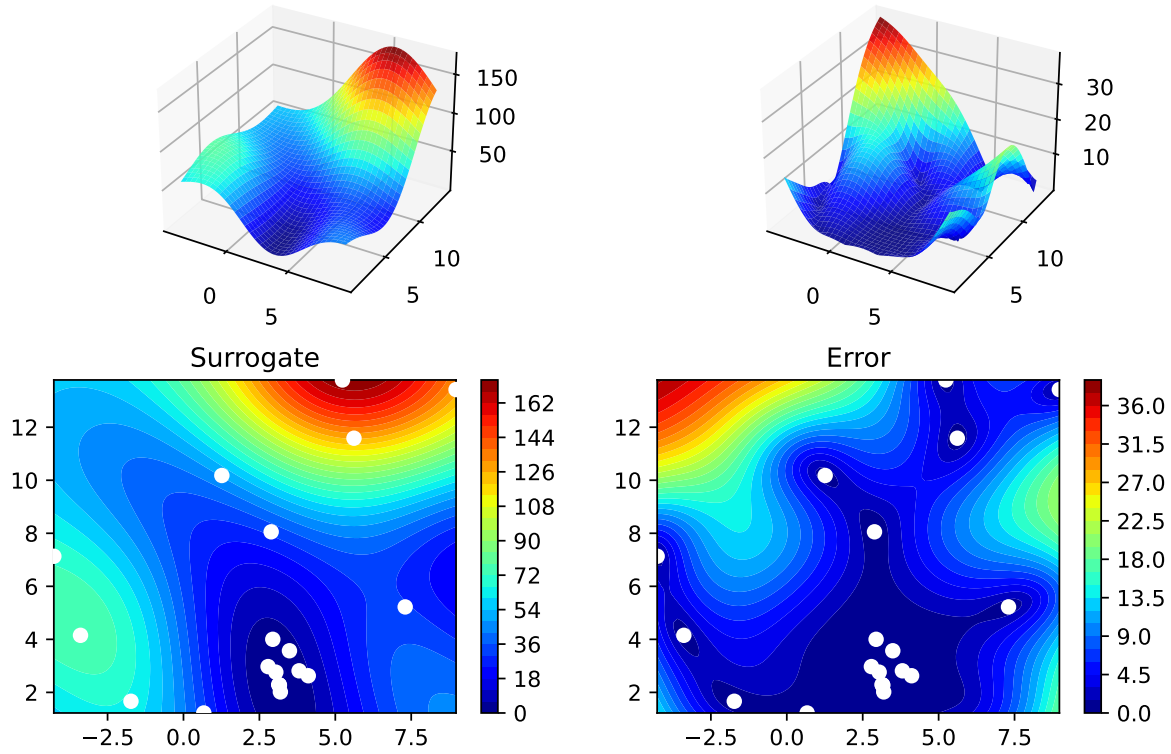
[['x0', 3.135528626303215], ['x1', 2.2926027772585886]]
```

4.1.4 Show the Progress and the Surrogate

```
spot_2.plot_progress(log_y=True)
```




```
spot_2.surrogate.plot()
```



4.2 Example: Using Surrogates From scikit-learn

- Default is the `spotPython` (i.e., the internal) `kriging` surrogate.

- It can be called explicitely and passed to `Spot`.

```
from spotPython.build.kriging import Kriging
S_0 = Kriging(name='kriging', seed=123)
```

- Alternatively, models from `scikit-learn` can be selected, e.g., Gaussian Process, RBFs, Regression Trees, etc.

```
# Needed for the sklearn surrogates:
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn import linear_model
from sklearn import tree
import pandas as pd
```

- Here are some additional models that might be useful later:

```
S_Tree = DecisionTreeRegressor(random_state=0)
S_LM = linear_model.LinearRegression()
S_Ridge = linear_model.Ridge()
S_RF = RandomForestRegressor(max_depth=2, random_state=0)
```

4.2.1 GaussianProcessRegressor as a Surrogate

- To use a Gaussian Process model from `sklearn`, that is similar to `spotPython`'s `Kriging`, we can proceed as follows:

```
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
S_GP = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
```

- The scikit-learn GP model `S_GP` is selected for `Spot` as follows:

  `surrogate = S_GP`

- We can check the kind of surogate model with the command `isinstance`:

```
isinstance(S_GP, GaussianProcessRegressor)
```

```
True
```

```
isinstance(S_0, Kriging)
```

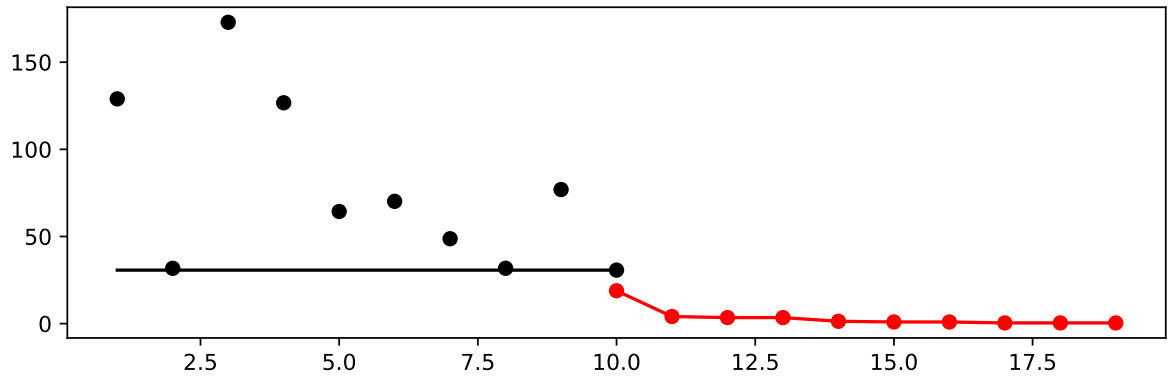
```
True
```

- Similar to the `Spot` run with the internal `Kriging` model, we can call the run with the `scikit-learn` surrogate:

```
fun = analytical(seed=123).fun_branin
spot_2_GP = spot.Spot(fun=fun,
                      lower = lower,
                      upper = upper,
                      fun_evals = 20,
                      seed=123,
                      design_control={"init_size": 10},
                      surrogate = S_GP)
spot_2_GP.run()
```

```
<spotPython.spot.spot.Spot at 0x164d637c0>
```

```
spot_2_GP.plot_progress()
```




```
spot_2_GP.print_results()
```

```
min y: 0.39821939809704077
x0: 3.14976322931894
x1: 2.272032569093181

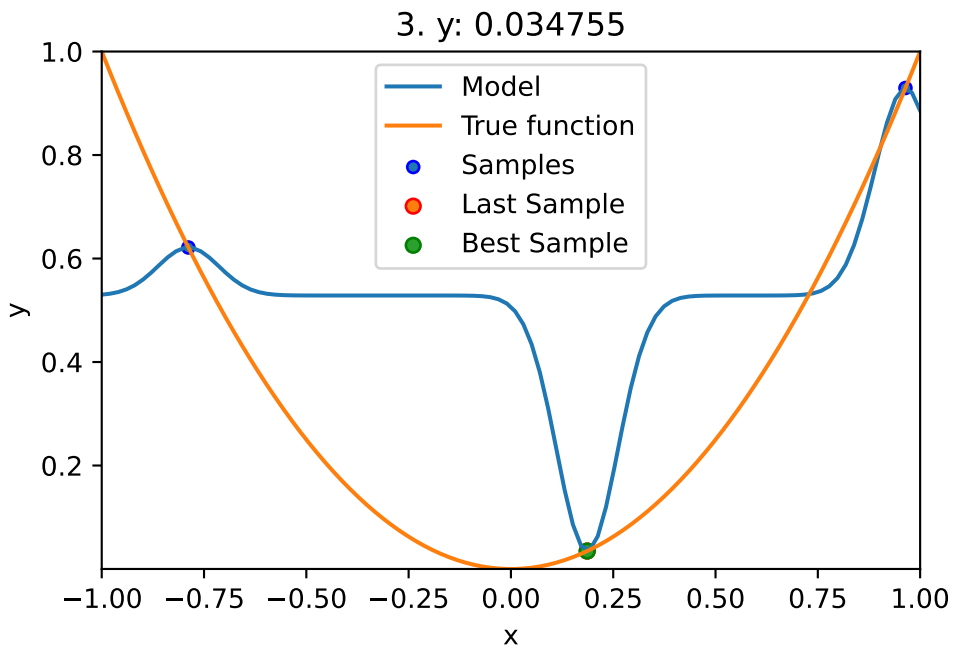
[['x0', 3.14976322931894], ['x1', 2.272032569093181]]
```

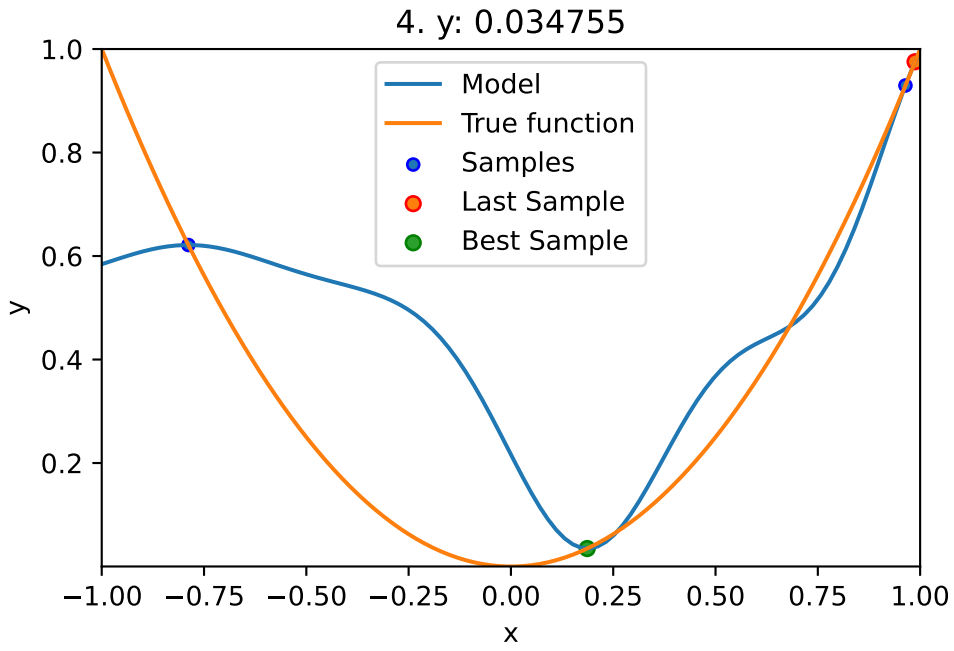
4.3 Example: One-dimensional Sphere Function With `spotPython`'s Kriging

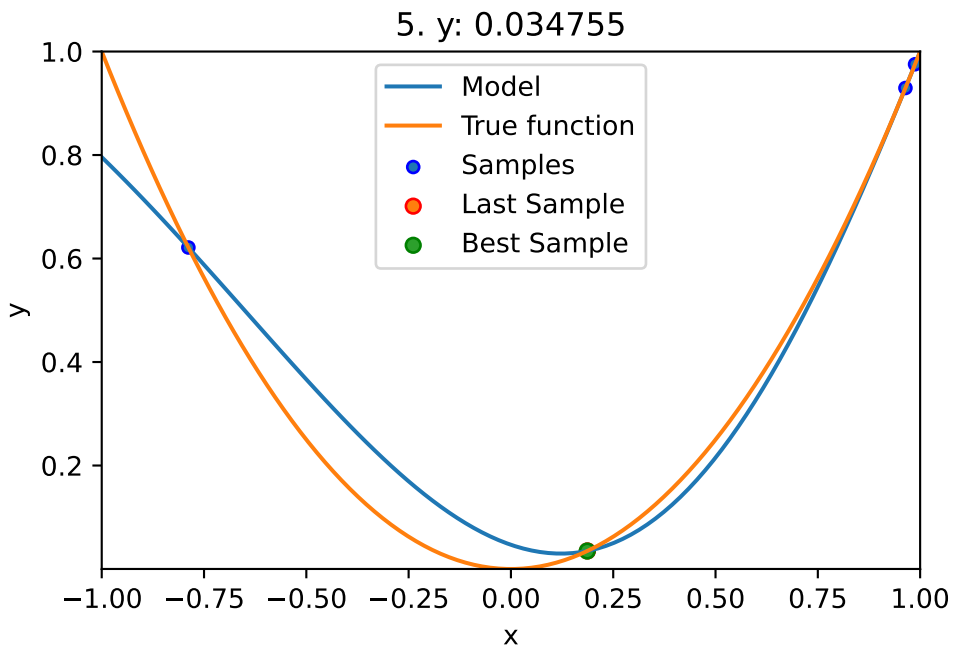
- In this example, we will use an one-dimensional function, which allows us to visualize the optimization process.
  - `show_models= True` is added to the argument list.

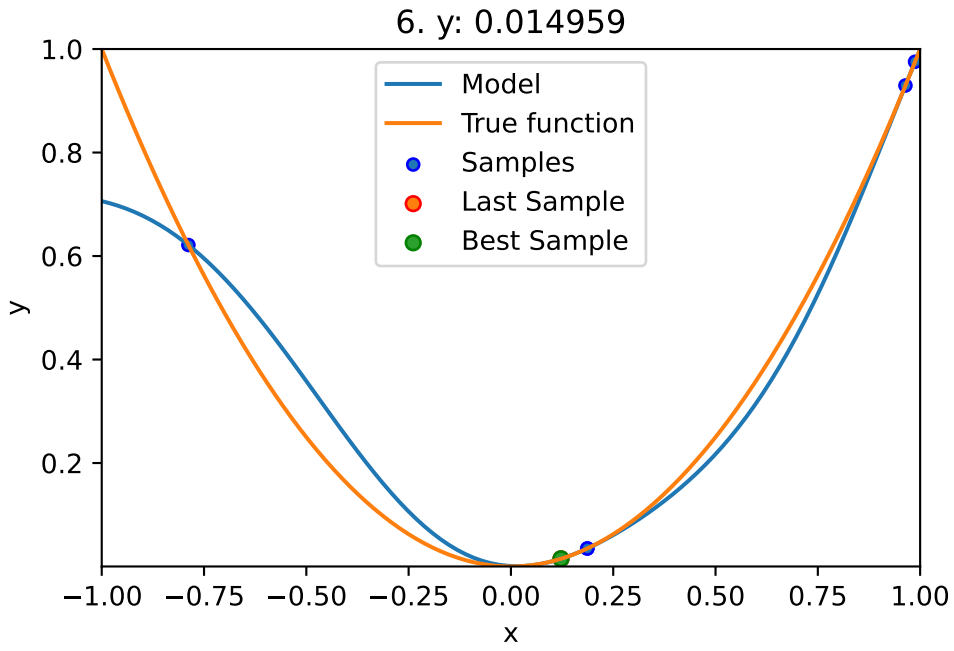
```
from spotPython.fun.objectivefunctions import analytical
lower = np.array([-1])
upper = np.array([1])
fun = analytical(seed=123).fun_sphere
```

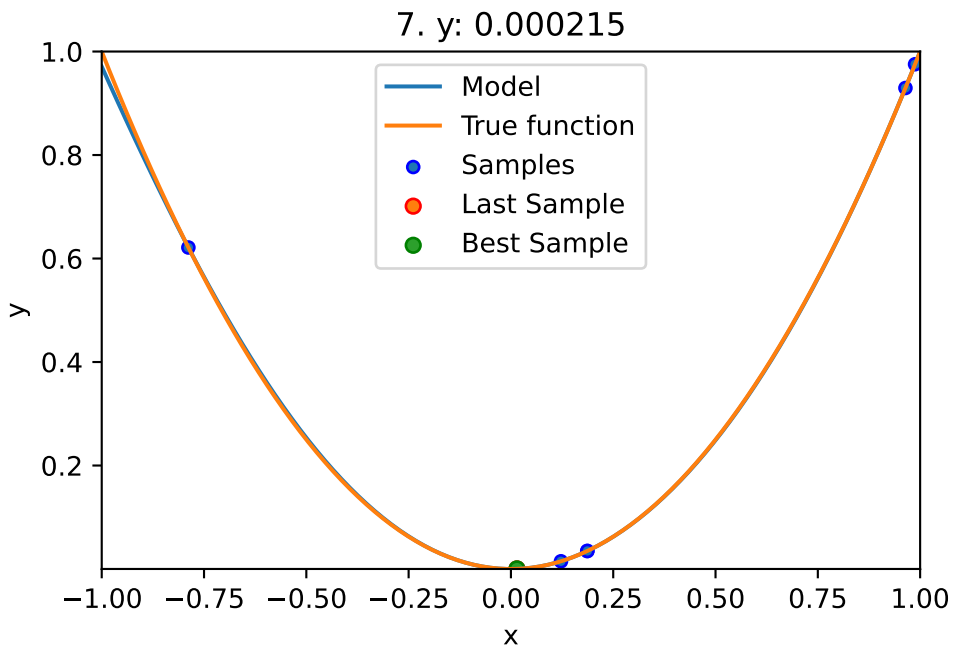
```
spot_1 = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = 10,
                   max_time = inf,
                   seed=123,
                   show_models= True,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   design_control={"init_size": 3},)
spot_1.run()
```

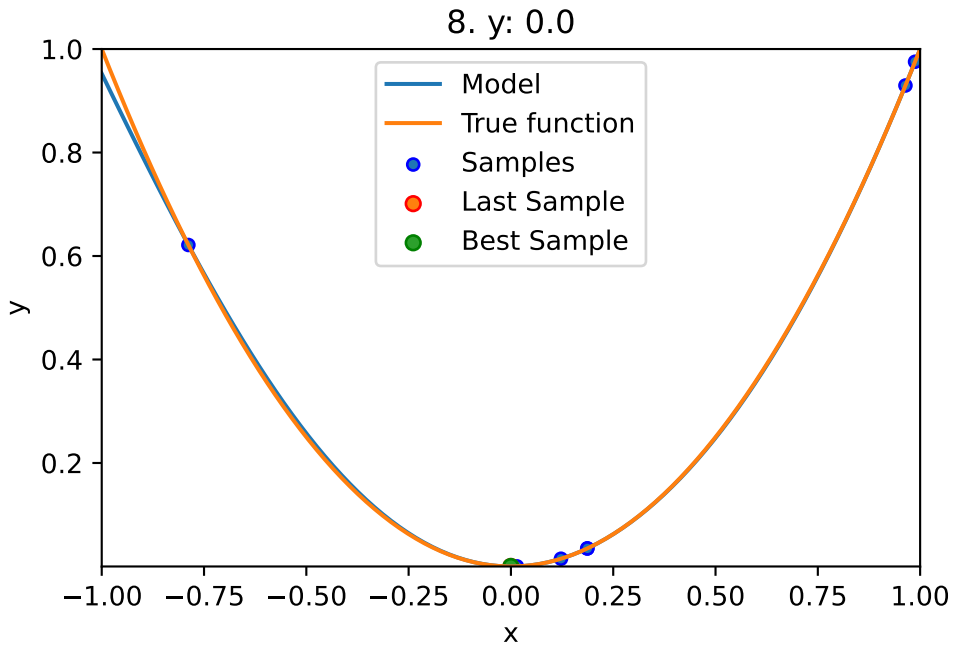

3. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

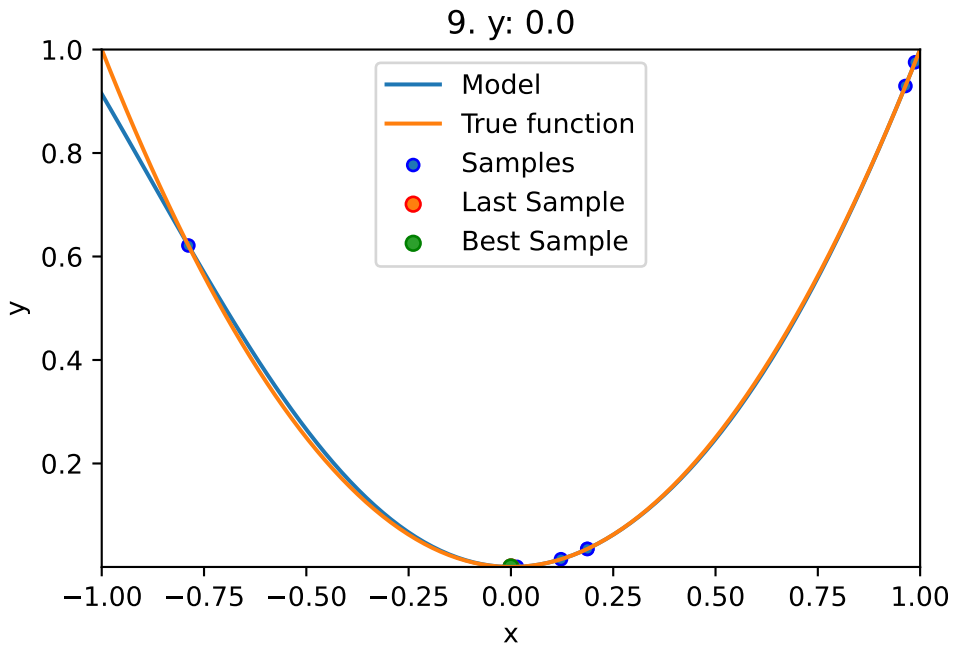

4. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

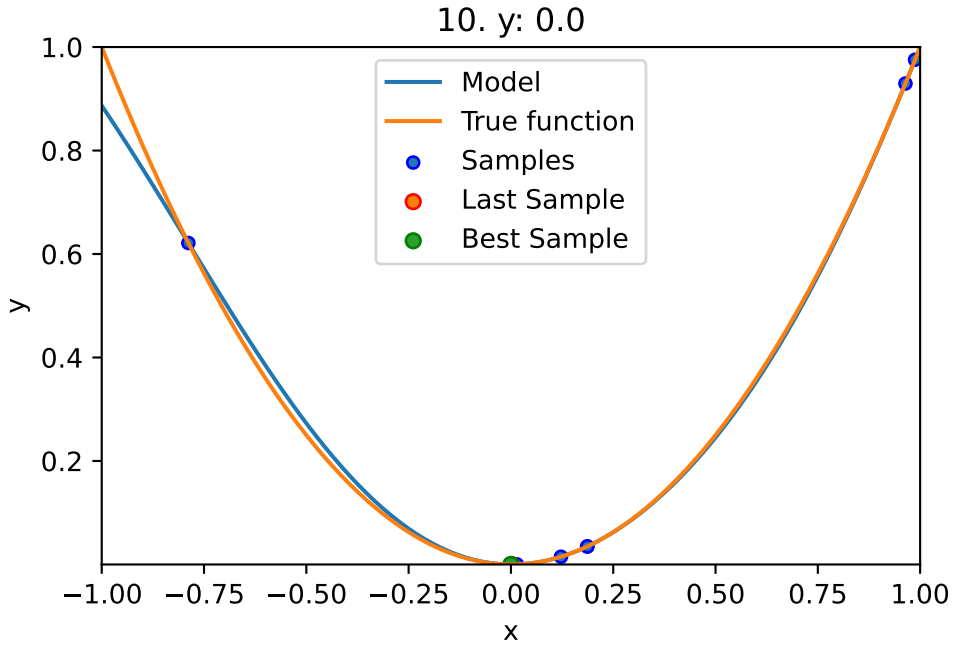

5. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


6. y: 0.014959
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


7. y: 0.000215
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


8. y: 0.0
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x






```
<spotPython.spot.spot.Spot at 0x164d63010>
```

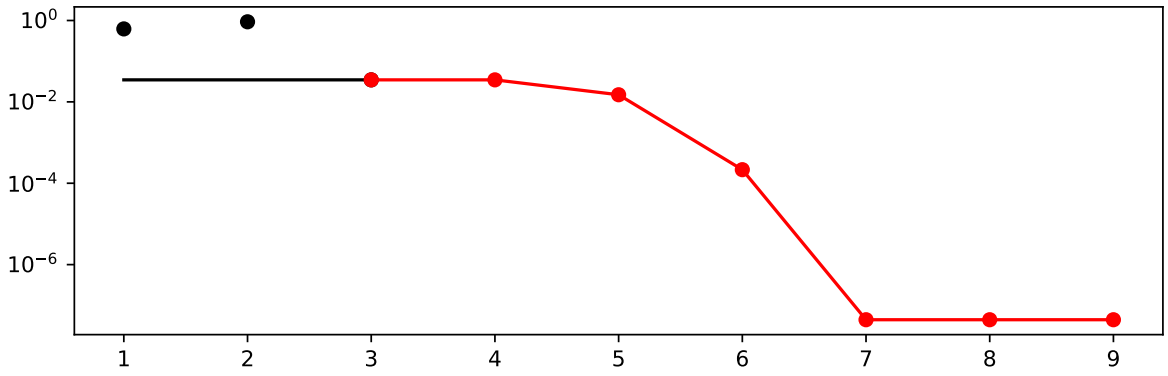
4.3.1 Results

```
spot_1.print_results()
```

```
min y: 4.41925228274096e-08
x0: -0.00021022017702259125

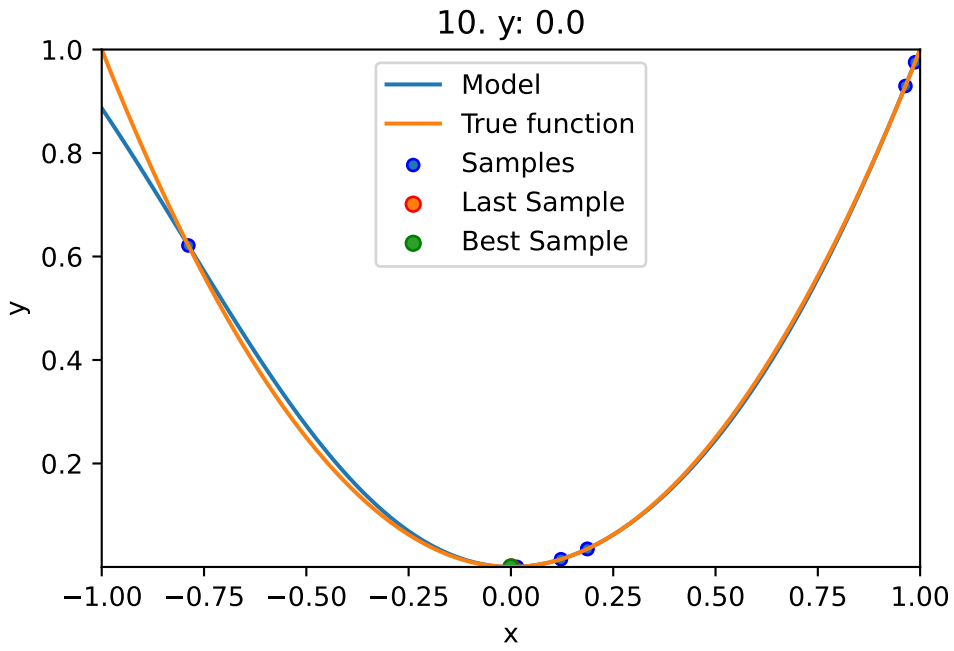
[['x0', -0.00021022017702259125]]
```

```
spot_1.plot_progress(log_y=True)
```



- The method `plot_model` plots the final surrogate:

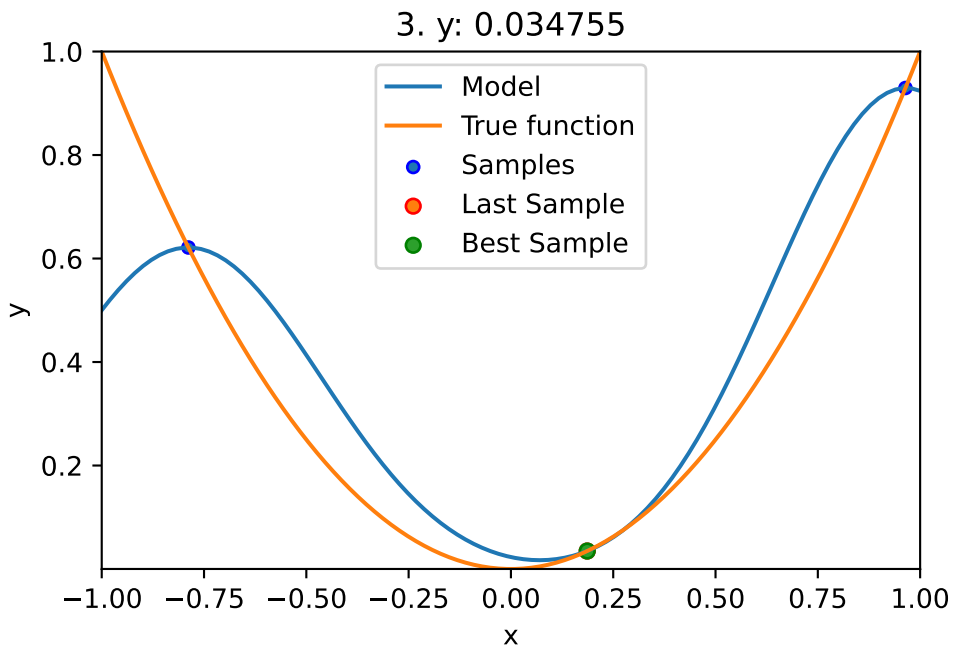
```
spot_1.plot_model()
```

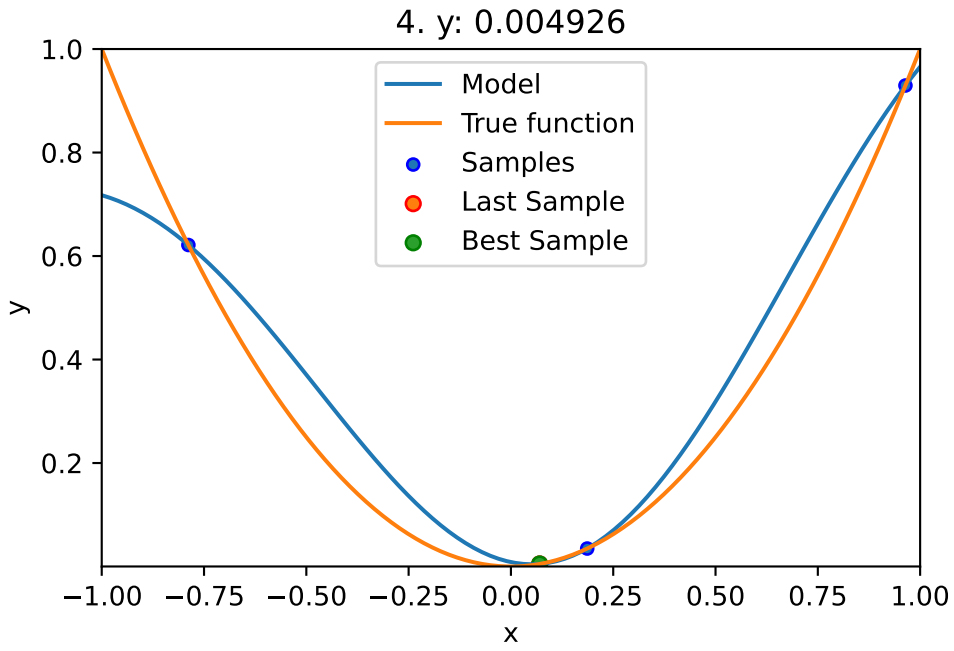


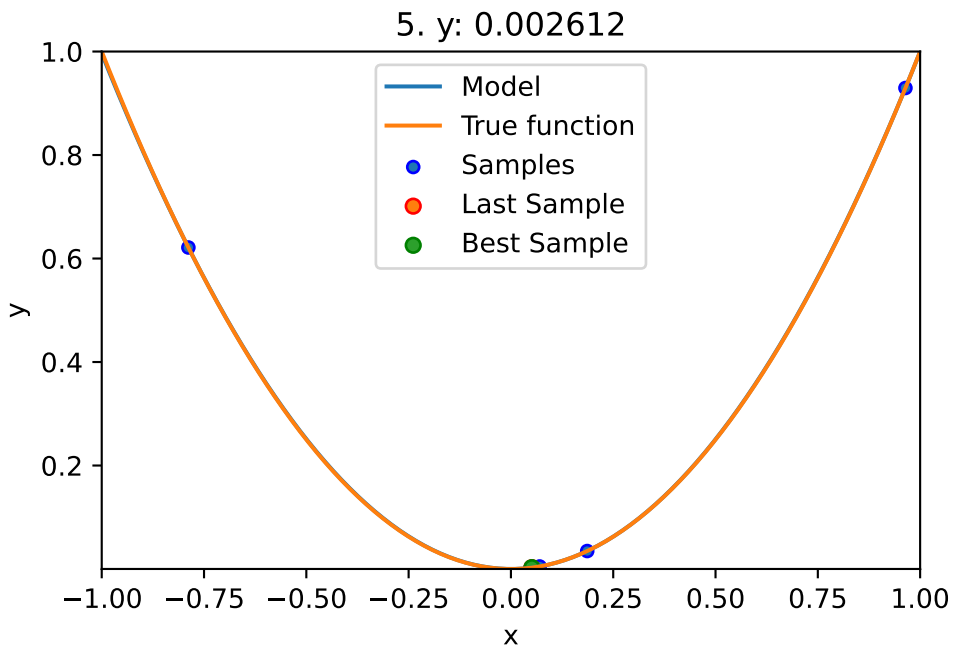
4.4 Example: `Sklearn` Model GaussianProcess

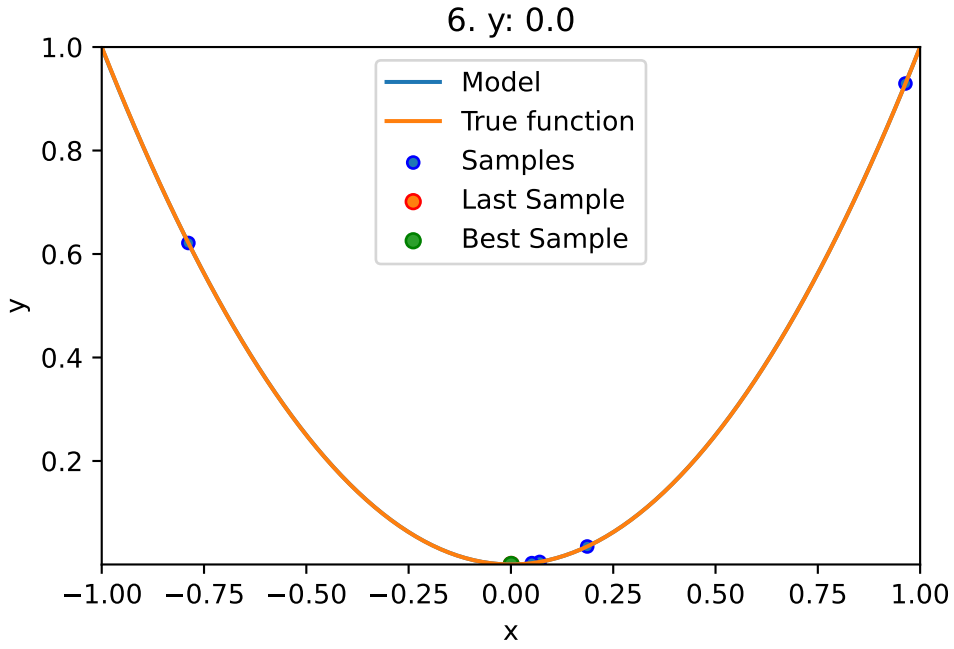
- This example visualizes the search process on the `GaussianProcessRegression` surrogate from `sklearn`.
- Therefore `surrogate = S_GP` is added to the argument list.

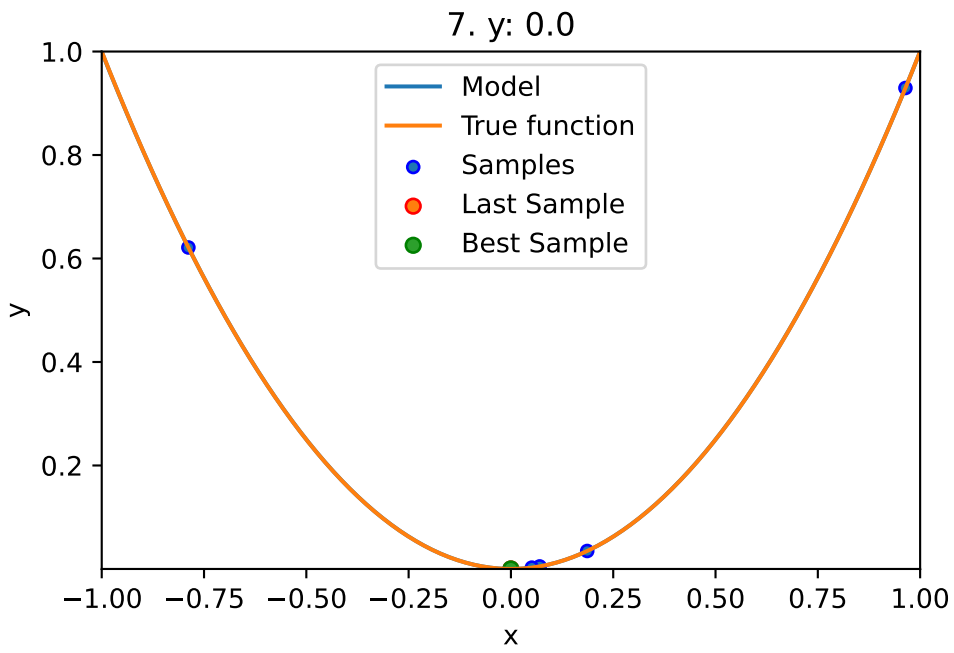
```
fun = analytical(seed=123).fun_sphere
spot_1_GP = spot.Spot(fun=fun,
                      lower = lower,
                      upper = upper,
                      fun_evals = 10,
                      max_time = inf,
                      seed=123,
                      show_models= True,
                      design_control={"init_size": 3},
                      surrogate = S_GP)
spot_1_GP.run()
```

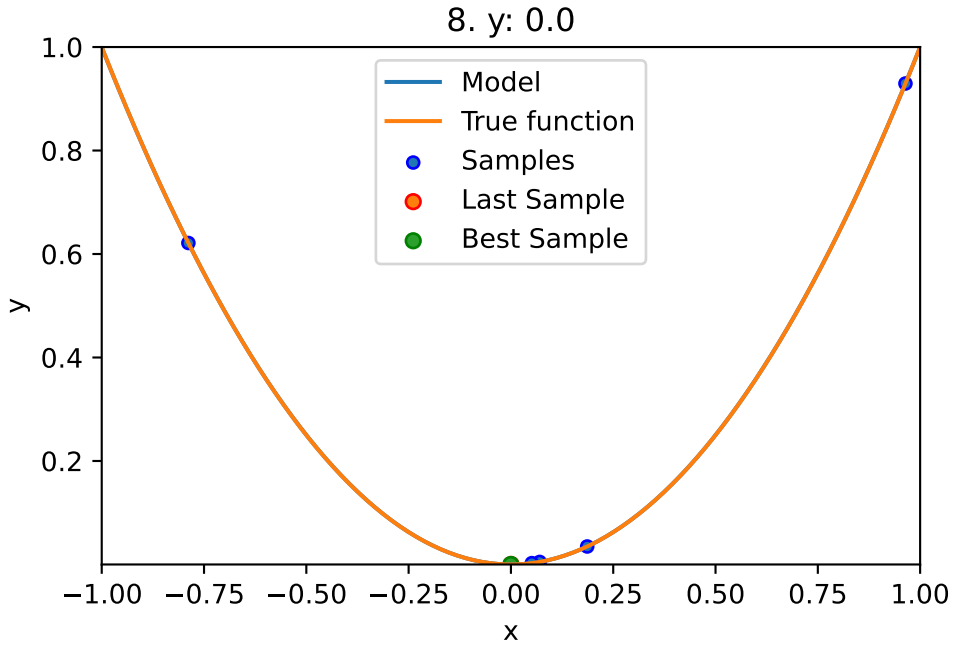

3. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

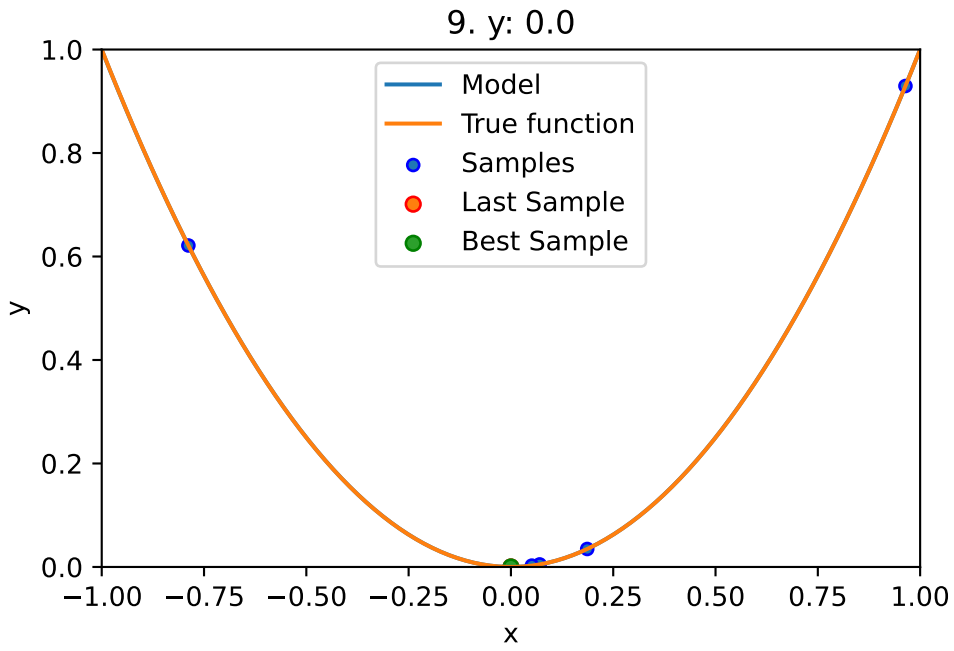

4. y: 0.004926
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

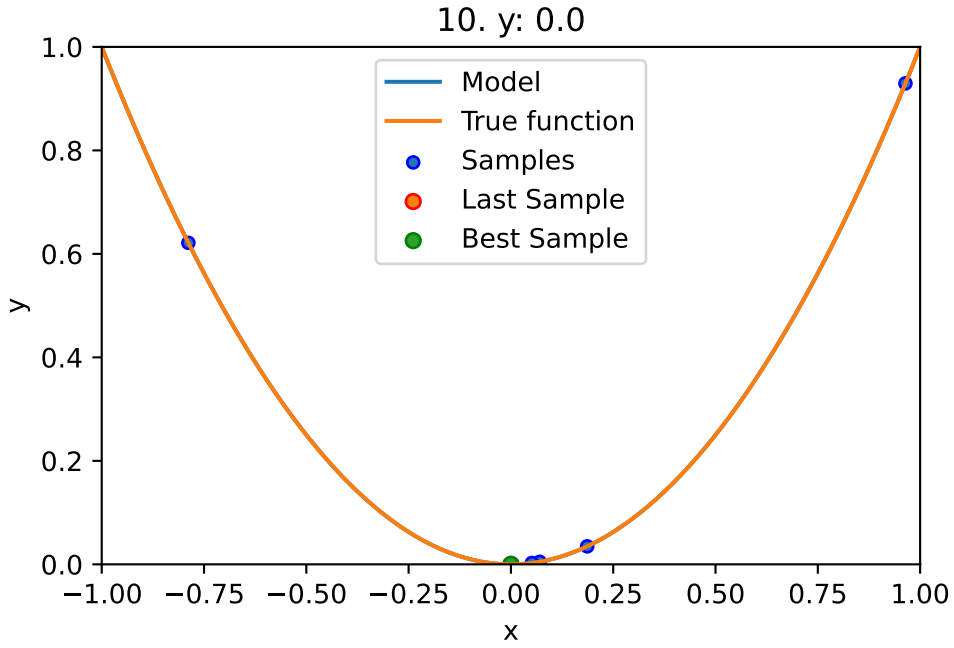

5. y: 0.002612
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


6. y: 0.0
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


7. y: 0.0
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


8. y: 0.0
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x





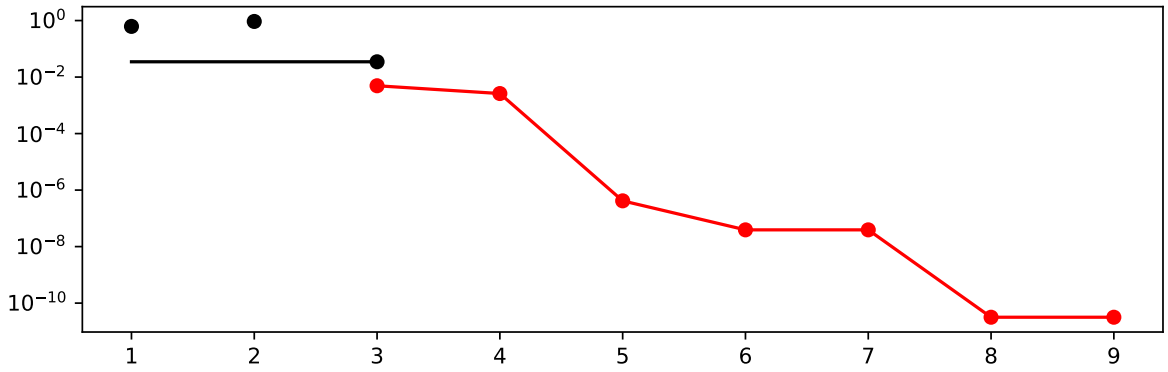

```
<spotPython.spot.spot.Spot at 0x2a05ddf00>
```

```
spot_1_GP.print_results()
```

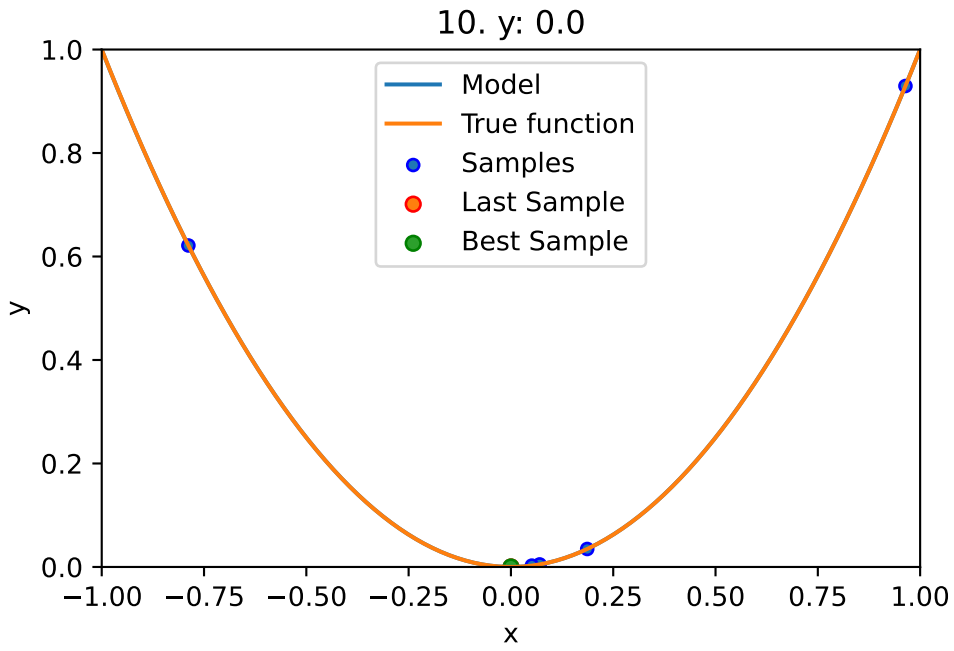
```
min y: 3.1635674949756653e-11
x0: -5.62455997832334e-06

[['x0', -5.62455997832334e-06]]
```

```
spot_1_GP.plot_progress(log_y=True)
```




```
spot_1_GP.plot_model()
```



4.5 Exercises

4.5.1 `DecisionTreeRegressor`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.5.2 `RandomForestRegressor`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.5.3 `linear_model.LinearRegression`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.5.4 `linear_model.Ridge`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.6 Exercise 2

- Compare the performance of the five different surrogates on both objective functions:
  - `spotPython`'s internal Kriging
  - `DecisionTreeRegressor`
  - `RandomForestRegressor`
  - `linear_model.LinearRegression`
  - `linear_model.Ridge`

5 Sequential Parameter Optimization: Using `scipy` Optimizers

This notebook describes how different optimizers form the `scipy optimize` package can be used on the surrogate. The optimization algorithms are available from https://docs.scipy.org/doc/scipy/reference/optimize.html

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
from scipy.optimize import dual_annealing
from scipy.optimize import basinhopping
import matplotlib.pyplot as plt
```

5.1 The Objective Function Branin

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula.
- Here we will use the Branin function. The 2-dim Branin function is

$$y = a * (x2 - b * x1 * *2 + c * x1 - r) * *2 + s * (1 - t) * cos(x1) + s,$$

where values of a, b, c, r, s and t are: $a = 1, b = 5.1/(4 * pi * *2), c = 5/pi, r = 6, s = 10$ and $t = 1/(8 * pi)$.

- It has three global minima:

$f(x) = 0.397887$ at $(-\pi, 12.275)$, $(\pi, 2.275)$, and $(9.42478, 2.475)$.

- Input Domain: This function is usually evaluated on the square x1 in [-5, 10] x x2 in [0, 15].

```
from spotPython.fun.objectivefunctions import analytical
lower = np.array([-5,-0])
upper = np.array([10,15])
```

```
fun = analytical(seed=123).fun_branin
```

5.2 The Optimizer

- Differential Evalution from the `scikit.optimize` package, see https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.differential_evolution.html#scipy.optimize.differential_evolution is the default optimizer for the search on the surrogate.
- Other optimiers that are available in `spotPython`:
  - `dual_annealing`
  - `direct`
  - `shgo`
  - `basinhopping`, see https://docs.scipy.org/doc/scipy/reference/optimize.html#global-optimization.
- These can be selected as follows:

  `surrogate_control = "model_optimizer": differential_evolution`
- We will use `differential_evolution`.
- The optimizer can use `1000` evaluations. This value will be passed to the `differential_evolution` method, which has the argument `maxiter` (int). It defines the maximum number of generations over which the entire differential evolution population is evolved, see https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.differential_evolution.html#scipy.optimize.differential_evolution

```
spot_de = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = 20,
                    max_time = inf,
                    seed=125,
                    noise=False,
```

```
                    show_models= False,
                    design_control={"init_size": 10},
                    surrogate_control={"n_theta": 2,
                                       "model_optimizer": differential_evolution,
                                       "model_fun_evals": 1000,
                                       })
spot_de.run()
```

```
<spotPython.spot.spot.Spot at 0x107a70880>
```

5.3 Print the Results

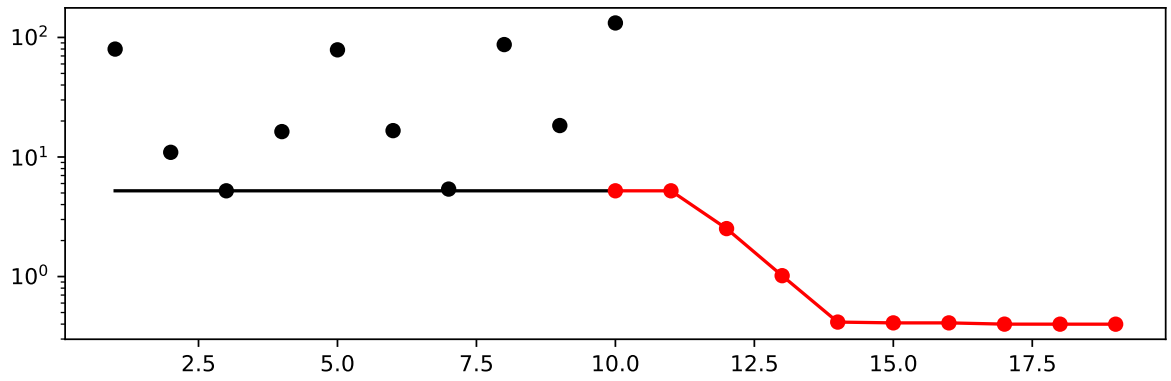
```
spot_de.print_results()
```

```
min y: 0.39951958110619046
x0: -3.1570201165683587
x1: 12.289980569430284

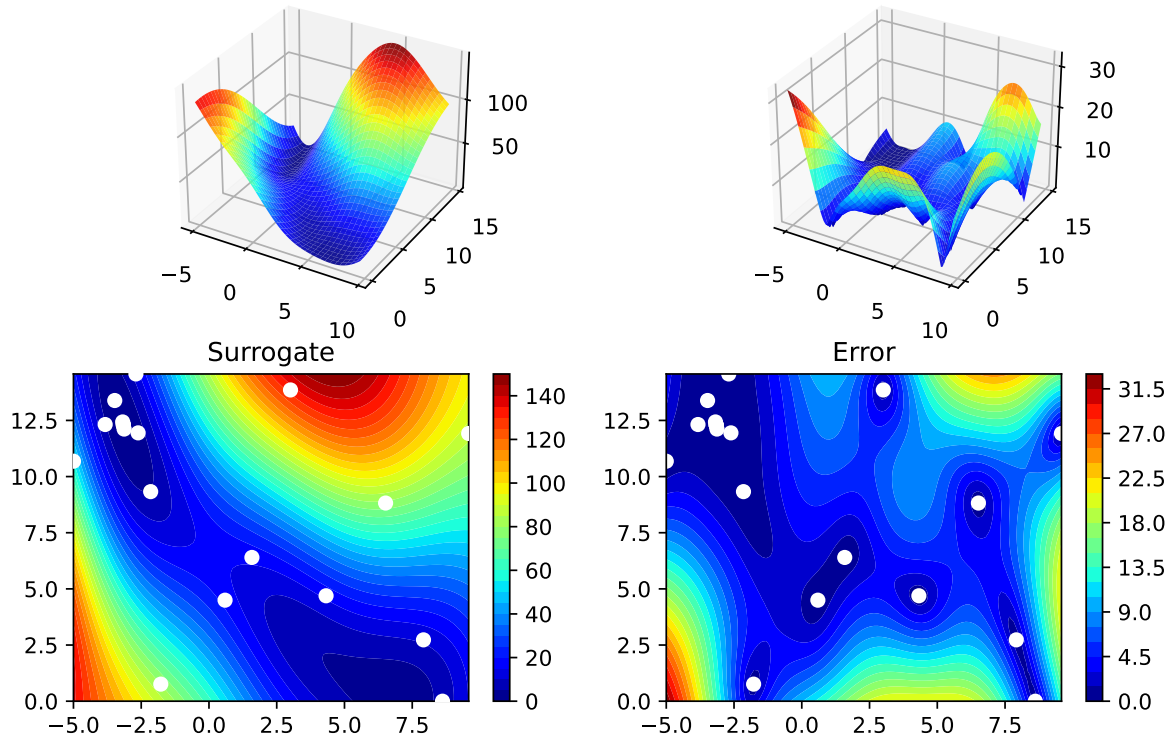
[['x0', -3.1570201165683587], ['x1', 12.289980569430284]]
```

5.4 Show the Progress

```
spot_de.plot_progress(log_y=True)
```



```
spot_de.surrogate.plot()
```



5.5 Exercises

5.5.1 `dual_annealing`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.2 `direct`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.3 `shgo`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.4 `basinhopping`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.5 Performance Comparison

Compare the performance and run time of the 5 different optimizers:

```
* `differential_evolution`
* `dual_annealing`
*  `direct`
* `shgo`
* `basinhopping`.
```

The Branin function has three global minima:

- $f(x) = 0.397887$ at
  - $(-\pi, 12.275)$,
  - $(\pi, 2.275)$, and
  - $(9.42478, 2.475)$.

- Which optima are found by the optimizers? Does the `seed` change this behavior?

6 Sequential Parameter Optimization: Gaussian Process Models

- This notebook analyzes differences between
  - the `Kriging` implementation in `spotPython` and
  - the `GaussianProcessRegressor` in `scikit-learn`.

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.design.spacefilling import spacefilling
from spotPython.spot import spot
from spotPython.build.kriging import Kriging
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
import math as m
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
```

6.1 Gaussian Processes Regression: Basic Introductory `scikit-learn` Example

- This is the example from scikit-learn: https://scikit-learn.org/stable/auto_examples/gaussian_process/pl
- After fitting our model, we see that the hyperparameters of the kernel have been optimized.
- Now, we will use our kernel to compute the mean prediction of the full dataset and plot the 95% confidence interval.

6.1.1 Train and Test Data

```
X = np.linspace(start=0, stop=10, num=1_000).reshape(-1, 1)
y = np.squeeze(X * np.sin(X))
rng = np.random.RandomState(1)
training_indices = rng.choice(np.arange(y.size), size=6, replace=False)
X_train, y_train = X[training_indices], y[training_indices]
```

6.1.2 Building the Surrogate With `Sklearn`

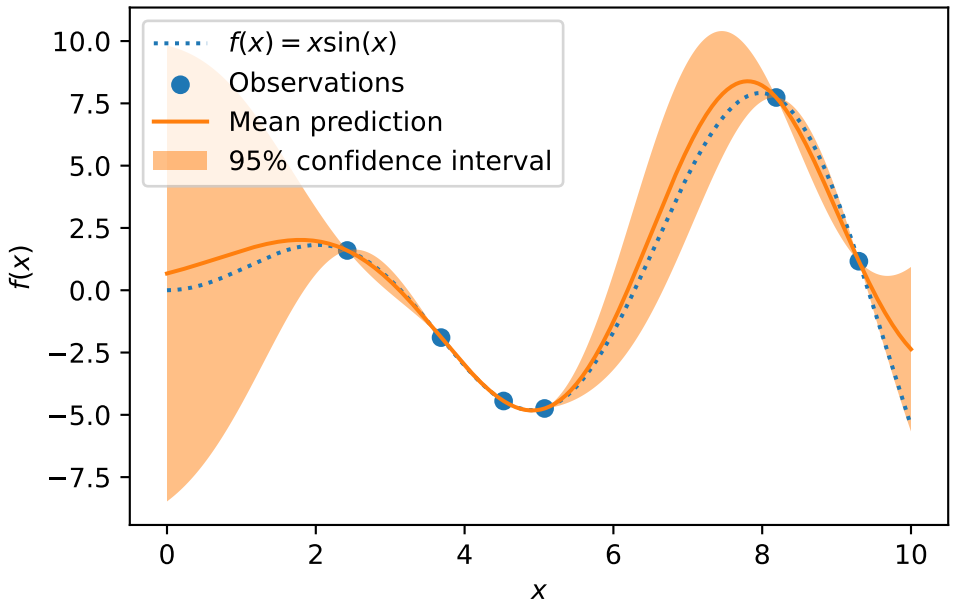
- The model building with `sklearn` consisits of three steps:
    1. Instantiating the model, then
    2. fitting the model (using `fit`), and
    3. making predictions (using `predict`)

```
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
gaussian_process = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gaussian_process.fit(X_train, y_train)
mean_prediction, std_prediction = gaussian_process.predict(X, return_std=True)
```

6.1.3 Plotting the `Sklearn`Model

```
plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
    mean_prediction - 1.96 * std_prediction,
    mean_prediction + 1.96 * std_prediction,
    alpha=0.5,
    label=r"95% confidence interval",
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("sk-learn Version: Gaussian process regression on noise-free dataset")
```

sk-learn Version: Gaussian process regression on noise-free dataset



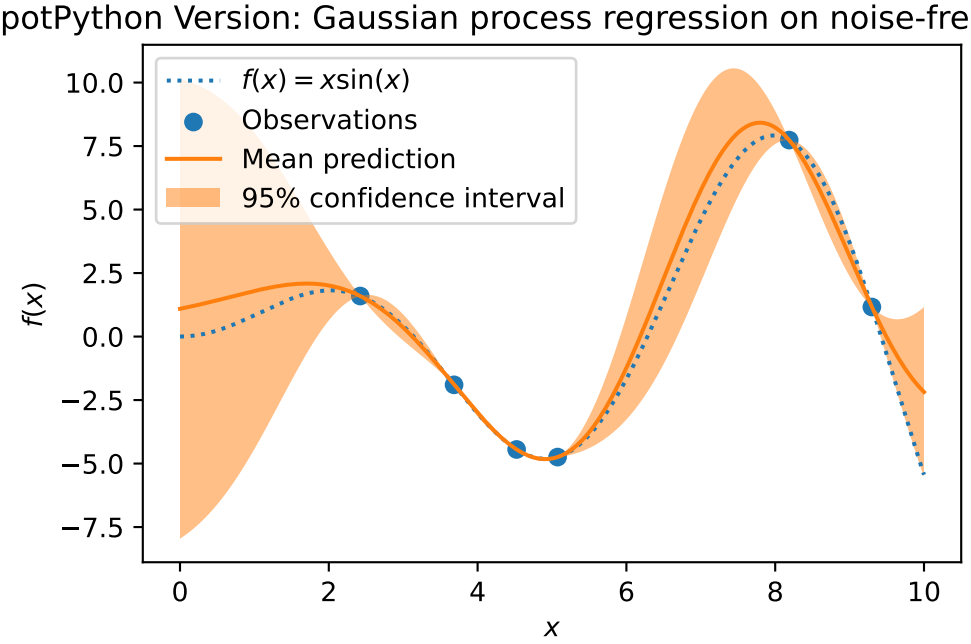
6.1.4 The `spotPython` Version

- The `spotPython` version is very similar:
  1. Instantiating the model, then
  2. fitting the model and
  3. making predictions (using `predict`).

```
S = Kriging(name='kriging',  seed=123, log_level=50, cod_type="norm")
S.fit(X_train, y_train)
S_mean_prediction, S_std_prediction, S_ei = S.predict(X, return_val="all")
```

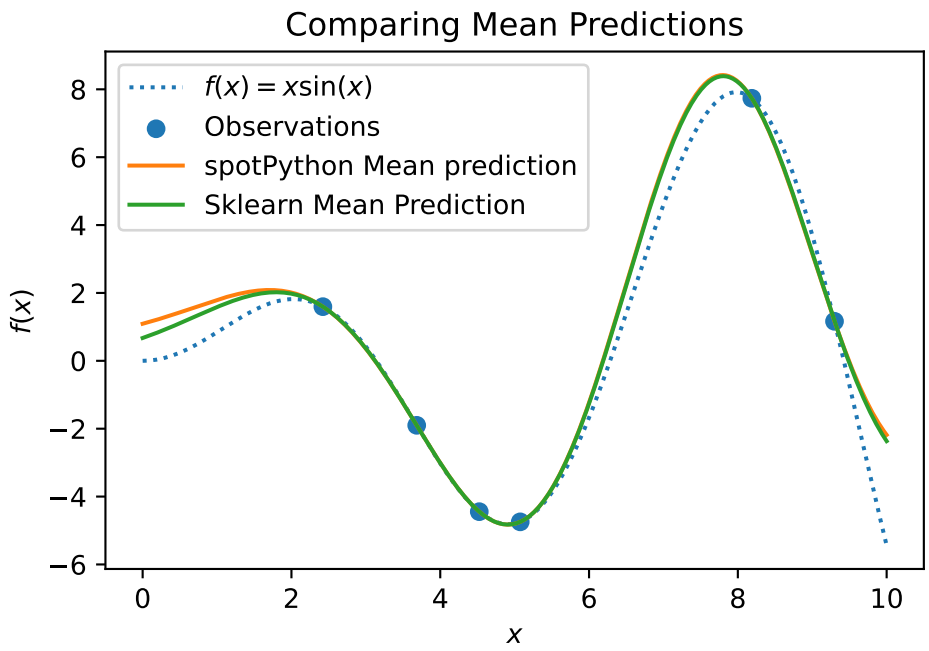
```
plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, S_mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
    S_mean_prediction - 1.96 * S_std_prediction,
    S_mean_prediction + 1.96 * S_std_prediction,
    alpha=0.5,
    label=r"95% confidence interval",
```

```
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("spotPython Version: Gaussian process regression on noise-free dataset")
```



6.1.5 Visualizing the Differences Between the `spotPython` and the `sklearn` Model Fits

```
plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, S_mean_prediction, label="spotPython Mean prediction")
plt.plot(X, mean_prediction, label="Sklearn Mean Prediction")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Comparing Mean Predictions")
```



6.2 Exercises

6.2.1 `Schonlau Example Function`

- The Schonlau Example Function is based on sample points only (there is no analytical function description available):

```
X = np.linspace(start=0, stop=13, num=1_000).reshape(-1, 1)
X_train = np.array([1., 2., 3., 4., 12.]).reshape(-1,1)
y_train = np.array([0., -1.75, -2, -0.5, 5.])
```

- Describe the function.
- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Since there is no analytical function available, you might be interested in adding some points and describe the effects.

6.2.2 `Forrester Example Function`

- The Forrester Example Function is defined as follows:

f(x) = (6x- 2)^2 sin(12x-4) for x in [0,1].

- Data points are generated as follows:

```
X = np.linspace(start=-0.5, stop=1.5, num=1_000).reshape(-1, 1)
X_train = np.array([0.0, 0.175, 0.225, 0.3, 0.35, 0.375, 0.5,1]).reshape(-1,1)
fun = analytical().fun_forrester
fun_control = {"sigma": 0.1,
               "seed": 123}
y = fun(X, fun_control=fun_control)
y_train = fun(X_train, fun_control=fun_control)
```

- Describe the function.
- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Modify the noise level (`"sigma"`), e.g., use a value of `0.2`, and compare the two models.

```
fun_control = {"sigma": 0.2}
```

6.2.3 `fun_runge` Function (1-dim)

- The Runge function is defined as follows:

  f(x) = 1/ (1 + sum(x_i))^2

- Data points are generated as follows:

```
gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = {"sigma": 0.025,
               "seed": 123}
X_train = gen.scipy_lhd(10, lower=lower, upper = upper).reshape(-1,1)
y_train = fun(X, fun_control=fun_control)
X = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
y = fun(X, fun_control=fun_control)
```

- Describe the function.

- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Modify the noise level (`"sigma"`), e.g., use a value of `0.05`, and compare the two models.

```
fun_control = {"sigma": 0.5}
```

6.2.4 `fun_cubed (1-dim)`

- The Cubed function is defined as follows:

  `np.sum(X[i]** 3)`

- Data points are generated as follows:

```
gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_cubed
fun_control = {"sigma": 0.025,
               "seed": 123}
X_train = gen.scipy_lhd(10, lower=lower, upper = upper).reshape(-1,1)
y_train = fun(X, fun_control=fun_control)
X = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
y = fun(X, fun_control=fun_control)
```

- Describe the function.
- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Modify the noise level (`"sigma"`), e.g., use a value of `0.05`, and compare the two models.

```
fun_control = {"sigma": 0.05}
```

6.2.5 The Effect of Noise

How does the behavior of the `spotPython` fit changes when the argument `noise` is set to `True`, i.e.,

```
S = Kriging(name='kriging',  seed=123, n_theta=1, noise=True)
```

is used?

7 Expected Improvement

7.1 Example: `Spot` and the 1-dim Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

7.1.1 The Objective Function: 1-dim Sphere

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = x^2$$

```
fun = analytical().fun_sphere
```

```
fun = analytical().fun_sphere
fun_control = {"sigma": 0,
               "seed": 123}
```

- The size of the `lower` bound vector determines the problem dimension.
- Here we will use `np.array([-1])`, i.e., a one-dim function.

```
spot_1 = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([1]))
```

```
spot_1.run()
```

```
<spotPython.spot.spot.Spot at 0x15a763b50>
```

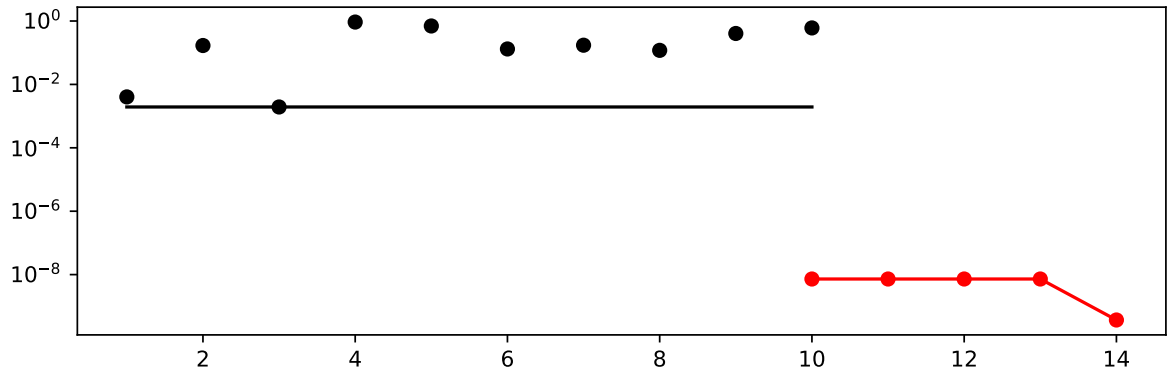
7.1.2 Results

```
spot_1.print_results()
```

```
min y: 3.696886711914087e-10
x0: 1.922728975158508e-05

[['x0', 1.922728975158508e-05]]
```

```
spot_1.plot_progress(log_y=True)
```

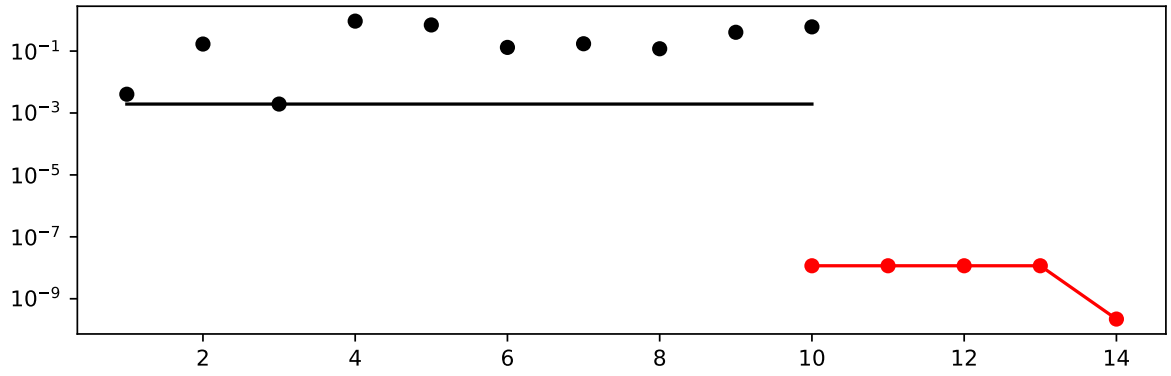


7.2 Same, but with EI as infill_criterion

```
spot_1_ei = spot.Spot(fun=fun,
                    lower = np.array([-1]),
                    upper = np.array([1]),
                    infill_criterion = "ei")
spot_1_ei.run()
```

```
<spotPython.spot.spot.Spot at 0x15fee73d0>
```

```
spot_1_ei.plot_progress(log_y=True)
```




```
spot_1_ei.print_results()
```

```
min y: 2.207887258868953e-10
x0: 1.4858961130809088e-05

[['x0', 1.4858961130809088e-05]]
```

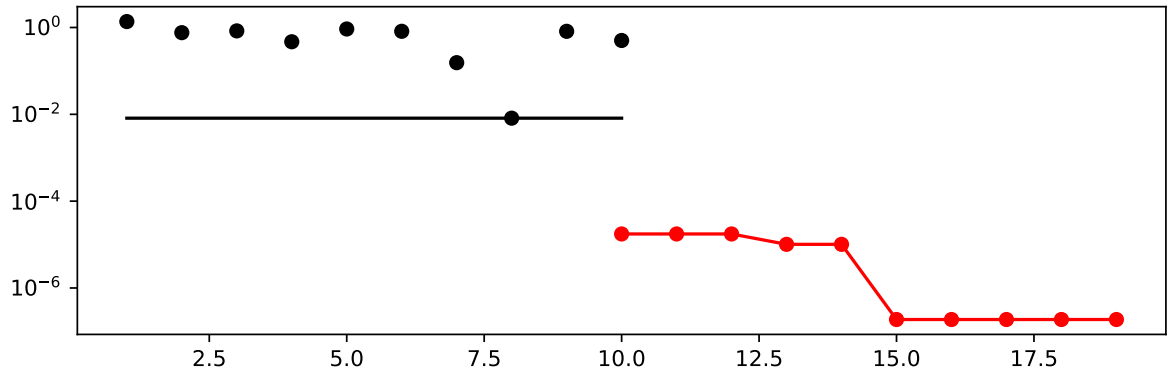
7.3 Non-isotropic Kriging

```
spot_2_ei_noniso = spot.Spot(fun=fun,
                    lower = np.array([-1, -1]),
                    upper = np.array([1, 1]),
                    fun_evals = 20,
                    fun_repeats = 1,
                    max_time = inf,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type=["num"],
                    infill_criterion = "ei",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models=True,
                    fun_control = fun_control,
```

```
                    design_control={"init_size": 10,
                                    "repeats": 1},
                    surrogate_control={"noise": False,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": 2,
                                       "model_optimizer": differential_evolution,
                                       "model_fun_evals": 1000,
                                       })
spot_2_ei_noniso.run()
```

```
<spotPython.spot.spot.Spot at 0x1694c5fc0>
```

```
spot_2_ei_noniso.plot_progress(log_y=True)
```

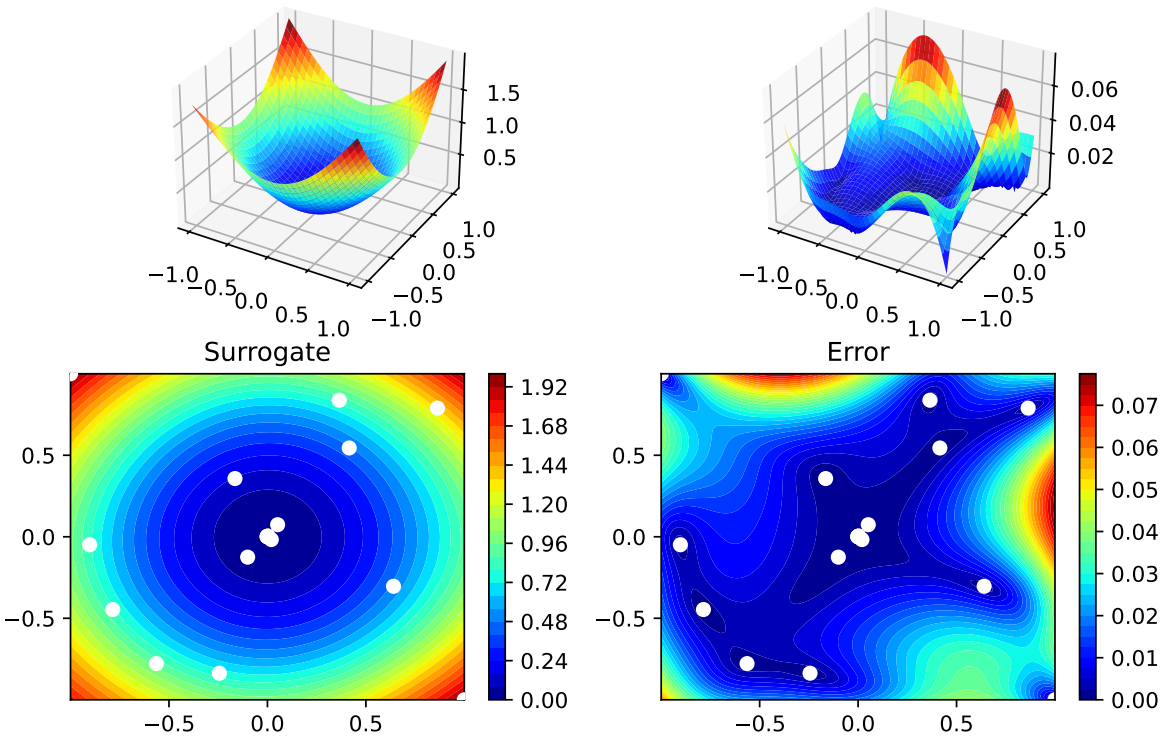



```
spot_2_ei_noniso.print_results()
```

```
min y: 1.8779971830281702e-07
x0: -0.0002783721390529846
x1: 0.0003321274913371111

[['x0', -0.0002783721390529846], ['x1', 0.0003321274913371111]]
```

```
spot_2_ei_noniso.surrogate.plot()
```



7.4 Using `sklearn` Surrogates

7.4.1 The spot Loop

The `spot` loop consists of the following steps:

1. Init: Build initial design X
2. Evaluate initial design on real objective f: $y = f(X)$
3. Build surrogate: $S = S(X, y)$
4. Optimize on surrogate: $X_0 = \text{optimize}(S)$
5. Evaluate on real objective: $y_0 = f(X_0)$
6. Impute (Infill) new points: $X = X \cup X_0$, $y = y \cup y_0$.
7. Got 3.

The `spot` loop is implemented in `R` as follows:

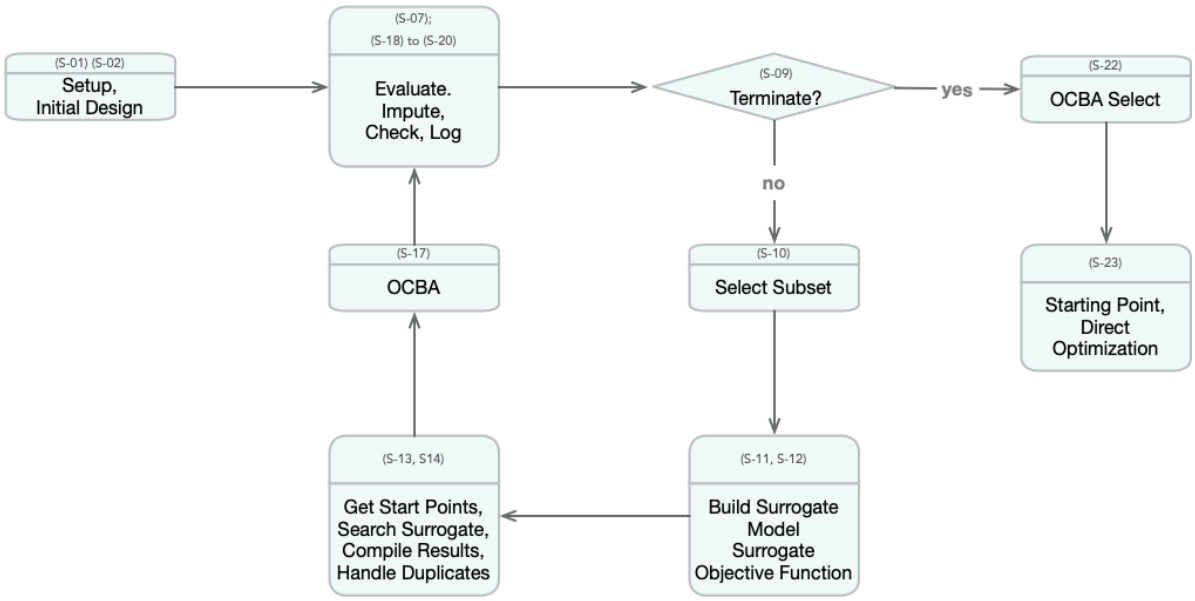


Figure 7.1: Visual representation of the model based search with SPOT. Taken from: Bartz-Beielstein, T., and Zaefferer, M. Hyperparameter tuning approaches. In Hyperparameter Tuning for Machine and Deep Learning with R - A Practical Guide, E. Bartz, T. Bartz-Beielstein, M. Zaefferer, and O. Mersmann, Eds. Springer, 2022, ch. 4, pp. 67–114.

7.4.2 spot: The Initial Model

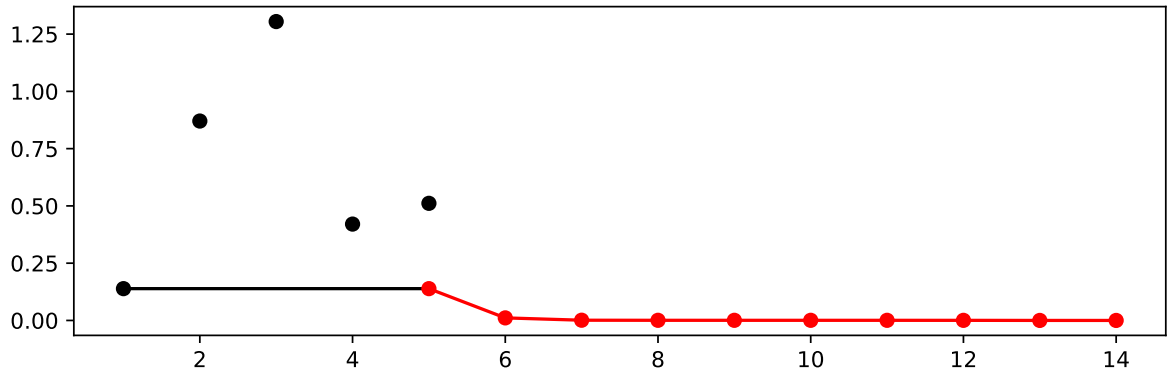
7.4.2.1 Example: Modifying the initial design size

This is the "Example: Modifying the initial design size" from Chapter 4.5.1 in [bart21i].

```
spot_ei = spot.Spot(fun=fun,
                    lower = np.array([-1,-1]),
                    upper= np.array([1,1]),
                    design_control={"init_size": 5})
spot_ei.run()
```

```
<spotPython.spot.spot.Spot at 0x16b5c6d10>
```

```
spot_ei.plot_progress()
```




```
np.min(spot_1.y), np.min(spot_ei.y)
```

```
(3.696886711914087e-10, 1.7928640814182596e-05)
```

7.4.3 Init: Build Initial Design

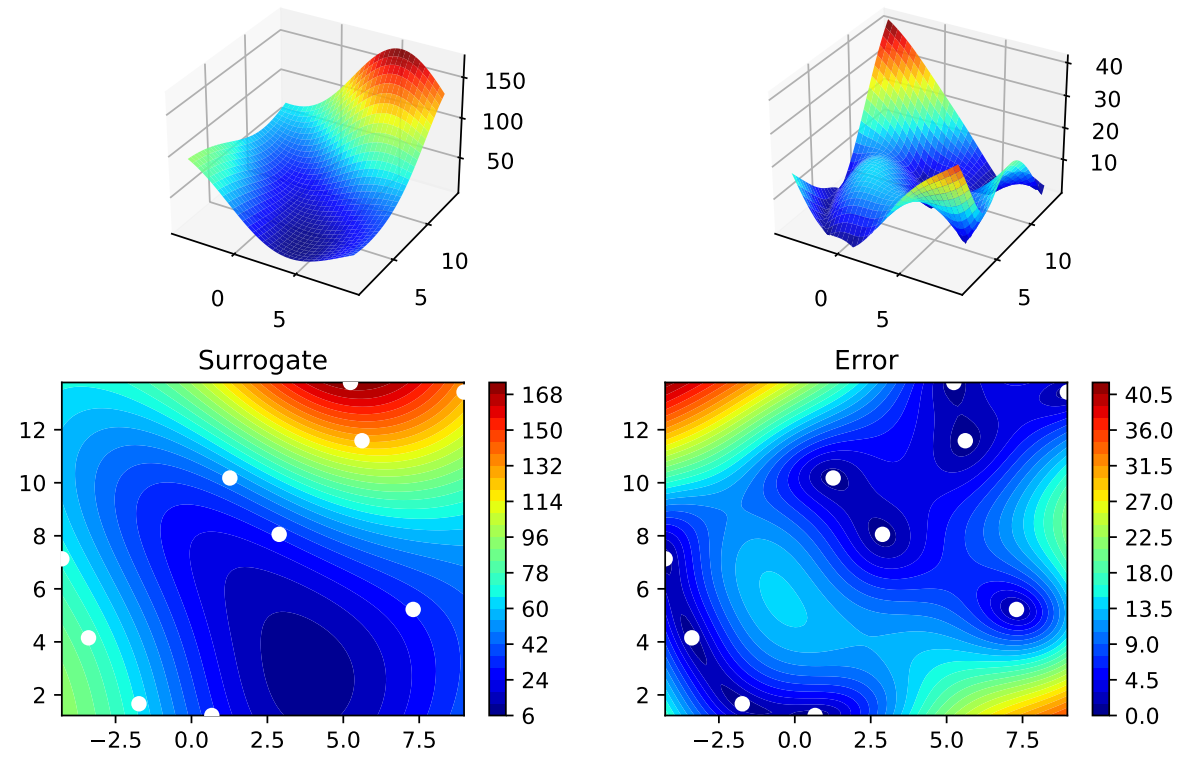
```
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
from spotPython.fun.objectivefunctions import analytical
gen = spacefilling(2)
```

```
rng = np.random.RandomState(1)
lower = np.array([-5,-0])
upper = np.array([10,15])
fun = analytical().fun_branin
fun_control = {"sigma": 0,
               "seed": 123}

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
```

```
[[ 8.97647221 13.41926847]
 [ 0.66946019  1.22344228]
 [ 5.23614115 13.78185824]
 [ 5.6149825  11.5851384 ]
 [-1.72963184  1.66516096]
 [-4.26945568  7.1325531 ]
 [ 1.26363761 10.17935555]
 [ 2.88779942  8.05508969]
 [-3.39111089  4.15213772]
 [ 7.30131231  5.22275244]]
[128.95676449  31.73474356 172.89678121 126.71295908  64.34349975
  70.16178611  48.71407916  31.77322887  76.91788181  30.69410529]
```

```
S = Kriging(name='kriging',  seed=123)
S.fit(X, y)
S.plot()
```




```
gen = spacefilling(2, seed=123)
X0 = gen.scipy_lhd(3)
gen = spacefilling(2, seed=345)
X1 = gen.scipy_lhd(3)
X2 = gen.scipy_lhd(3)
gen = spacefilling(2, seed=123)
X3 = gen.scipy_lhd(3)
X0, X1, X2, X3
```

```
(array([[0.77254938, 0.31539299],
        [0.59321338, 0.93854273],
        [0.27469803, 0.3959685 ]]),
 array([[0.78373509, 0.86811887],
        [0.06692621, 0.6058029 ],
        [0.41374778, 0.00525456]]),
 array([[0.121357  , 0.69043832],
        [0.41906219, 0.32838498],
        [0.86742658, 0.52910374]]),
```

```
array([[0.77254938, 0.31539299],
       [0.59321338, 0.93854273],
       [0.27469803, 0.3959685 ]]))
```

7.4.4 Evaluate

7.4.5 Build Surrogate

7.4.6 A Simple Predictor

The code below shows how to use a simple model for prediction.

- Assume that only two (very costly) measurements are available:
  1. f(0) = 0.5
  2. f(2) = 2.5
- We are interested in the value at $x_0 = 1$, i.e., $f(x_0 = 1)$, but cannot run an additional, third experiment.

```
from sklearn import linear_model
X = np.array([[0], [2]])
y = np.array([0.5, 2.5])
S_lm = linear_model.LinearRegression()
S_lm = S_lm.fit(X, y)
X0 = np.array([[1]])
y0 = S_lm.predict(X0)
print(y0)
```

```
[1.5]
```

- Central Idea:
  - Evaluation of the surrogate model `S_lm` is much cheaper (or / and much faster) than running the real-world experiment f.

7.5 Gaussian Processes regression: basic introductory example

This example was taken from scikit-learn. After fitting our model, we see that the hyperparameters of the kernel have been optimized. Now, we will use our kernel to compute the mean prediction of the full dataset and plot the 95% confidence interval.

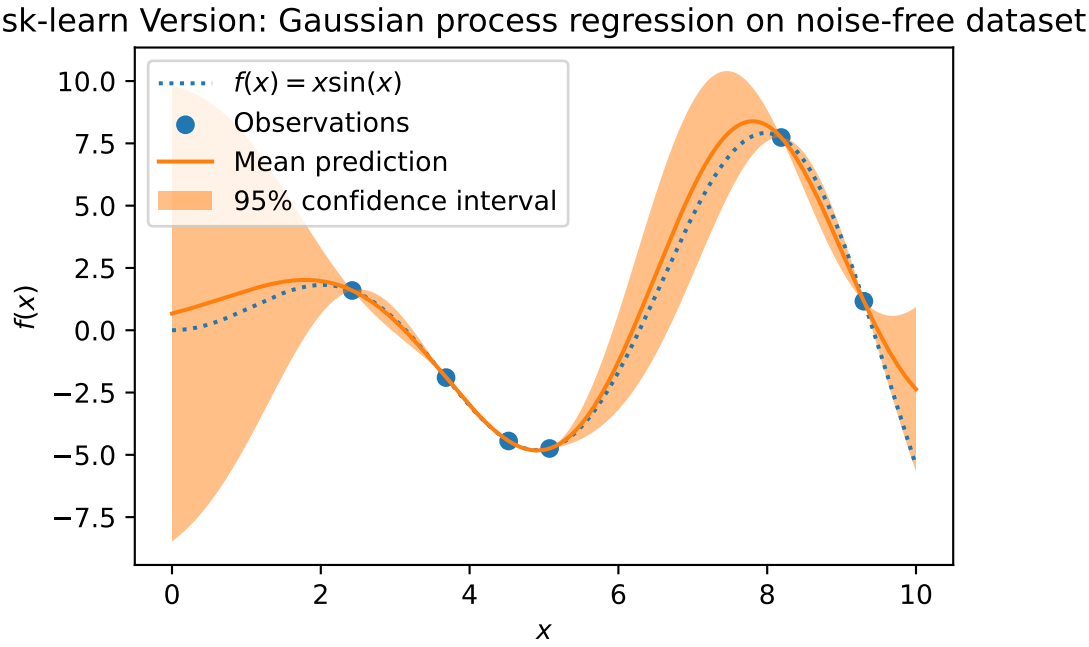
```
import numpy as np
import matplotlib.pyplot as plt
import math as m
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF

X = np.linspace(start=0, stop=10, num=1_000).reshape(-1, 1)
y = np.squeeze(X * np.sin(X))
rng = np.random.RandomState(1)
training_indices = rng.choice(np.arange(y.size), size=6, replace=False)
X_train, y_train = X[training_indices], y[training_indices]

kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
gaussian_process = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gaussian_process.fit(X_train, y_train)
gaussian_process.kernel_

mean_prediction, std_prediction = gaussian_process.predict(X, return_std=True)

plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
    mean_prediction - 1.96 * std_prediction,
    mean_prediction + 1.96 * std_prediction,
    alpha=0.5,
    label=r"95% confidence interval",
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("sk-learn Version: Gaussian process regression on noise-free dataset")
```




```
from spotPython.build.kriging import Kriging
import numpy as np
import matplotlib.pyplot as plt
rng = np.random.RandomState(1)
X = np.linspace(start=0, stop=10, num=1_000).reshape(-1, 1)
y = np.squeeze(X * np.sin(X))
training_indices = rng.choice(np.arange(y.size), size=6, replace=False)
X_train, y_train = X[training_indices], y[training_indices]

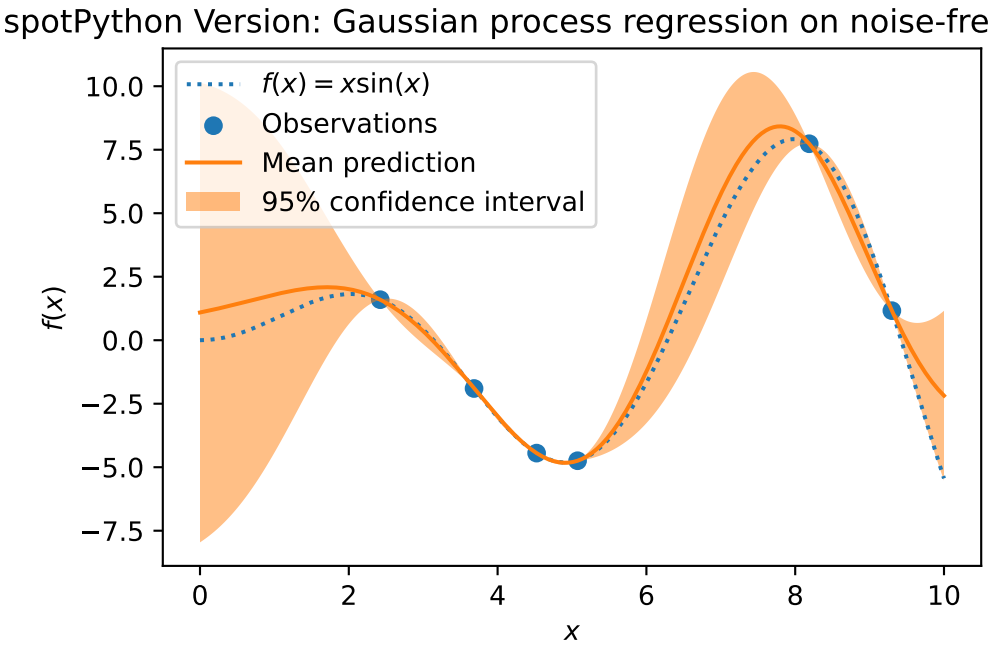

S = Kriging(name='kriging',  seed=123, log_level=50, cod_type="norm")
S.fit(X_train, y_train)

mean_prediction, std_prediction, ei = S.predict(X, return_val="all")

std_prediction

plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
plt.fill_between(
```

```
    X.ravel(),
    mean_prediction - 1.96 * std_prediction,
    mean_prediction + 1.96 * std_prediction,
    alpha=0.5,
    label=r"95% confidence interval",
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("spotPython Version: Gaussian process regression on noise-free dataset")
```



7.6 The Surrogate: Using scikit-learn models

Default is the internal `kriging` surrogate.

```
S_0 = Kriging(name='kriging', seed=123)
```

Models from `scikit-learn` can be selected, e.g., Gaussian Process:

```
# Needed for the sklearn surrogates:
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn import linear_model
from sklearn import tree
import pandas as pd
```

```
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
S_GP = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
```

- and many more:

```
S_Tree = DecisionTreeRegressor(random_state=0)
S_LM = linear_model.LinearRegression()
S_Ridge = linear_model.Ridge()
S_RF = RandomForestRegressor(max_depth=2, random_state=0)
```

- The scikit-learn GP model `S_GP` is selected.

```
S = S_GP
```

```
isinstance(S, GaussianProcessRegressor)
```

```
True
```

```
from spotPython.fun.objectivefunctions import analytical
fun = analytical().fun_branin
lower = np.array([-5,-0])
upper = np.array([10,15])
design_control={"init_size": 5}
surrogate_control={
            "infill_criterion": None,
            "n_points": 1,
        }
spot_GP = spot.Spot(fun=fun, lower = lower, upper= upper, surrogate=S,
                    fun_evals = 15, noise = False, log_level = 50,
                    design_control=design_control,
                    surrogate_control=surrogate_control)
```

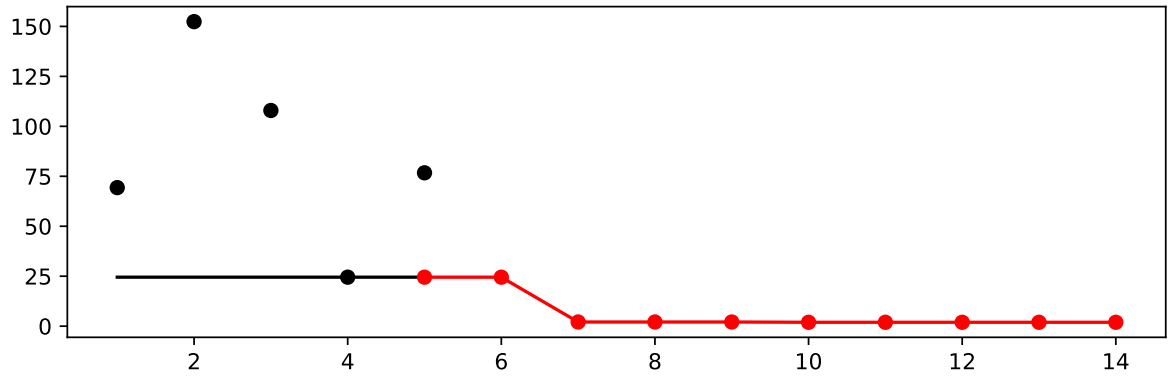
```
spot_GP.run()
```

```
<spotPython.spot.spot.Spot at 0x16b716710>
```

```
spot_GP.y
```

```
array([ 69.32459936, 152.38491454, 107.92560483,  24.51465459,
        76.73500031,  86.3042577 , 128.1584069 ,   2.0848684 ,
         5.65023665,   2.59664684,   1.94316346,   1.94350862,
        12.83580716,  21.55925114,   1.94238966])
```

```
spot_GP.plot_progress()
```




```
spot_GP.print_results()
```

```
min y: 1.9423896629538913
x0: 9.999794212305758
x1: 2.984757626104978

[['x0', 9.999794212305758], ['x1', 2.984757626104978]]
```

7.7 Additional Examples

```
# Needed for the sklearn surrogates:
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn import linear_model
from sklearn import tree
import pandas as pd
```

```
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
S_GP = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
```

```
from spotPython.build.kriging import Kriging
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot

S_K = Kriging(name='kriging',
              seed=123,
              log_level=50,
              infill_criterion = "y",
              n_theta=1,
              noise=False,
              cod_type="norm")
fun = analytical().fun_sphere
lower = np.array([-1,-1])
upper = np.array([1,1])

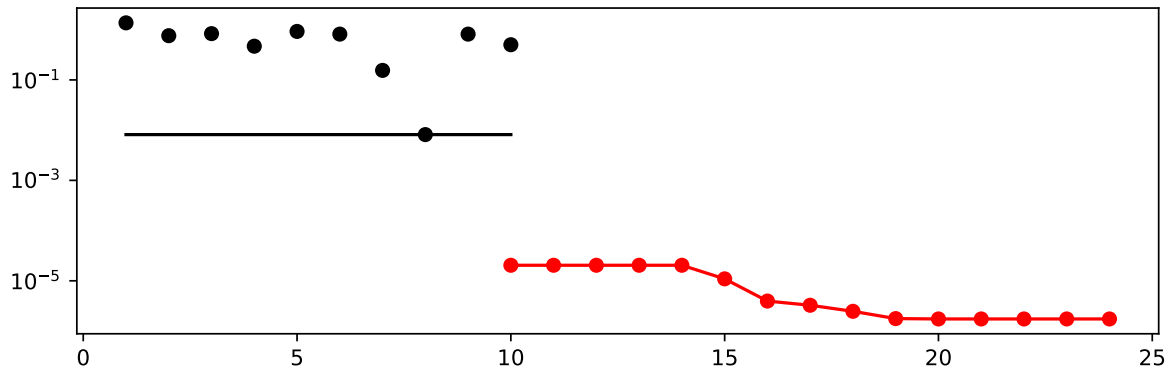
design_control={"init_size": 10}
surrogate_control={
            "n_points": 1,
        }
spot_S_K = spot.Spot(fun=fun,
                     lower = lower,
                     upper= upper,
                     surrogate=S_K,
                     fun_evals = 25,
                     noise = False,
                     log_level = 50,
```

```
                    design_control=design_control,
                    surrogate_control=surrogate_control)

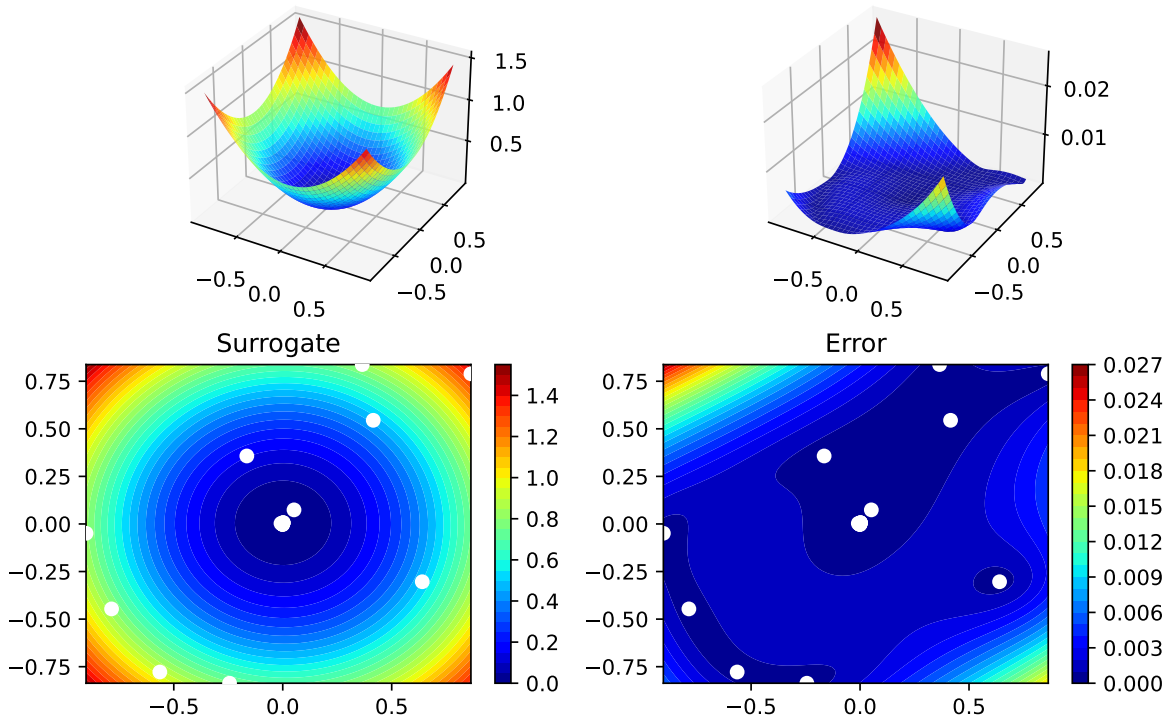
spot_S_K.run()
```

```
<spotPython.spot.spot.Spot at 0x16d33f700>
```

```
spot_S_K.plot_progress(log_y=True)
```




```
spot_S_K.surrogate.plot()
```




```
spot_S_K.print_results()
```

```
min y: 1.7395335905335862e-06
x0: -0.0013044072412622557
x1: 0.0001950777780173277

[['x0', -0.0013044072412622557], ['x1', 0.0001950777780173277]]
```

7.7.1 Optimize on Surrogate

7.7.2 Evaluate on Real Objective

7.7.3 Impute / Infill new Points

7.8 Tests

```
import numpy as np
from spotPython.spot import spot
from spotPython.fun.objectivefunctions import analytical

fun_sphere = analytical().fun_sphere
spot_1 = spot.Spot(
    fun=fun_sphere,
    lower=np.array([-1, -1]),
    upper=np.array([1, 1]),
    n_points = 2
)

# (S-2) Initial Design:
spot_1.X = spot_1.design.scipy_lhd(
    spot_1.design_control["init_size"], lower=spot_1.lower, upper=spot_1.upper
)
print(spot_1.X)

# (S-3): Eval initial design:
spot_1.y = spot_1.fun(spot_1.X)
print(spot_1.y)

spot_1.surrogate.fit(spot_1.X, spot_1.y)
X0 = spot_1.suggest_new_X()
print(X0)
assert X0.size == spot_1.n_points * spot_1.k
```

```
[[ 0.86352963  0.7892358 ]
 [-0.24407197 -0.83687436]
 [ 0.36481882  0.8375811 ]
 [ 0.415331    0.54468512]
 [-0.56395091 -0.77797854]
 [-0.90259409 -0.04899292]]
```

```
 [-0.16484832  0.35724741]
 [ 0.05170659  0.07401196]
 [-0.78548145 -0.44638164]
 [ 0.64017497 -0.30363301]]
[1.36857656 0.75992983 0.83463487 0.46918172 0.92329124 0.8170764
 0.15480068 0.00815134 0.81623768 0.502017  ]
[[0.00160553 0.00428429]
 [0.00160553 0.00428429]]
```

7.9 EI: The Famous Schonlau Example

```
X_train0 = np.array([1, 2, 3, 4, 12]).reshape(-1,1)
X_train = np.linspace(start=0, stop=10, num=5).reshape(-1, 1)
```

```
from spotPython.build.kriging import Kriging
import numpy as np
import matplotlib.pyplot as plt

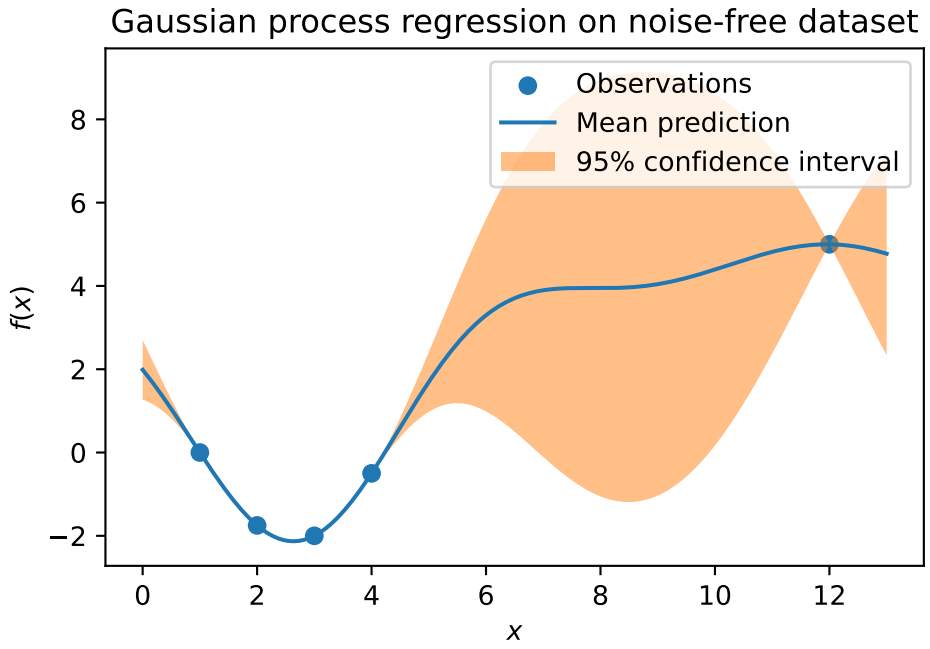
X_train = np.array([1., 2., 3., 4., 12.]).reshape(-1,1)
y_train = np.array([0., -1.75, -2, -0.5, 5.])

S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False, cod_type="nor
S.fit(X_train, y_train)

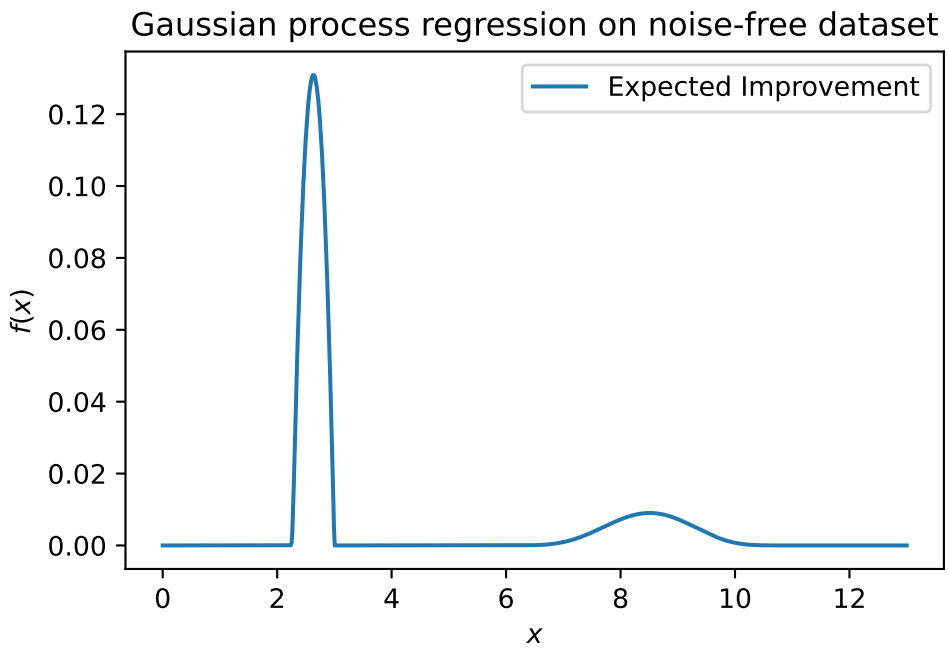
X = np.linspace(start=0, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
if True:
    plt.fill_between(
        X.ravel(),
        mean_prediction - 2 * std_prediction,
        mean_prediction + 2 * std_prediction,
        alpha=0.5,
        label=r"95% confidence interval",
    )
plt.legend()
plt.xlabel("$x$")
```

```
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```




```
#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
# plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, -ei, label="Expected Improvement")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```




```
S.log
```

```
{'negLnLike': array([1.20788205]),
 'theta': array([1.09276]),
 'p': array([2.]),
 'Lambda': array([None], dtype=object)}
```

7.10 EI: The Forrester Example

```
from spotPython.build.kriging import Kriging
import numpy as np
import matplotlib.pyplot as plt
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot

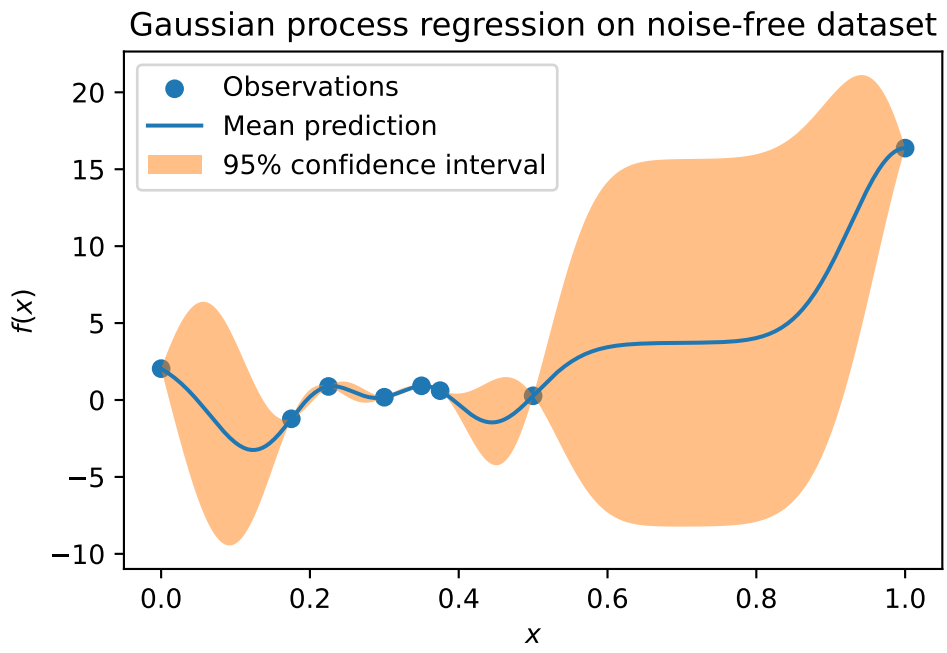
# exact x locations are unknown:
X_train = np.array([0.0, 0.175, 0.225, 0.3, 0.35, 0.375, 0.5,1]).reshape(-1,1)
```

```
fun = analytical().fun_forrester
fun_control = {"sigma": 1.0,
               "seed": 123}
y_train = fun(X_train, fun_control=fun_control)

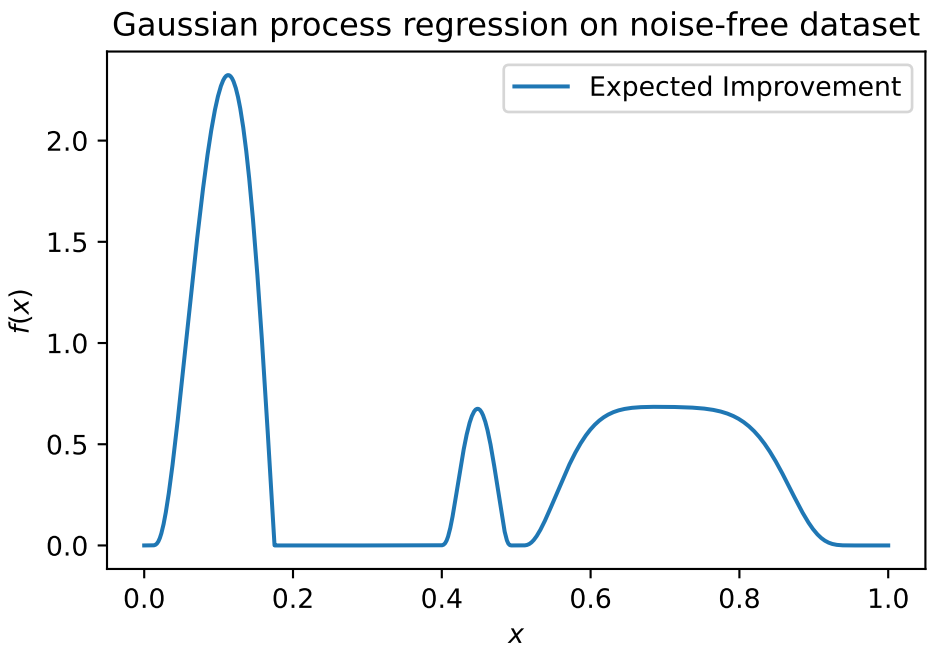
S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False, cod_type="nor
S.fit(X_train, y_train)

X = np.linspace(start=0, stop=1, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
if True:
    plt.fill_between(
        X.ravel(),
        mean_prediction - 2 * std_prediction,
        mean_prediction + 2 * std_prediction,
        alpha=0.5,
        label=r"95% confidence interval",
    )
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```




```
#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
# plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, -ei, label="Expected Improvement")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```



7.11 Noise

```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_sphere
fun_control = {"sigma": 2,
               "seed": 125}
X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
```

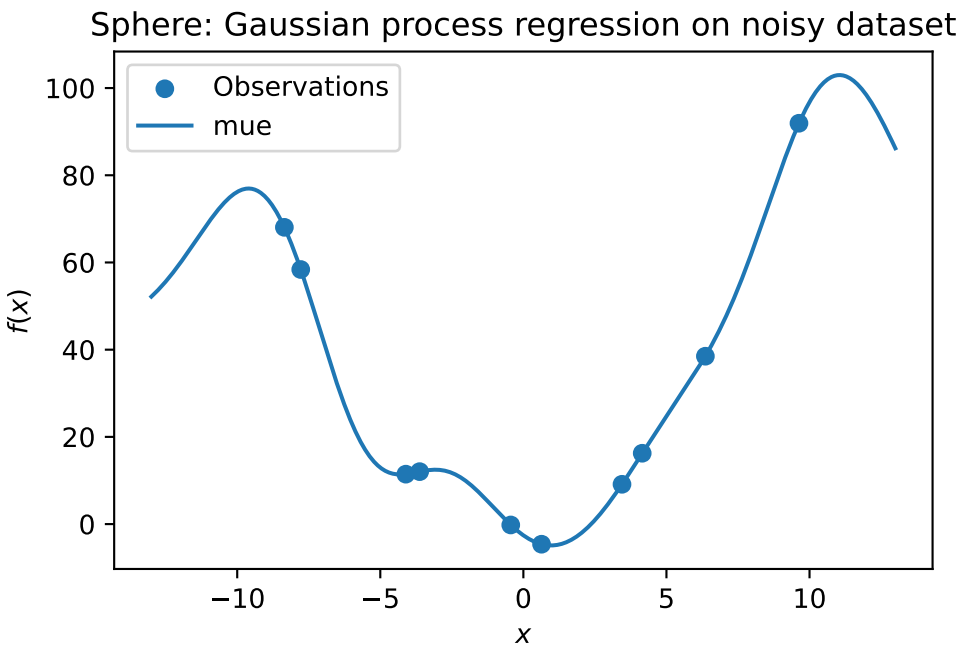
```
print(y)
y.shape
X_train = X.reshape(-1,1)
y_train = y

S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=False)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression on noisy dataset")
```

```
[[ 0.63529627]
 [-4.10764204]
 [-0.44071975]
 [ 9.63125638]
 [-8.3518118 ]
 [-3.62418901]
 [ 4.15331   ]
 [ 3.4468512 ]
 [ 6.36049088]
 [-7.77978539]]
[-4.61635371 11.44873209 -0.19988024 91.92791676 68.05926244 12.02926818
 16.2470957   9.12729929 38.4987029  58.38469104]
```




```
S.log
```

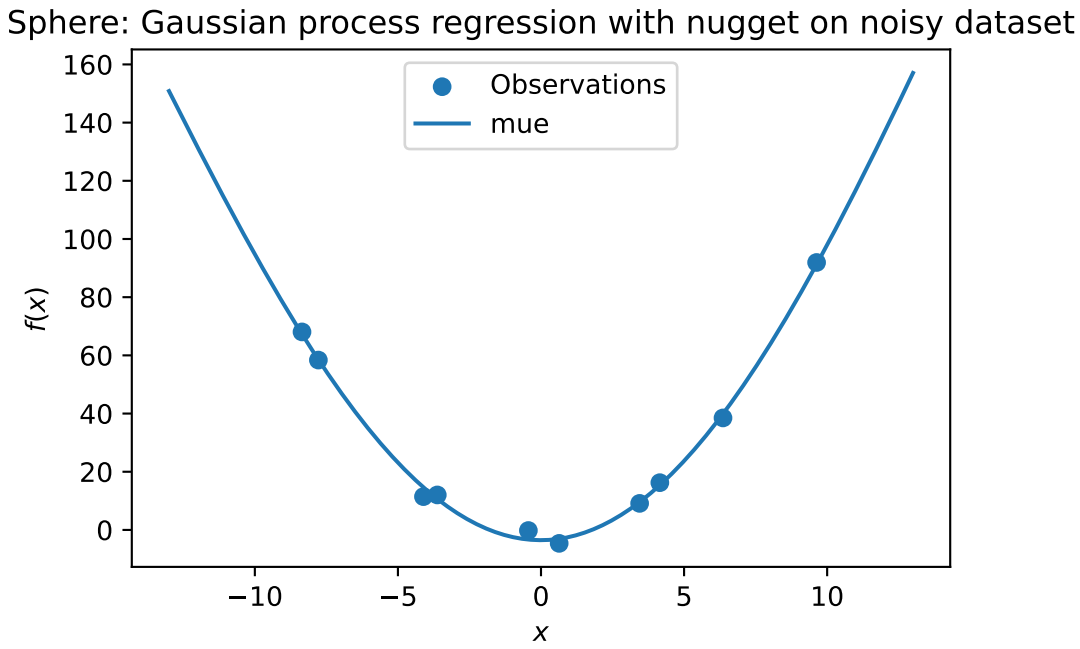
```
{'negLnLike': array([24.69806131]),
 'theta': array([1.31023943]),
 'p': array([2.]),
 'Lambda': array([None], dtype=object)}
```

```
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
```

```
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression with nugget on noisy dataset")
```




```
S.log
```

```
{'negLnLike': array([22.14095646]),
 'theta': array([-0.32527397]),
 'p': array([2.]),
 'Lambda': array([9.08815007e-05])}
```

7.12 Cubic Function

```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
```

```
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_cubed
fun_control = {"sigma": 10,
               "seed": 123}

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
y.shape
X_train = X.reshape(-1,1)
y_train = y

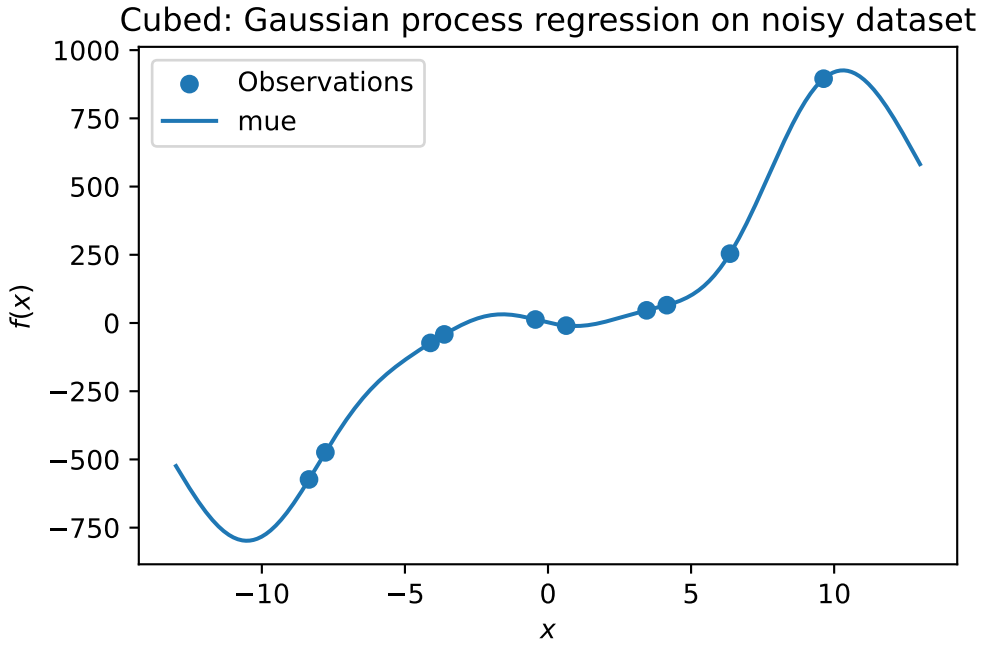
S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Cubed: Gaussian process regression on noisy dataset")
```

```
[[ 0.63529627]
 [-4.10764204]
 [-0.44071975]
 [ 9.63125638]
 [-8.3518118 ]
 [-3.62418901]
 [ 4.15331   ]
 [ 3.4468512 ]
 [ 6.36049088]
```

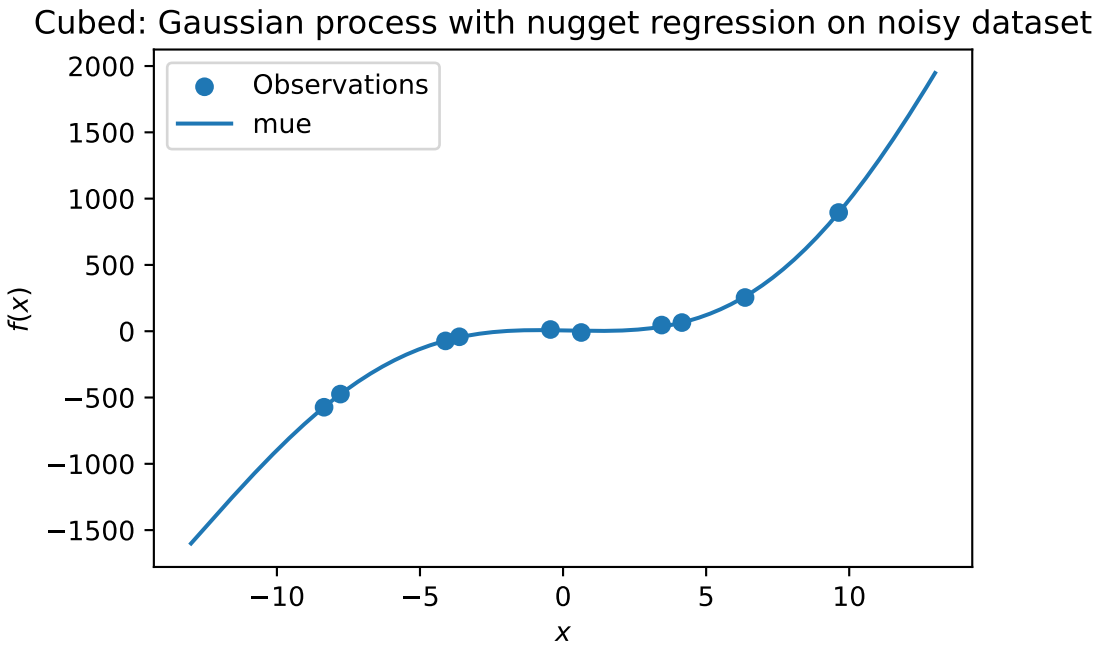
```
 [-7.77978539]]
[  -9.63480707  -72.98497325   12.7936499   895.34567477 -573.35961837
  -41.83176425   65.27989461   46.37081417  254.1530734  -474.09587355]
```




```
S = Kriging(name='kriging',  seed=123, log_level=0, n_theta=1, noise=True)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Cubed: Gaussian process with nugget regression on noisy dataset")
```




```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = {"sigma": 0.25,
               "seed": 123}

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
y.shape
```

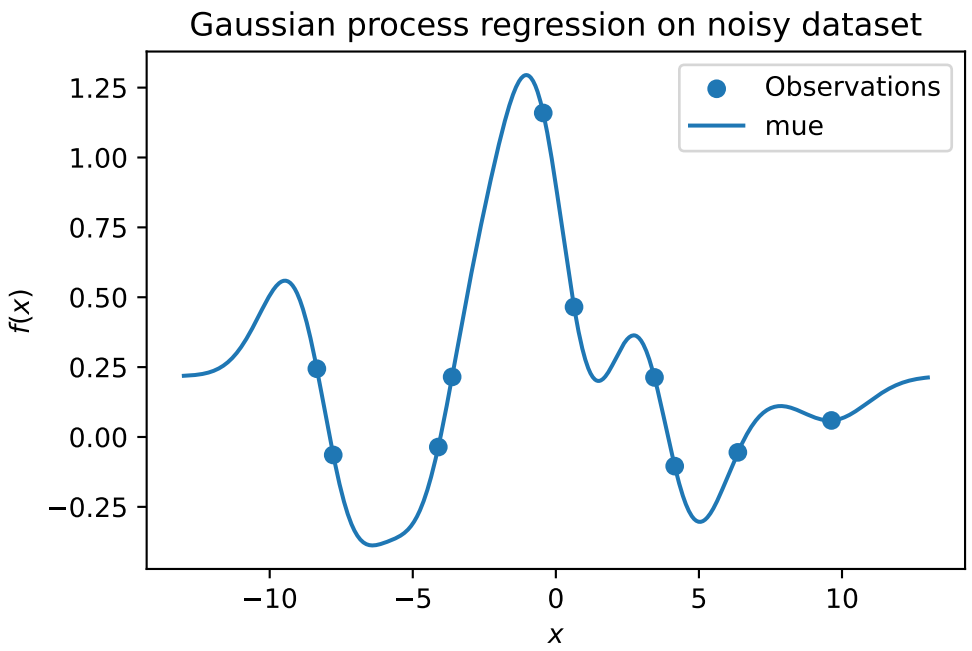
```
X_train = X.reshape(-1,1)
y_train = y

S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noisy dataset")
```

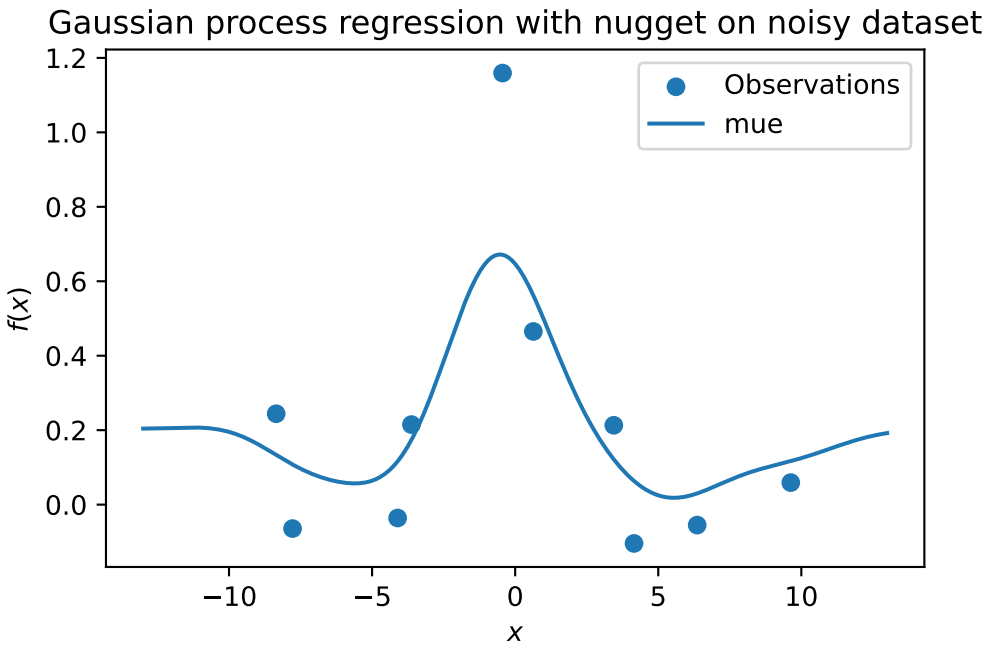
```
[[ 0.63529627]
 [-4.10764204]
 [-0.44071975]
 [ 9.63125638]
 [-8.3518118 ]
 [-3.62418901]
 [ 4.15331   ]
 [ 3.4468512 ]
 [ 6.36049088]
 [-7.77978539]]
[ 0.46517267 -0.03599548  1.15933822  0.05915901  0.24419145  0.21502359
 -0.10432134  0.21312309 -0.05502681 -0.06434374]
```




```
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression with nugget on noisy dataset")
```



7.13 Factors

```
["num"] * 3
```

```
['num', 'num', 'num']
```

```
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
from spotPython.fun.objectivefunctions import analytical
import numpy as np
```

```
gen = spacefilling(2)
n = 30
rng = np.random.RandomState(1)
lower = np.array([-5,-0])
upper = np.array([10,15])
fun = analytical().fun_branin_factor
#fun = analytical(sigma=0).fun_sphere
```

```
X0 = gen.scipy_lhd(n, lower=lower, upper = upper)
X1 = np.random.randint(low=1, high=3, size=(n,))
X = np.c_[X0, X1]
y = fun(X)
S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=3, noise=False, var_type=["nu
S.fit(X, y)
Sf = Kriging(name='kriging',  seed=123, log_level=50, n_theta=3, noise=False, var_type=["n
Sf.fit(X, y)
n = 50
X0 = gen.scipy_lhd(n, lower=lower, upper = upper)
X1 = np.random.randint(low=1, high=3, size=(n,))
X = np.c_[X0, X1]
y = fun(X)
s=np.sum(np.abs(S.predict(X)[0] - y))
sf=np.sum(np.abs(Sf.predict(X)[0] - y))
sf - s
```

```
-193.01351282220276
```

```
# vars(S)
```

```
# vars(Sf)
```

8 Hyperparameter Tuning and Noise

This chapter demonstrates how noisy functions can be handled by `Spot`.

8.1 Example: `Spot` and the Noisy Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
```

```
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '10-sklearn' + "_" + HOSTNAME + "_" + str(start_time).split(".", 1)[0].r
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
10-sklearn_bartz09_2023-06-19_02-25-15
```

8.1.1 The Objective Function: Noisy Sphere

- The `spotPython` package provides several classes of objective functions.

- We will use an analytical objective function with noise, i.e., a function that can be described by a (closed) formula:

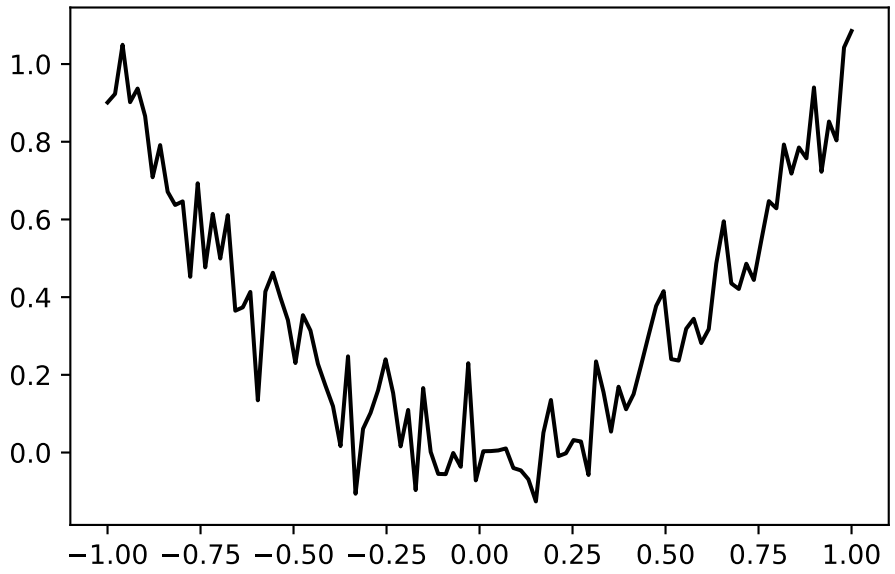
$$f(x) = x^2 + \epsilon$$

- Since `sigma` is set to `0.1`, noise is added to the function:

```
fun = analytical().fun_sphere
fun_control = {"sigma": 0.1,
               "seed": 123}
```

- A plot illustrates the noise:

```
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x, fun_control=fun_control)
plt.figure()
plt.plot(x,y, "k")
plt.show()
```

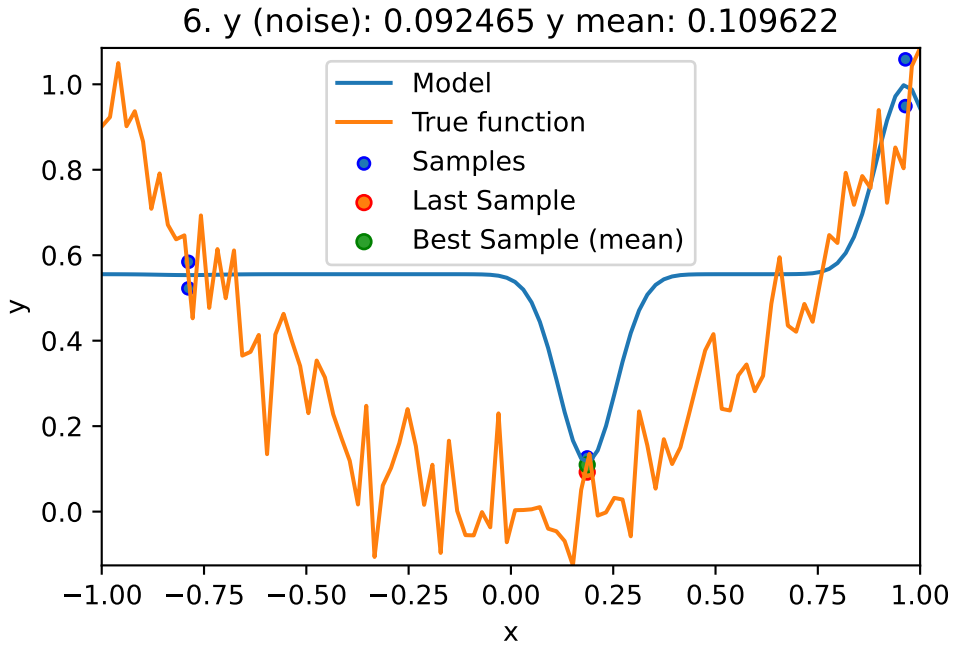


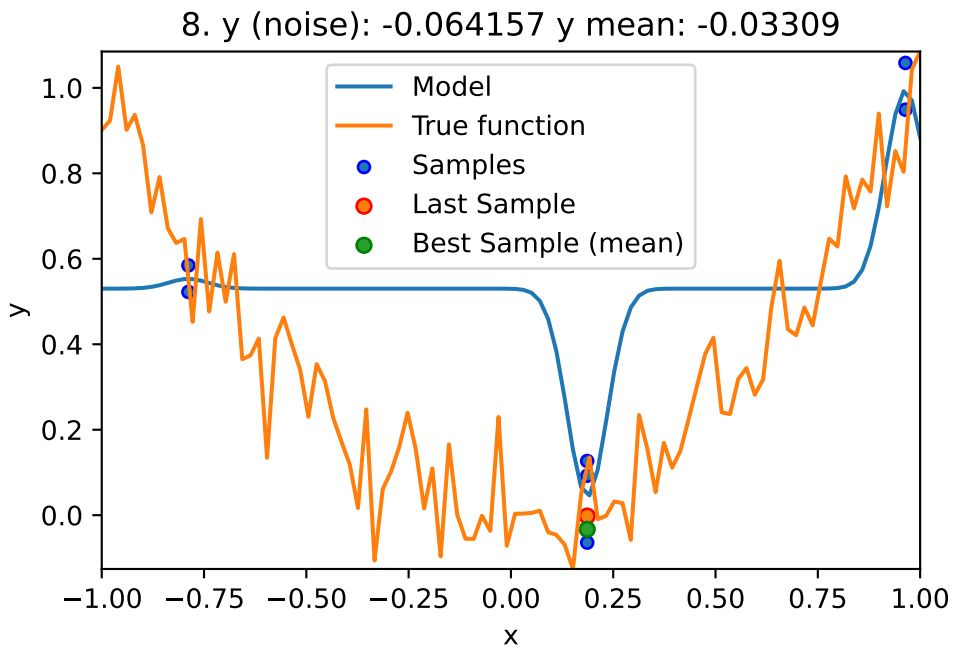
`Spot` is adopted as follows to cope with noisy functions:

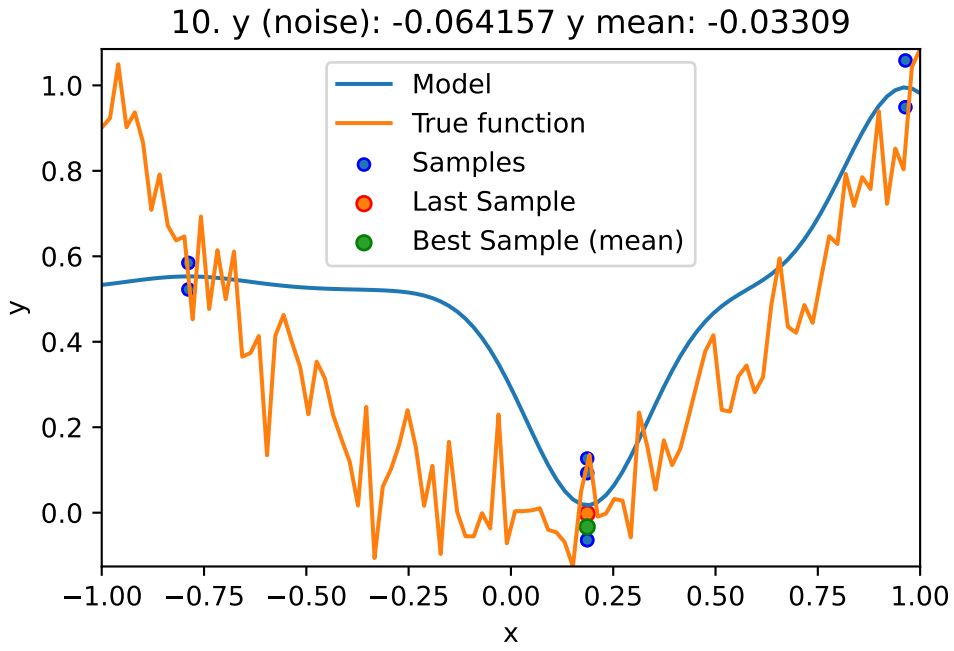
1. `fun_repeats` is set to a value larger than 1 (here: 2)
2. `noise` is set to `true`. Therefore, a nugget (`Lambda`) term is added to the correlation matrix
3. `init size` (of the `design_control` dictionary) is set to a value larger than 1 (here: 2)

```
spot_1_noisy = spot.Spot(fun=fun,
                    lower = np.array([-1]),
                    upper = np.array([1]),
                    fun_evals = 10,
                    fun_repeats = 2,
                    noise = True,
                    seed=123,
                    show_models=True,
                    fun_control = fun_control,
                    design_control={"init_size": 3,
                                    "repeats": 2},
                    surrogate_control={"noise": True})
```

```
spot_1_noisy.run()
```








```
<spotPython.spot.spot.Spot at 0x16a68b880>
```

8.2 Print the Results

```
spot_1_noisy.print_results()
```

```
min y: -0.06415721594238855
x0: 0.18642671238960512
min mean y: -0.03309048099839016
x0: 0.18642671238960512
```

```
[['x0', 0.18642671238960512], ['x0', 0.18642671238960512]]
```

```
spot_1_noisy.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

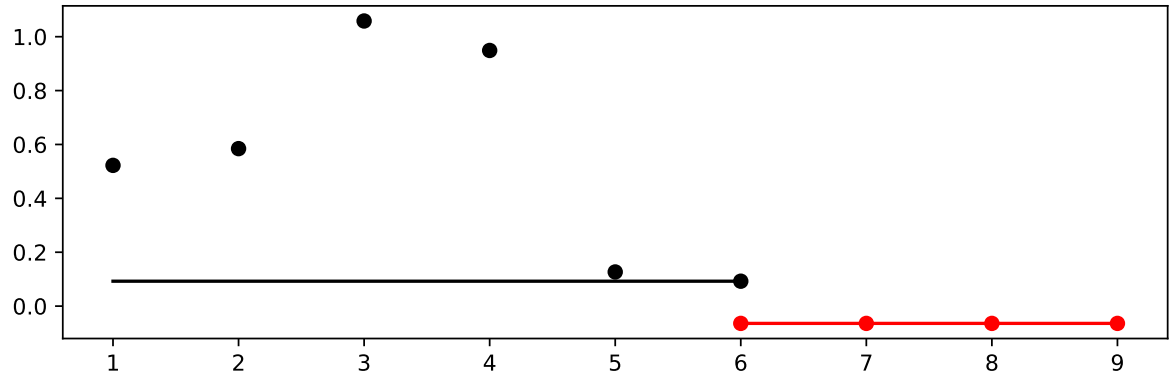


Figure 8.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

8.3 Noise and Surrogates: The Nugget Effect

8.3.1 The Noisy Sphere

8.3.1.1 The Data

- We prepare some data first:

```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

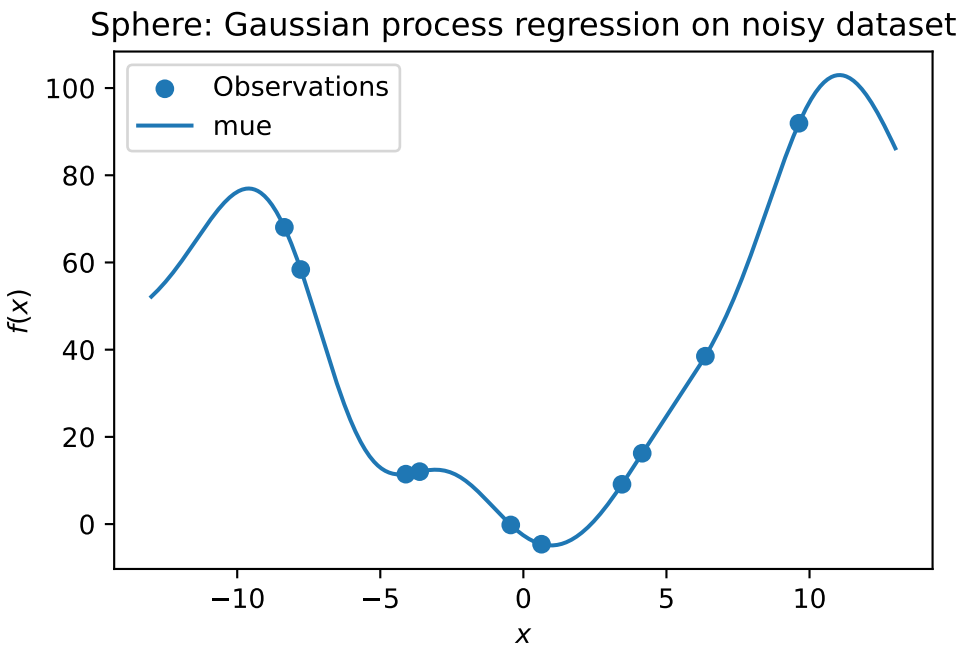
gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_sphere
fun_control = {"sigma": 2,
               "seed": 125}
X = gen.scipy_lhd(10, lower=lower, upper = upper)
y = fun(X, fun_control=fun_control)
X_train = X.reshape(-1,1)
y_train = y
```

- A surrogate without nugget is fitted to these data:

```
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=False)
S.fit(X_train, y_train)

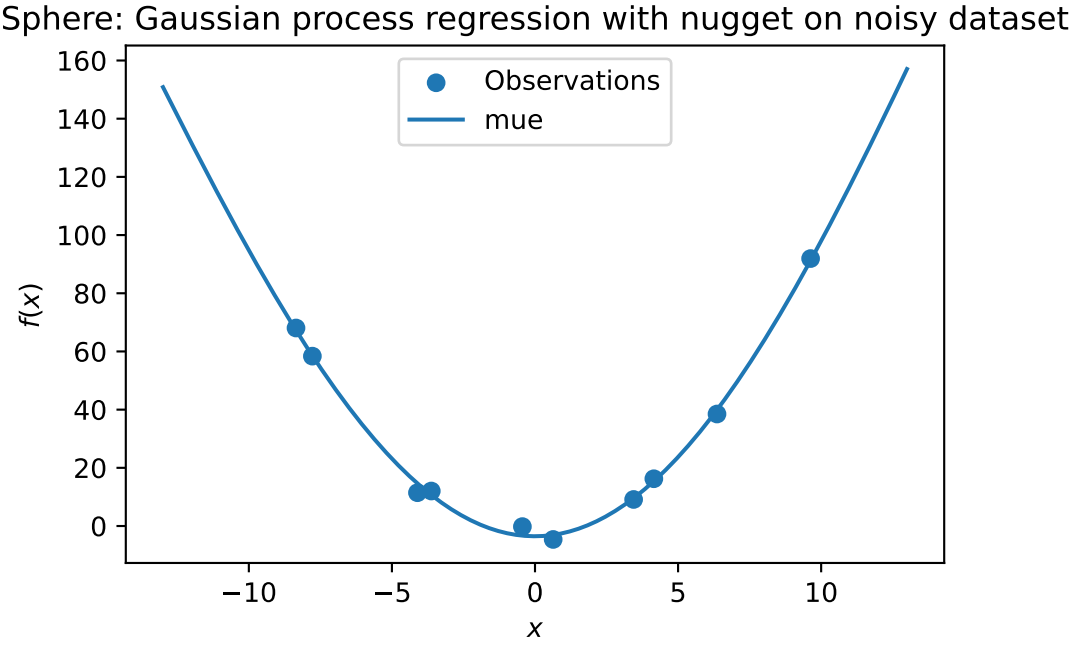
X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression on noisy dataset")
```



- In comparison to the surrogate without nugget, we fit a surrogate with nugget to the data:

```
S_nug = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S_nug.fit(X_train, y_train)
X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S_nug.predict(X_axis, return_val="all")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression with nugget on noisy dataset")
```



- The value of the nugget term can be extracted from the model as follows:

```
S.Lambda
```

```
S_nug.Lambda
```

```
9.088150066416743e-05
```

- We see:
  - the first model `S` has no nugget,
  - whereas the second model has a nugget value (`Lambda`) larger than zero.

8.4 Exercises

8.4.1 Noisy `fun_cubed`

- Analyse the effect of noise on the `fun_cubed` function with the following settings:

```
fun = analytical().fun_cubed
fun_control = {"sigma": 10,
```

```
                "seed": 123}
lower = np.array([-10])
upper = np.array([10])
```

8.4.2 `fun_runge`

- Analyse the effect of noise on the `fun_runge` function with the following settings:

```
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = {"sigma": 0.25,
                "seed": 123}
```

8.4.3 `fun_forrester`

- Analyse the effect of noise on the `fun_forrester` function with the following settings:

```
lower = np.array([0])
upper = np.array([1])
fun = analytical().fun_forrester
fun_control = {"sigma": 5,
                "seed": 123}
```

8.4.4 `fun_xsin`

- Analyse the effect of noise on the `fun_xsin` function with the following settings:

```
lower = np.array([-1.])
upper = np.array([1.])
fun = analytical().fun_xsin
fun_control = {"sigma": 0.5,
                "seed": 123}
```

9 Handling Noise: Optimal Computational Budget Allocation in Spot

This notebook demonstrates how noisy functions can be handled with OCBA by Spot.

9.1 Example: Spot, OCBA, and the Noisy Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

9.1.1 The Objective Function: Noisy Sphere

The spotPython package provides several classes of objective functions. We will use an analytical objective function with noise, i.e., a function that can be described by a (closed) formula:

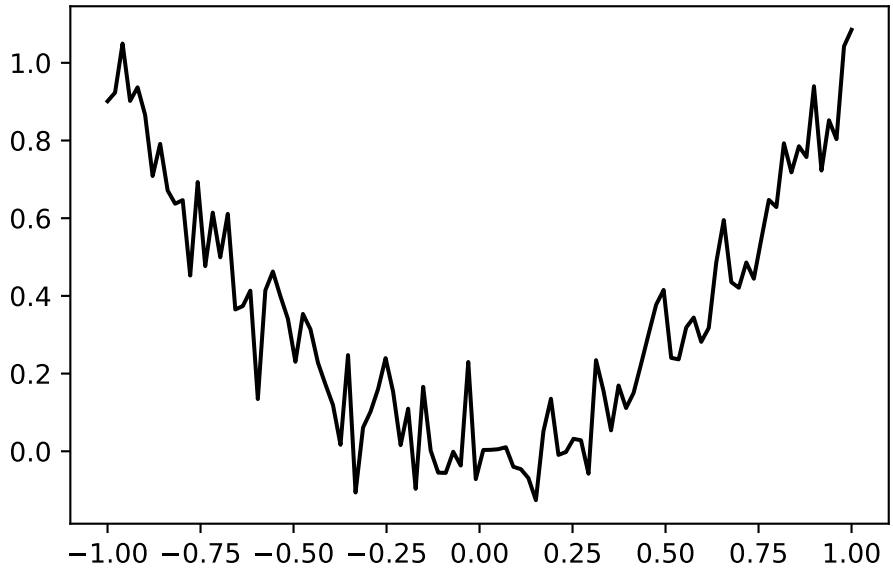
$$f(x) = x^2 + \epsilon$$

Since sigma is set to 0.1, noise is added to the function:

```
fun = analytical().fun_sphere
fun_control = {"sigma": 0.1,
               "seed": 123}
```

A plot illustrates the noise:

```
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x, fun_control=fun_control)
plt.figure()
plt.plot(x,y, "k")
plt.show()
```



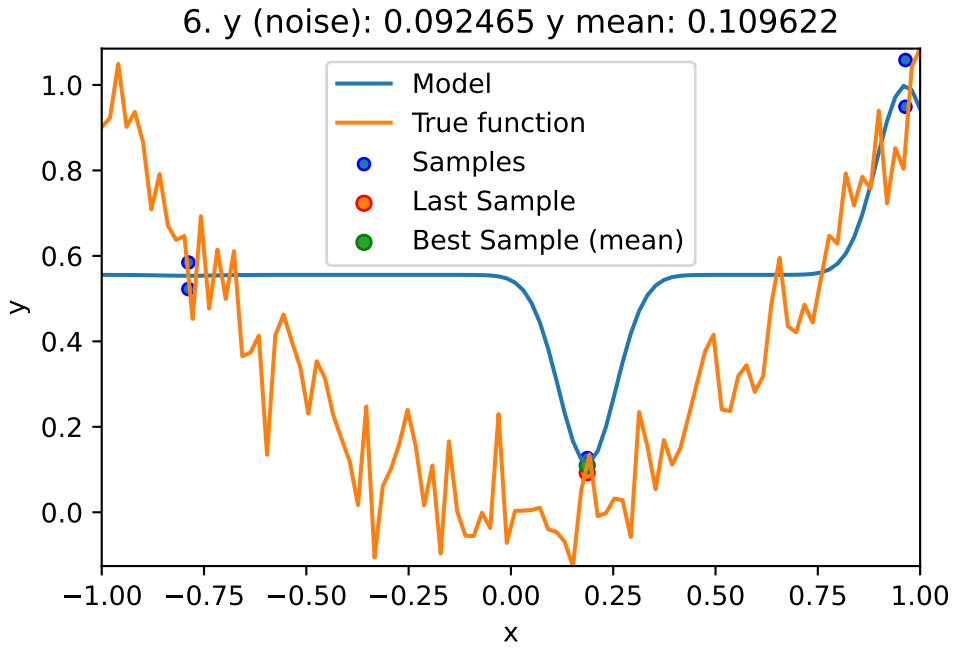
`Spot` is adopted as follows to cope with noisy functions:

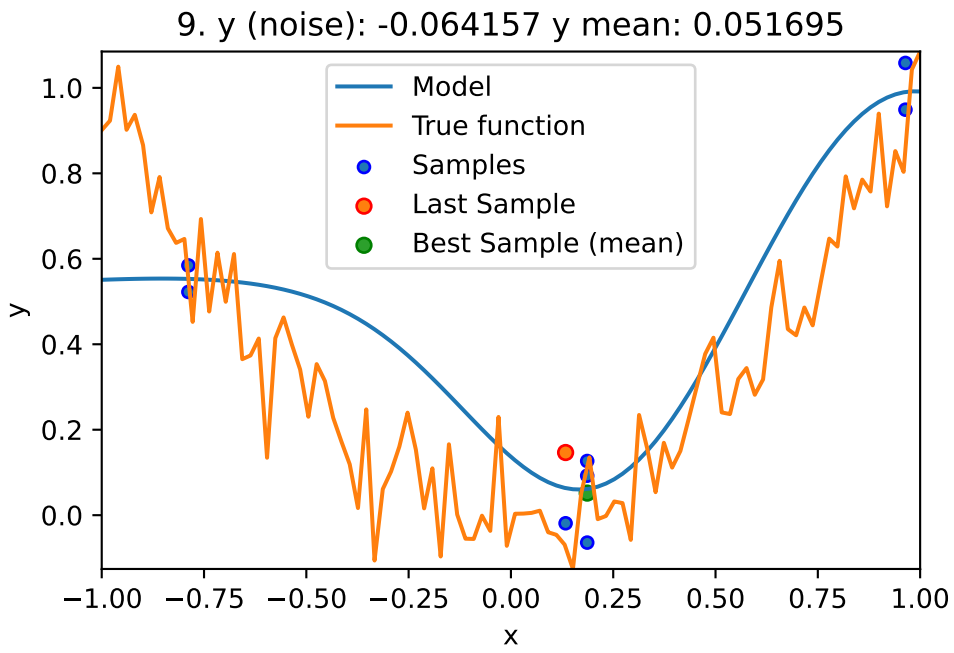
1. `fun_repeats` is set to a value larger than 1 (here: 2)
2. `noise` is set to `true`. Therefore, a nugget (`Lambda`) term is added to the correlation matrix
3. `init size` (of the `design_control` dictionary) is set to a value larger than 1 (here: 2)

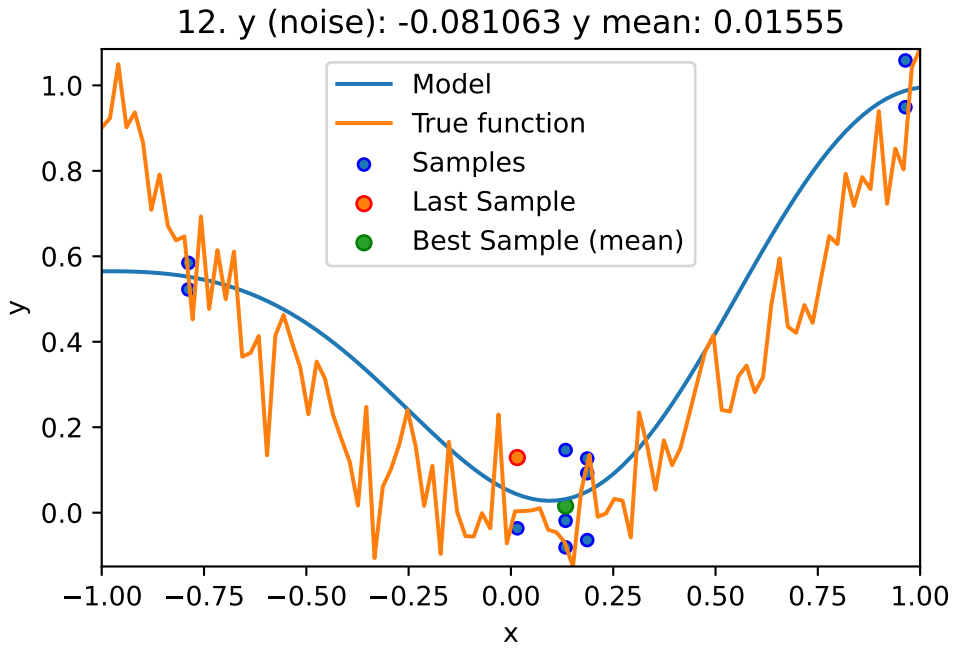
```
spot_1_noisy = spot.Spot(fun=fun,
                    lower = np.array([-1]),
                    upper = np.array([1]),
                    fun_evals = 50,
                    fun_repeats = 2,
                    infill_criterion="ei",
                    noise = True,
                    tolerance_x=0.0,
                    ocba_delta = 1,
                    seed=123,
```

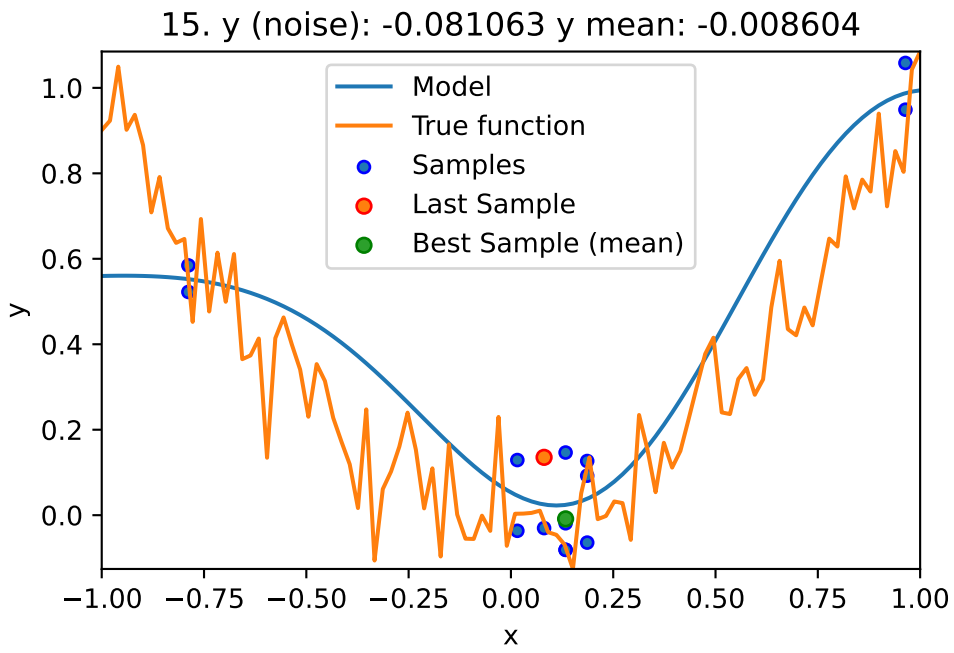
```
                    show_models=True,
                    fun_control = fun_control,
                    design_control={"init_size": 3,
                                    "repeats": 2},
                    surrogate_control={"noise": True})
```

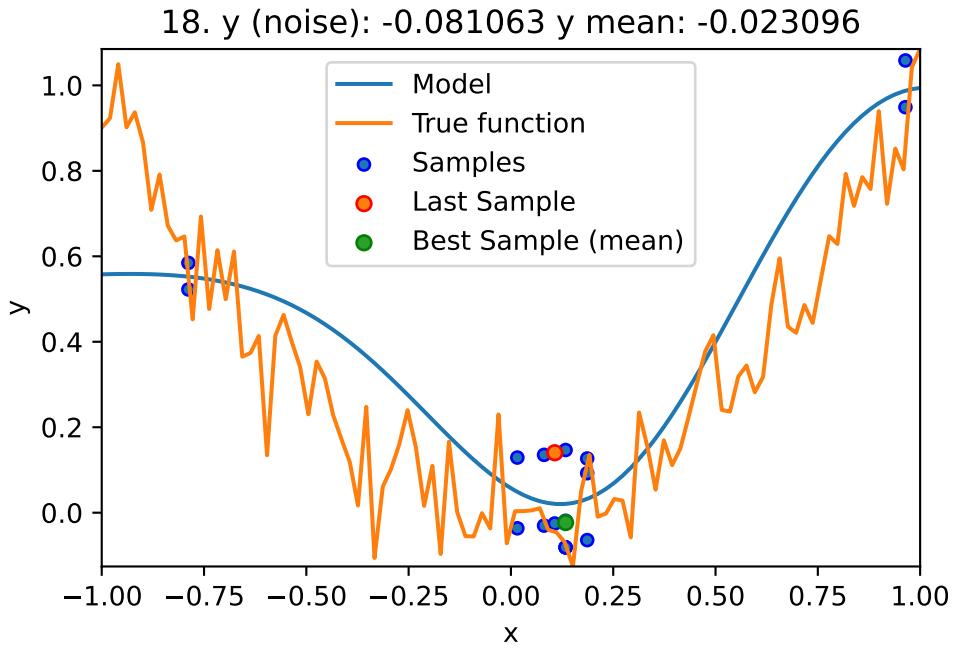
```
spot_1_noisy.run()
```

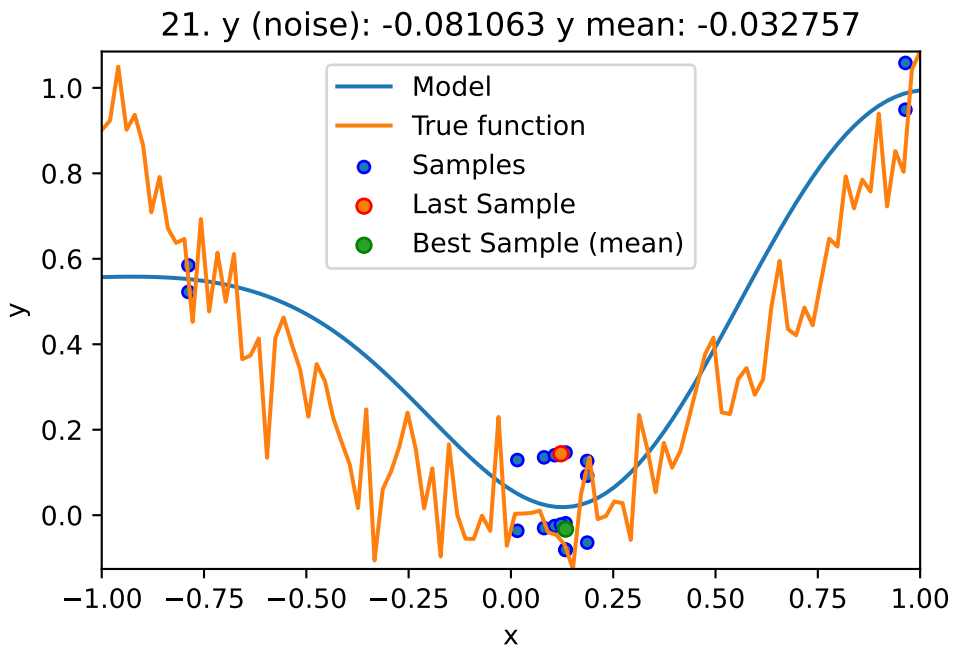


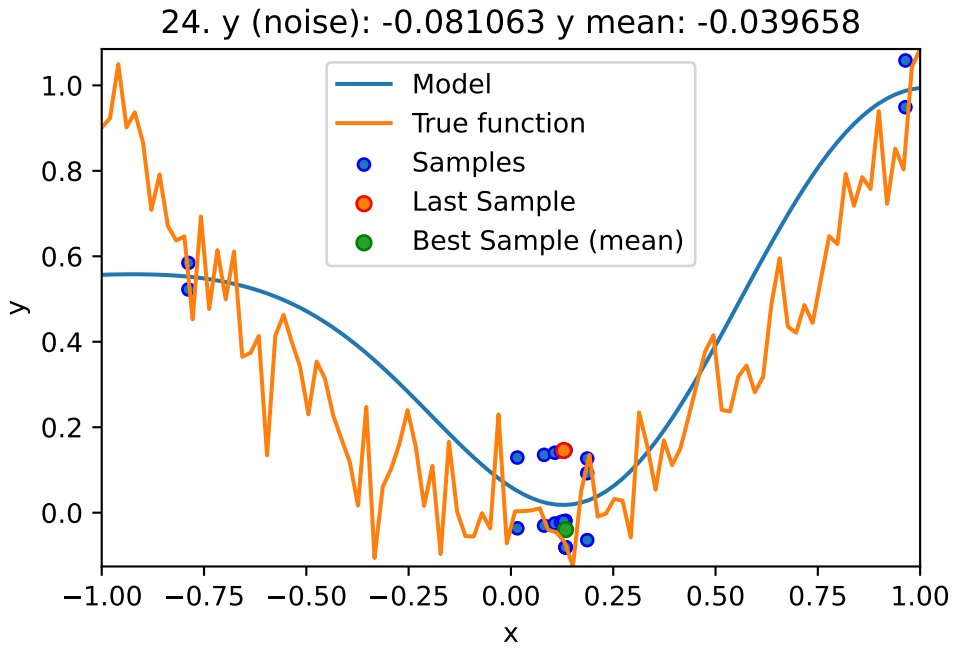

9. y (noise): -0.064157 y mean: 0.051695
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

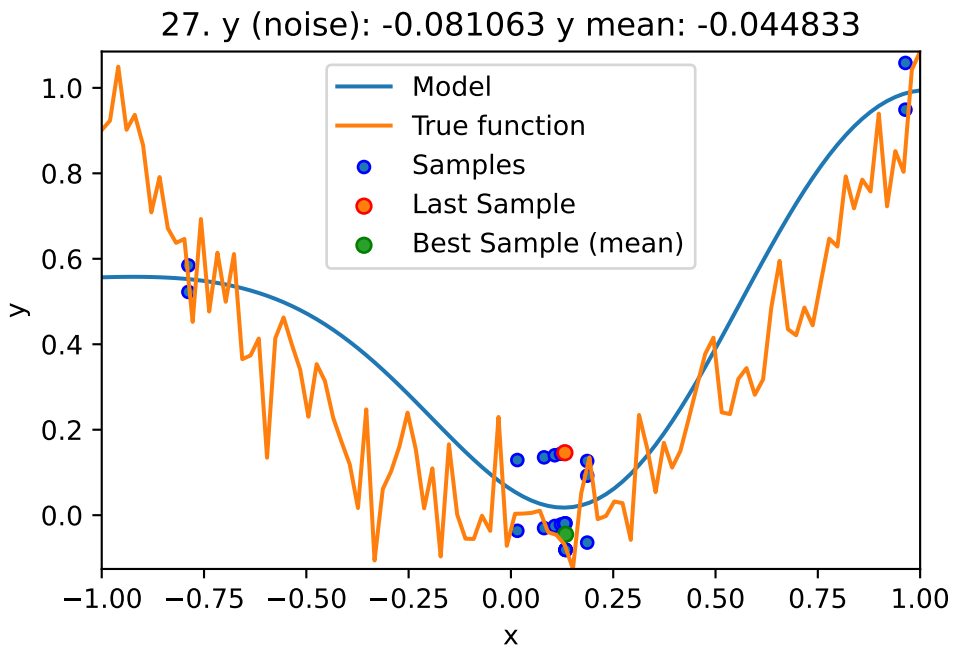

12. y (noise): -0.081063 y mean: 0.01555
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

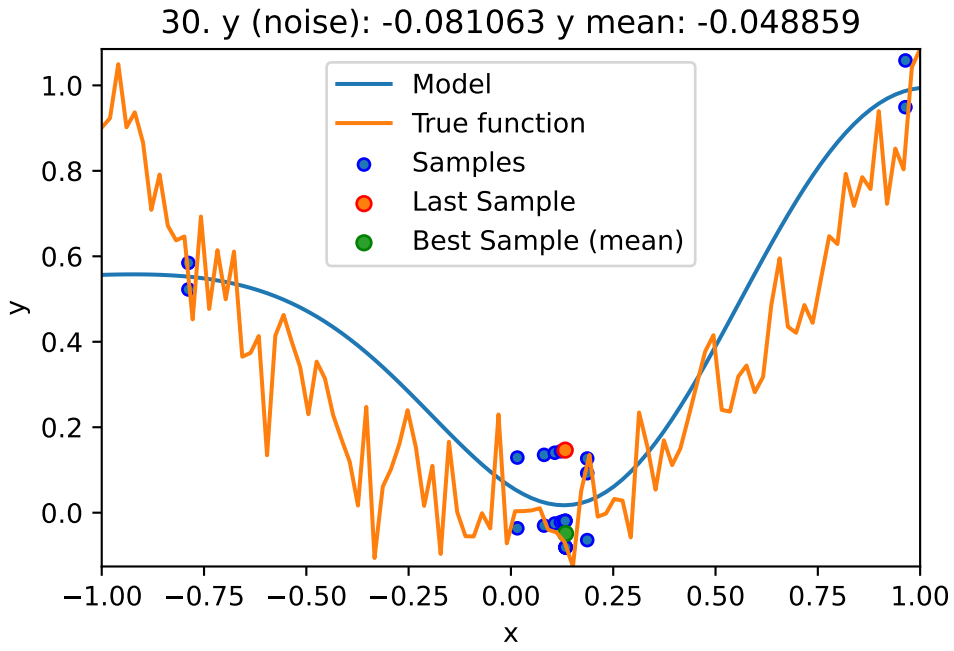

15. y (noise): -0.081063 y mean: -0.008604
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

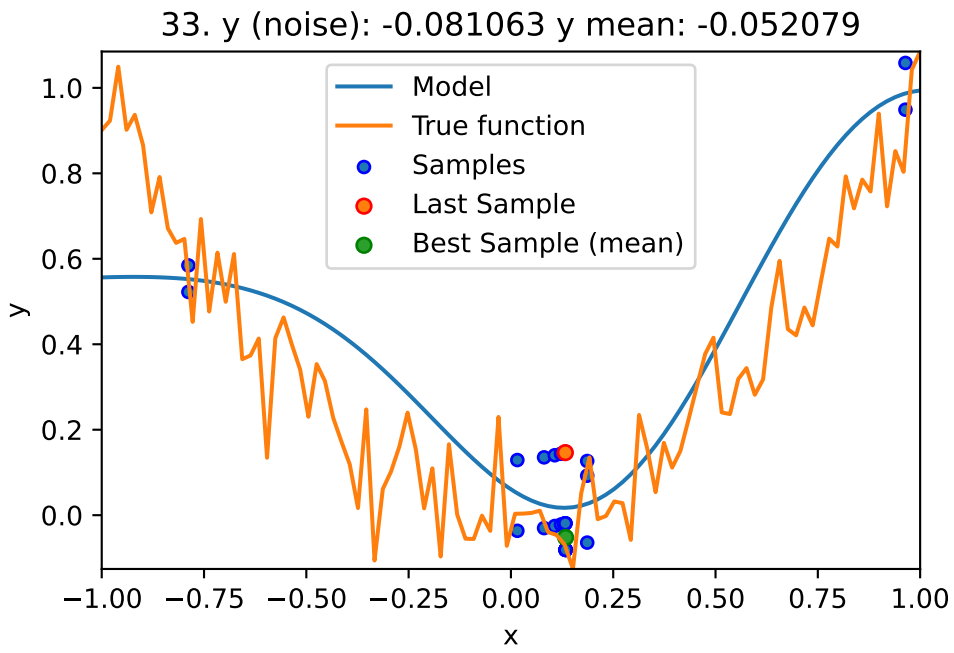

18. y (noise): -0.081063 y mean: -0.023096
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

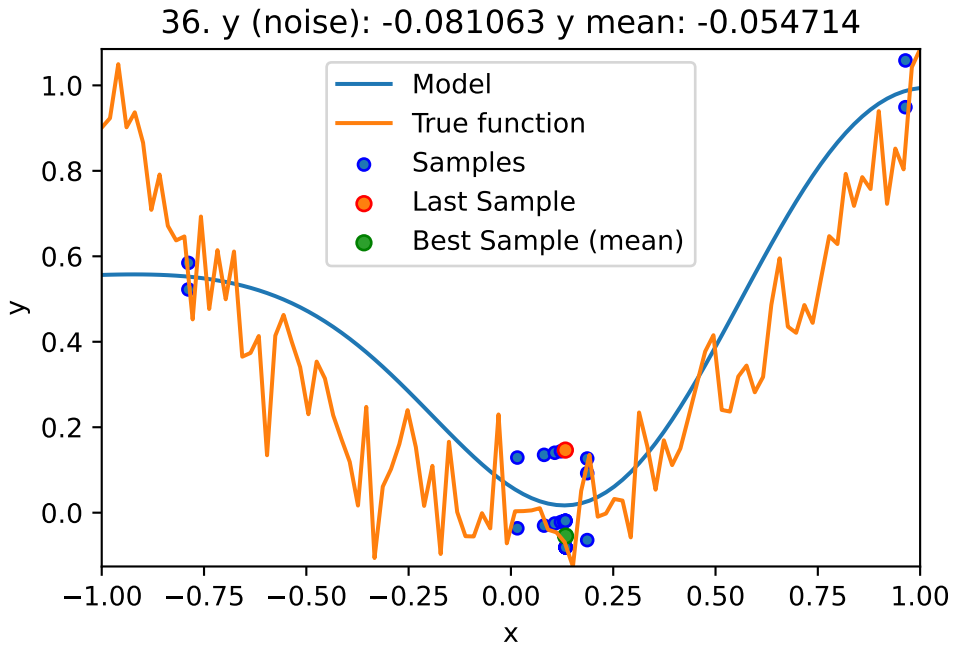

21. y (noise): -0.081063 y mean: -0.032757
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

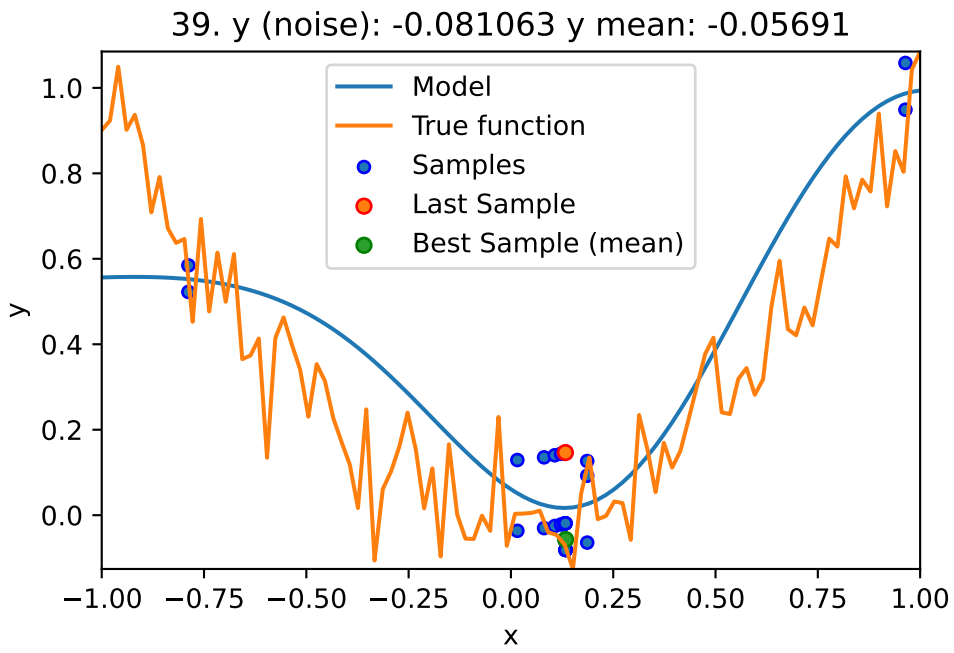

24. y (noise): -0.081063 y mean: -0.039658
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

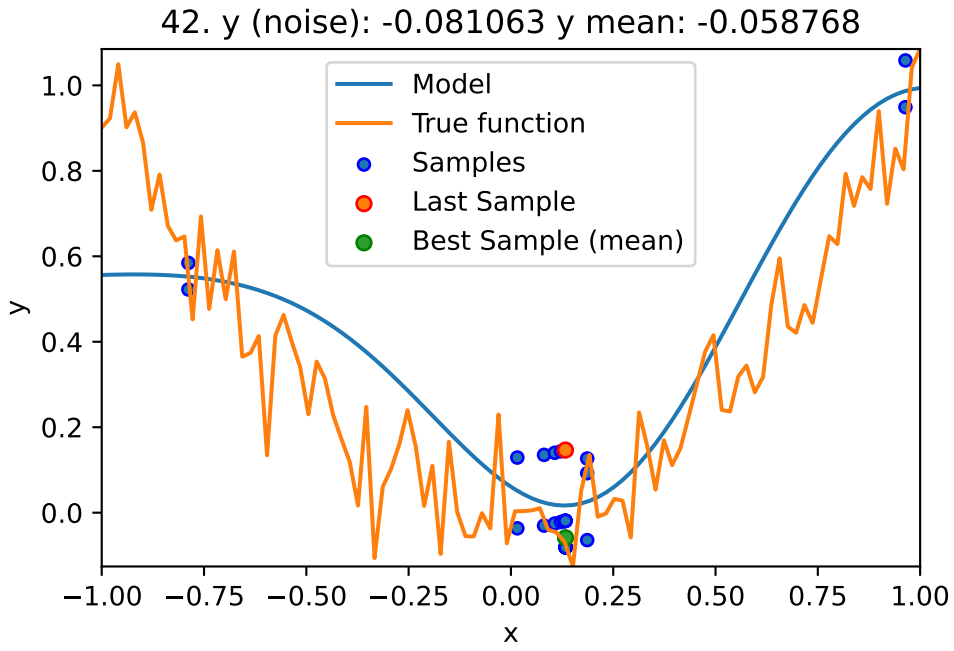

27. y (noise): -0.081063 y mean: -0.044833
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

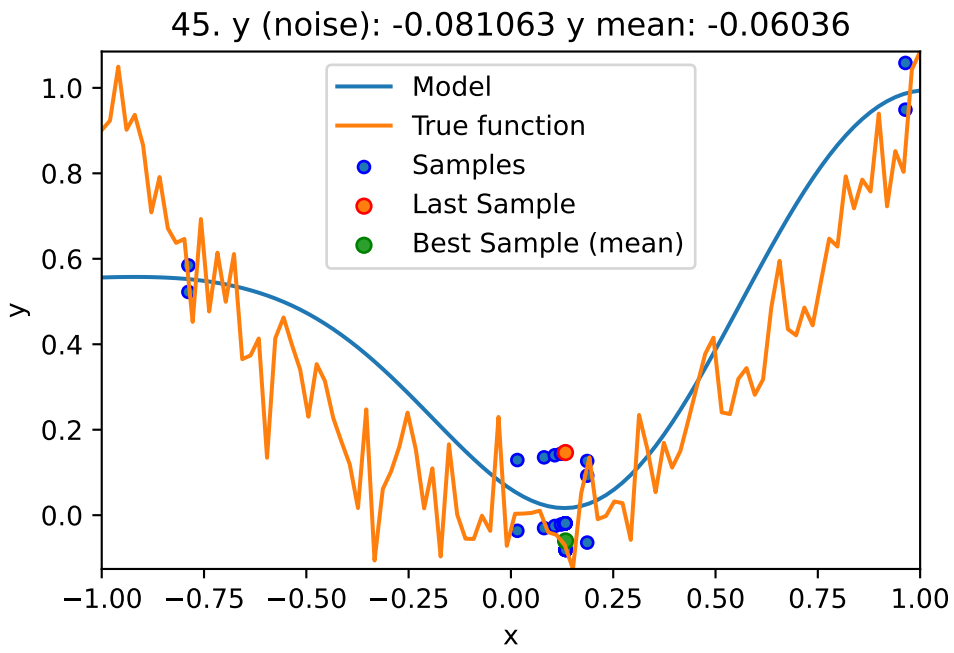

30. y (noise): -0.081063 y mean: -0.048859
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

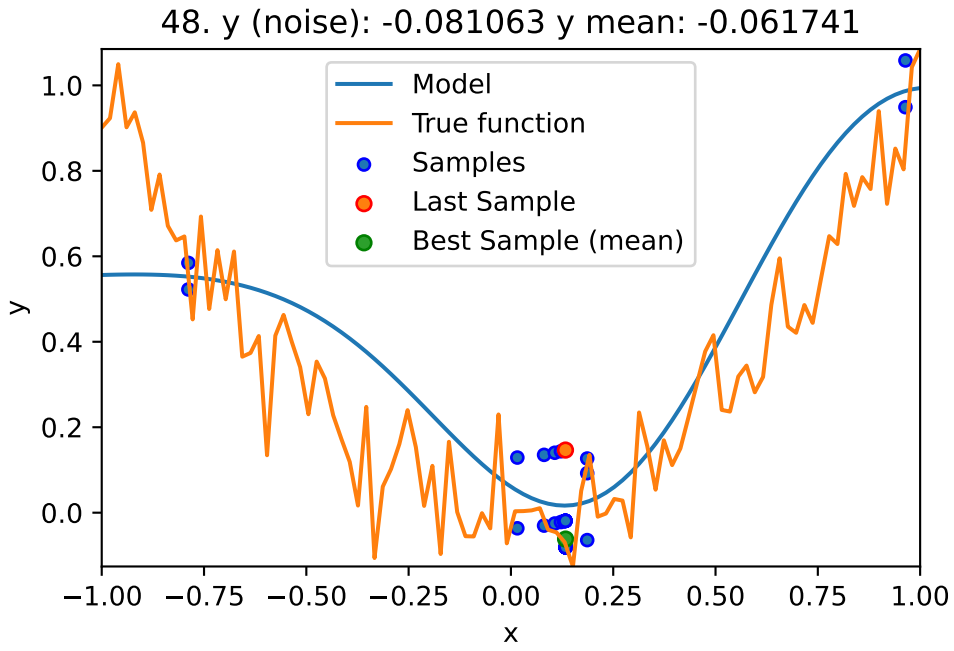

33. y (noise): -0.081063 y mean: -0.052079
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

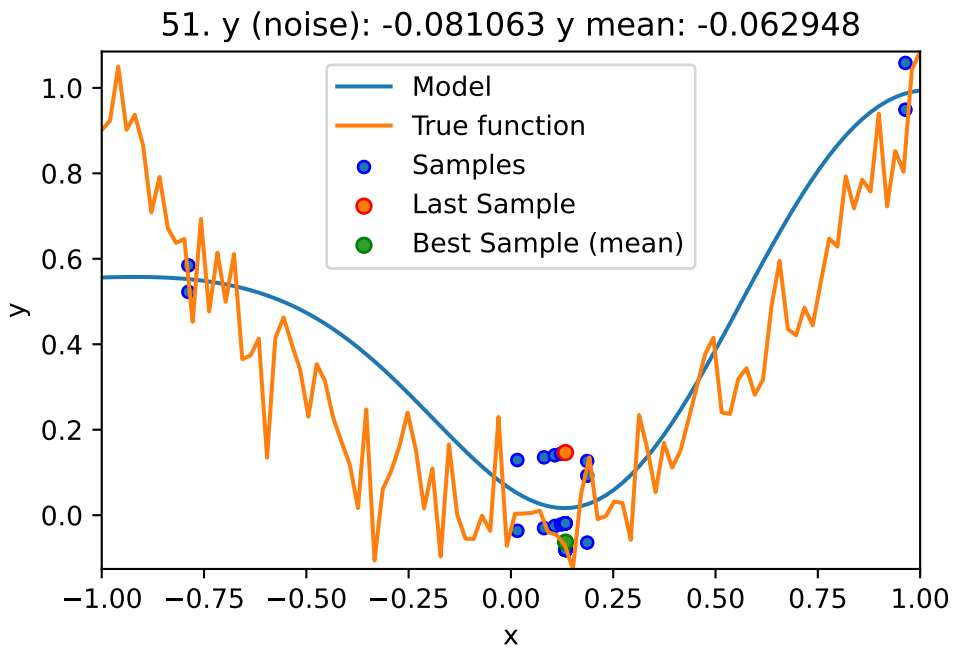

36. y (noise): -0.081063 y mean: -0.054714
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00


39. y (noise): -0.081063 y mean: -0.05691
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00


42. y (noise): -0.081063 y mean: -0.058768
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00


45. y (noise): -0.081063 y mean: -0.06036
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00


48. y (noise): -0.081063 y mean: -0.061741
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00




```
<spotPython.spot.spot.Spot at 0x16c0eb700>
```

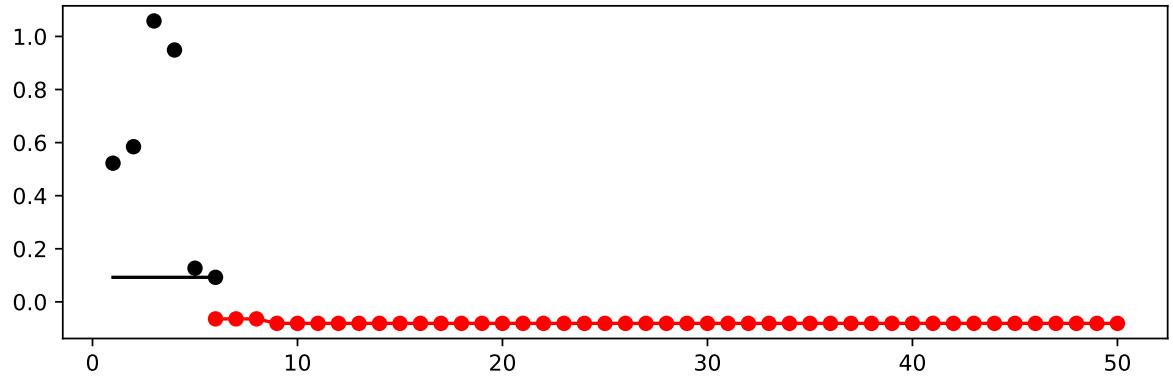
9.2 Print the Results

```
spot_1_noisy.print_results()
```

```
min y: -0.08106318979661208
x0: 0.1335999447536301
min mean y: -0.06294830660588041
x0: 0.1335999447536301

[['x0', 0.1335999447536301], ['x0', 0.1335999447536301]]
```

```
spot_1_noisy.plot_progress(log_y=False)
```



9.3 Noise and Surrogates: The Nugget Effect

9.3.1 The Noisy Sphere

9.3.1.1 The Data

We prepare some data first:

```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

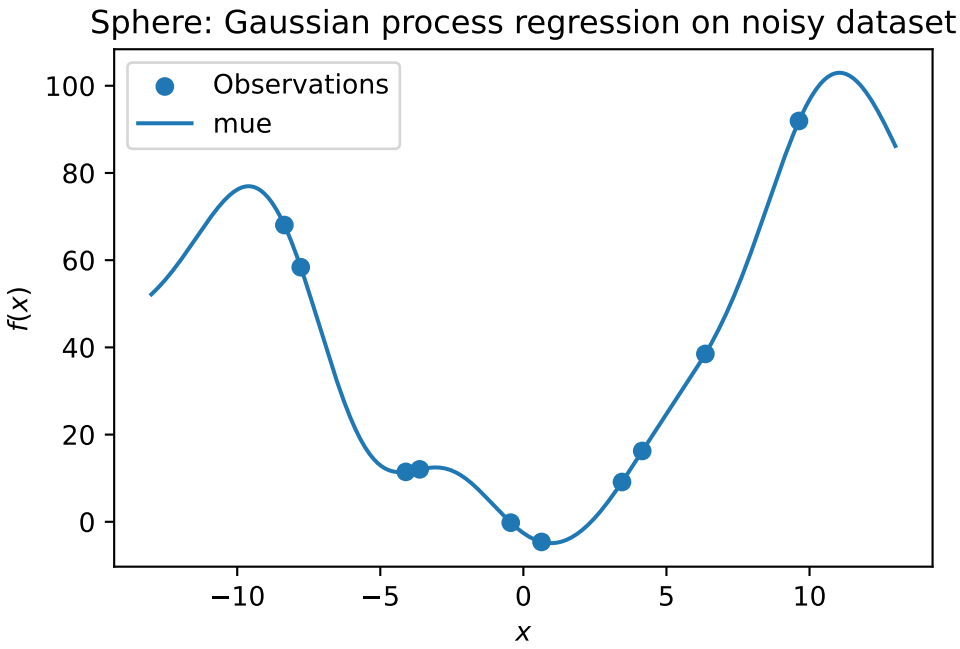
gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_sphere
fun_control = {"sigma": 2,
               "seed": 125}
X = gen.scipy_lhd(10, lower=lower, upper = upper)
y = fun(X, fun_control=fun_control)
X_train = X.reshape(-1,1)
y_train = y
```

A surrogate without nugget is fitted to these data:

```
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=False)
S.fit(X_train, y_train)

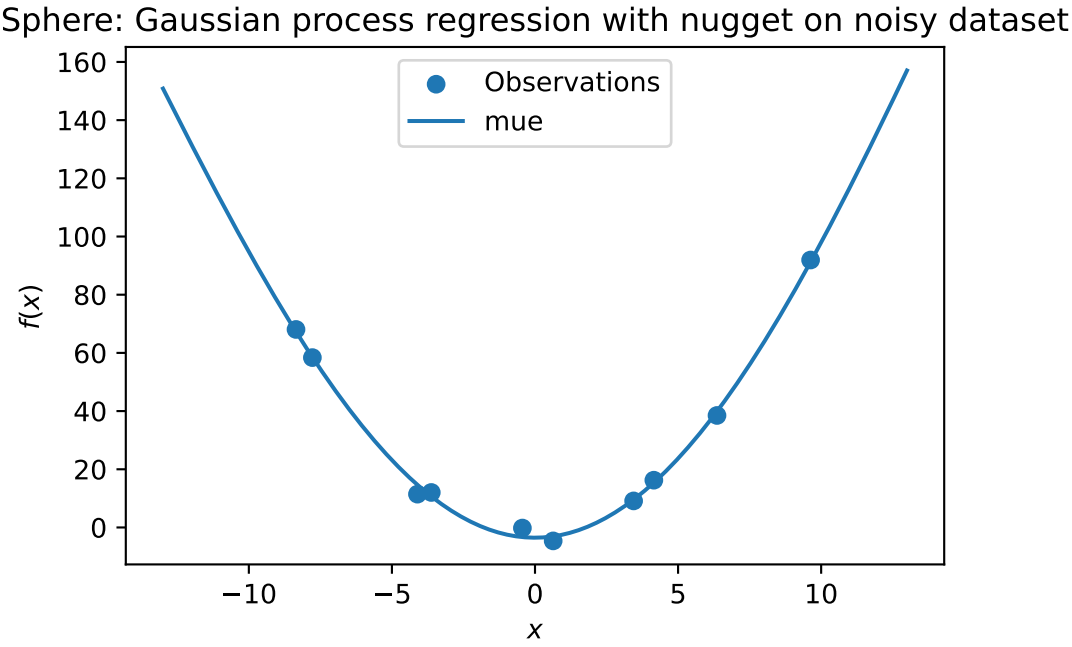
X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression on noisy dataset")
```



In comparison to the surrogate without nugget, we fit a surrogate with nugget to the data:

```
S_nug = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S_nug.fit(X_train, y_train)
X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S_nug.predict(X_axis, return_val="all")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression with nugget on noisy dataset")
```



The value of the nugget term can be extracted from the model as follows:

```
S.Lambda
```

```
S_nug.Lambda
```

```
9.088150066416743e-05
```

We see:

- the first model `S` has no nugget,
- whereas the second model has a nugget value (`Lambda`) larger than zero.

9.4 Exercises

9.4.1 Noisy `fun_cubed`

Analyse the effect of noise on the `fun_cubed` function with the following settings:

```
fun = analytical().fun_cubed
fun_control = {"sigma": 10,
               "seed": 123}
lower = np.array([-10])
upper = np.array([10])
```

9.4.2 `fun_runge`

Analyse the effect of noise on the `fun_runge` function with the following settings:

```
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = {"sigma": 0.25,
               "seed": 123}
```

9.4.3 `fun_forrester`

Analyse the effect of noise on the `fun_forrester` function with the following settings:

```
lower = np.array([0])
upper = np.array([1])
fun = analytical().fun_forrester
fun_control = {"sigma": 5,
               "seed": 123}
```

9.4.4 `fun_xsin`

Analyse the effect of noise on the `fun_xsin` function with the following settings:

```
lower = np.array([-1.])
upper = np.array([1.])
fun = analytical().fun_xsin
fun_control = {"sigma": 0.5,
               "seed": 123}
```

```
spot_1_noisy.mean_y.shape[0]
```

```
18
```

10 HPT: sklearn SVC on Moons Data

This document refers to the following software versions:

- python: 3.10.10

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93
```

```
Note: you may need to restart the kernel to use updated packages.
```

spotPython can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of spotPython from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

10.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time and the initial design size.

```
MAX_TIME = 1
INIT_SIZE = 5
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '10-sklearn' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(INIT_
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
10-sklearn_bartz09_1min_5init_2023-06-19_02-26-52
```

10.2 Step 2: Initialization of the Empty `fun_control` Dictionary

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/10_spot_hpt_sklearn_classification")
```

10.3 Step 3: SKlearn Load Data (Classification)

Randomly generate classification data.

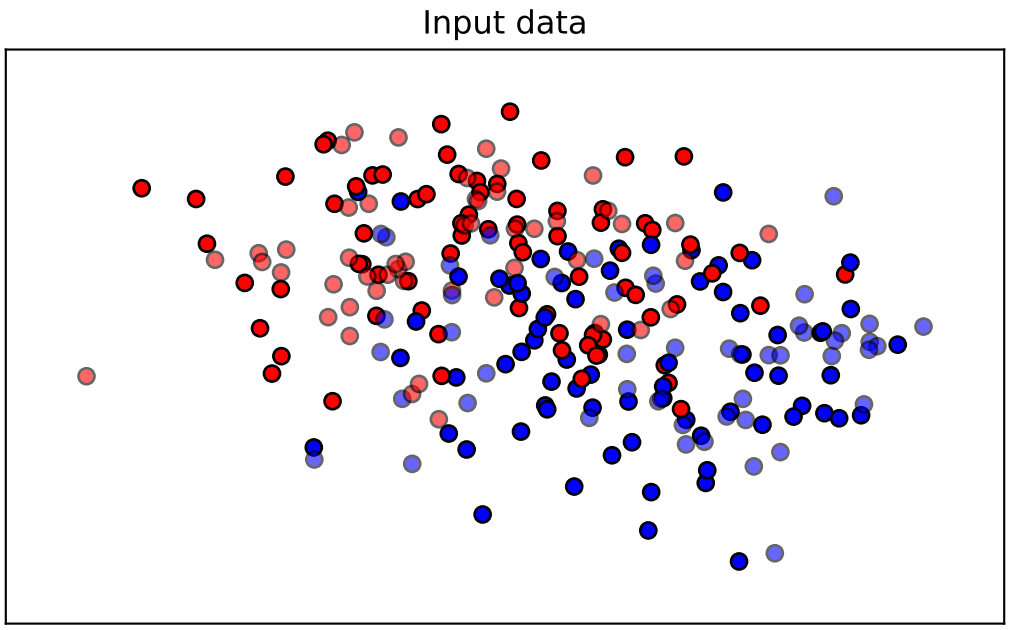
```
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.datasets import make_moons, make_circles, make_classification
n_features = 2
n_samples = 250
target_column = "y"
```

```
ds =  make_moons(n_samples, noise=0.5, random_state=0)
X, y = ds
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.4, random_state=42
)
train = pd.DataFrame(np.hstack((X_train, y_train.reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, y_test.reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
train.head()
```

	x1	x2	y
0	1.083978	-1.246111	1.0
1	0.074916	0.868104	0.0
2	-1.668535	0.751752	0.0
3	1.286597	1.454165	0.0
4	1.387021	0.448355	1.0

```
import matplotlib.pyplot as plt
from matplotlib.colors import ListedColormap

x_min, x_max = X[:, 0].min() - 0.5, X[:, 0].max() + 0.5
y_min, y_max = X[:, 1].min() - 0.5, X[:, 1].max() + 0.5
cm = plt.cm.RdBu
cm_bright = ListedColormap(["#FF0000", "#0000FF"])
ax = plt.subplot(1, 1, 1)
ax.set_title("Input data")
# Plot the training points
ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap=cm_bright, edgecolors="k")
# Plot the testing points
ax.scatter(
    X_test[:, 0], X_test[:, 1], c=y_test, cmap=cm_bright, alpha=0.6, edgecolors="k"
)
ax.set_xlim(x_min, x_max)
ax.set_ylim(y_min, y_max)
ax.set_xticks(())
ax.set_yticks(())
plt.tight_layout()
plt.show()
```




```
n_samples = len(train)
# add the dataset to the fun_control
fun_control.update({"data": None, # dataset,
                "train": train,
                "test": test,
                "n_samples": n_samples,
                "target_column": target_column})
```

10.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

```
prep_model = None
fun_control.update({"prep_model": prep_model})
```

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
from sklearn.preprocessing import StandardScaler
prep_model = StandardScaler()
fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

```
# categorical_columns = []
# one_hot_encoder = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
# prep_model = ColumnTransformer(
#         transformers=[
#             ("categorical", one_hot_encoder, categorical_columns),
#         ],
#         remainder=StandardScaler(),
#     )
```

10.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
# core_model = RandomForestClassifier
core_model = SVC
```

```
  # core_model = LogisticRegression
  # core_model = KNeighborsClassifier
  # core_model = GradientBoostingClassifier
  fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=SklearnHyperDict,
                                filename=None)
```

Now `fun_control` has the information from the JSON file. The corresponding entries for the `core_model` class are shown below.

```
  fun_control['core_model_hyper_dict']
```

```
{'C': {'type': 'float',
  'default': 1.0,
  'transform': 'None',
  'lower': 0.1,
  'upper': 10.0},
 'kernel': {'levels': ['linear', 'poly', 'rbf', 'sigmoid'],
  'type': 'factor',
  'default': 'rbf',
  'transform': 'None',
  'core_model_parameter_type': 'str',
  'lower': 0,
  'upper': 3},
 'degree': {'type': 'int',
  'default': 3,
  'transform': 'None',
  'lower': 3,
  'upper': 3},
 'gamma': {'levels': ['scale', 'auto'],
  'type': 'factor',
  'default': 'scale',
  'transform': 'None',
  'core_model_parameter_type': 'str',
  'lower': 0,
  'upper': 1},
 'coef0': {'type': 'float',
  'default': 0.0,
  'transform': 'None',
  'lower': 0.0,
  'upper': 0.0},
```

```
 'shrinking': {'levels': [0, 1],
  'type': 'factor',
  'default': 0,
  'transform': 'None',
  'core_model_parameter_type': 'bool',
  'lower': 0,
  'upper': 1},
 'probability': {'levels': [0, 1],
  'type': 'factor',
  'default': 0,
  'transform': 'None',
  'core_model_parameter_type': 'bool',
  'lower': 0,
  'upper': 1},
 'tol': {'type': 'float',
  'default': 0.001,
  'transform': 'None',
  'lower': 0.0001,
  'upper': 0.01},
 'cache_size': {'type': 'float',
  'default': 200,
  'transform': 'None',
  'lower': 100,
  'upper': 400},
 'break_ties': {'levels': [0, 1],
  'type': 'factor',
  'default': 0,
  'transform': 'None',
  'core_model_parameter_type': 'bool',
  'lower': 0,
  'upper': 1}}
```

10.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

10.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the `modify_hyper_parameter_bounds` method. For example, to change the `tol` hyperparameter of the `SVC` model to the interval [1e-3, 1e-2], the following code can be used:

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
fun_control = modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])
# fun_control = modify_hyper_parameter_bounds(fun_control, "min_samples_split", bounds=[3,
#fun_control = modify_hyper_parameter_bounds(fun_control, "merit_preprune", bounds=[0, 0])
fun_control["core_model_hyper_dict"]["tol"]
```

```
{'type': 'float',
 'default': 0.001,
 'transform': 'None',
 'lower': 0.001,
 'upper': 0.01}
```

10.6.2 Modify hyperparameter of type factor

Factors can be modified with the `modify_hyper_parameter_levels` function. For example, to exclude the `sigmoid` kernel from the tuning, the `kernel` hyperparameter of the `SVC` model can be modified as follows:

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["linear", "poly", "rbf
fun_control["core_model_hyper_dict"]["kernel"]
```

```
{'levels': ['linear', 'poly', 'rbf'],
 'type': 'factor',
 'default': 'rbf',
 'transform': 'None',
 'core_model_parameter_type': 'str',
 'lower': 0,
 'upper': 2}
```

10.6.3 Optimizers

Optimizers are described in Section 14.6.1.

10.7 Step 7: Selection of the Objective (Loss) Function

There are two metrics:

1. `metric_river` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `metric_sklearn` is used for the sklearn based evaluation.

```
from sklearn.metrics import mean_absolute_error, accuracy_score, roc_curve, roc_auc_score,
fun_control.update({
                "metric_sklearn": log_loss,
                })
```

10.7.1 Predict Classes or Class Probabilities

If the key `"predict_proba"` is set to `True`, the class probabilities are predicted. `False` is the default, i.e., the classes are predicted.

```
fun_control.update({
                "predict_proba": False,
                })
```

10.8 Step 8: Calling the SPOT Function

10.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name        | type   | default   |   lower |   upper | transform   |
|-------------|--------|-----------|---------|---------|-------------|
| C           | float  | 1.0       |   0.1   |   10    | None        |
| kernel      | factor | rbf       |   0     |    2    | None        |
| degree      | int    | 3         |   3     |    3    | None        |
| gamma       | factor | scale     |   0     |    1    | None        |
| coef0       | float  | 0.0       |   0     |    0    | None        |
| shrinking   | factor | 0         |   0     |    1    | None        |
| probability | factor | 0         |   0     |    1    | None        |
| tol         | float  | 0.001     |   0.001 |    0.01 | None        |
| cache_size  | float  | 200.0     | 100     |  400    | None        |
| break_ties  | factor | 0         |   0     |    1    | None        |
```

10.8.2 The Objective Function

The objective function is selected next. It implements an interface from `sklearn`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

10.8.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=SklearnHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
array([[1.e+00, 2.e+00, 3.e+00, 0.e+00, 0.e+00, 0.e+00, 0.e+00, 1.e-03,
        2.e+02, 0.e+00]])
```

10.8.4 Starting the Hyperparameter Tuning

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
spotPython tuning: 5.691103166702708 [----------] 2.78%

spotPython tuning: 5.691103166702708 [----------] 4.59%

spotPython tuning: 5.691103166702708 [#---------] 6.10%

spotPython tuning: 5.691103166702708 [#---------] 7.54%
```

```
spotPython tuning: 5.691103166702708 [#---------] 8.97%

spotPython tuning: 5.691103166702708 [#---------] 11.38%

spotPython tuning: 5.691103166702708 [#---------] 13.68%

spotPython tuning: 5.691103166702708 [##--------] 15.88%

spotPython tuning: 5.691103166702708 [##--------] 18.18%

spotPython tuning: 5.691103166702708 [##--------] 20.41%

spotPython tuning: 5.691103166702708 [##--------] 22.86%

spotPython tuning: 5.691103166702708 [###-------] 25.44%

spotPython tuning: 5.691103166702708 [###-------] 33.91%

spotPython tuning: 5.691103166702708 [#####-----] 45.79%

spotPython tuning: 5.691103166702708 [######----] 58.45%

spotPython tuning: 5.691103166702708 [#######---] 71.14%

spotPython tuning: 5.691103166702708 [########--] 83.66%

spotPython tuning: 5.691103166702708 [##########] 95.99%

spotPython tuning: 5.691103166702708 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x28d897040>
```

10.9 Step 9: Results

```
SAVE = False
LOAD = False

if SAVE:
    result_file_name = "res_" + experiment_name + ".pkl"
    with open(result_file_name, 'wb') as f:
        pickle.dump(spot_tuner, f)

if LOAD:
    result_file_name = "res_ch10-friedman-hpt-0_maans03_60min_20init_1K_2023-04-14_10-11-1
    with open(result_file_name, 'rb') as f:
        spot_tuner =  pickle.load(f)
```

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

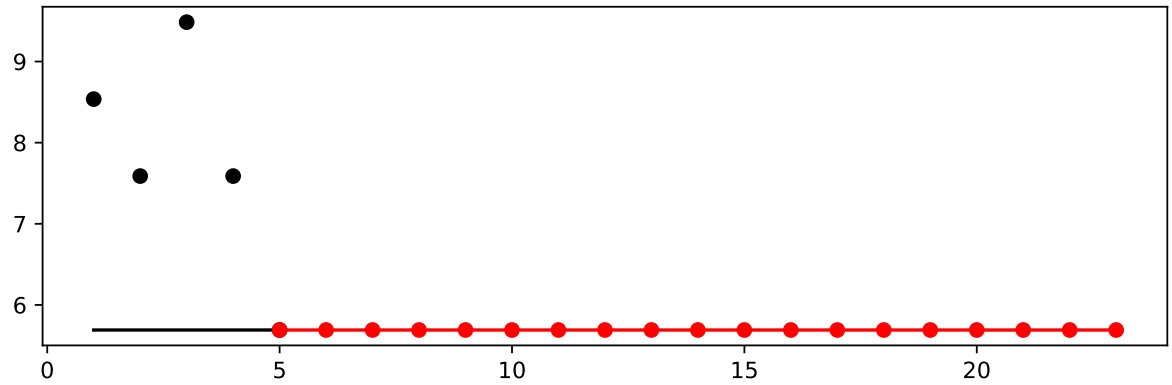


Figure 10.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

```
print(gen_design_table(fun_control=fun_control,
    spot=spot_tuner))
```

```
| name        | type   | default   |   lower |   upper |               tuned | transform
|-------------|--------|-----------|---------|---------|---------------------|------------
```

C	float	1.0	0.1	10.0	3.6280771109650245	None
kernel	factor	rbf	0.0	2.0	1.0	None
degree	int	3	3.0	3.0	3.0	None
gamma	factor	scale	0.0	1.0	0.0	None
coef0	float	0.0	0.0	0.0	0.0	None
shrinking	factor	0	0.0	1.0	1.0	None
probability	factor	0	0.0	1.0	0.0	None
tol	float	0.001	0.001	0.01	0.006642600916881275	None
cache_size	float	200.0	100.0	400.0	202.03372626175258	None
break_ties	factor	0	0.0	1.0	1.0	None

10.9.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

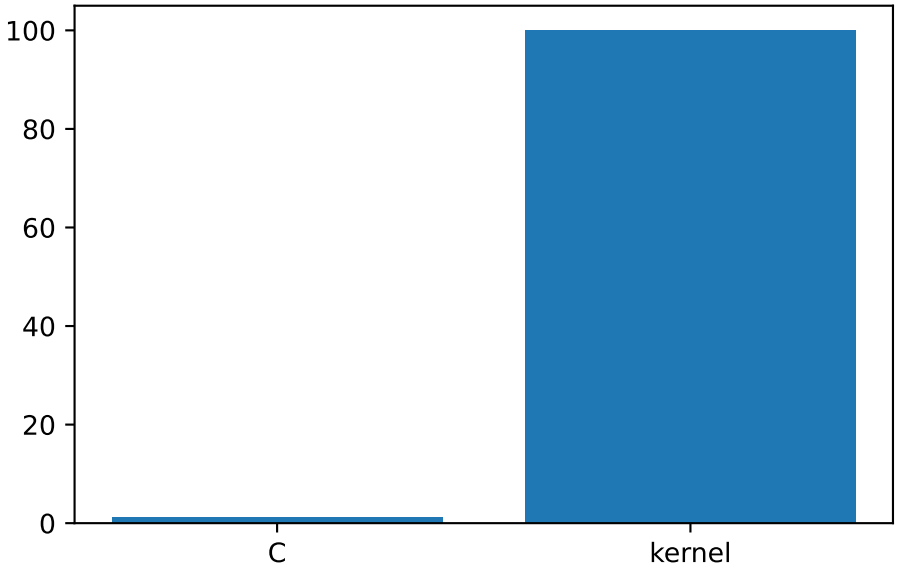


Figure 10.2: Variable importance plot, threshold 0.025.

10.9.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'C': 1.0,
 'kernel': 'rbf',
 'degree': 3,
 'gamma': 'scale',
 'coef0': 0.0,
 'shrinking': 0,
 'probability': 0,
 'tol': 0.001,
 'cache_size': 200.0,
 'break_ties': 0}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('standardscaler', StandardScaler()),
                ('svc',
                 SVC(break_ties=0, cache_size=200.0, probability=0,
                     shrinking=0))])
```

10.9.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[3.62807711e+00 1.00000000e+00 3.00000000e+00 0.00000000e+00
  0.00000000e+00 1.00000000e+00 0.00000000e+00 6.64260092e-03
  2.02033726e+02 1.00000000e+00]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

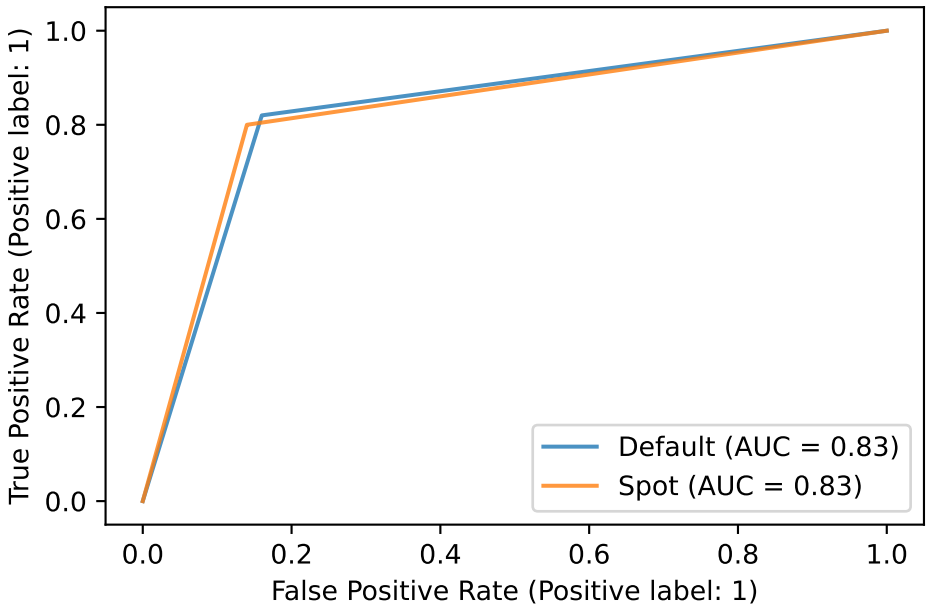
```
[{'C': 3.6280771109650245,
  'kernel': 'poly',
  'degree': 3,
  'gamma': 'scale',
  'coef0': 0.0,
  'shrinking': 1,
  'probability': 0,
  'tol': 0.006642600916881275,
  'cache_size': 202.03372626175258,
  'break_ties': 1}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

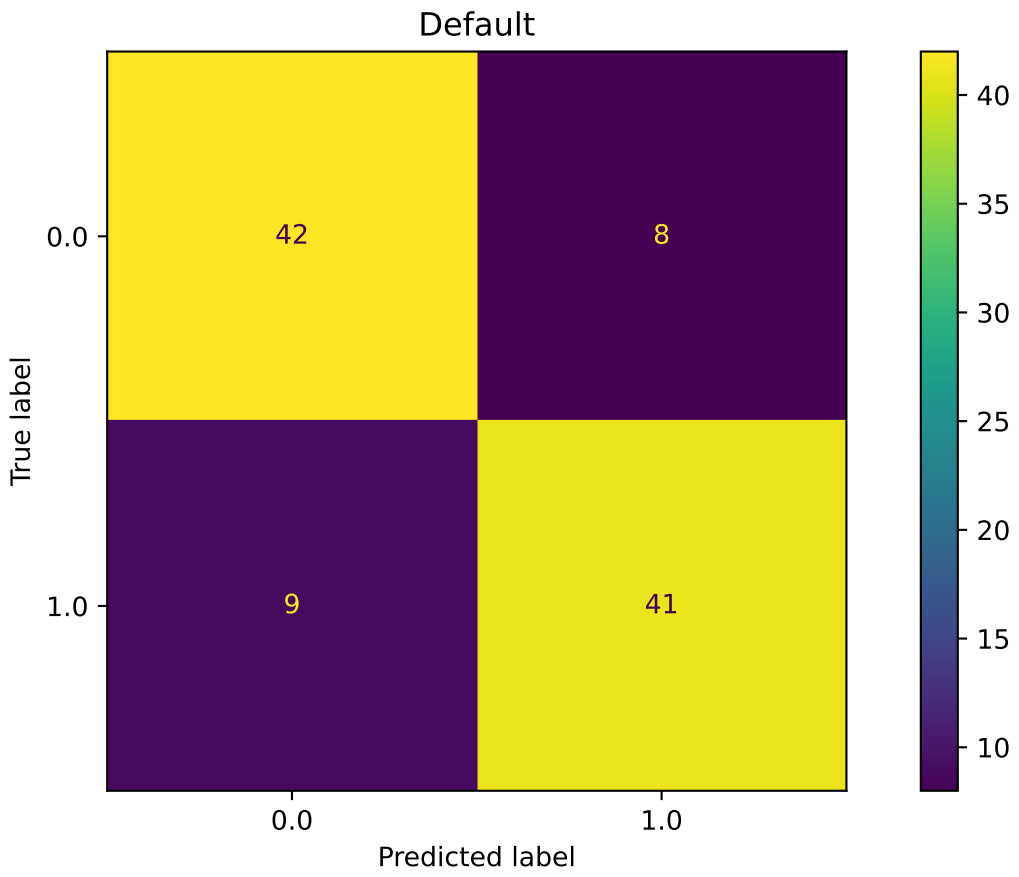
```
Pipeline(steps=[('standardscaler', StandardScaler()),
                ('svc',
                 SVC(C=3.6280771109650245, break_ties=1,
                     cache_size=202.03372626175258, kernel='poly',
                     probability=0, shrinking=1, tol=0.006642600916881275))])
```

10.9.4 Plot: Compare Predictions

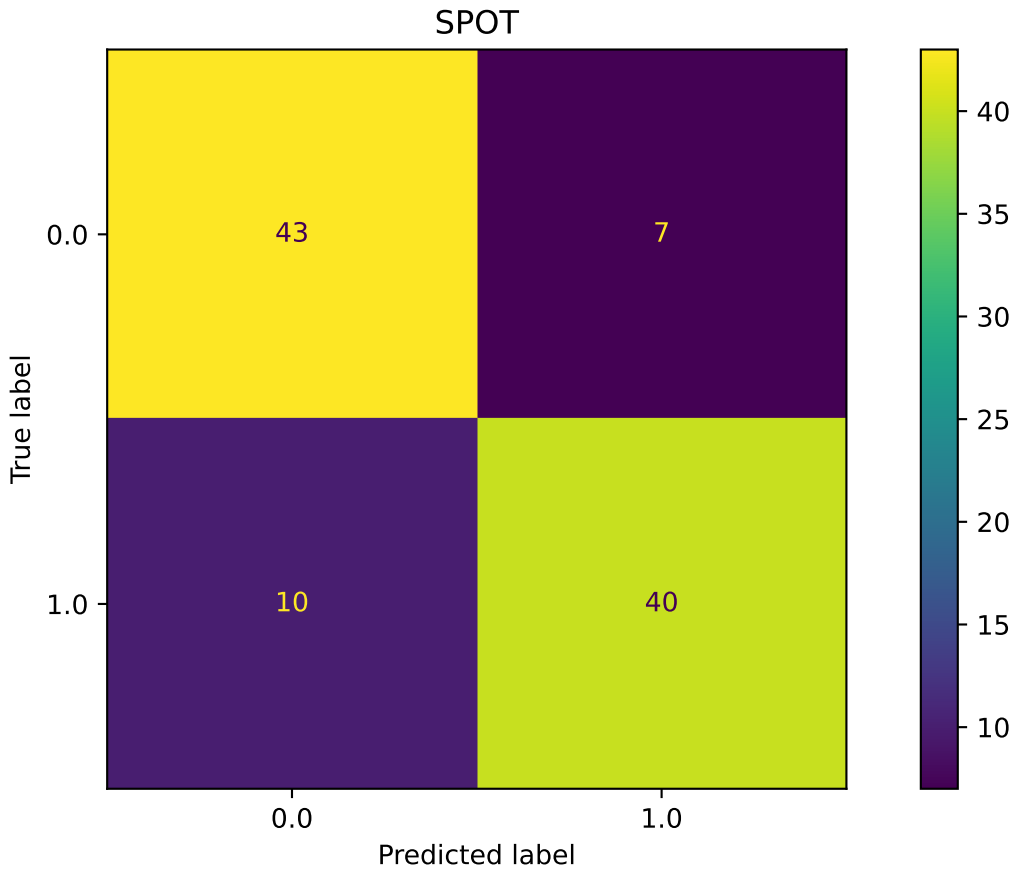
```
from spotPython.plot.validation import plot_roc
plot_roc([model_default, model_spot], fun_control, model_names=["Default", "Spot"])
```




```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```




```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```



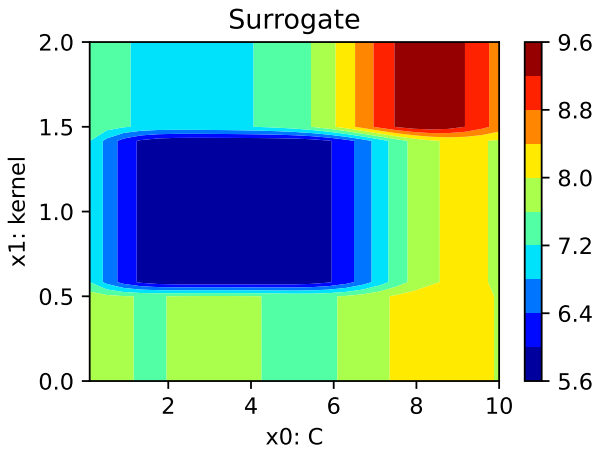

```
min(spot_tuner.y), max(spot_tuner.y)
```

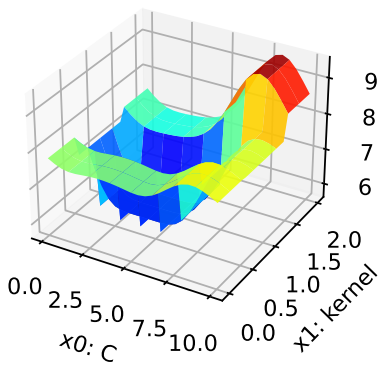
```
(5.691103166702708, 9.485171944504513)
```

10.9.5 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
C:  1.1399176173997725
kernel:  100.0
```





10.9.6 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

10.9.7 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

11 HPT: PyTorch With fashionMNIST

In this tutorial, we will show how `spotPython` can be integrated into the `PyTorch` training workflow.

This document refers to the following software versions:

- `python`: 3.10.10
- `torch`: 2.0.1
- `torchvision`: 0.15.0

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

11.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size and the device that is used.

Caution: Run time and initial design size should be increased for real experiments

- MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
- INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.

Note: Device selection

- The device can be selected by setting the variable `DEVICE`.
- Since we are using a simple neural net, the setting `"cpu"` is preferred (on Mac).
- If you have a GPU, you can use `"cuda:0"` instead.
- If DEVICE is set to `None`, `spotPython` will automatically select the device.
  - This might result in `"mps"` on Macs, which is not the best choice for simple neural nets.

```
MAX_TIME = 1
INIT_SIZE = 5
DEVICE = "cpu" # "cuda:0"
```

```
from spotPython.utils.device import getDevice
DEVICE = getDevice(DEVICE)
print(DEVICE)
```

```
cpu
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '11-torch' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(INIT_SI
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
11-torch_bartz09_1min_5init_2023-06-19_02-34-00
```

11.2 Step 2: Initialization of the Empty `fun_control` Dictionary

`spotPython` uses a Python dictionary for storing the information required for the hyperparameter tuning process, which was described in Section 14.2.

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/11_spot_hpt_torch_fashion_mnist",
    device=DEVICE)
```

11.3 Step 3: PyTorch Data Loading

11.3.1 Load fashionMNIST Data

```
from torchvision import datasets, transforms
from torchvision.transforms import ToTensor
def load_data(data_dir="./data"):
    # Download training data from open datasets.
    training_data = datasets.FashionMNIST(
        root=data_dir,
        train=True,
        download=True,
        transform=ToTensor(),
    )
    # Download test data from open datasets.
    test_data = datasets.FashionMNIST(
        root=data_dir,
        train=False,
        download=True,
        transform=ToTensor(),
    )
    return training_data, test_data
```

```
train, test = load_data()
train.data.shape, test.data.shape
```

```
(torch.Size([60000, 28, 28]), torch.Size([10000, 28, 28]))
```

```
n_samples = len(train)
# add the dataset to the fun_control
fun_control.update({"data": None,
                "train": train,
                "test": test,
                "n_samples": n_samples,
                "target_column": None})
```

11.4 Step 4: Specification of the Preprocessing Model

After the training and test data are specified and added to the `fun_control` dictionary, `spotPython` allows the specification of a data preprocessing pipeline, e.g., for the scaling of the data or for the one-hot encoding of categorical variables, see Section 14.4. This feature is not used here, so we do not change the default value (which is `None`).

11.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

`spotPython` implements a class which is similar to the class described in the PyTorch tutorial. The class is called `Net_fashionMNIST` and is implemented in the file `netfashionMNIST.py`. The class is imported here.

```
from torch import nn
import spotPython.torch.netcore as netcore


class Net_fashionMNIST(netcore.Net_Core):
    def __init__(self, l1, l2, lr_mult, batch_size, epochs, k_folds, patience, optimizer,
        super(Net_fashionMNIST, self).__init__(
            lr_mult=lr_mult,
            batch_size=batch_size,
            epochs=epochs,
```

```
            k_folds=k_folds,
            patience=patience,
            optimizer=optimizer,
            sgd_momentum=sgd_momentum,
        )
        self.flatten = nn.Flatten()
        self.linear_relu_stack = nn.Sequential(
            nn.Linear(28 * 28, l1),
            nn.ReLU(),
            nn.Linear(l1, l2),
            nn.ReLU(),
            nn.Linear(l2, 10)
        )

    def forward(self, x):
        x = self.flatten(x)
        logits = self.linear_relu_stack(x)
        return logits
```

This class inherits from the class `Net_Core` which is implemented in the file `netcore.py`, see Section 14.5.1.

```
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.torch.netfashionMNIST import Net_fashionMNIST
from spotPython.hyperparameters.values import add_core_model_to_fun_control
fun_control = add_core_model_to_fun_control(core_model=Net_fashionMNIST,
                                fun_control=fun_control,
                                hyper_dict=TorchHyperDict,
                                filename=None)
```

11.5.1 The Search Space

11.5.2 Configuring the Search Space With spotPython

11.5.2.1 The `hyper_dict` Hyperparameters for the Selected Algorithm

`spotPython` uses `JSON` files for the specification of the hyperparameters, which were described in Section 14.5.5.

The corresponding entries for the `core_model` class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'l1': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 9},
 'l2': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 9},
 'lr_mult': {'type': 'float',
  'default': 1.0,
  'transform': 'None',
  'lower': 0.1,
  'upper': 10.0},
 'batch_size': {'type': 'int',
  'default': 4,
  'transform': 'transform_power_2_int',
  'lower': 1,
  'upper': 4},
 'epochs': {'type': 'int',
  'default': 3,
  'transform': 'transform_power_2_int',
  'lower': 3,
  'upper': 4},
 'k_folds': {'type': 'int',
  'default': 1,
  'transform': 'None',
  'lower': 1,
  'upper': 1},
 'patience': {'type': 'int',
  'default': 5,
  'transform': 'None',
  'lower': 2,
  'upper': 10},
 'optimizer': {'levels': ['Adadelta',
   'Adagrad',
   'Adam',
   'AdamW',
   'SparseAdam',
```

```
   'Adamax',
   'ASGD',
   'NAdam',
   'RAdam',
   'RMSprop',
   'Rprop',
   'SGD'],
  'type': 'factor',
  'default': 'SGD',
  'transform': 'None',
  'core_model_parameter_type': 'str',
  'lower': 0,
  'upper': 12},
 'sgd_momentum': {'type': 'float',
  'default': 0.0,
  'transform': 'None',
  'lower': 0.0,
  'upper': 1.0}}
```

11.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

11.6.1 Modify hyperparameter of type numeric and integer (boolean)

The hyperparameter `k_folds` is not used, it is de-activated here by setting the lower and upper bound to the same value.

Caution: Small net size, number of epochs, and patience for demonstration purposes

- Net sizes `l1` and `l2` as well as `epochs` and `patience` are set to small values for demonstration purposes. These values are too small for a real application.
- More resonable values are, e.g.:
  - `fun_control = modify_hyper_parameter_bounds(fun_control, "l1", bounds=[2, 7])`
  - `fun_control = modify_hyper_parameter_bounds(fun_control,`

```
    "epochs", bounds=[7, 9]) and
- fun_control = modify_hyper_parameter_bounds(fun_control,
  "patience", bounds=[2, 7])
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
fun_control = modify_hyper_parameter_bounds(fun_control, "k_folds", bounds=[0, 0])
fun_control = modify_hyper_parameter_bounds(fun_control, "patience", bounds=[2, 2])
fun_control = modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[2, 3])
fun_control = modify_hyper_parameter_bounds(fun_control, "l1", bounds=[2, 5])
fun_control = modify_hyper_parameter_bounds(fun_control, "l2", bounds=[2, 5])
```

11.6.2 Modify hyperparameter of type factor

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer",["Adam", "AdamW", "Ad
```

11.6.3 Optimizers

Optimizers are described in Section 14.6.1.

```
fun_control = modify_hyper_parameter_bounds(fun_control,
    "lr_mult", bounds=[1e-3, 1e-3])
fun_control = modify_hyper_parameter_bounds(fun_control,
    "sgd_momentum", bounds=[0.9, 0.9])
```

11.7 Step 7: Selection of the Objective (Loss) Function

11.7.1 Evaluation

The evaluation procedure requires the specification of two elements:

1. the way how the data is split into a train and a test set and
2. the loss function (and a metric).

These are described in Section 19.7.1.

The key `"loss_function"` specifies the loss function which is used during the optimization, see Section 14.7.5.

We will use CrossEntropy loss for the multiclass-classification task.

```
from torch.nn import CrossEntropyLoss
loss_function = CrossEntropyLoss()
fun_control.update({
        "loss_function": loss_function,
        "shuffle": True,
        "eval":  "train_hold_out"
        })
```

11.7.2 Metric

```
from torchmetrics import Accuracy
metric_torch = Accuracy(task="multiclass", num_classes=10).to(fun_control["device"])
fun_control.update({"metric_torch": metric_torch})
```

11.8 Step 8: Calling the SPOT Function

11.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name          | type    | default    |   lower |   upper | transform              |
|---------------|---------|------------|---------|---------|------------------------|
```

l1	int	5	2	5	transform_power_2_int
l2	int	5	2	5	transform_power_2_int
lr_mult	float	1.0	0.001	0.001	None
batch_size	int	4	1	4	transform_power_2_int
epochs	int	3	2	3	transform_power_2_int
k_folds	int	1	0	0	None
patience	int	5	2	2	None
optimizer	factor	SGD	0	3	None
sgd_momentum	float	0.0	0.9	0.9	None

11.8.2 The Objective Function `fun_torch`

The objective function `fun_torch` is selected next. It implements an interface from `PyTorch`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypertorch import HyperTorch
fun = HyperTorch().fun_torch
```

11.8.3 Starting the Hyperparameter Tuning

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
```

```
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
config: {'l1': 16, 'l2': 8, 'lr_mult': 0.001, 'batch_size': 16, 'epochs': 8, 'k_folds': 0, 'p
Epoch: 1 |

MulticlassAccuracy: 0.1395833343267441 | Loss: 2.2910702989896139 | Acc: 0.1395833333333333.
Epoch: 2 |

MulticlassAccuracy: 0.1887083351612091 | Loss: 2.2610746043523151 | Acc: 0.1887083333333333.
Epoch: 3 |

MulticlassAccuracy: 0.1938333362340927 | Loss: 2.2349918131828308 | Acc: 0.1938333333333333.
Epoch: 4 |

MulticlassAccuracy: 0.2007916718721390 | Loss: 2.2061429832776387 | Acc: 0.2007916666666667.
Epoch: 5 |

MulticlassAccuracy: 0.2020833343267441 | Loss: 2.1774697759946187 | Acc: 0.2020833333333333.
Epoch: 6 |

MulticlassAccuracy: 0.2025416642427444 | Loss: 2.1493491821289061 | Acc: 0.2025416666666667.
Epoch: 7 |

MulticlassAccuracy: 0.2015833407640457 | Loss: 2.1234116615454357 | Acc: 0.2015833333333333.
Epoch: 8 |
```

```
MulticlassAccuracy: 0.2035000026226044 | Loss: 2.0989609602292378 | Acc: 0.2035000000000000.
Returned to Spot: Validation loss: 2.098960960229238

config: {'l1': 8, 'l2': 8, 'lr_mult': 0.001, 'batch_size': 8, 'epochs': 4, 'k_folds': 0, 'pat
Epoch: 1 |


MulticlassAccuracy: 0.0995416641235352 | Loss: 2.3227417463461557 | Acc: 0.0995416666666667.
Epoch: 2 |


MulticlassAccuracy: 0.0995416641235352 | Loss: 2.3156459696292879 | Acc: 0.0995416666666667.
Epoch: 3 |


MulticlassAccuracy: 0.0995416641235352 | Loss: 2.3093050432999931 | Acc: 0.0995416666666667.
Epoch: 4 |


MulticlassAccuracy: 0.0999583303928375 | Loss: 2.3032854072252911 | Acc: 0.0999583333333333.
Returned to Spot: Validation loss: 2.303285407225291

config: {'l1': 32, 'l2': 16, 'lr_mult': 0.001, 'batch_size': 2, 'epochs': 8, 'k_folds': 0, 'p
Epoch: 1 |


MulticlassAccuracy: 0.2719583213329315 | Loss: 2.1422173360188803 | Acc: 0.2719583333333334.
Epoch: 2 |


MulticlassAccuracy: 0.3155833184719086 | Loss: 1.9287186470131079 | Acc: 0.3155833333333333.
Epoch: 3 |


MulticlassAccuracy: 0.3675000071525574 | Loss: 1.6976838712344566 | Acc: 0.3675000000000000.
Epoch: 4 |


MulticlassAccuracy: 0.4343749880790710 | Loss: 1.4833368577162425 | Acc: 0.4343750000000000.
Epoch: 5 |


MulticlassAccuracy: 0.5630833506584167 | Loss: 1.3038433362829189 | Acc: 0.5630833333333334.
Epoch: 6 |


MulticlassAccuracy: 0.5956666469573975 | Loss: 1.1723824600316584 | Acc: 0.5956666666666667.
Epoch: 7 |
```

```
MulticlassAccuracy: 0.6169166564941406 | Loss: 1.0750376099298398 | Acc: 0.6169166666666667.
Epoch: 8 |

MulticlassAccuracy: 0.6428750157356262 | Loss: 1.0028487622166673 | Acc: 0.6428750000000000.
Returned to Spot: Validation loss: 1.0028487622166673

config: {'l1': 4, 'l2': 8, 'lr_mult': 0.001, 'batch_size': 4, 'epochs': 4, 'k_folds': 0, 'pat
Epoch: 1 |

MulticlassAccuracy: 0.1016250029206276 | Loss: 2.2951913241545361 | Acc: 0.1016250000000000.
Epoch: 2 |

MulticlassAccuracy: 0.0960833355784416 | Loss: 2.2737737801869708 | Acc: 0.0960833333333333.
Epoch: 3 |

MulticlassAccuracy: 0.1021666675806046 | Loss: 2.2533710262775419 | Acc: 0.1021666666666667.
Epoch: 4 |

MulticlassAccuracy: 0.1210833340883255 | Loss: 2.2334476508696874 | Acc: 0.1210833333333333.
Returned to Spot: Validation loss: 2.2334476508696874

config: {'l1': 16, 'l2': 32, 'lr_mult': 0.001, 'batch_size': 8, 'epochs': 8, 'k_folds': 0, 'p
Epoch: 1 |

MulticlassAccuracy: 0.1032499969005585 | Loss: 2.2762544226646422 | Acc: 0.1032500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.2049583345651627 | Loss: 2.2346506589253745 | Acc: 0.2049583333333333.
Epoch: 3 |

MulticlassAccuracy: 0.1946666687726974 | Loss: 2.1924666829903923 | Acc: 0.1946666666666667.
Epoch: 4 |

MulticlassAccuracy: 0.1942083388566971 | Loss: 2.1497441027164461 | Acc: 0.1942083333333333.
Epoch: 5 |

MulticlassAccuracy: 0.1945416629314423 | Loss: 2.1075240010420480 | Acc: 0.1945416666666667.
Epoch: 6 |
```

```
MulticlassAccuracy: 0.1961666643619537 | Loss: 2.0650026981433234 | Acc: 0.1961666666666667.
Epoch: 7 |

MulticlassAccuracy: 0.2014999985694885 | Loss: 2.0221298006772996 | Acc: 0.2015000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.2169999927282333 | Loss: 1.9782093891302746 | Acc: 0.2170000000000000.
Returned to Spot: Validation loss: 1.9782093891302746


config: {'l1': 8, 'l2': 16, 'lr_mult': 0.001, 'batch_size': 8, 'epochs': 8, 'k_folds': 0, 'pa
Epoch: 1 |

MulticlassAccuracy: 0.0982916653156281 | Loss: 2.2982495419979094 | Acc: 0.0982916666666667.
Epoch: 2 |

MulticlassAccuracy: 0.0982916653156281 | Loss: 2.2705754169623056 | Acc: 0.0982916666666667.
Epoch: 3 |

MulticlassAccuracy: 0.0982916653156281 | Loss: 2.2382629959980647 | Acc: 0.0982916666666667.
Epoch: 4 |

MulticlassAccuracy: 0.1042499989271164 | Loss: 2.2041005131006242 | Acc: 0.1042500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.1448333263397217 | Loss: 2.1684542604287467 | Acc: 0.1448333333333333.
Epoch: 6 |

MulticlassAccuracy: 0.1692083328962326 | Loss: 2.1305531595547995 | Acc: 0.1692083333333333.
Epoch: 7 |

MulticlassAccuracy: 0.1992083340883255 | Loss: 2.0902105062007905 | Acc: 0.1992083333333333.
Epoch: 8 |

MulticlassAccuracy: 0.2788749933242798 | Loss: 2.0482383878628414 | Acc: 0.2788750000000000.
Returned to Spot: Validation loss: 2.0482383878628414
spotPython tuning: 1.0028487622166673 [####------] 44.27%
```

```
config: {'l1': 16, 'l2': 16, 'lr_mult': 0.001, 'batch_size': 2, 'epochs': 4, 'k_folds': 0, '
Epoch: 1 |

MulticlassAccuracy: 0.1944999992847443 | Loss: 2.2520305745303633 | Acc: 0.1945000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.2562916576862335 | Loss: 2.1541367422242961 | Acc: 0.2562916666666666.
Epoch: 3 |

MulticlassAccuracy: 0.3050416707992554 | Loss: 2.0353351381421088 | Acc: 0.3050416666666667.
Epoch: 4 |

MulticlassAccuracy: 0.3342083394527435 | Loss: 1.9166675697068374 | Acc: 0.3342083333333333.
Returned to Spot: Validation loss: 1.9166675697068374
spotPython tuning: 1.0028487622166673 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x17fc53af0>
```

11.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

11.10 Step 10: Results

After the hyperparameter tuning run is finished, the results can be analyzed as described in Section 14.10.

```
SAVE = False
LOAD = False

if SAVE:
    result_file_name = "res_" + experiment_name + ".pkl"
    with open(result_file_name, 'wb') as f:
        pickle.dump(spot_tuner, f)

if LOAD:
```

```
    result_file_name = "ADD THE NAME here, e.g.: res_ch10-friedman-hpt-0_maans03_60min_20i
    with open(result_file_name, 'rb') as f:
        spot_tuner =  pickle.load(f)
```

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

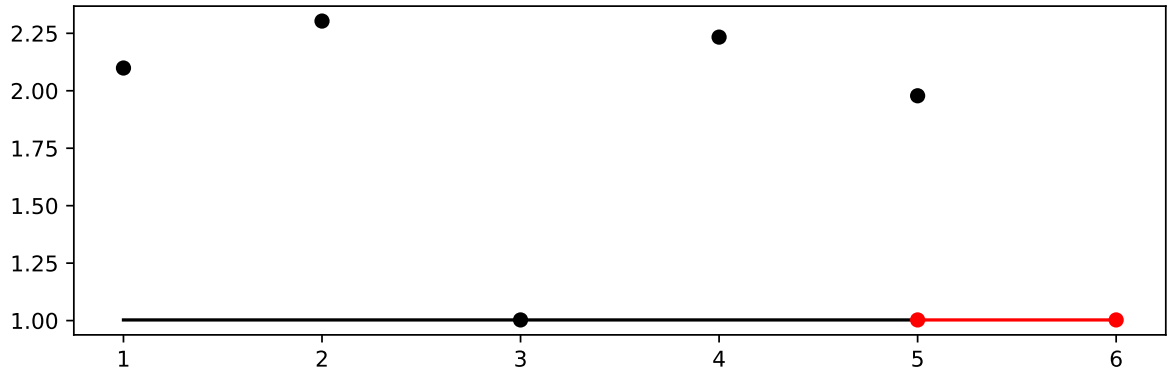


Figure 11.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

```
print(gen_design_table(fun_control=fun_control,
    spot=spot_tuner))
```

name	type	default	lower	upper	tuned	transform
l1	int	5	2.0	5.0	5.0	transform_power_2_int
l2	int	5	2.0	5.0	4.0	transform_power_2_int
lr_mult	float	1.0	0.001	0.001	0.001	None
batch_size	int	4	1.0	4.0	1.0	transform_power_2_int
epochs	int	3	2.0	3.0	3.0	transform_power_2_int
k_folds	int	1	0.0	0.0	0.0	None
patience	int	5	2.0	2.0	2.0	None
optimizer	factor	SGD	0.0	3.0	3.0	None
sgd_momentum	float	0.0	0.9	0.9	0.9	None

11.10.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

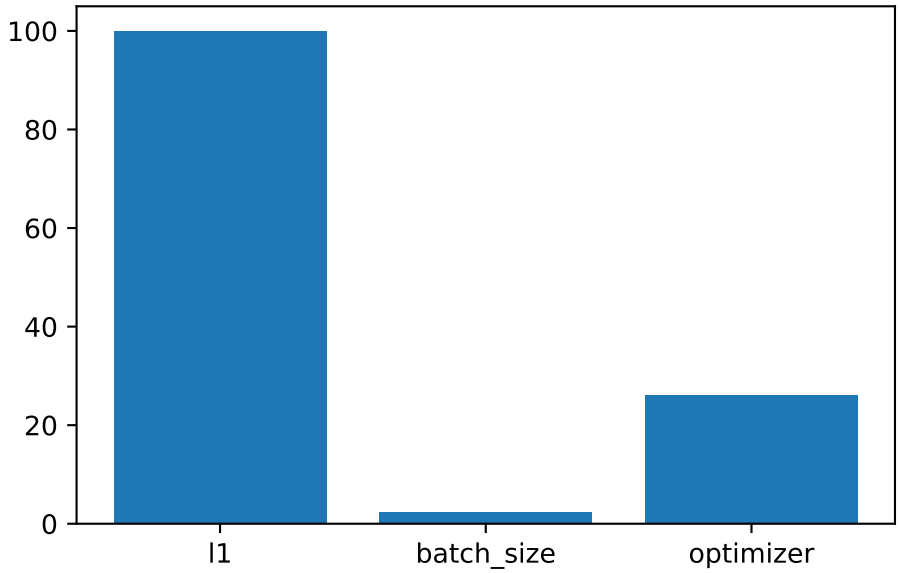


Figure 11.2: Variable importance plot, threshold 0.025.

11.10.2 Get the Tuned Architecture (SPOT Results)

The architecture of the `spotPython` model can be obtained by the following code:

```
from spotPython.hyperparameters.values import get_one_core_model_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
model_spot = get_one_core_model_from_X(X, fun_control)
model_spot
```

```
Net_fashionMNIST(
  (flatten): Flatten(start_dim=1, end_dim=-1)
  (linear_relu_stack): Sequential(
    (0): Linear(in_features=784, out_features=32, bias=True)
    (1): ReLU()
    (2): Linear(in_features=32, out_features=16, bias=True)
    (3): ReLU()
    (4): Linear(in_features=16, out_features=10, bias=True)
```

```
  )
)
```

11.10.3 Get Default Hyperparameters

```
fc = fun_control
fc.update({"core_model_hyper_dict":
    hyper_dict[fun_control["core_model"].__name__]})
model_default = get_one_core_model_from_X(X_start, fun_control=fc)
model_default
```

```
Net_fashionMNIST(
  (flatten): Flatten(start_dim=1, end_dim=-1)
  (linear_relu_stack): Sequential(
    (0): Linear(in_features=784, out_features=32, bias=True)
    (1): ReLU()
    (2): Linear(in_features=32, out_features=32, bias=True)
    (3): ReLU()
    (4): Linear(in_features=32, out_features=10, bias=True)
  )
)
```

11.10.4 Evaluation of the Default and the Tuned Architectures

The method `train_tuned` takes a model architecture without trained weights and trains this model with the train data. The train data is split into train and validation data. The validation data is used for early stopping. The trained model weights are saved as a dictionary.

```
from spotPython.torch.traintest import train_tuned
train_tuned(net=model_default, train_dataset=train, shuffle=True,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        device = fun_control["device"],
        show_batch_interval=1_000_000,
        path=None,
        task=fun_control["task"])
```

```
Epoch: 1 |
```

```
MulticlassAccuracy: 0.3391666710376740 | Loss: 2.0737699147065483 | Acc: 0.3391666666666667.
Epoch: 2 |

MulticlassAccuracy: 0.4791249930858612 | Loss: 1.5249479449590047 | Acc: 0.4791250000000000.
Epoch: 3 |

MulticlassAccuracy: 0.6147916913032532 | Loss: 1.1953332616488139 | Acc: 0.6147916666666666.
Epoch: 4 |

MulticlassAccuracy: 0.6680416464805603 | Loss: 1.0364151503245036 | Acc: 0.6680416666666666.
Epoch: 5 |

MulticlassAccuracy: 0.6905000209808350 | Loss: 0.9377396509448688 | Acc: 0.6905000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.7003750205039978 | Loss: 0.8730384647846222 | Acc: 0.7003750000000000.
Epoch: 7 |

MulticlassAccuracy: 0.7117083072662354 | Loss: 0.8279227907458941 | Acc: 0.7117083333333334.
Epoch: 8 |

MulticlassAccuracy: 0.7172083258628845 | Loss: 0.7946865118145943 | Acc: 0.7172083333333333.
Returned to Spot: Validation loss: 0.7946865118145943
```

```
from spotPython.torch.traintest import test_tuned
test_tuned(net=model_default, test_dataset=test,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=False,
        device = fun_control["device"],
        task=fun_control["task"])
```

```
MulticlassAccuracy: 0.7125999927520752 | Loss: 0.8081323936939240 | Acc: 0.7126000000000000.
Final evaluation: Validation loss: 0.808132393693924
Final evaluation: Validation metric: 0.7125999927520752
---------------------------------------------

(0.808132393693924, nan, tensor(0.7126))
```

The following code trains the model `model_spot`. If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be saved to this file.

```
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=True,
        device = fun_control["device"],
        path=None,
        task=fun_control["task"])
```

```
Epoch: 1 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.232

MulticlassAccuracy: 0.3914583325386047 | Loss: 1.9770964104533195 | Acc: 0.3914583333333334.
Epoch: 2 |

Batch: 10000. Batch Size: 2. Training Loss (running): 1.882

MulticlassAccuracy: 0.4615833461284637 | Loss: 1.6711871655707558 | Acc: 0.4615833333333333.
Epoch: 3 |

Batch: 10000. Batch Size: 2. Training Loss (running): 1.598

MulticlassAccuracy: 0.5159583091735840 | Loss: 1.4528864771264294 | Acc: 0.5159583333333333.
Epoch: 4 |

Batch: 10000. Batch Size: 2. Training Loss (running): 1.398

MulticlassAccuracy: 0.5601249933242798 | Loss: 1.2964802738521248 | Acc: 0.5601250000000000.
Epoch: 5 |

Batch: 10000. Batch Size: 2. Training Loss (running): 1.260

MulticlassAccuracy: 0.5947083234786987 | Loss: 1.1789221649660417 | Acc: 0.5947083333333333.
Epoch: 6 |

Batch: 10000. Batch Size: 2. Training Loss (running): 1.143
```

```
MulticlassAccuracy: 0.6173333525657654 | Loss: 1.0856274762209506 | Acc: 0.6173333333333333.
Epoch: 7 |

Batch: 10000. Batch Size: 2. Training Loss (running): 1.055

MulticlassAccuracy: 0.6342083215713501 | Loss: 1.0114365832787007 | Acc: 0.6342083333333334.
Epoch: 8 |

Batch: 10000. Batch Size: 2. Training Loss (running): 0.979

MulticlassAccuracy: 0.6452500224113464 | Loss: 0.9519951666158935 | Acc: 0.6452500000000000.
Returned to Spot: Validation loss: 0.9519951666158935
```

```
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = fun_control["device"],
            task=fun_control["task"])
```

```
MulticlassAccuracy: 0.6423000097274780 | Loss: 0.9578003666810692 | Acc: 0.6423000000000000.
Final evaluation: Validation loss: 0.9578003666810692
Final evaluation: Validation metric: 0.642300009727478
---------------------------------------------
```

```
(0.9578003666810692, nan, tensor(0.6423))
```

11.10.5 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
l1:  100.0
batch_size:  2.3422106092726107
optimizer:  26.08413824178054
```

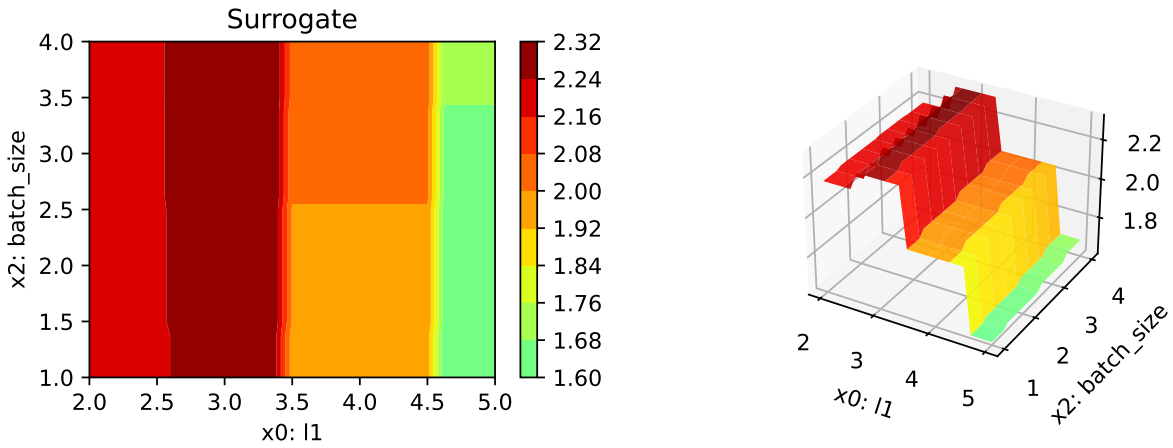
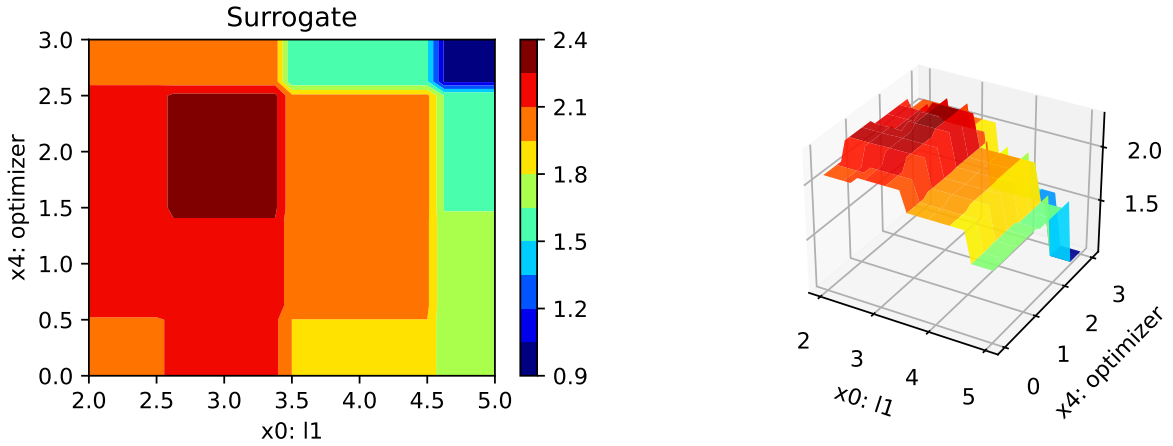
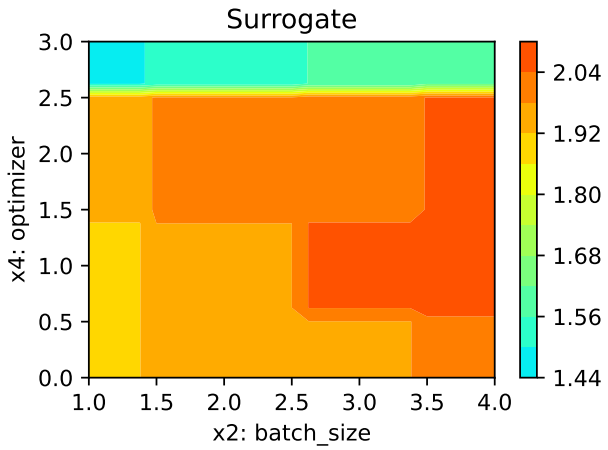
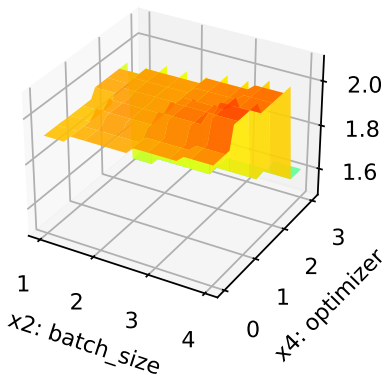


Figure 11.3: Contour plots.







11.10.6 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

Parallel coordinates plots

```
Unable to display output for mime type(s): text/html
```

11.10.7 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

12 HPT: PyTorch With cifar10 Data

In this tutorial, we will show how `spotPython` can be integrated into the `PyTorch` training workflow.

This document refers to the following software versions:

- `python`: 3.10.10
- `torch`: 2.0.1
- `torchvision`: 0.15.0

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

12.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size and the device that is used.

Caution: Run time and initial design size should be increased for real experiments

- MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
- INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.

Note: Device selection

- The device can be selected by setting the variable `DEVICE`.
- Since we are using a simple neural net, the setting `"cpu"` is preferred (on Mac).
- If you have a GPU, you can use `"cuda:0"` instead.
- If DEVICE is set to `None`, `spotPython` will automatically select the device.
  - This might result in `"mps"` on Macs, which is not the best choice for simple neural nets.

```
MAX_TIME = 1
INIT_SIZE = 5
DEVICE = "cpu" # "cuda:0" None
```

```
from spotPython.utils.device import getDevice
DEVICE = getDevice(DEVICE)
print(DEVICE)
```

```
cpu
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '12-torch' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(INIT_SI
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
12-torch_bartz09_1min_5init_2023-06-19_02-50-41
```

12.2 Step 2: Initialization of the Empty `fun_control` Dictionary

`spotPython` uses a Python dictionary for storing the information required for the hyperparameter tuning process, which was described in Section 14.2.

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/12_spot_hpt_torch_cifar10",
    device=DEVICE)
```

12.3 Step 3: PyTorch Data Loading

12.3.1 Load Data Cifar10 Data

```
from torchvision import datasets, transforms
import torchvision
def load_data(data_dir="./data"):
    transform = transforms.Compose([
        transforms.ToTensor(),
        transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))
    ])

    trainset = torchvision.datasets.CIFAR10(
        root=data_dir, train=True, download=True, transform=transform)

    testset = torchvision.datasets.CIFAR10(
        root=data_dir, train=False, download=True, transform=transform)

    return trainset, testset
train, test = load_data()
```

```
Files already downloaded and verified
```

```
Files already downloaded and verified
```

- Since this works fine, we can add the data loading to the `fun_control` dictionary:

```
n_samples = len(train)
# add the dataset to the fun_control
fun_control.update({"data": None, # dataset,
                "train": train,
                "test": test,
                "n_samples": n_samples,
                "target_column": None})
```

12.4 Step 4: Specification of the Preprocessing Model

After the training and test data are specified and added to the `fun_control` dictionary, `spotPython` allows the specification of a data preprocessing pipeline, e.g., for the scaling of the data or for the one-hot encoding of categorical variables, see Section 14.4. This feature is not used here, so we do not change the default value (which is `None`).

12.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

12.5.1 Implementing a Configurable Neural Network With spotPython

`spotPython` includes the `Net_CIFAR10` class which is implemented in the file `netcifar10.py`. The class is imported here.

This class inherits from the class `Net_Core` which is implemented in the file `netcore.py`, see Section 14.5.1.

```
from spotPython.torch.netcifar10 import Net_CIFAR10
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
fun_control = add_core_model_to_fun_control(core_model=Net_CIFAR10,
                                fun_control=fun_control,
                                hyper_dict=TorchHyperDict,
                                filename=None)
```

12.5.2 The Search Space

12.5.3 Configuring the Search Space With spotPython

12.5.3.1 The `hyper_dict` Hyperparameters for the Selected Algorithm

`spotPython` uses `JSON` files for the specification of the hyperparameters, which were described in Section 14.5.5.

The corresponding entries for the `core_model` class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'l1': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 9},
 'l2': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 9},
 'lr_mult': {'type': 'float',
  'default': 1.0,
  'transform': 'None',
  'lower': 0.1,
  'upper': 10.0},
 'batch_size': {'type': 'int',
  'default': 4,
  'transform': 'transform_power_2_int',
  'lower': 1,
  'upper': 4},
 'epochs': {'type': 'int',
  'default': 3,
  'transform': 'transform_power_2_int',
  'lower': 3,
  'upper': 4},
 'k_folds': {'type': 'int',
  'default': 1,
  'transform': 'None',
  'lower': 1,
```

```
 'upper': 1},
'patience': {'type': 'int',
 'default': 5,
 'transform': 'None',
 'lower': 2,
 'upper': 10},
'optimizer': {'levels': ['Adadelta',
  'Adagrad',
  'Adam',
  'AdamW',
  'SparseAdam',
  'Adamax',
  'ASGD',
  'NAdam',
  'RAdam',
  'RMSprop',
  'Rprop',
  'SGD'],
 'type': 'factor',
 'default': 'SGD',
 'transform': 'None',
 'class_name': 'torch.optim',
 'core_model_parameter_type': 'str',
 'lower': 0,
 'upper': 12},
'sgd_momentum': {'type': 'float',
 'default': 0.0,
 'transform': 'None',
 'lower': 0.0,
 'upper': 1.0}}
```

12.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

12.6.1 Step 5: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

12.6.1.1 Modify Hyperparameters of Type numeric and integer (boolean)

The hyperparameter `k_folds` is not used, it is de-activated here by setting the lower and upper bound to the same value.

> Caution: Small net size, number of epochs, and patience for demonstration purposes
>
> - Net sizes `l1` and `l2` as well as `epochs` and `patience` are set to small values for demonstration purposes. These values are too small for a real application.
> - More resonable values are, e.g.:
>   - `fun_control = modify_hyper_parameter_bounds(fun_control, "l1", bounds=[2, 7])`
>   - `fun_control = modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[7, 9])` and
>   - `fun_control = modify_hyper_parameter_bounds(fun_control, "patience", bounds=[2, 7])`

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
fun_control = modify_hyper_parameter_bounds(fun_control, "k_folds", bounds=[0, 0])
fun_control = modify_hyper_parameter_bounds(fun_control, "patience", bounds=[2, 2])
fun_control = modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[2, 3])
fun_control = modify_hyper_parameter_bounds(fun_control, "l1", bounds=[2, 5])
fun_control = modify_hyper_parameter_bounds(fun_control, "l2", bounds=[2, 5])
```

12.6.2 Modify hyperparameter of type factor

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer",["Adam", "AdamW", "Ad
```

12.6.3 Optimizers

Optimizers can be selected as described in Section 19.6.2.

Optimizers are described in Section 14.6.1.

```
fun_control = modify_hyper_parameter_bounds(fun_control,
    "lr_mult", bounds=[1e-3, 1e-3])
fun_control = modify_hyper_parameter_bounds(fun_control,
    "sgd_momentum", bounds=[0.9, 0.9])
```

12.7 Step 7: Selection of the Objective (Loss) Function

12.7.1 Evaluation

The evaluation procedure requires the specification of two elements:

1. the way how the data is split into a train and a test set and
2. the loss function (and a metric).

These are described in Section 19.7.1.

The key `"loss_function"` specifies the loss function which is used during the optimization, see Section 14.7.5.

We will use CrossEntropy loss for the multiclass-classification task.

```
from torch.nn import CrossEntropyLoss
loss_function = CrossEntropyLoss()
fun_control.update({
        "loss_function": loss_function,
        "shuffle": True,
        "eval":  "train_hold_out"
        })
```

12.7.2 Metric

```
import torchmetrics
metric_torch = torchmetrics.Accuracy(task="multiclass",
     num_classes=10).to(fun_control["device"])
fun_control.update({"metric_torch": metric_torch})
```

12.8 Step 8: Calling the SPOT Function

12.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name          | type   | default   |   lower |   upper | transform             |
|---------------|--------|-----------|---------|---------|-----------------------|
| l1            | int    | 5         |   2     |   5     | transform_power_2_int |
| l2            | int    | 5         |   2     |   5     | transform_power_2_int |
| lr_mult       | float  | 1.0       |   0.001 |   0.001 | None                  |
| batch_size    | int    | 4         |   1     |   4     | transform_power_2_int |
| epochs        | int    | 3         |   2     |   3     | transform_power_2_int |
| k_folds       | int    | 1         |   0     |   0     | None                  |
| patience      | int    | 5         |   2     |   2     | None                  |
| optimizer     | factor | SGD       |   0     |   3     | None                  |
| sgd_momentum  | float  | 0.0       |   0.9   |   0.9   | None                  |
```

12.8.2 The Objective Function `fun_torch`

The objective function `fun_torch` is selected next. It implements an interface from `PyTorch`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypertorch import HyperTorch
fun = HyperTorch().fun_torch
```

12.8.3 Starting the Hyperparameter Tuning

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
config: {'l1': 16, 'l2': 8, 'lr_mult': 0.001, 'batch_size': 16, 'epochs': 8, 'k_folds': 0, '
Epoch: 1 |

MulticlassAccuracy: 0.0951500013470650 | Loss: 2.3132577299118040 | Acc: 0.0951500000000000.
Epoch: 2 |
```

```
MulticlassAccuracy: 0.0979000031948090 | Loss: 2.3118295257568358 | Acc: 0.0979000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.0984499976038933 | Loss: 2.3107973091125489 | Acc: 0.0984500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.0979499965906143 | Loss: 2.3097029823303221 | Acc: 0.0979500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.0974999964237213 | Loss: 2.3084314373016359 | Acc: 0.0975000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.0978000015020370 | Loss: 2.3069485197067259 | Acc: 0.0978000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.0994499996304512 | Loss: 2.3052204282760620 | Acc: 0.0994500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.1077999994158745 | Loss: 2.3031790950775148 | Acc: 0.1078000000000000.
Returned to Spot: Validation loss: 2.303179095077515

config: {'l1': 8, 'l2': 8, 'lr_mult': 0.001, 'batch_size': 8, 'epochs': 4, 'k_folds': 0, 'pat
Epoch: 1 |

MulticlassAccuracy: 0.1019499972462654 | Loss: 2.3290661005973816 | Acc: 0.1019500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.0920000001788139 | Loss: 2.3277609358787537 | Acc: 0.0920000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.0856499969959259 | Loss: 2.3266119544029236 | Acc: 0.0856500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.0936999991536140 | Loss: 2.3255103428840638 | Acc: 0.0937000000000000.
Returned to Spot: Validation loss: 2.3255103428840638

config: {'l1': 32, 'l2': 16, 'lr_mult': 0.001, 'batch_size': 2, 'epochs': 8, 'k_folds': 0, 'p
Epoch: 1 |
```

```
MulticlassAccuracy: 0.1010999977588654 | Loss: 2.3073783339738845 | Acc: 0.1011000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.1086999997496605 | Loss: 2.2941057253479959 | Acc: 0.1087000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.1623499989509583 | Loss: 2.2612908222079278 | Acc: 0.1623500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1683499962091446 | Loss: 2.2120475108027460 | Acc: 0.1683500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.1793999969959259 | Loss: 2.1673231732010843 | Acc: 0.1794000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.2073999941349030 | Loss: 2.1304403829693794 | Acc: 0.2074000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.2124000042676926 | Loss: 2.1028314747035504 | Acc: 0.2124000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.2163500040769577 | Loss: 2.0804890911757945 | Acc: 0.2163500000000000.
Returned to Spot: Validation loss: 2.0804890911757945

config: {'l1': 4, 'l2': 8, 'lr_mult': 0.001, 'batch_size': 4, 'epochs': 4, 'k_folds': 0, 'pa
Epoch: 1 |

MulticlassAccuracy: 0.0993499979376793 | Loss: 2.3089312206268309 | Acc: 0.0993500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.0978500023484230 | Loss: 2.3069013849258422 | Acc: 0.0978500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.0964500010013580 | Loss: 2.3048164315223696 | Acc: 0.0964500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1124999970197678 | Loss: 2.3030379461765289 | Acc: 0.1125000000000000.
Returned to Spot: Validation loss: 2.303037946176529

config: {'l1': 16, 'l2': 32, 'lr_mult': 0.001, 'batch_size': 8, 'epochs': 8, 'k_folds': 0, '
Epoch: 1 |
```

```
MulticlassAccuracy: 0.1054000034928322 | Loss: 2.3139406742095949 | Acc: 0.1054000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.1093000024557114 | Loss: 2.3129244773864746 | Acc: 0.1093000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.1137500032782555 | Loss: 2.3119277452468872 | Acc: 0.1137500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1186999976634979 | Loss: 2.3108698651313784 | Acc: 0.1187000000000000.
Epoch: 5 |

MulticlassAccuracy: 0.1224000006914139 | Loss: 2.3096745619773866 | Acc: 0.1224000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.1256500035524368 | Loss: 2.3082214976310729 | Acc: 0.1256500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.1280000060796738 | Loss: 2.3064146327018737 | Acc: 0.1280000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.1294499933719635 | Loss: 2.3041261745452881 | Acc: 0.1294500000000000.
Returned to Spot: Validation loss: 2.304126174545288


config: {'l1': 8, 'l2': 16, 'lr_mult': 0.001, 'batch_size': 8, 'epochs': 8, 'k_folds': 0, 'pa
Epoch: 1 |

MulticlassAccuracy: 0.1017500013113022 | Loss: 2.3090413111686705 | Acc: 0.1017500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.1014999970793724 | Loss: 2.3063754611015321 | Acc: 0.1015000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.1022500023245811 | Loss: 2.3024991001129149 | Acc: 0.1022500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1098999977111816 | Loss: 2.2978994737625120 | Acc: 0.1099000000000000.
Epoch: 5 |
```

```
MulticlassAccuracy: 0.1268000006675720 | Loss: 2.2934811944007873 | Acc: 0.1268000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.1454499959945679 | Loss: 2.2888825453758241 | Acc: 0.1454500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.1518999934196472 | Loss: 2.2838717328071594 | Acc: 0.1519000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.1623000055551529 | Loss: 2.2781795486450194 | Acc: 0.1623000000000000.
Returned to Spot: Validation loss: 2.2781795486450194
spotPython tuning: 2.0804890911757945 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2bbce6d10>
```

12.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

12.10 Step 10: Results

After the hyperparameter tuning run is finished, the results can be analyzed as described in Section 14.10.

```
SAVE = False
LOAD = False

if SAVE:
    result_file_name = "res_" + experiment_name + ".pkl"
    with open(result_file_name, 'wb') as f:
        pickle.dump(spot_tuner, f)

if LOAD:
    result_file_name = "ADD THE NAME here, e.g.: res_ch10-friedman-hpt-0_maans03_60min_20i
    with open(result_file_name, 'rb') as f:
        spot_tuner =  pickle.load(f)
```

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

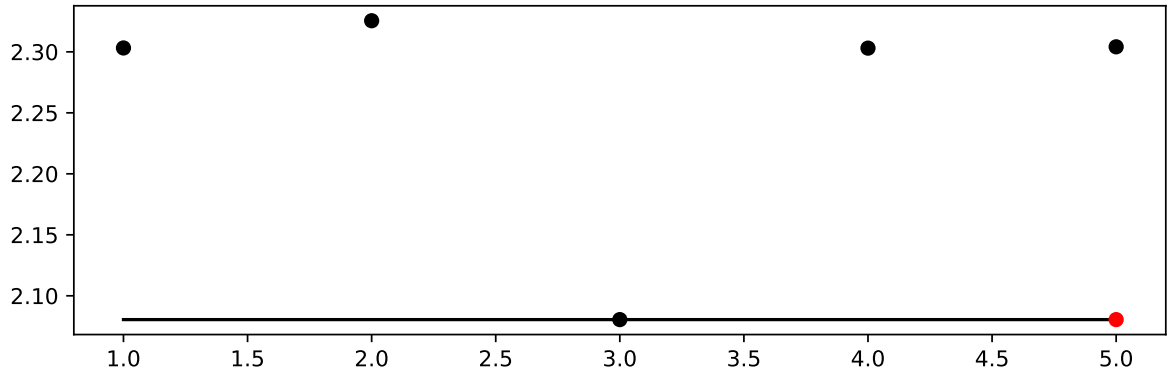


Figure 12.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

```
print(gen_design_table(fun_control=fun_control,
    spot=spot_tuner))
```

name	type	default	lower	upper	tuned	transform	
l1	int	5	2.0	5.0	5.0	transform_power_2_int	
l2	int	5	2.0	5.0	4.0	transform_power_2_int	
lr_mult	float	1.0	0.001	0.001	0.001	None	
batch_size	int	4	1.0	4.0	1.0	transform_power_2_int	
epochs	int	3	2.0	3.0	3.0	transform_power_2_int	
k_folds	int	1	0.0	0.0	0.0	None	
patience	int	5	2.0	2.0	2.0	None	
optimizer	factor	SGD	0.0	3.0	3.0	None	
sgd_momentum	float	0.0	0.9	0.9	0.9	None	

12.10.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

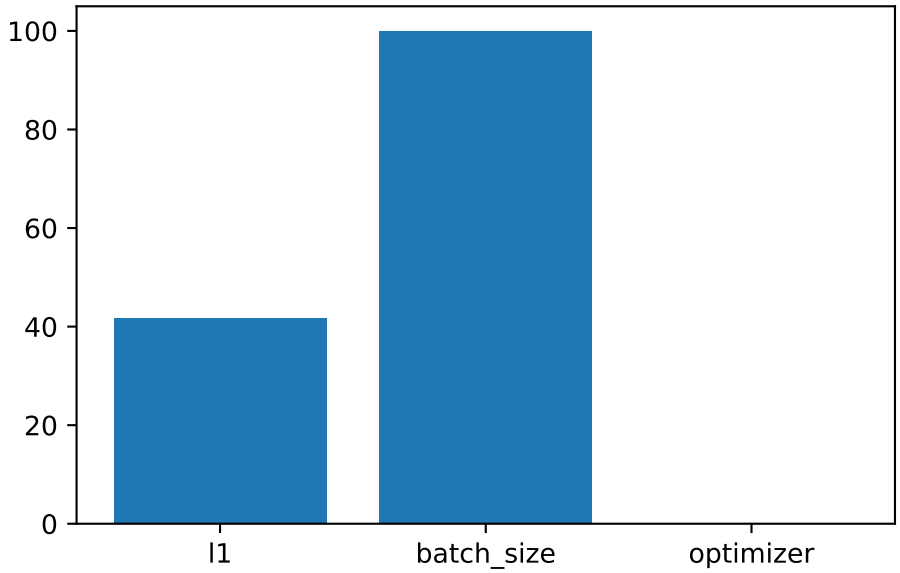


Figure 12.2: Variable importance plot, threshold 0.025.

12.10.2 Get the Tuned Architecture (SPOT Results)

The architecture of the `spotPython` model can be obtained by the following code:

```
from spotPython.hyperparameters.values import get_one_core_model_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
model_spot = get_one_core_model_from_X(X, fun_control)
model_spot
```

```
Net_CIFAR10(
  (conv1): Conv2d(3, 6, kernel_size=(5, 5), stride=(1, 1))
  (pool): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
  (conv2): Conv2d(6, 16, kernel_size=(5, 5), stride=(1, 1))
  (fc1): Linear(in_features=400, out_features=32, bias=True)
  (fc2): Linear(in_features=32, out_features=16, bias=True)
  (fc3): Linear(in_features=16, out_features=10, bias=True)
)
```

12.10.3 Evaluation of the Tuned Architecture

```
from spotPython.torch.traintest import (
    train_tuned,
    test_tuned,
    )
```

```
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=True,
        device = fun_control["device"],
        path=None,
        task=fun_control["task"],)
```

```
Epoch: 1 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.308

MulticlassAccuracy: 0.1005500033497810 | Loss: 2.3031486242294310 | Acc: 0.1005500000000000.
Epoch: 2 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.300

MulticlassAccuracy: 0.1138999983668327 | Loss: 2.2927414273738860 | Acc: 0.1139000000000000.
Epoch: 3 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.287

MulticlassAccuracy: 0.1597000062465668 | Loss: 2.2735267727375033 | Acc: 0.1597000000000000.
Epoch: 4 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.266

MulticlassAccuracy: 0.2150499969720840 | Loss: 2.2502061260223387 | Acc: 0.2150500000000000.
Epoch: 5 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.243
```

```
MulticlassAccuracy: 0.2282000035047531 | Loss: 2.2223145659089090 | Acc: 0.2282000000000000.
Epoch: 6 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.213

MulticlassAccuracy: 0.2391999959945679 | Loss: 2.1825061973452566 | Acc: 0.2392000000000000.
Epoch: 7 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.167

MulticlassAccuracy: 0.2432000041007996 | Loss: 2.1375639670968054 | Acc: 0.2432000000000000.
Epoch: 8 |

Batch: 10000. Batch Size: 2. Training Loss (running): 2.129

MulticlassAccuracy: 0.2525500059127808 | Loss: 2.0974310400962830 | Acc: 0.2525500000000000.
Returned to Spot: Validation loss: 2.097431040096283
```

If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be loaded from this file.

```
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = fun_control["device"],
            task=fun_control["task"],)
```

```
MulticlassAccuracy: 0.2560999989509583 | Loss: 2.0896654647111892 | Acc: 0.2561000000000000.
Final evaluation: Validation loss: 2.089665464711189
Final evaluation: Validation metric: 0.25609999895095825
---------------------------------------------


(2.089665464711189, nan, tensor(0.2561))
```

12.10.4 Cross-validated Evaluations

Caution: Cross-validated Evaluations

- The number of folds is set to 1 by default.
- Here it was changed to 3 for demonstration purposes.
- Set the number of folds to a reasonable value, e.g., 10.
- This can be done by setting the `k_folds` attribute of the model as follows:
- `setattr(model_spot, "k_folds", 10)`

```
from spotPython.torch.traintest import evaluate_cv
# modify k-kolds:
setattr(model_spot, "k_folds", 3)
df_eval, df_preds, df_metrics = evaluate_cv(net=model_spot,
            dataset=fun_control["data"],
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            task=fun_control["task"],
            writer=fun_control["writer"],
            writerId="model_spot_cv",
            device = fun_control["device"])
```

```
Error in Net_Core. Call to evaluate_cv() failed. err=TypeError("Expected sequence or array-li
```

```
metric_name = type(fun_control["metric_torch"]).__name__
print(f"loss: {df_eval}, Cross-validated {metric_name}: {df_metrics}")
```

```
loss: nan, Cross-validated MulticlassAccuracy: nan
```

12.10.5 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
l1:  41.759595356993984
batch_size:  100.0
optimizer:  0.035981536916571195
```

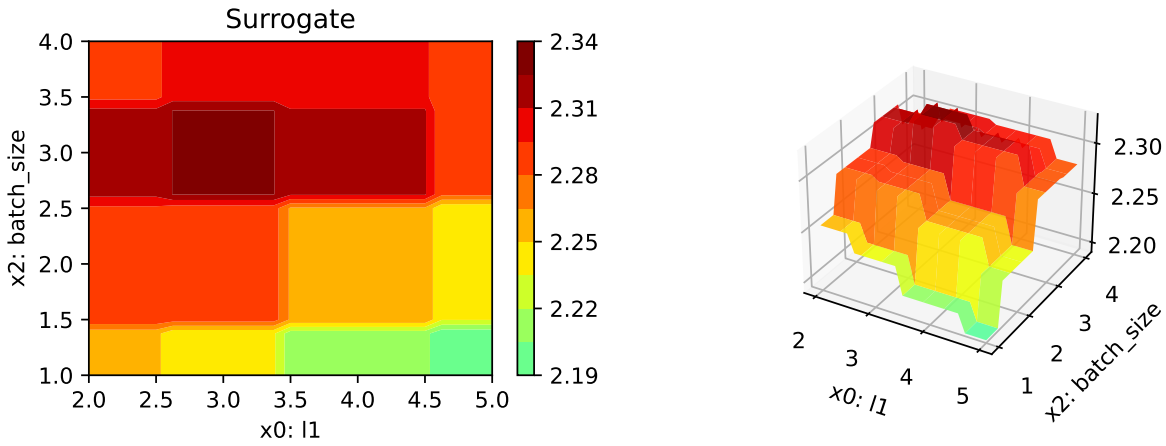
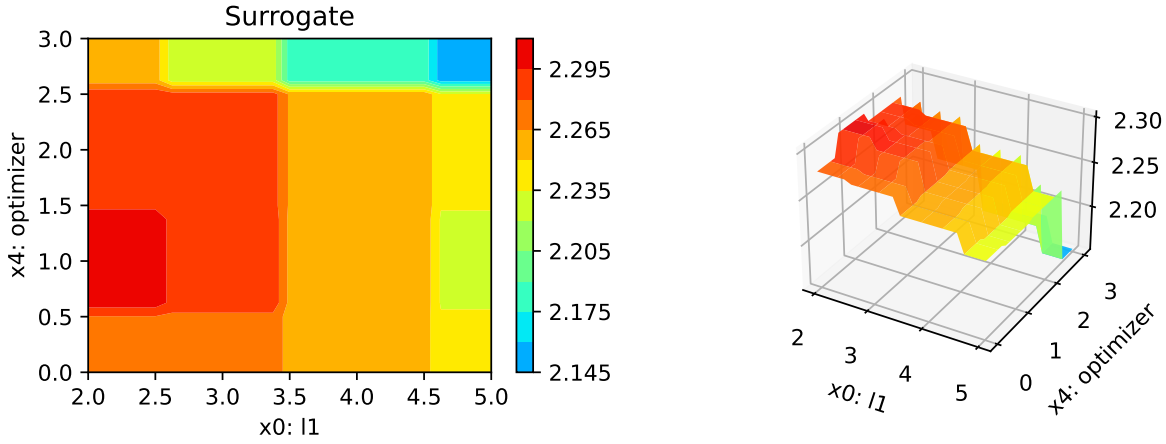
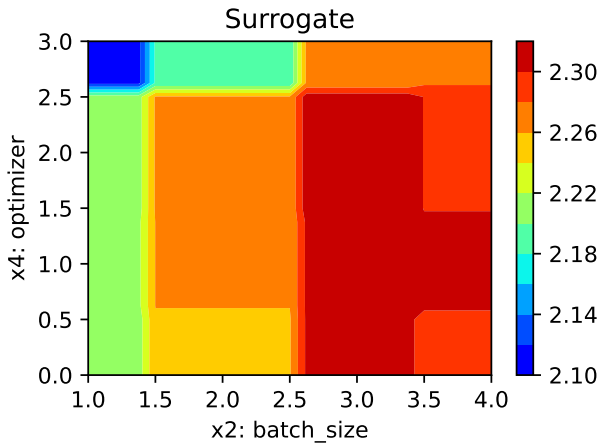
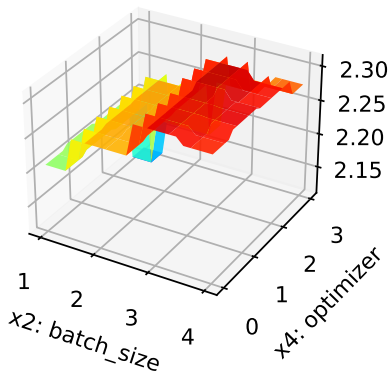


Figure 12.3: Contour plots.







12.10.6 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

Parallel coordinates plots

```
Unable to display output for mime type(s): text/html
```

12.10.7 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

13 HPT: River

River is a Python library for online machine learning (Montiel et al. 2021). It aims to be the most user-friendly library for doing machine learning on streaming data. River is the result of a merger between creme and scikit-multiflow.

13.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size and the device that is used.

> Caution: Run time and initial design size should be increased for real experiments
>
> - MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
> - INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.
> - K is set to 0.1 for demonstration purposes. For real experiments, this should be increased to at least 1.

```
MAX_TIME = 1
INIT_SIZE = 5
K = .1
```

```
10-river_bartz09_1min_5init_2023-06-19_03-04-54
```

13.1.1 `river` Hyperparameter Tuning: HATR with Friedman Drift Data

- This notebook exemplifies hyperparameter tuning with SPOT (spotPython and spotRiver).
- The hyperparameter software SPOT was developed in R (statistical programming language), see Open Access book "Hyperparameter Tuning for Machine and Deep Learning with R - A Practical Guide", available here: https://link.springer.com/book/10.1007/978-981-19-5170-1.

- This notebook demonstrates hyperparameter tuning for `river`. It is based on the notebook "Incremental decision trees in river: the Hoeffding Tree case", see: https://riverml.xyz/0.15.0/recipes/on-hoeffding-trees/#42-regression-tree-splitters.
- Here we will use the river `HTR` and `HATR` functions as in "Incremental decision trees in river: the Hoeffding Tree case", see: https://riverml.xyz/0.15.0/recipes/on-hoeffding-trees/#42-regression-tree-splitters.

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

13.2 Step 2: Initialization of the `fun_control` Dictionary

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="regression",
 tensorboard_path=None)
```

13.3 Step 3: Load the Friedman Drift Data

```
horizon = 7*24
k = K
n_total = int(k*100_000)
n_samples = n_total
p_1 = int(k*25_000)
p_2 = int(k*50_000)
position=(p_1, p_2)
n_train = 1_000
a = n_train + p_1 - 12
b = a + 12
```

- Since we also need a `river` version of the data below for plotting the model, the corresponding data set is generated here. Note: `spotRiver` uses the `train` and `test` data sets, while `river` uses the `X` and `y` data sets

```
from river.datasets import synth
import pandas as pd
dataset = synth.FriedmanDrift(
   drift_type='gra',
   position=position,
     seed=123
)
data_dict = {key: [] for key in list(dataset.take(1))[0][0].keys()}
data_dict["y"] = []
for x, y in dataset.take(n_total):
    for key, value in x.items():
        data_dict[key].append(value)
    data_dict["y"].append(y)
df = pd.DataFrame(data_dict)
# Add column names x1 until x10 to the first 10 columns of the dataframe and the column na
df.columns = [f"x{i}" for i in range(1, 11)] + ["y"]

train = df[:n_train]
test = df[n_train:]
target_column = "y"
#
fun_control.update({"data": None, # dataset,
                "train": train,
                "test": test,
                "n_samples": n_samples,
                "target_column": target_column})
```

13.4 Step 4: Specification of the Preprocessing Model

```
from river import preprocessing
prep_model = preprocessing.StandardScaler()
fun_control.update({"prep_model": prep_model})
```

13.5 Step 5: Select `algorithm` and `core_model_hyper_dict`

- The `river` model (`HATR`) is selected.
- Furthermore, the corresponding hyperparameters, see: https://riverml.xyz/0.15.0/api/tree/HoeffdingTreeRegressor/ are selected (incl. type information, names, and bounds).
- The corresponding hyperparameter dictionary is added to the `fun_control` dictionary.
- Alternatively, you can load a local hyper_dict. Simply set `river_hyper_dict.json` as the filename. If `filename`is set to `None`, the hyper_dict is loaded from the `spotRiver` package.

```
from river.tree import HoeffdingAdaptiveTreeRegressor
from spotRiver.data.river_hyper_dict import RiverHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
core_model  = HoeffdingAdaptiveTreeRegressor
fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=RiverHyperDict,
                                filename=None)
```

The corresponding entries for the `core_model` class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'grace_period': {'type': 'int',
  'default': 200,
  'transform': 'None',
  'lower': 10,
  'upper': 1000},
 'max_depth': {'type': 'int',
  'default': 20,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 20},
 'delta': {'type': 'float',
  'default': 1e-07,
  'transform': 'None',
  'lower': 1e-08,
  'upper': 1e-06},
 'tau': {'type': 'float',
  'default': 0.05,
  'transform': 'None',
  'lower': 0.01,
```

```
 'upper': 0.1},
'leaf_prediction': {'levels': ['mean', 'model', 'adaptive'],
 'type': 'factor',
 'default': 'mean',
 'transform': 'None',
 'core_model_parameter_type': 'str',
 'lower': 0,
 'upper': 2},
'leaf_model': {'levels': ['LinearRegression', 'PARegressor', 'Perceptron'],
 'type': 'factor',
 'default': 'LinearRegression',
 'transform': 'None',
 'class_name': 'river.linear_model',
 'core_model_parameter_type': 'instance()',
 'lower': 0,
 'upper': 2},
'model_selector_decay': {'type': 'float',
 'default': 0.95,
 'transform': 'None',
 'lower': 0.9,
 'upper': 0.99},
'splitter': {'levels': ['EBSTSplitter', 'TEBSTSplitter', 'QOSplitter'],
 'type': 'factor',
 'default': 'EBSTSplitter',
 'transform': 'None',
 'class_name': 'river.tree.splitter',
 'core_model_parameter_type': 'instance()',
 'lower': 0,
 'upper': 2},
'min_samples_split': {'type': 'int',
 'default': 5,
 'transform': 'None',
 'lower': 2,
 'upper': 10},
'bootstrap_sampling': {'levels': [0, 1],
 'type': 'factor',
 'default': 0,
 'transform': 'None',
 'core_model_parameter_type': 'bool',
 'lower': 0,
 'upper': 1},
'drift_window_threshold': {'type': 'int',
 'default': 300,
```

```
 'transform': 'None',
 'lower': 100,
 'upper': 500},
'switch_significance': {'type': 'float',
 'default': 0.05,
 'transform': 'None',
 'lower': 0.01,
 'upper': 0.1},
'binary_split': {'levels': [0, 1],
 'type': 'factor',
 'default': 0,
 'transform': 'None',
 'core_model_parameter_type': 'bool',
 'lower': 0,
 'upper': 1},
'max_size': {'type': 'float',
 'default': 500.0,
 'transform': 'None',
 'lower': 100.0,
 'upper': 1000.0},
'memory_estimate_period': {'type': 'int',
 'default': 1000000,
 'transform': 'None',
 'lower': 100000,
 'upper': 1000000},
'stop_mem_management': {'levels': [0, 1],
 'type': 'factor',
 'default': 0,
 'transform': 'None',
 'core_model_parameter_type': 'bool',
 'lower': 0,
 'upper': 1},
'remove_poor_attrs': {'levels': [0, 1],
 'type': 'factor',
 'default': 0,
 'transform': 'None',
 'core_model_parameter_type': 'bool',
 'lower': 0,
 'upper': 1},
'merit_preprune': {'levels': [0, 1],
 'type': 'factor',
 'default': 0,
 'transform': 'None',
```

```
'core_model_parameter_type': 'bool',
'lower': 0,
'upper': 1}}
```

13.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

13.6.1 Modify hyperparameter of type factor

```
# fun_control = modify_hyper_parameter_levels(fun_control, "leaf_model", ["LinearRegressio
# fun_control["core_model_hyper_dict"]
```

13.6.2 Modify hyperparameter of type numeric and integer (boolean)

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
fun_control = modify_hyper_parameter_bounds(fun_control, "delta", bounds=[1e-10, 1e-6])
# fun_control = modify_hyper_parameter_bounds(fun_control, "min_samples_split", bounds=[3,
fun_control = modify_hyper_parameter_bounds(fun_control, "merit_preprune", [0, 0])
```

13.7 Step 7: Selection of the Objective (Loss) Function

There are three metrics:

1. `metric_river` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `metric_sklearn` is used for the sklearn based evaluation via `eval_oml_horizon`.
3. `metric_torch` is used for the pytorch based evaluation.

```
import numpy as np
from river import metrics
from sklearn.metrics import mean_absolute_error


from spotRiver.fun.hyperriver import HyperRiver
fun = HyperRiver(seed=123, log_level=50).fun_oml_horizon
weights = np.array([1, 1/1000, 1/1000])*10_000.0
horizon = 7*24
```

```
oml_grace_period = 2
step = 100
weight_coeff = 1.0

fun_control.update({
                "horizon": horizon,
                "oml_grace_period": oml_grace_period,
                "weights": weights,
                "step": step,
                "log_level": 50,
                "weight_coeff": weight_coeff,
                "metric_river": metrics.MAE(),
                "metric_sklearn": mean_absolute_error
                })
```

13.8 Step 8: Calling the SPOT Function

13.8.1 Prepare the SPOT Parameters

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
from spotPython.hyperparameters.values import (
    get_var_type,
    get_var_name,
    get_bound_values
    )
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})

lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name                   | type   | default          |      lower |    upper | transform
|------------------------|--------|------------------|------------|----------|--------------
```

```
| grace_period           | int    | 200              |     10      | 1000      | None
| max_depth              | int    | 20               |      2      |   20      | transform_powe
| delta                  | float  | 1e-07            |      1e-10  |    1e-06  | None
| tau                    | float  | 0.05             |      0.01   |    0.1    | None
| leaf_prediction        | factor | mean             |      0      |    2      | None
| leaf_model             | factor | LinearRegression |      0      |    2      | None
| model_selector_decay   | float  | 0.95             |      0.9    |    0.99   | None
| splitter               | factor | EBSTSplitter     |      0      |    2      | None
| min_samples_split      | int    | 5                |      2      |   10      | None
| bootstrap_sampling     | factor | 0                |      0      |    1      | None
| drift_window_threshold | int    | 300              |    100      |  500      | None
| switch_significance    | float  | 0.05             |      0.01   |    0.1    | None
| binary_split           | factor | 0                |      0      |    1      | None
| max_size               | float  | 500.0            |    100      | 1000      | None
| memory_estimate_period | int    | 1000000          | 100000      |    1e+06  | None
| stop_mem_management    | factor | 0                |      0      |    1      | None
| remove_poor_attrs      | factor | 0                |      0      |    1      | None
| merit_preprune         | factor | 0                |      0      |    0      | None
```

13.8.2 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=RiverHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
```

```
from spotPython.spot import spot
from math import inf
import numpy as np
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
```

```
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
spotPython tuning: 2.145751611487961 [##--------] 15.43%

spotPython tuning: 2.145751611487961 [###-------] 34.06%

spotPython tuning: 2.145751611487961 [#####-----] 51.79%

spotPython tuning: 2.145751611487961 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2a6e36b00>
```

13.9 Step 9: Results

```
import pickle
SAVE = False
LOAD = False

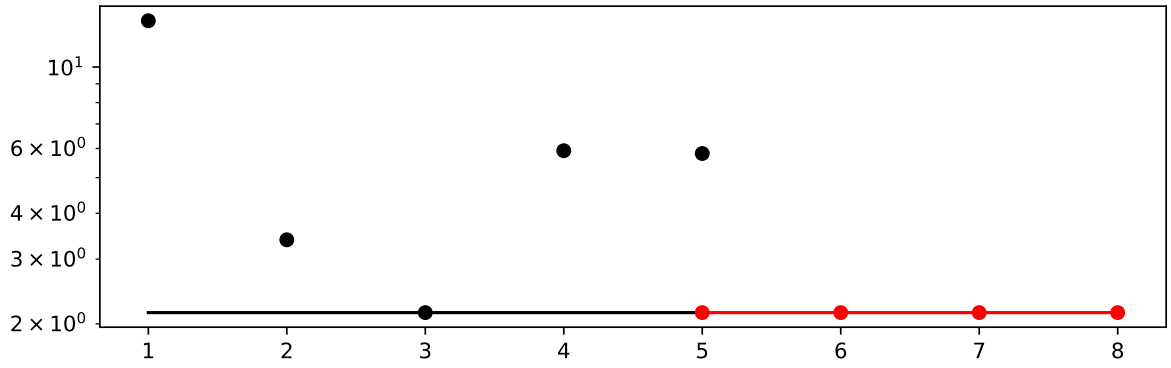
if SAVE:
    result_file_name = "res_" + experiment_name + ".pkl"
```

```
    with open(result_file_name, 'wb') as f:
        pickle.dump(spot_tuner, f)

if LOAD:
    result_file_name = "res_ch10-friedman-hpt-0_maans03_60min_20init_1K_2023-04-14_10-11-1
    with open(result_file_name, 'rb') as f:
        spot_tuner =  pickle.load(f)
```

- Show the Progress of the hyperparameter tuning:

```
spot_tuner.plot_progress(log_y=True, filename="./figures/" + experiment_name+"_progress.pd
```



- Print the Results

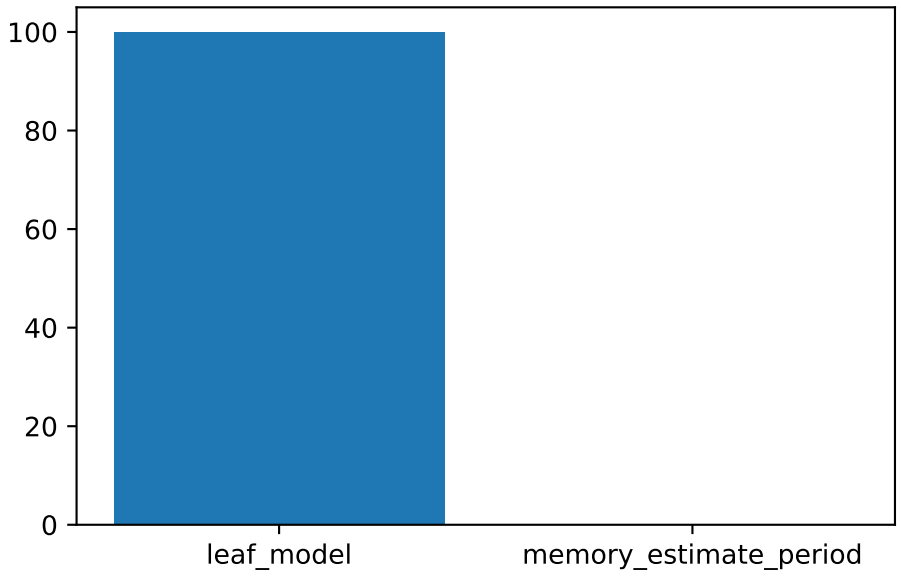
```
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

name	type	default	lower	upper	
grace_period	int	200	10.0	1000.0	
max_depth	int	20	2.0	20.0	
delta	float	1e-07	1e-10	1e-06	4.068723023437
tau	float	0.05	0.01	0.1	0.0484260091
leaf_prediction	factor	mean	0.0	2.0	
leaf_model	factor	LinearRegression	0.0	2.0	
model_selector_decay	float	0.95	0.9	0.99	0.970713237
splitter	factor	EBSTSplitter	0.0	2.0	
min_samples_split	int	5	2.0	10.0	
bootstrap_sampling	factor	0	0.0	1.0	
drift_window_threshold	int	300	100.0	500.0	

| switch_significance | float | 0.05 | 0.01 | 0.1 | 0.040370639
| binary_split | factor | 0 | 0.0 | 1.0 |
| max_size | float | 500.0 | 100.0 | 1000.0 | 454.140654
| memory_estimate_period | int | 1000000 | 100000.0 | 1000000.0 | 9
stop_mem_management	factor	0	0.0	1.0
remove_poor_attrs	factor	0	0.0	1.0
merit_preprune	factor	0	0.0	0.0

13.9.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.0025, filename="./figures/" + experiment_name+"_imp
```



13.9.2 Build and Evaluate HTR Model with Tuned Hyperparameters

```
m = test.shape[0]
a = int(m/2)-50
b = int(m/2)
```

13.9.3 The Large Data Set (k=0.2)

> Caution: Increased Friedman-Drift Data Set
>
> - The Friedman-Drift Data Set is increased by a factor of two to show the transferability of the hyperparameter tuning results.
> - Larger values of `k` lead to a longer run time.

```
horizon = 7*24
k = .2
n_total = int(k*100_000)
n_samples = n_total
p_1 = int(k*25_000)
p_2 = int(k*50_000)
position=(p_1, p_2)
n_train = 1_000
a = n_train + p_1 - 12
b = a + 12
dataset = synth.FriedmanDrift(
   drift_type='gra',
   position=position,
     seed=123
)
data_dict = {key: [] for key in list(dataset.take(1))[0][0].keys()}
data_dict["y"] = []
for x, y in dataset.take(n_total):
    for key, value in x.items():
        data_dict[key].append(value)
    data_dict["y"].append(y)
df = pd.DataFrame(data_dict)
# Add column names x1 until x10 to the first 10 columns of the dataframe and the column na
df.columns = [f"x{i}" for i in range(1, 11)] + ["y"]

train = df[:n_train]
test = df[n_train:]
target_column = "y"
#
fun_control.update({"data": None, # dataset,
                "train": train,
                "test": test,
                "n_samples": n_samples,
```

```
                "target_column": target_column})
```

13.9.4 Get Default Hyperparameters

```
# fun_control was modified, we generate a new one with the original
# default hyperparameters
from spotPython.hyperparameters.values import get_one_core_model_from_X
fc = fun_control
fc.update({"core_model_hyper_dict":
    hyper_dict[fun_control["core_model"].__name__]})
model_default = get_one_core_model_from_X(X_start, fun_control=fc)
model_default
```

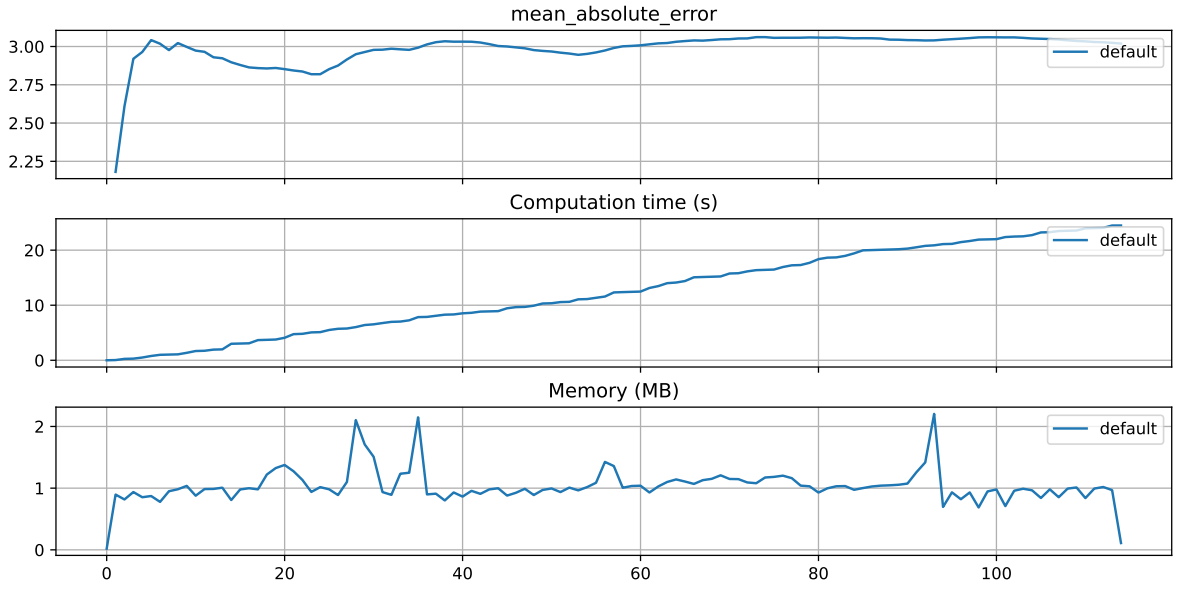
```
HoeffdingAdaptiveTreeRegressor (
  grace_period=200
  max_depth=1048576
  delta=1e-07
  tau=0.05
  leaf_prediction="mean"
  leaf_model=LinearRegression (
    optimizer=SGD (
      lr=Constant (
        learning_rate=0.01
      )
    )
    loss=Squared ()
    l2=0.
    l1=0.
    intercept_init=0.
    intercept_lr=Constant (
      learning_rate=0.01
    )
    clip_gradient=1e+12
    initializer=Zeros ()
  )
  model_selector_decay=0.95
  nominal_attributes=None
  splitter=EBSTSplitter ()
  min_samples_split=5
  bootstrap_sampling=0
```

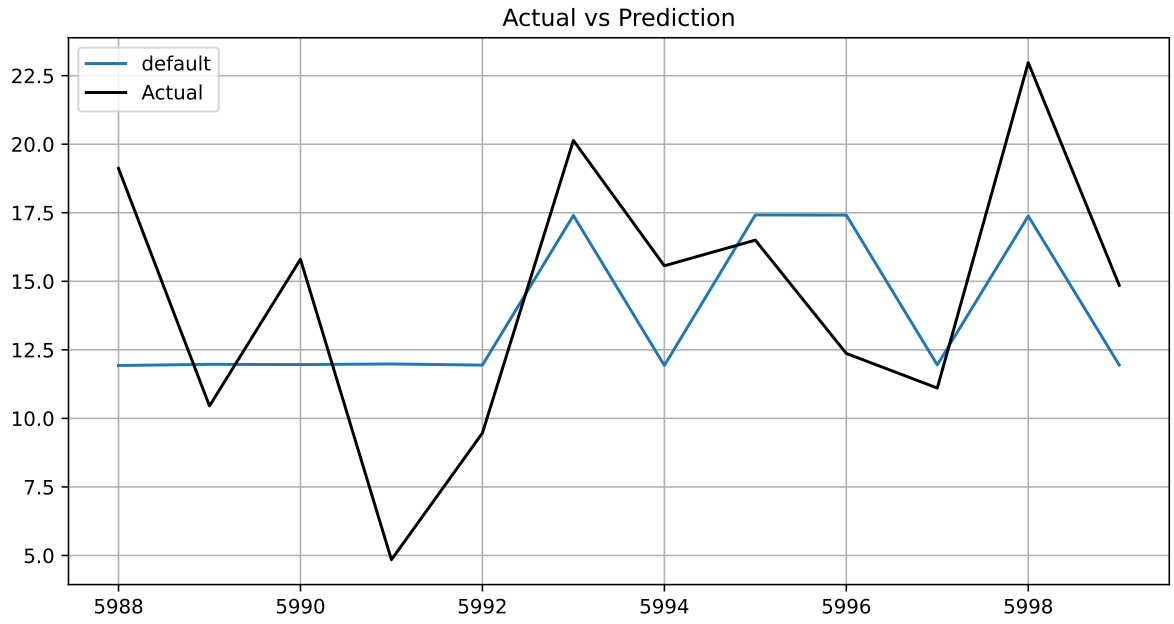
```
  drift_window_threshold=300
  drift_detector=ADWIN (
    delta=0.002
    clock=32
    max_buckets=5
    min_window_length=5
    grace_period=10
  )
  switch_significance=0.05
  binary_split=0
  max_size=500.
  memory_estimate_period=1000000
  stop_mem_management=0
  remove_poor_attrs=0
  merit_preprune=0
  seed=None
)
```

```
from spotRiver.evaluation.eval_bml import eval_oml_horizon

df_eval_default, df_true_default = eval_oml_horizon(
                    model=model_default,
                    train=fun_control["train"],
                    test=fun_control["test"],
                    target_column=fun_control["target_column"],
                    horizon=fun_control["horizon"],
                    oml_grace_period=fun_control["oml_grace_period"],
                    metric=fun_control["metric_sklearn"],
                )
```

```
from spotRiver.evaluation.eval_bml import plot_bml_oml_horizon_metrics, plot_bml_oml_horiz
df_labels=["default"]
plot_bml_oml_horizon_metrics(df_eval = [df_eval_default], log_y=False, df_labels=df_labels
plot_bml_oml_horizon_predictions(df_true = [df_true_default[a:b]], target_column=target_co
```


mean_absolute_error
default
3.00
2.75
2.50
2.25
Computation time (s)
default
20
10
0
Memory (MB)
default
2
1
0
0
20
40
60
80
100


Actual vs Prediction
default
Actual
22.5
20.0
17.5
15.0
12.5
10.0
7.5
5.0
5988
5990
5992
5994
5996
5998

13.9.5 Get SPOT Results

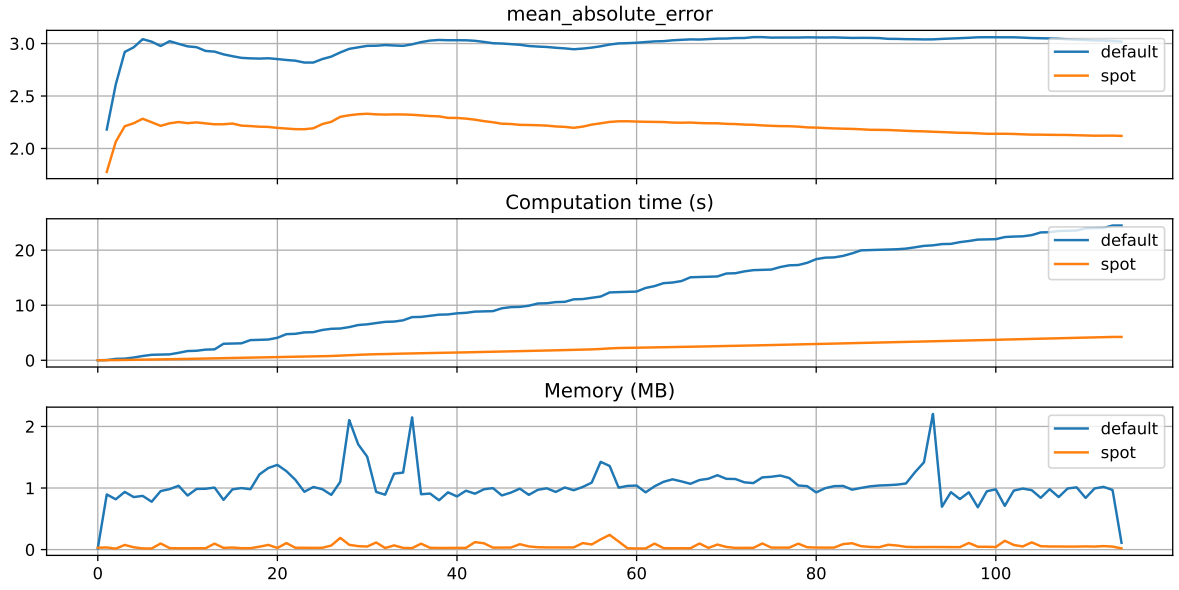
```
from spotPython.hyperparameters.values import get_one_core_model_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
model_spot = get_one_core_model_from_X(X, fun_control)
model_spot
```

```
HoeffdingAdaptiveTreeRegressor (
  grace_period=657
  max_depth=256
  delta=4e-08
  tau=0.048426
  leaf_prediction="adaptive"
  leaf_model=LinearRegression (
    optimizer=SGD (
      lr=Constant (
        learning_rate=0.01
      )
    )
    loss=Squared ()
    l2=0.
    l1=0.
    intercept_init=0.
    intercept_lr=Constant (
      learning_rate=0.01
    )
    clip_gradient=1e+12
    initializer=Zeros ()
  )
  model_selector_decay=0.970713
  nominal_attributes=None
  splitter=QOSplitter (
    radius=0.25
    allow_multiway_splits=False
  )
  min_samples_split=5
  bootstrap_sampling=1
  drift_window_threshold=166
  drift_detector=ADWIN (
    delta=0.002
    clock=32
    max_buckets=5
```

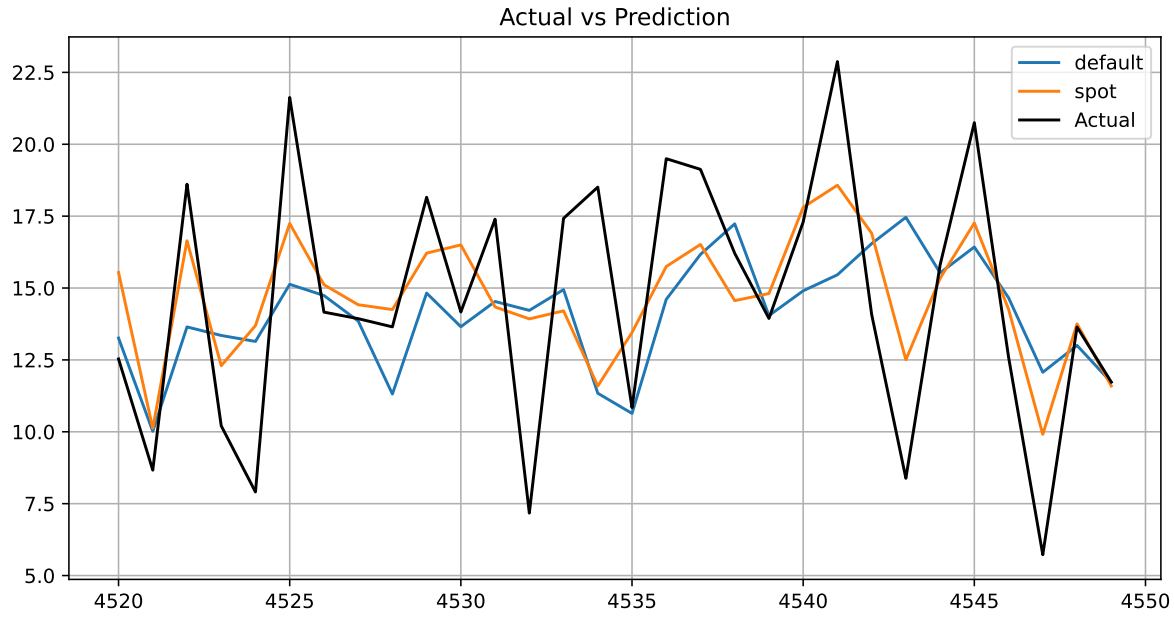
```
    min_window_length=5
    grace_period=10
  )
  switch_significance=0.040371
  binary_split=0
  max_size=454.140654
  memory_estimate_period=910594
  stop_mem_management=1
  remove_poor_attrs=1
  merit_preprune=0
  seed=None
)
```

```
df_eval_spot, df_true_spot = eval_oml_horizon(
                    model=model_spot,
                    train=fun_control["train"],
                    test=fun_control["test"],
                    target_column=fun_control["target_column"],
                    horizon=fun_control["horizon"],
                    oml_grace_period=fun_control["oml_grace_period"],
                    metric=fun_control["metric_sklearn"],
                )
```

```
df_labels=["default", "spot"]
plot_bml_oml_horizon_metrics(df_eval = [df_eval_default, df_eval_spot], log_y=False, df_la
```

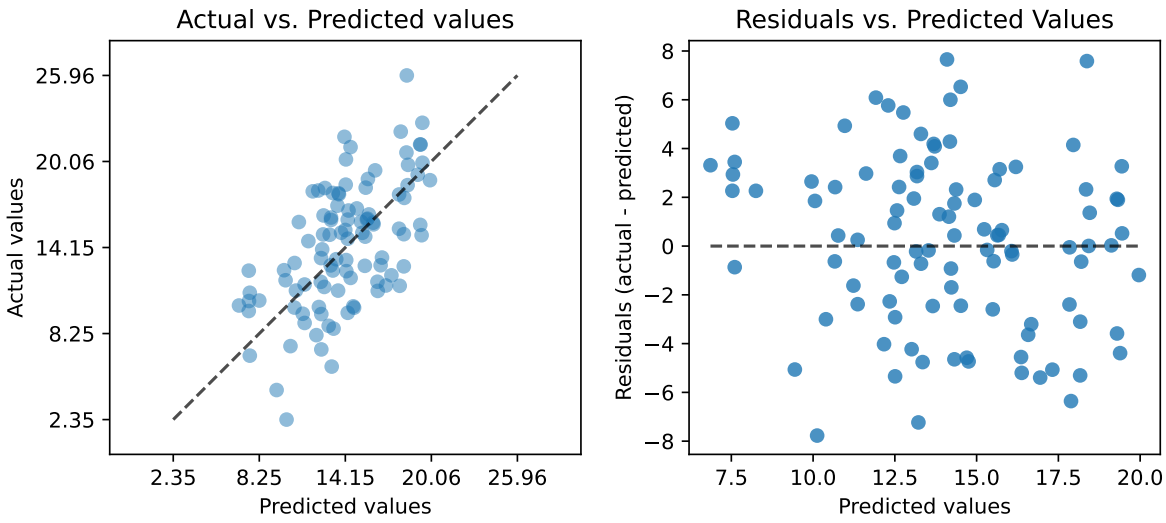



```
a = int(m/2)+20
b = int(m/2)+50
plot_bml_oml_horizon_predictions(df_true = [df_true_default[a:b], df_true_spot[a:b]], targ
```

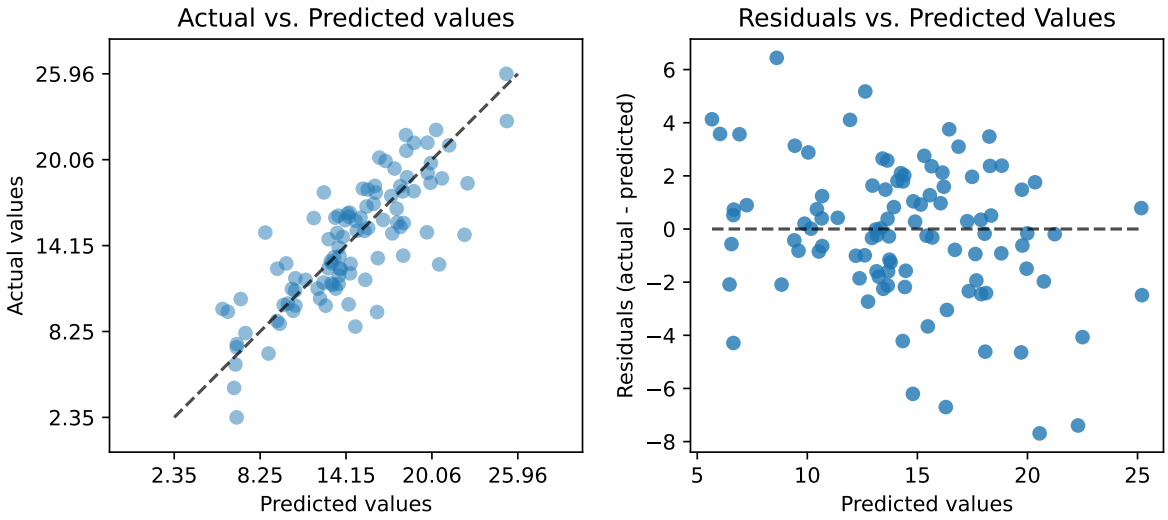


```
from spotPython.plot.validation import plot_actual_vs_predicted
plot_actual_vs_predicted(y_test=df_true_default["y"], y_pred=df_true_default["Prediction"]
plot_actual_vs_predicted(y_test=df_true_spot["y"], y_pred=df_true_spot["Prediction"], titl
```

Default



SPOT



13.9.6 Visualize Regression Trees

```
dataset_f = dataset.take(n_total)
for x, y in dataset_f:
    model_default.learn_one(x, y)
```

Caution: Large Trees

- Since the trees are large, the visualization is suppressed by default.
- To visualize the trees, uncomment the following line.

```
# model_default.draw()
```

```
model_default.summary
```

```
{'n_nodes': 35,
 'n_branches': 17,
 'n_leaves': 18,
 'n_active_leaves': 96,
 'n_inactive_leaves': 0,
 'height': 6,
 'total_observed_weight': 39002.0,
 'n_alternate_trees': 21,
 'n_pruned_alternate_trees': 6,
 'n_switch_alternate_trees': 2}
```

13.9.7 Spot Model

```
dataset_f = dataset.take(n_total)
for x, y in dataset_f:
    model_spot.learn_one(x, y)
```

Caution: Large Trees

- Since the trees are large, the visualization is suppressed by default.
- To visualize the trees, uncomment the following line.

```
# model_spot.draw()
```

```
model_spot.summary
```

```
{'n_nodes': 25,
 'n_branches': 12,
 'n_leaves': 13,
 'n_active_leaves': 55,
 'n_inactive_leaves': 0,
 'height': 6,
 'total_observed_weight': 39002.0,
 'n_alternate_trees': 24,
 'n_pruned_alternate_trees': 10,
 'n_switch_alternate_trees': 0}
```

```
from spotPython.utils.eda import compare_two_tree_models
print(compare_two_tree_models(model_default, model_spot))
```

```
| Parameter                |   Default |   Spot |
|--------------------------|-----------|--------|
| n_nodes                  |        35 |     25 |
| n_branches               |        17 |     12 |
| n_leaves                 |        18 |     13 |
| n_active_leaves          |        96 |     55 |
| n_inactive_leaves        |         0 |      0 |
| height                   |         6 |      6 |
| total_observed_weight    |     39002 |  39002 |
| n_alternate_trees        |        21 |     24 |
| n_pruned_alternate_trees |         6 |     10 |
| n_switch_alternate_trees |         2 |      0 |
```

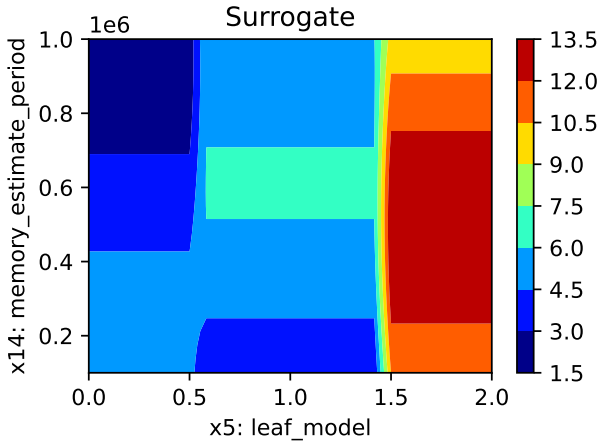
```
min(spot_tuner.y), max(spot_tuner.y)
```

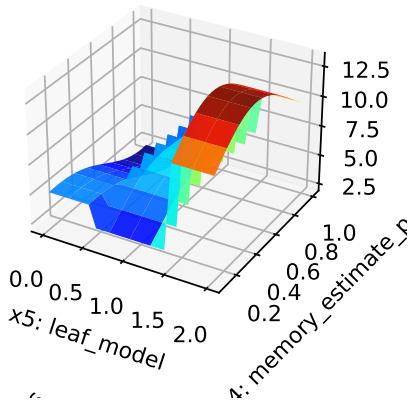
```
(2.145751611487961, 13.362638642210635)
```

13.9.8 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
leaf_model:  100.0
memory_estimate_period:  0.1638816497501305
```





13.9.9 Parallel Coordinates Plots

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

13.9.10 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
```

```
for i in range(n-1):
    for j in range(i+1, n):
        spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

14 HPT: PyTorch With spotPython and Ray Tune on CIFAR10

In this tutorial, we will show how spotPython can be integrated into the PyTorch training workflow. It is based on the tutorial "Hyperparameter Tuning with Ray Tune" from the PyTorch documentation (PyTorch 2023a), which is an extension of the tutorial "Training a Classifier" (PyTorch 2023b) for training a CIFAR10 image classifier.

This document refers to the following software versions:

- python: 3.10.10
- torch: 2.0.1
- torchvision: 0.15.0

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

spotPython can be installed via pip[1].

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of spotPython from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

[1]Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

Results that refer to the `Ray Tune` package are taken from https://PyTorch.org/tutorials/beginner/hyperparameter_tuning_tutorial.html[2].

14.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size and the device that is used.

> Caution: Run time and initial design size should be increased for real experiments
>
> - MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
> - INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.

> Note: Device selection
>
> - The device can be selected by setting the variable `DEVICE`.
> - Since we are using a simple neural net, the setting `"cpu"` is preferred (on Mac).
> - If you have a GPU, you can use `"cuda:0"` instead.
> - If DEVICE is set to `None`, `spotPython` will automatically select the device.
>   - This might result in `"mps"` on Macs, which is not the best choice for simple neural nets.

```
MAX_TIME = 10
INIT_SIZE = 5
DEVICE = "cpu" # "cuda:0"
```

```
from spotPython.utils.device import getDevice
DEVICE = getDevice(DEVICE)
print(DEVICE)
```

```
cpu
```

```
import os
import copy
import socket
```

[2]We were not able to install `Ray Tune` on our system. Therefore, we used the results from the `PyTorch` tutorial.

```
import warnings
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '14-torch' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(INIT_SI
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
warnings.filterwarnings("ignore")
```

```
14-torch_bartz09_10min_5init_2023-06-19_03-33-31
```

14.2 Step 2: Initialization of the `fun_control` Dictionary

`spotPython` uses a Python dictionary for storing the information required for the hyperparameter tuning process. This dictionary is called `fun_control` and is initialized with the function `fun_control_init`. The function `fun_control_init` returns a skeleton dictionary. The dictionary is filled with the required information for the hyperparameter tuning process. It stores the hyperparameter tuning settings, e.g., the deep learning network architecture that should be tuned, the classification (or regression) problem, and the data that is used for the tuning. The dictionary is used as an input for the SPOT function.

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/14_spot_ray_hpt_torch_cifar10",
    device=DEVICE,)
```

14.3 Step 3: PyTorch Data Loading

The data loading process is implemented in the same manner as described in the Section "Data loaders" in PyTorch (2023a). The data loaders are wrapped into the function

`load_data_cifar10` which is identical to the function `load_data` in PyTorch (2023a). A global data directory is used, which allows sharing the data directory between different trials. The method `load_data_cifar10` is part of the `spotPython` package and can be imported from `spotPython.data.torchdata`.

In the following step, the test and train data are added to the dictionary `fun_control`.

```
from spotPython.data.torchdata import load_data_cifar10
train, test = load_data_cifar10()
n_samples = len(train)
# add the dataset to the fun_control
fun_control.update({
    "train": train,
    "test": test,
    "n_samples": n_samples})
```

```
Files already downloaded and verified
```

```
Files already downloaded and verified
```

14.4 Step 4: Specification of the Preprocessing Model

After the training and test data are specified and added to the `fun_control` dictionary, `spotPython` allows the specification of a data preprocessing pipeline, e.g., for the scaling of the data or for the one-hot encoding of categorical variables. The preprocessing model is called `prep_model` ("preparation" or pre-processing) and includes steps that are not subject to the hyperparameter tuning process. The preprocessing model is specified in the `fun_control` dictionary. The preprocessing model can be implemented as a `sklearn` pipeline. The following code shows a typical preprocessing pipeline:

```
categorical_columns = ["cities", "colors"]
one_hot_encoder = OneHotEncoder(handle_unknown="ignore",
                                sparse_output=False)
prep_model = ColumnTransformer(
        transformers=[
            ("categorical", one_hot_encoder, categorical_columns),
        ],
        remainder=StandardScaler(),
    )
```

Because the Ray Tune (`ray[tune]`) hyperparameter tuning as described in PyTorch (2023a) does not use a preprocessing model, the preprocessing model is set to `None` here.

```
prep_model = None
fun_control.update({"prep_model": prep_model})
```

14.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The same neural network model as implemented in the section "Configurable neural network" of the `PyTorch` tutorial (PyTorch 2023a) is used here. We will show the implementation from PyTorch (2023a) in Section 14.5.0.1 first, before the extended implementation with `spotPython` is shown in Section 14.5.0.2.

14.5.0.1 Implementing a Configurable Neural Network With Ray Tune

We used the same hyperparameters that are implemented as configurable in the `PyTorch` tutorial. We specify the layer sizes, namely `l1` and `l2`, of the fully connected layers:

```
class Net(nn.Module):
    def __init__(self, l1=120, l2=84):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(3, 6, 5)
        self.pool = nn.MaxPool2d(2, 2)
        self.conv2 = nn.Conv2d(6, 16, 5)
        self.fc1 = nn.Linear(16 * 5 * 5, l1)
        self.fc2 = nn.Linear(l1, l2)
        self.fc3 = nn.Linear(l2, 10)

    def forward(self, x):
        x = self.pool(F.relu(self.conv1(x)))
        x = self.pool(F.relu(self.conv2(x)))
        x = x.view(-1, 16 * 5 * 5)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

The learning rate, i.e., `lr`, of the optimizer is made configurable, too:

```
optimizer = optim.SGD(net.parameters(), lr=config["lr"], momentum=0.9)
```

14.5.0.2 Implementing a Configurable Neural Network With spotPython

`spotPython` implements a class which is similar to the class described in the `PyTorch` tutorial. The class is called `Net_CIFAR10` and is implemented in the file `netcifar10.py`.

```
from torch import nn
import torch.nn.functional as F
import spotPython.torch.netcore as netcore


class Net_CIFAR10(netcore.Net_Core):
    def __init__(self, l1, l2, lr_mult, batch_size, epochs, k_folds, patience,
    optimizer, sgd_momentum):
        super(Net_CIFAR10, self).__init__(
            lr_mult=lr_mult,
            batch_size=batch_size,
            epochs=epochs,
            k_folds=k_folds,
            patience=patience,
            optimizer=optimizer,
            sgd_momentum=sgd_momentum,
        )
        self.conv1 = nn.Conv2d(3, 6, 5)
        self.pool = nn.MaxPool2d(2, 2)
        self.conv2 = nn.Conv2d(6, 16, 5)
        self.fc1 = nn.Linear(16 * 5 * 5, l1)
        self.fc2 = nn.Linear(l1, l2)
        self.fc3 = nn.Linear(l2, 10)

    def forward(self, x):
        x = self.pool(F.relu(self.conv1(x)))
        x = self.pool(F.relu(self.conv2(x)))
        x = x.view(-1, 16 * 5 * 5)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

14.5.1 The `Net_Core` class

`Net_CIFAR10` inherits from the class `Net_Core` which is implemented in the file `netcore.py`. It implements the additional attributes that are common to all neural network models. The `Net_Core` class is implemented in the file `netcore.py`. It implements hyperparameters as attributes, that are not used by the `core_model`, e.g.:

- optimizer (`optimizer`),
- learning rate (`lr`),
- batch size (`batch_size`),
- epochs (`epochs`),
- k_folds (`k_folds`), and
- early stopping criterion "patience" (`patience`).

Users can add further attributes to the class. The class `Net_Core` is shown below.

```
from torch import nn


class Net_Core(nn.Module):
    def __init__(self, lr_mult, batch_size, epochs, k_folds, patience,
        optimizer, sgd_momentum):
        super(Net_Core, self).__init__()
        self.lr_mult = lr_mult
        self.batch_size = batch_size
        self.epochs = epochs
        self.k_folds = k_folds
        self.patience = patience
        self.optimizer = optimizer
        self.sgd_momentum = sgd_momentum
```

14.5.2 Comparison of the Approach Described in the PyTorch Tutorial With spotPython

Comparing the class `Net` from the `PyTorch` tutorial and the class `Net_CIFAR10` from `spotPython`, we see that the class `Net_CIFAR10` has additional attributes and does not inherit from `nn` directly. It adds an additional class, `Net_core`, that takes care of additional attributes that are common to all neural network models, e.g., the learning rate multiplier `lr_mult` or the batch size `batch_size`.

`spotPython`'s `core_model` implements an instance of the `Net_CIFAR10` class. In addition to the basic neural network model, the `core_model` can use these additional attributes. `spotPython`

provides methods for handling these additional attributes to guarantee 100% compatibility with the `PyTorch` classes. The method `add_core_model_to_fun_control` adds the hyperparameters and additional attributes to the `fun_control` dictionary. The method is shown below.

```
from spotPython.torch.netcifar10 import Net_CIFAR10
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
core_model = Net_CIFAR10
fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=TorchHyperDict,
                                filename=None)
```

14.5.3 The Search Space: Hyperparameters

In Section 14.5.4, we first describe how to configure the search space with `ray[tune]` (as shown in PyTorch (2023a)) and then how to configure the search space with `spotPython` in -14.

14.5.4 Configuring the Search Space With Ray Tune

Ray Tune's search space can be configured as follows (PyTorch 2023a):

```
config = {
    "l1": tune.sample_from(lambda _: 2**np.random.randint(2, 9)),
    "l2": tune.sample_from(lambda _: 2**np.random.randint(2, 9)),
    "lr": tune.loguniform(1e-4, 1e-1),
    "batch_size": tune.choice([2, 4, 8, 16])
}
```

The `tune.sample_from()` function enables the user to define sample methods to obtain hyperparameters. In this example, the `l1` and `l2` parameters should be powers of 2 between 4 and 256, so either 4, 8, 16, 32, 64, 128, or 256. The `lr` (learning rate) should be uniformly sampled between 0.0001 and 0.1. Lastly, the batch size is a choice between 2, 4, 8, and 16.

At each trial, `ray[tune]` will randomly sample a combination of parameters from these search spaces. It will then train a number of models in parallel and find the best performing one among these. `ray[tune]` uses the `ASHAScheduler` which will terminate bad performing trials early.

14.5.5 Configuring the Search Space With spotPython

14.5.5.1 The `hyper_dict` Hyperparameters for the Selected Algorithm

`spotPython` uses `JSON` files for the specification of the hyperparameters. Users can specify their individual `JSON` files, or they can use the `JSON` files provided by `spotPython`. The `JSON` file for the `core_model` is called `torch_hyper_dict.json`.

In contrast to `ray[tune]`, `spotPython` can handle numerical, boolean, and categorical hyperparameters. They can be specified in the `JSON` file in a similar way as the numerical hyperparameters as shown below. Each entry in the `JSON` file represents one hyperparameter with the following structure: `type`, `default`, `transform`, `lower`, and `upper`.

```
  "factor_hyperparameter": {
      "levels": ["A", "B", "C"],
      "type": "factor",
      "default": "B",
      "transform": "None",
      "core_model_parameter_type": "str",
      "lower": 0,
      "upper": 2},
```

The corresponding entries for the core_model‘ class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'l1': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 9},
 'l2': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 9},
 'lr_mult': {'type': 'float',
  'default': 1.0,
  'transform': 'None',
  'lower': 0.1,
  'upper': 10.0},
 'batch_size': {'type': 'int',
```

```
 'default': 4,
 'transform': 'transform_power_2_int',
 'lower': 1,
 'upper': 4},
'epochs': {'type': 'int',
 'default': 3,
 'transform': 'transform_power_2_int',
 'lower': 3,
 'upper': 4},
'k_folds': {'type': 'int',
 'default': 1,
 'transform': 'None',
 'lower': 1,
 'upper': 1},
'patience': {'type': 'int',
 'default': 5,
 'transform': 'None',
 'lower': 2,
 'upper': 10},
'optimizer': {'levels': ['Adadelta',
  'Adagrad',
  'Adam',
  'AdamW',
  'SparseAdam',
  'Adamax',
  'ASGD',
  'NAdam',
  'RAdam',
  'RMSprop',
  'Rprop',
  'SGD'],
 'type': 'factor',
 'default': 'SGD',
 'transform': 'None',
 'class_name': 'torch.optim',
 'core_model_parameter_type': 'str',
 'lower': 0,
 'upper': 12},
'sgd_momentum': {'type': 'float',
 'default': 0.0,
 'transform': 'None',
 'lower': 0.0,
 'upper': 1.0}}
```

14.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

Ray tune (PyTorch 2023a) does not provide a way to change the specified hyperparameters without re-compilation. However, `spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions are described in the following.

14.6.0.1 Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

After specifying the model, the corresponding hyperparameters, their types and bounds are loaded from the `JSON` file `torch_hyper_dict.json`. After loading, the user can modify the hyperparameters, e.g., the bounds. `spotPython` provides a simple rule for de-activating hyperparameters: If the lower and the upper bound are set to identical values, the hyperparameter is de-activated. This is useful for the hyperparameter tuning, because it allows to specify a hyperparameter in the `JSON` file, but to de-activate it in the `fun_control` dictionary. This is done in the next step.

14.6.0.2 Modify Hyperparameters of Type numeric and integer (boolean)

Since the hyperparameter `k_folds` is not used in the `PyTorch` tutorial, it is de-activated here by setting the lower and upper bound to the same value. Note, `k_folds` is of type "integer".

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
fun_control = modify_hyper_parameter_bounds(fun_control,
    "batch_size", bounds=[1, 5])
fun_control = modify_hyper_parameter_bounds(fun_control,
    "k_folds", bounds=[0, 0])
fun_control = modify_hyper_parameter_bounds(fun_control,
    "patience", bounds=[3, 3])
```

14.6.0.3 Modify Hyperparameter of Type factor

In a similar manner as for the numerical hyperparameters, the categorical hyperparameters can be modified. New configurations can be chosen by adding or deleting levels. For example, the hyperparameter `optimizer` can be re-configured as follows:

In the following setting, two optimizers (`"SGD"` and `"Adam"`) will be compared during the `spotPython` hyperparameter tuning. The hyperparameter `optimizer` is active.

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control,
     "optimizer", ["SGD", "Adam"])
```

The hyperparameter `optimizer` can be de-activated by choosing only one value (level), here: `"SGD"`.

```
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer", ["SGD"])
```

As discussed in Section 14.6.1, there are some issues with the LBFGS optimizer. Therefore, the usage of the LBFGS optimizer is not deactivated in `spotPython` by default. However, the LBFGS optimizer can be activated by adding it to the list of optimizers. `Rprop` was removed, because it does perform very poorly (as some pre-tests have shown). However, it can also be activated by adding it to the list of optimizers. Since `SparseAdam` does not support dense gradients, `Adam` was used instead. Therefore, there are 10 default optimizers:

```
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer",
    ["Adadelta", "Adagrad", "Adam", "AdamW", "Adamax", "ASGD",
    "NAdam", "RAdam", "RMSprop", "SGD"])
```

14.6.1 Optimizers

Table 14.1 shows some of the optimizers available in `PyTorch`:

a denotes (0.9,0.999), b (0.5,1.2), and c (1e-6, 50), respectively. R denotes `required, but unspecified`. "m" denotes `momentum`, "w_d" `weight_decay`, "d" `dampening`, "n" `nesterov`, "r" `rho`, "l_s" `learning rate for scaling delta`, "l_d" `lr_decay`, "b" `betas`, "l" `lambd`, "a" `alpha`, "m_d" for `momentum_decay`, "e" `etas`, and "s_s" for `step_sizes`.

Table 14.1: Optimizers available in PyTorch (selection). The default values are shown in the table.

Optimizer	lr	m	w_d	d	n	r	l_s	l_d	b	l	a	m_d	e	s_s
Adadelta	-	-	0.	-	-	0.9	1.	-	-	-	-	-	-	-
Adagrad	1e-2	-	0.	-	-	-	-	0.	-	-	-	-	-	-
Adam	1e-3	-	0.	-	-	-	-	-	a	-	-	-	-	-
AdamW	1e-3	-	1e-2	-	-	-	-	-	a	-	-	-	-	-
SparseAdam	1e-3	-	-	-	-	-	-	-	a	-	-	-	-	-
Adamax	2e-3	-	0.	-	-	-	-	-	a	-	-	-	-	-

Optimizer	lr	m	w_d	d	n	r	l_s	l_d	b	l	a	m_d	e	s_s
ASGD	1e-2	.9	0.	-	F	-	-	-	-	1e-4	.75	-	-	-
LBFGS	1.	-	-	-	-	-	-	-	-	-	-	-	-	-
NAdam	2e-3	-	0.	-	-	-	-	-	a	-	-	0	-	-
RAdam	1e-3	-	0.	-	-	-	-	-	a	-	-	-	-	-
RMSprop	1e-2	0.	0.	-	-	-	-	-	a	-	-	-	-	-
Rprop	1e-2	-	-	-	-	-	-	-	-	-	b	c	-	-
SGD	R	0.	0.	0.	F	-	-	-	-	-	-	-	-	-

`spotPython` implements an `optimization` handler that maps the optimizer names to the corresponding `PyTorch` optimizers.

A note on LBFGS

We recommend deactivating `PyTorch`'s LBFGS optimizer, because it does not perform very well. The `PyTorch` documentation, see https://pytorch.org/docs/stable/generated/torch.optim.LBFGS.html#torch.optim.LBFGS, states:

> This is a very memory intensive optimizer (it requires additional `param_bytes * (history_size + 1)` bytes). If it doesn't fit in memory try reducing the history size, or use a different algorithm.

Furthermore, the LBFGS optimizer is not compatible with the `PyTorch` tutorial. The reason is that the LBFGS optimizer requires the `closure` function, which is not implemented in the `PyTorch` tutorial. Therefore, the `LBFGS` optimizer is recommended here. Since there are ten optimizers in the portfolio, it is not recommended tuning the hyperparameters that effect one single optimizer only.

A note on the learning rate

`spotPython` provides a multiplier for the default learning rates, `lr_mult`, because optimizers use different learning rates. Using a multiplier for the learning rates might enable a simultaneous tuning of the learning rates for all optimizers. However, this is not recommended, because the learning rates are not comparable across optimizers. Therefore, we recommend fixing the learning rate for all optimizers if multiple optimizers are used. This can be done by setting the lower and upper bounds of the learning rate multiplier to the same value as shown below.
Thus, the learning rate, which affects the `SGD` optimizer, will be set to a fixed value. We choose the default value of `1e-3` for the learning rate, because it is used in other `PyTorch` examples (it is also the default value used by `spotPython` as defined in the `optimizer_handler()` method). We recommend tuning the learning rate later, when a

reduced set of optimizers is fixed. Here, we will demonstrate how to select in a screening phase the optimizers that should be used for the hyperparameter tuning.

For the same reason, we will fix the `sgd_momentum` to `0.9`.

```
fun_control = modify_hyper_parameter_bounds(fun_control,
    "lr_mult", bounds=[1.0, 1.0])
fun_control = modify_hyper_parameter_bounds(fun_control,
    "sgd_momentum", bounds=[0.9, 0.9])
```

14.7 Step 7: Selection of the Objective (Loss) Function

14.7.1 Evaluation: Data Splitting

The evaluation procedure requires the specification of the way how the data is split into a train and a test set and the loss function (and a metric). As a default, `spotPython` provides a standard hold-out data split and cross validation.

14.7.2 Hold-out Data Split

If a hold-out data split is used, the data will be partitioned into a training, a validation, and a test data set. The split depends on the setting of the `eval` parameter. If `eval` is set to `train_hold_out`, one data set, usually the original training data set, is split into a new training and a validation data set. The training data set is used for training the model. The validation data set is used for the evaluation of the hyperparameter configuration and early stopping to prevent overfitting. In this case, the original test data set is not used.

> **Note**
>
> `spotPython` returns the hyperparameters of the machine learning and deep learning models, e.g., number of layers, learning rate, or optimizer, but not the model weights. Therefore, after the SPOT run is finished, the corresponding model with the optimized architecture has to be trained again with the best hyperparameter configuration. The training is performed on the training data set. The test data set is used for the final evaluation of the model.
> Summarizing, the following splits are performed in the hold-out setting:
>
> 1. Run `spotPython` with `eval` set to `train_hold_out` to determine the best hyperparameter configuration.
> 2. Train the model with the best hyperparameter configuration ("architecture") on

the training data set: `train_tuned(model_spot, train, "model_spot.pt")`.
3. Test the model on the test data: `test_tuned(model_spot, test, "model_spot.pt")`

These steps will be exemplified in the following sections.

In addition to this `hold-out` setting, `spotPython` provides another hold-out setting, where an explicit test data is specified by the user that will be used as the validation set. To choose this option, the `eval` parameter is set to `test_hold_out`. In this case, the training data set is used for the model training. Then, the explicitly defined test data set is used for the evaluation of the hyperparameter configuration (the validation).

14.7.3 Cross-Validation

The cross validation setting is used by setting the `eval` parameter to `train_cv` or `test_cv`. In both cases, the data set is split into k folds. The model is trained on $k-1$ folds and evaluated on the remaining fold. This is repeated k times, so that each fold is used exactly once for evaluation. The final evaluation is performed on the test data set. The cross validation setting is useful for small data sets, because it allows to use all data for training and evaluation. However, it is computationally expensive, because the model has to be trained k times.

Note

Combinations of the above settings are possible, e.g., cross validation can be used for training and hold-out for evaluation or *vice versa*. Also, cross validation can be used for training and testing. Because cross validation is not used in the `PyTorch` tutorial (PyTorch 2023a), it is not considered further here.

14.7.4 Overview of the Evaluation Settings

14.7.4.1 Settings for the Hyperparameter Tuning

An overview of the training evaluations is shown in Table 14.2. `"train_cv"` and `"test_cv"` use `sklearn.model_selection.KFold()` internally. More details on the data splitting are provided in Section 21.14 (in the Appendix).

Table 14.2: Overview of the evaluation settings.

eval	train	test	function	comment
"train_hold_out"	✓		train_one_epoch(), validate_one_epoch() for early stopping	splits the train data set internally
"test_hold_out"	✓	✓	train_one_epoch(), validate_one_epoch() for early stopping	use the test data set for validate_one_epoch()
"train_cv"	✓		evaluate_cv(net, train)	CV using the train data set
"test_cv"		✓	evaluate_cv(net, test)	CV using the test data set . Identical to "train_cv", uses only test data.

14.7.4.2 Settings for the Final Evaluation of the Tuned Architecture

14.7.4.2.1 Training of the Tuned Architecture

`train_tuned(model, train)`: train the model with the best hyperparameter configuration (or simply the default) on the training data set. It splits the `train`data into new `train` and `validation` sets using `create_train_val_data_loaders()`, which calls `torch.utils.data.random_split()` internally. Currently, 60% of the data is used for training and 40% for validation. The `train` data is used for training the model with `train_hold_out()`. The `validation` data is used for early stopping using `validate_fold_or_hold_out()` on the `validation` data set.

14.7.4.2.2 Testing of the Tuned Architecture

`test_tuned(model, test)`: test the model on the test data set. No data splitting is performed. The (trained) model is evaluated using the `validate_fold_or_hold_out()` function. Note: During training, `"shuffle"` is set to `True`, whereas during testing, `"shuffle"` is set to `False`.

Section 21.14.1.4 describes the final evaluation of the tuned architecture.

```
fun_control.update({
    "eval": "train_hold_out",
    "path": "torch_model.pt",
    "shuffle": True})
```

14.7.5 Evaluation: Loss Functions and Metrics

The key `"loss_function"` specifies the loss function which is used during the optimization. There are several different loss functions under `PyTorch`'s `nn` package. For example, a simple loss is `MSELoss`, which computes the mean-squared error between the output and the target. In this tutorial we will use `CrossEntropyLoss`, because it is also used in the `PyTorch` tutorial.

```
from torch.nn import CrossEntropyLoss
loss_function = CrossEntropyLoss()
fun_control.update({"loss_function": loss_function})
```

In addition to the loss functions, `spotPython` provides access to a large number of metrics.

- The key `"metric_sklearn"` is used for metrics that follow the `scikit-learn` conventions.
- The key `"river_metric"` is used for the river based evaluation (Montiel et al. 2021) via `eval_oml_iter_progressive`, and
- the key `"metric_torch"` is used for the metrics from `TorchMetrics`.

`TorchMetrics` is a collection of more than 90 PyTorch metrics, see https://torchmetrics.readthedocs.io/en/latest/. Because the `PyTorch` tutorial uses the accuracy as metric, we use the same metric here. Currently, accuracy is computed in the tutorial's example code. We will use `TorchMetrics` instead, because it offers more flexibilty, e.g., it can be used for regression and classification. Furthermore, `TorchMetrics` offers the following advantages:

```
* A standardized interface to increase reproducibility
* Reduces Boilerplate
* Distributed-training compatible
* Rigorously tested
* Automatic accumulation over batches
* Automatic synchronization between multiple devices
```

Therefore, we set

```
import torchmetrics
metric_torch = torchmetrics.Accuracy(task="multiclass", num_classes=10).to(fun_control["de
fun_control.update({"metric_torch": metric_torch})
```

14.8 Step 8: Calling the SPOT Function

14.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`.

```
from spotPython.hyperparameters.values import (
    get_var_type,
    get_var_name,
    get_bound_values
    )
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})

lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

Now, the dictionary `fun_control` contains all information needed for the hyperparameter tuning. Before the hyperparameter tuning is started, it is recommended to take a look at the experimental design. The method `gen_design_table` generates a design table as follows:

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name          | type   | default   |   lower |   upper | transform             |
|---------------|--------|-----------|---------|---------|-----------------------|
| l1            | int    | 5         |     2   |     9   | transform_power_2_int |
| l2            | int    | 5         |     2   |     9   | transform_power_2_int |
| lr_mult       | float  | 1.0       |     1   |     1   | None                  |
| batch_size    | int    | 4         |     1   |     5   | transform_power_2_int |
| epochs        | int    | 3         |     3   |     4   | transform_power_2_int |
| k_folds       | int    | 1         |     0   |     0   | None                  |
| patience      | int    | 5         |     3   |     3   | None                  |
| optimizer     | factor | SGD       |     0   |     9   | None                  |
| sgd_momentum  | float  | 0.0       |     0.9 |     0.9 | None                  |
```

This allows to check if all information is available and if the information is correct. **?@tbl-design** shows the experimental design for the hyperparameter tuning. The table shows the

hyperparameters, their types, default values, lower and upper bounds, and the transformation function. The transformation function is used to transform the hyperparameter values from the unit hypercube to the original domain. The transformation function is applied to the hyperparameter values before the evaluation of the objective function. Hyperparameter transformations are shown in the column "transform", e.g., the `l1` default is `5`, which results in the value $2^5 = 32$ for the network, because the transformation `transform_power_2_int` was selected in the `JSON` file. The default value of the `batch_size` is set to `4`, which results in a batch size of $2^4 = 16$.

14.8.2 The Objective Function `fun_torch`

The objective function `fun_torch` is selected next. It implements an interface from `PyTorch`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypertorch import HyperTorch
fun = HyperTorch().fun_torch
```

14.8.3 Using Default Hyperparameters or Results from Previous Runs

We add the default setting to the initial design:

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=TorchHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
```

14.8.4 Starting the Hyperparameter Tuning

The `spotPython` hyperparameter tuning is started by calling the `Spot` function. Here, we will run the tuner for approximately 30 minutes (`max_time`). Note: the initial design is always evaluated in the `spotPython` run. As a consequence, the run may take longer than specified by `max_time`, because the evaluation time of initial design (here: `init_size`, 10 points) is performed independently of `max_time`. During the run, results from the training is shown. These results can be visualized with Tensorboard as will be shown in Section 14.9.

```
from spotPython.spot import spot
from math import inf
import numpy as np
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
```

```
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
config: {'l1': 128, 'l2': 8, 'lr_mult': 1.0, 'batch_size': 32, 'epochs': 16, 'k_folds': 0, '
Epoch: 1 |

MulticlassAccuracy: 0.3716000020503998 | Loss: 1.6777605989456177 | Acc: 0.3716000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4320000112056732 | Loss: 1.5005067241668701 | Acc: 0.4320000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.4627999961376190 | Loss: 1.4282591786384582 | Acc: 0.4628000000000000.
Epoch: 4 |
```

```
MulticlassAccuracy: 0.4885500073432922 | Loss: 1.3688855980873107 | Acc: 0.4885500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5167999863624573 | Loss: 1.3167984383583069 | Acc: 0.5168000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5378999710083008 | Loss: 1.2682793026924133 | Acc: 0.5379000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5465000271797180 | Loss: 1.2487945146560668 | Acc: 0.5465000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5631999969482422 | Loss: 1.2205491739273071 | Acc: 0.5632000000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5613999962806702 | Loss: 1.2304849659919739 | Acc: 0.5614000000000000.
Epoch: 10 |

MulticlassAccuracy: 0.5752500295639038 | Loss: 1.1978971423149110 | Acc: 0.5752500000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5883499979972839 | Loss: 1.1682895747184754 | Acc: 0.5883500000000000.
Epoch: 12 |

MulticlassAccuracy: 0.5803499817848206 | Loss: 1.2077535195350646 | Acc: 0.5803500000000000.
Epoch: 13 |

MulticlassAccuracy: 0.5759999752044678 | Loss: 1.2306316658020020 | Acc: 0.5760000000000000.
Epoch: 14 |

MulticlassAccuracy: 0.5906000137329102 | Loss: 1.1822338700294495 | Acc: 0.5906000000000000.
Early stopping at epoch 13
Returned to Spot: Validation loss: 1.1822338700294495

config: {'l1': 16, 'l2': 16, 'lr_mult': 1.0, 'batch_size': 8, 'epochs': 8, 'k_folds': 0, 'pat
Epoch: 1 |

MulticlassAccuracy: 0.4542500078678131 | Loss: 1.5091321352601050 | Acc: 0.4542500000000000.
Epoch: 2 |
```

```
MulticlassAccuracy: 0.4963499903678894 | Loss: 1.4083931375503540 | Acc: 0.4963500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5075500011444092 | Loss: 1.3952710754871369 | Acc: 0.5075499999999999.
Epoch: 4 |

MulticlassAccuracy: 0.5388500094413757 | Loss: 1.2818053160846234 | Acc: 0.5388500000000001.
Epoch: 5 |

MulticlassAccuracy: 0.5512499809265137 | Loss: 1.2799427218079567 | Acc: 0.5512500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5591999888420105 | Loss: 1.2349592106938363 | Acc: 0.5592000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5665000081062317 | Loss: 1.2287030029177666 | Acc: 0.5665000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5521000027656555 | Loss: 1.2753997170805931 | Acc: 0.5521000000000000.
Returned to Spot: Validation loss: 1.275399717080593

config: {'l1': 256, 'l2': 128, 'lr_mult': 1.0, 'batch_size': 2, 'epochs': 16, 'k_folds': 0,
Epoch: 1 |

MulticlassAccuracy: 0.1001000031828880 | Loss: 2.3082210160255432 | Acc: 0.1001000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.1024499982595444 | Loss: 2.3105591154098510 | Acc: 0.1024500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.0992500036954880 | Loss: 2.3095418009757998 | Acc: 0.0992500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1027500033378601 | Loss: 2.3071149304151537 | Acc: 0.1027500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.0991000011563301 | Loss: 2.3067904354810715 | Acc: 0.0991000000000000.
Epoch: 6 |
```

```
MulticlassAccuracy: 0.0999500006437302 | Loss: 2.3113588804483416 | Acc: 0.0999500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.0991000011563301 | Loss: 2.3086068964004518 | Acc: 0.0991000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.0988999977707863 | Loss: 2.3113879865884779 | Acc: 0.0989000000000000.
Early stopping at epoch 7
Returned to Spot: Validation loss: 2.311387986588478

config: {'l1': 8, 'l2': 32, 'lr_mult': 1.0, 'batch_size': 4, 'epochs': 8, 'k_folds': 0, 'pati
Epoch: 1 |

MulticlassAccuracy: 0.4166499972343445 | Loss: 1.5726691699266433 | Acc: 0.4166500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4670000076293945 | Loss: 1.4920029521405698 | Acc: 0.4670000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5202500224113464 | Loss: 1.3516685632601380 | Acc: 0.5202500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5358499884605408 | Loss: 1.3217709792330861 | Acc: 0.5358500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5334500074386597 | Loss: 1.3406620404675602 | Acc: 0.5334500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5503000020980835 | Loss: 1.2966141935270279 | Acc: 0.5503000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5745499730110168 | Loss: 1.2292844279039652 | Acc: 0.5745500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5806000232696533 | Loss: 1.2071203859100119 | Acc: 0.5806000000000000.
Returned to Spot: Validation loss: 1.207120385910012

config: {'l1': 64, 'l2': 512, 'lr_mult': 1.0, 'batch_size': 16, 'epochs': 16, 'k_folds': 0,
Epoch: 1 |
```

```
MulticlassAccuracy: 0.4485999941825867 | Loss: 1.4967560271263123 | Acc: 0.4486000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4823000133037567 | Loss: 1.4261294353008269 | Acc: 0.4823000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5031999945640564 | Loss: 1.3617523387908936 | Acc: 0.5032000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5171499848365784 | Loss: 1.3235158298015595 | Acc: 0.5171500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5337499976158142 | Loss: 1.2952653534412384 | Acc: 0.5337499999999999.
Epoch: 6 |

MulticlassAccuracy: 0.5358999967575073 | Loss: 1.2782614757061004 | Acc: 0.5359000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5461500287055969 | Loss: 1.2658197217941285 | Acc: 0.5461500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5529000163078308 | Loss: 1.2501332284450530 | Acc: 0.5528999999999999.
Epoch: 9 |

MulticlassAccuracy: 0.5569999814033508 | Loss: 1.2343813209533692 | Acc: 0.5570000000000001.
Epoch: 10 |

MulticlassAccuracy: 0.5604500174522400 | Loss: 1.2296385282993316 | Acc: 0.5604500000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5650500059127808 | Loss: 1.2153698269367219 | Acc: 0.5650500000000001.
Epoch: 12 |

MulticlassAccuracy: 0.5697500109672546 | Loss: 1.2049174281597137 | Acc: 0.5697500000000000.
Epoch: 13 |

MulticlassAccuracy: 0.5668500065803528 | Loss: 1.2107061998367310 | Acc: 0.5668500000000000.
Epoch: 14 |
```

```
MulticlassAccuracy: 0.5727999806404114 | Loss: 1.1986185997486114 | Acc: 0.5728000000000000.
Epoch: 15 |

MulticlassAccuracy: 0.5730000138282776 | Loss: 1.1946961738824844 | Acc: 0.5730000000000000.
Epoch: 16 |

MulticlassAccuracy: 0.5774499773979187 | Loss: 1.1870610105276107 | Acc: 0.5774500000000000.
Returned to Spot: Validation loss: 1.1870610105276107


config: {'l1': 128, 'l2': 16, 'lr_mult': 1.0, 'batch_size': 32, 'epochs': 16, 'k_folds': 0,
Epoch: 1 |

MulticlassAccuracy: 0.4137000143527985 | Loss: 1.5898399522781372 | Acc: 0.4137000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4796000123023987 | Loss: 1.4382932362556458 | Acc: 0.4796000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5036000013351440 | Loss: 1.3805855596542358 | Acc: 0.5036000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5412499904632568 | Loss: 1.2722473503112792 | Acc: 0.5412500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5504000186920166 | Loss: 1.2480867130279540 | Acc: 0.5504000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5694000124931335 | Loss: 1.2153308080673217 | Acc: 0.5694000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5759999752044678 | Loss: 1.1881502468109131 | Acc: 0.5760000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5806999802589417 | Loss: 1.1821760972976685 | Acc: 0.5807000000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5892000198364258 | Loss: 1.1729242265701294 | Acc: 0.5891999999999999.
Epoch: 10 |
```

```
MulticlassAccuracy: 0.5850499868392944 | Loss: 1.1787366871833802 | Acc: 0.5850500000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5993000268936157 | Loss: 1.1413288003444673 | Acc: 0.5993000000000001.
Epoch: 12 |

MulticlassAccuracy: 0.6014500260353088 | Loss: 1.1668504621505738 | Acc: 0.6014500000000000.
Epoch: 13 |

MulticlassAccuracy: 0.6021999716758728 | Loss: 1.1557737874984741 | Acc: 0.6022000000000000.
Epoch: 14 |

MulticlassAccuracy: 0.5997999906539917 | Loss: 1.1702202931880952 | Acc: 0.5998000000000000.
Early stopping at epoch 13
Returned to Spot: Validation loss: 1.1702202931880952

spotPython tuning: 1.1702202931880952 [###-------] 25.93%


config: {'l1': 128, 'l2': 512, 'lr_mult': 1.0, 'batch_size': 32, 'epochs': 16, 'k_folds': 0,
Epoch: 1 |

MulticlassAccuracy: 0.4648999869823456 | Loss: 1.4701293358802796 | Acc: 0.4649000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.5274500250816345 | Loss: 1.3237315242767334 | Acc: 0.5274500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5690500140190125 | Loss: 1.2135559646606446 | Acc: 0.5690499999999999.
Epoch: 4 |

MulticlassAccuracy: 0.5766500234603882 | Loss: 1.1901183177947998 | Acc: 0.5766500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5976499915122986 | Loss: 1.1567914697647095 | Acc: 0.5976500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5945000052452087 | Loss: 1.1695243903160095 | Acc: 0.5945000000000000.
Epoch: 7 |
```

```
MulticlassAccuracy: 0.6041499972343445 | Loss: 1.1281628733634950 | Acc: 0.6041500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.6075000166893005 | Loss: 1.1357142903327941 | Acc: 0.6075000000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5954999923706055 | Loss: 1.1975024526596070 | Acc: 0.5955000000000000.
Epoch: 10 |

MulticlassAccuracy: 0.6201999783515930 | Loss: 1.1172574646949769 | Acc: 0.6202000000000000.
Epoch: 11 |

MulticlassAccuracy: 0.6057999730110168 | Loss: 1.2158279525756837 | Acc: 0.6058000000000000.
Epoch: 12 |

MulticlassAccuracy: 0.6096500158309937 | Loss: 1.1873015019416808 | Acc: 0.6096500000000000.
Epoch: 13 |

MulticlassAccuracy: 0.6156499981880188 | Loss: 1.2245036499977111 | Acc: 0.6156500000000000.
Early stopping at epoch 12
Returned to Spot: Validation loss: 1.224503649997711
spotPython tuning: 1.1702202931880952 [#####-----] 50.51%


config: {'l1': 128, 'l2': 4, 'lr_mult': 1.0, 'batch_size': 32, 'epochs': 16, 'k_folds': 0, '
Epoch: 1 |

MulticlassAccuracy: 0.2649500072002411 | Loss: 1.8519469415664673 | Acc: 0.2649500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.3759500086307526 | Loss: 1.6833340278625488 | Acc: 0.3759500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.4282500147819519 | Loss: 1.5327493906021119 | Acc: 0.4282500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.4458500146865845 | Loss: 1.4759345014572143 | Acc: 0.4458500000000000.
Epoch: 5 |
```

```
MulticlassAccuracy: 0.4708999991416931 | Loss: 1.4370097077369690 | Acc: 0.4709000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.4718999862670898 | Loss: 1.4181426862716675 | Acc: 0.4719000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.4939500093460083 | Loss: 1.3904836480140685 | Acc: 0.4939500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.4995500147342682 | Loss: 1.3769942201614380 | Acc: 0.4995500000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5084499716758728 | Loss: 1.3722874144554138 | Acc: 0.5084500000000000.
Epoch: 10 |

MulticlassAccuracy: 0.5225999951362610 | Loss: 1.3297592091560364 | Acc: 0.5226000000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5249000191688538 | Loss: 1.3007804115295409 | Acc: 0.5249000000000000.
Epoch: 12 |

MulticlassAccuracy: 0.5105000138282776 | Loss: 1.3568648647308350 | Acc: 0.5105000000000000.
Epoch: 13 |

MulticlassAccuracy: 0.5199000239372253 | Loss: 1.3266702429771424 | Acc: 0.5199000000000000.
Epoch: 14 |

MulticlassAccuracy: 0.5394499897956848 | Loss: 1.2927523935317993 | Acc: 0.5394500000000000.
Epoch: 15 |

MulticlassAccuracy: 0.5360500216484070 | Loss: 1.3086393711090087 | Acc: 0.5360500000000000.
Epoch: 16 |

MulticlassAccuracy: 0.5379999876022339 | Loss: 1.3059302357673646 | Acc: 0.5380000000000000.
Returned to Spot: Validation loss: 1.3059302357673646
spotPython tuning: 1.1702202931880952 [########--] 80.14%


config: {'l1': 16, 'l2': 32, 'lr_mult': 1.0, 'batch_size': 8, 'epochs': 16, 'k_folds': 0, 'pa
Epoch: 1 |
```

```
MulticlassAccuracy: 0.0975499972701073 | Loss: 2.3062089468955995 | Acc: 0.0975500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.0998999997973442 | Loss: 2.3083316393852233 | Acc: 0.0999000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.1017000004649162 | Loss: 2.3034695069313051 | Acc: 0.1017000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1020999997854233 | Loss: 2.3041320311546327 | Acc: 0.1021000000000000.
Epoch: 5 |

MulticlassAccuracy: 0.1000500023365021 | Loss: 2.3084358304977415 | Acc: 0.1000500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.1020999997854233 | Loss: 2.3038669599533081 | Acc: 0.1021000000000000.
Early stopping at epoch 5
Returned to Spot: Validation loss: 2.303866959953308

spotPython tuning: 1.1702202931880952 [#########-] 89.35%


config: {'l1': 16, 'l2': 512, 'lr_mult': 1.0, 'batch_size': 32, 'epochs': 16, 'k_folds': 0,
Epoch: 1 |

MulticlassAccuracy: 0.4500499963760376 | Loss: 1.5282039699554444 | Acc: 0.4500500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4803999960422516 | Loss: 1.4396946838378906 | Acc: 0.4804000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.4852499961853027 | Loss: 1.4204688949584960 | Acc: 0.4852500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.4954499900341034 | Loss: 1.3889629602432252 | Acc: 0.4954500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5120000243186951 | Loss: 1.3607494637489319 | Acc: 0.5120000000000000.
Epoch: 6 |
```

```
MulticlassAccuracy: 0.5115000009536743 | Loss: 1.3528809277534486 | Acc: 0.5115000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5188000202178955 | Loss: 1.3332977566719055 | Acc: 0.5188000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5234000086784363 | Loss: 1.3171866333007813 | Acc: 0.5234000000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5331500172615051 | Loss: 1.3003805235862731 | Acc: 0.5331500000000000.
Epoch: 10 |

MulticlassAccuracy: 0.5362499952316284 | Loss: 1.2932402163505554 | Acc: 0.5362500000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5390999913215637 | Loss: 1.2862701608657836 | Acc: 0.5391000000000000.
Epoch: 12 |

MulticlassAccuracy: 0.5392000079154968 | Loss: 1.2832893109321595 | Acc: 0.5392000000000000.
Epoch: 13 |

MulticlassAccuracy: 0.5435000061988831 | Loss: 1.2712353020668030 | Acc: 0.5435000000000000.
Epoch: 14 |

MulticlassAccuracy: 0.5435500144958496 | Loss: 1.2644357828140258 | Acc: 0.5435500000000000.
Epoch: 15 |

MulticlassAccuracy: 0.5423499941825867 | Loss: 1.2824453946113585 | Acc: 0.5423500000000000.
Epoch: 16 |

MulticlassAccuracy: 0.5516499876976013 | Loss: 1.2494336812019349 | Acc: 0.5516500000000000.
Returned to Spot: Validation loss: 1.2494336812019349
spotPython tuning: 1.1702202931880952 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x28d6ab820>
```

14.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard.

14.9.1 Tensorboard: Start Tensorboard

Start TensorBoard through the command line to visualize data you logged. Specify the root log directory as used in `fun_control = fun_control_init(task="regression", tensorboard_path="runs/24_spot_torch_regression")` as the `tensorboard_path`. The argument logdir points to directory where TensorBoard will look to find event files that it can display. TensorBoard will recursively walk the directory structure rooted at logdir, looking for *.tfevents.* files.

```
tensorboard --logdir=runs
```

Go to the URL it provides or to http://localhost:6006/. The following figures show some screenshots of Tensorboard.

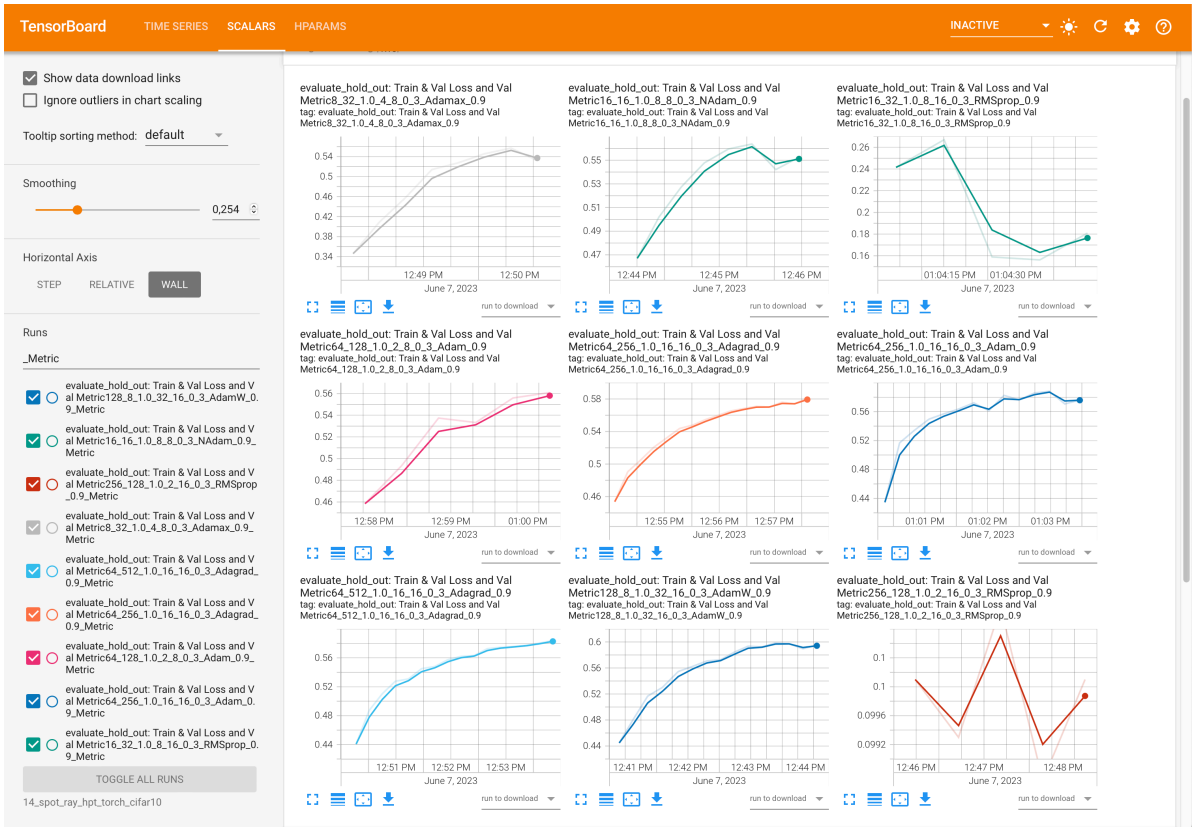


Figure 14.1: Tensorboard

Figure 14.2: Tensorboard

14.9.2 Saving the State of the Notebook

The state of the notebook can be saved and reloaded as follows:

```
import pickle
SAVE = False
LOAD = False

if SAVE:
    result_file_name = "res_" + experiment_name + ".pkl"
    with open(result_file_name, 'wb') as f:
        pickle.dump(spot_tuner, f)

if LOAD:
    result_file_name = "add_the_name_of_the_result_file_here.pkl"
    with open(result_file_name, 'rb') as f:
        spot_tuner =  pickle.load(f)
```

14.10 Step 10: Results

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

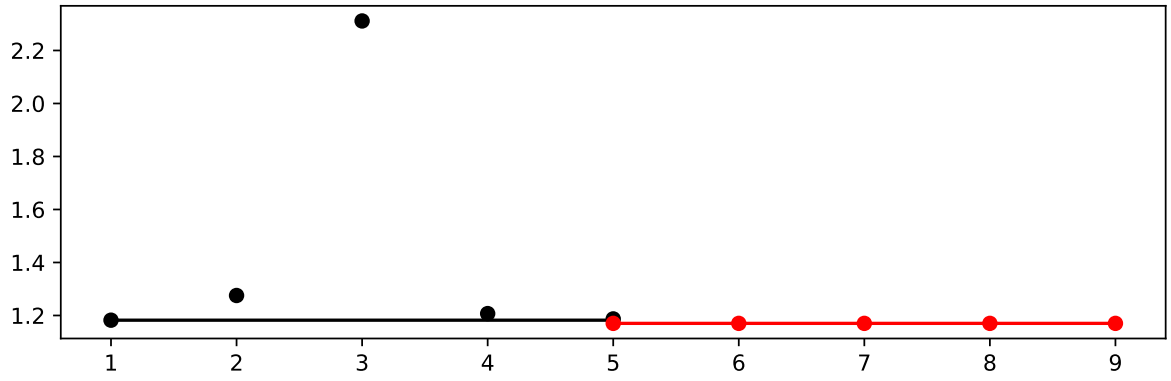


Figure 14.3: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

?@fig-progress shows a typical behaviour that can be observed in many hyperparameter studies (Bartz et al. 2022): the largest improvement is obtained during the evaluation of the initial design. The surrogate model based optimization-optimization with the surrogate refines the results. **?@fig-progress** also illustrates one major difference between `ray[tune]` as used in PyTorch (2023a) and `spotPython`: the `ray[tune]` uses a random search and will generate results similar to the *black* dots, whereas `spotPython` uses a surrogate model based optimization and presents results represented by *red* dots in **?@fig-progress**. The surrogate model based optimization is considered to be more efficient than a random search, because the surrogate model guides the search towards promising regions in the hyperparameter space.

In addition to the improved ("optimized") hyperparameter values, `spotPython` allows a statistical analysis, e.g., a sensitivity analysis, of the results. We can print the results of the hyperparameter tuning, see **?@tbl-results**. The table shows the hyperparameters, their types, default values, lower and upper bounds, and the transformation function. The column "tuned" shows the tuned values. The column "importance" shows the importance of the hyperparameters. The column "stars" shows the importance of the hyperparameters in stars. The importance is computed by the SPOT software.

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

```
| name         | type    | default   |   lower |   upper |   tuned | transform              |
|--------------|---------|-----------|---------|---------|---------|------------------------|--
| l1           | int     | 5         |     2.0 |     9.0 |     7.0 | transform_power_2_int  |
| l2           | int     | 5         |     2.0 |     9.0 |     4.0 | transform_power_2_int  |
| lr_mult      | float   | 1.0       |     1.0 |     1.0 |     1.0 | None                   |
| batch_size   | int     | 4         |     1.0 |     5.0 |     5.0 | transform_power_2_int  |
```

```
| epochs       | int    | 3         |     3.0 |     4.0 |     4.0 | transform_power_2_int |
| k_folds      | int    | 1         |     0.0 |     0.0 |     0.0 | None                  |
| patience     | int    | 5         |     3.0 |     3.0 |     3.0 | None                  |
| optimizer    | factor | SGD       |     0.0 |     9.0 |     3.0 | None                  |
| sgd_momentum | float  | 0.0       |     0.9 |     0.9 |     0.9 | None                  |
```

To visualize the most important hyperparameters, `spotPython` provides the function `plot_importance`. The following code generates the importance plot from **?@fig-importance**.

```
spot_tuner.plot_importance(threshold=0.025,
    filename="./figures/" + experiment_name+"_importance.png")
```

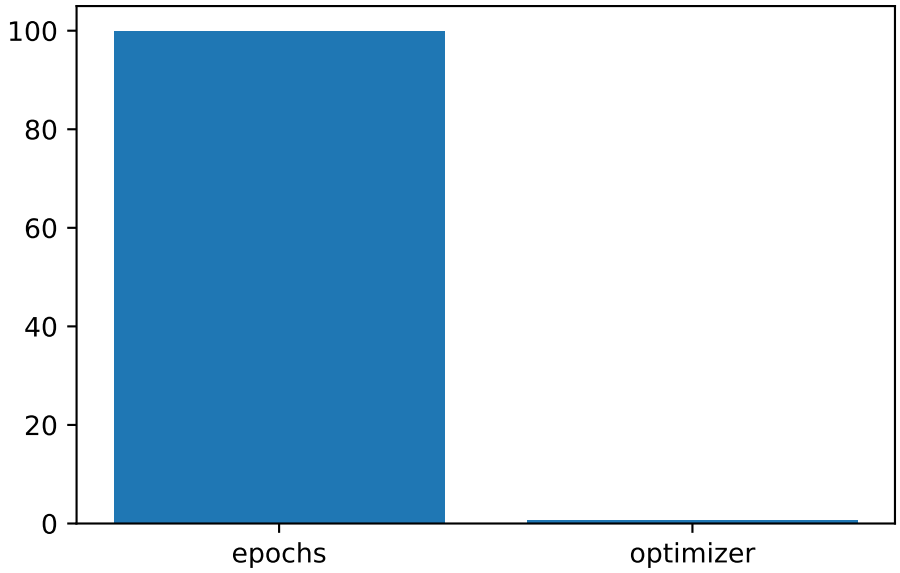


Figure 14.4: Variable importance plot, threshold 0.025.

14.10.1 Get the Tuned Architecture (SPOT Results)

The architecture of the `spotPython` model can be obtained as follows. First, the numerical representation of the hyperparameters are obtained, i.e., the numpy array `X` is generated. This array is then used to generate the model `model_spot` by the function `get_one_core_model_from_X`. The model `model_spot` has the following architecture:

```
from spotPython.hyperparameters.values import get_one_core_model_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
model_spot = get_one_core_model_from_X(X, fun_control)
model_spot
```

```
Net_CIFAR10(
  (conv1): Conv2d(3, 6, kernel_size=(5, 5), stride=(1, 1))
  (pool): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
  (conv2): Conv2d(6, 16, kernel_size=(5, 5), stride=(1, 1))
  (fc1): Linear(in_features=400, out_features=128, bias=True)
  (fc2): Linear(in_features=128, out_features=16, bias=True)
  (fc3): Linear(in_features=16, out_features=10, bias=True)
)
```

14.10.2 Get Default Hyperparameters

In a similar manner as in Section 14.10.1, the default hyperparameters can be obtained.

```
# fun_control was modified, we generate a new one with the original
# default hyperparameters
from spotPython.hyperparameters.values import get_one_core_model_from_X
fc = fun_control
fc.update({"core_model_hyper_dict":
    hyper_dict[fun_control["core_model"].__name__]})
model_default = get_one_core_model_from_X(X_start, fun_control=fc)
model_default
```

```
Net_CIFAR10(
  (conv1): Conv2d(3, 6, kernel_size=(5, 5), stride=(1, 1))
  (pool): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
  (conv2): Conv2d(6, 16, kernel_size=(5, 5), stride=(1, 1))
  (fc1): Linear(in_features=400, out_features=32, bias=True)
  (fc2): Linear(in_features=32, out_features=32, bias=True)
  (fc3): Linear(in_features=32, out_features=10, bias=True)
)
```

14.10.3 Evaluation of the Default Architecture

The method `train_tuned` takes a model architecture without trained weights and trains this model with the train data. The train data is split into train and validation data. The validation

data is used for early stopping. The trained model weights are saved as a dictionary.

This evaluation is similar to the final evaluation in PyTorch (2023a).

```
from spotPython.torch.traintest import (
    train_tuned,
    test_tuned,
    )
train_tuned(net=model_default, train_dataset=train, shuffle=True,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        device = fun_control["device"], show_batch_interval=1_000_000,
        path=None,
        task=fun_control["task"],)

test_tuned(net=model_default, test_dataset=test,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=False,
        device = fun_control["device"],
        task=fun_control["task"],)
```

```
Epoch: 1 |

MulticlassAccuracy: 0.1036999970674515 | Loss: 2.3042341236114501 | Acc: 0.1037000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.1106000021100044 | Loss: 2.3031450422286985 | Acc: 0.1106000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.1171500012278557 | Loss: 2.3022329263687134 | Acc: 0.1171500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1272000074386597 | Loss: 2.3012789381027221 | Acc: 0.1272000000000000.
Epoch: 5 |

MulticlassAccuracy: 0.1410499960184097 | Loss: 2.2999784152984617 | Acc: 0.1410500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.1469500064849854 | Loss: 2.2978194450378417 | Acc: 0.1469500000000000.
Epoch: 7 |
```

```
MulticlassAccuracy: 0.1459999978542328 | Loss: 2.2935358682632447 | Acc: 0.1460000000000000.
Epoch: 8 |


MulticlassAccuracy: 0.1375499963760376 | Loss: 2.2826718236923216 | Acc: 0.1375500000000000.
Returned to Spot: Validation loss: 2.2826718236923216


MulticlassAccuracy: 0.1374000012874603 | Loss: 2.2815687587738038 | Acc: 0.1374000000000000.
Final evaluation: Validation loss: 2.281568758773804
Final evaluation: Validation metric: 0.13740000128746033
------------------------------------------------


(2.281568758773804, nan, tensor(0.1374))
```

14.10.4 Evaluation of the Tuned Architecture

The following code trains the model `model_spot`.

If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be saved to this file.

If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be loaded from this file.

```
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=True,
        device = fun_control["device"],
        path=None,
        task=fun_control["task"],)
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = fun_control["device"],
            task=fun_control["task"],)
```

```
Epoch: 1 |


MulticlassAccuracy: 0.4389500021934509 | Loss: 1.5250833265304566 | Acc: 0.4389500000000000.
Epoch: 2 |
```

```
MulticlassAccuracy: 0.4782499969005585 | Loss: 1.4415405203819276 | Acc: 0.4782500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5252000093460083 | Loss: 1.3205223499298095 | Acc: 0.5252000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5540999770164490 | Loss: 1.2503223680496216 | Acc: 0.5541000000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5724499821662903 | Loss: 1.2086611101150513 | Acc: 0.5724500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5636500120162964 | Loss: 1.2337835314750671 | Acc: 0.5636500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5816000103950500 | Loss: 1.1978520113945008 | Acc: 0.5816000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5947999954223633 | Loss: 1.1535573720932006 | Acc: 0.5948000000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5975499749183655 | Loss: 1.1575893239021302 | Acc: 0.5975500000000000.
Epoch: 10 |

MulticlassAccuracy: 0.5904999971389771 | Loss: 1.1804296854019165 | Acc: 0.5905000000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5957499742507935 | Loss: 1.1608618884086608 | Acc: 0.5957500000000000.
Early stopping at epoch 10
Returned to Spot: Validation loss: 1.1608618884086608

MulticlassAccuracy: 0.6010000109672546 | Loss: 1.1575195035233665 | Acc: 0.6010000000000000.
Final evaluation: Validation loss: 1.1575195035233665
Final evaluation: Validation metric: 0.6010000109672546
---------------------------------------------

(1.1575195035233665, nan, tensor(0.6010))
```

14.10.5 Detailed Hyperparameter Plots

The contour plots in this section visualize the interactions of the three most important hyperparameters. Since some of these hyperparameters take fatorial or integer values, sometimes step-like fitness landcapes (or response surfaces) are generated. SPOT draws the interactions of the main hyperparameters by default. It is also possible to visualize all interactions.

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
epochs:  100.0
optimizer:  0.803179786530439
```

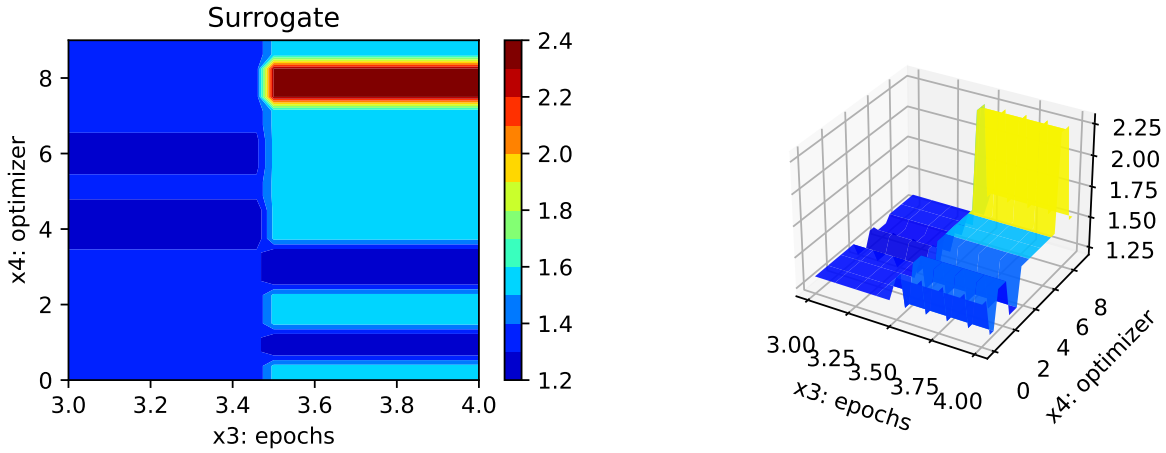


Figure 14.5: Contour plots.

The figures (**?@fig-contour**) show the contour plots of the loss as a function of the hyperparameters. These plots are very helpful for benchmark studies and for understanding neural networks. `spotPython` provides additional tools for a visual inspection of the results and give valuable insights into the hyperparameter tuning process. This is especially useful for model explainability, transparency, and trustworthiness. In addition to the contour plots, **?@fig-parallel** shows the parallel plot of the hyperparameters.

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

Parallel coordinates plots

```
Unable to display output for mime type(s): text/html
```

14.11 Summary and Outlook

This tutorial presents the hyperparameter tuning open source software `spotPython` for `PyTorch`. To show its basic features, a comparison with the "official" `PyTorch` hyperparameter tuning tutorial (PyTorch 2023a) is presented. Some of the advantages of `spotPython` are:

- Numerical and categorical hyperparameters.
- Powerful surrogate models.
- Flexible approach and easy to use.
- Simple JSON files for the specification of the hyperparameters.
- Extension of default and user specified network classes.
- Noise handling techniques.
- Interaction with `tensorboard`.

Currently, only rudimentary parallel and distributed neural network training is possible, but these capabilities will be extended in the future. The next version of `spotPython` will also include a more detailed documentation and more examples.

> **!** Important
>
> Important: This tutorial does not present a complete benchmarking study (Bartz-Beielstein et al. 2020). The results are only preliminary and highly dependent on the local configuration (hard- and software). Our goal is to provide a first impression of the performance of the hyperparameter tuning package `spotPython`. To demonstrate its capabilities, a quick comparison with `ray[tune]` was performed. `ray[tune]` was chosen, because it is presented as "an industry standard tool for distributed hyperparameter tuning." The results should be interpreted with care.

14.12 Appendix

14.12.1 Sample Output From Ray Tune's Run

The output from `ray[tune]` could look like this (PyTorch 2023b):

```
Number of trials: 10 (10 TERMINATED)
------+------+-------------+--------------+---------+------------+--------------------+
|   l1 |   l2 |          lr |   batch_size |    loss |   accuracy | training_iteration |
+------+------+-------------+--------------+---------+------------+--------------------|
|   64 |    4 | 0.00011629  |            2 | 1.87273 |     0.244  |                  2 |
|   32 |   64 | 0.000339763 |            8 | 1.23603 |     0.567  |                  8 |
|    8 |   16 | 0.00276249  |           16 | 1.1815  |     0.5836 |                 10 |
|    4 |   64 | 0.000648721 |            4 | 1.31131 |     0.5224 |                  8 |
|   32 |   16 | 0.000340753 |            8 | 1.26454 |     0.5444 |                  8 |
|    8 |    4 | 0.000699775 |            8 | 1.99594 |     0.1983 |                  2 |
|  256 |    8 | 0.0839654   |           16 | 2.3119  |     0.0993 |                  1 |
|   16 |  128 | 0.0758154   |           16 | 2.33575 |     0.1327 |                  1 |
|   16 |    8 | 0.0763312   |           16 | 2.31129 |     0.1042 |                  4 |
|  128 |   16 | 0.000124903 |            4 | 2.26917 |     0.1945 |                  1 |
+------+------+-------------+--------------+---------+------------+--------------------
Best trial config: {'l1': 8, 'l2': 16, 'lr': 0.00276249, 'batch_size': 16, 'data_dir': '..
Best trial final validation loss: 1.181501
Best trial final validation accuracy: 0.5836
Best trial test set accuracy: 0.5806
```

15 HPT: sklearn RandomForestClassifier VBDP Data

This document refers to the following software versions:

- `python`: 3.10.10

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93
```

```
Note: you may need to restart the kernel to use updated packages.
```

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

15.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time and the initial design size.

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '16-rf-sklearn' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(IN
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
16-rf-sklearn_bartz09_1min_5init_2023-06-19_04-02-41
```

```
import warnings
warnings.filterwarnings("ignore")
```

15.2 Step 2: Initialization of the Empty `fun_control` Dictionary

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/16_spot_hpt_sklearn_classification")
```

15.3 Step 3: PyTorch Data Loading

15.3.1 Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

15.3.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
# add the dataset to the fun_control
fun_control.update({"data": train_df, # full dataset,
                    "train": train,
                    "test": test,
                    "n_samples": n_samples,
                    "target_column": target_column})
```

15.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

```
prep_model = None
fun_control.update({"prep_model": prep_model})
```

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

```
# categorical_columns = []
# one_hot_encoder = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
# prep_model = ColumnTransformer(
#         transformers=[
#             ("categorical", one_hot_encoder, categorical_columns),
#         ],
#         remainder=StandardScaler(),
#     )
```

15.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

```
fun_control = add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)
```

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
core_model = RandomForestClassifier
# core_model = SVC
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=SklearnHyperDict,
                                filename=None)
```

Now `fun_control` has the information from the JSON file. The available hyperparameters are:

```
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
n_estimators
criterion
max_depth
min_samples_split
min_samples_leaf
min_weight_fraction_leaf
max_features
max_leaf_nodes
min_impurity_decrease
bootstrap
oob_score
```

15.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

15.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the `modify_hyper_parameter_bounds` method. For example, to change the `tol` hyperparameter of the `SVC` model to the interval [1e-3, 1e-2], the following code can be used:

```
fun_control = modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3,
1e-2])
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
# fun_control = modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])
```

15.6.2 Modify hyperparameter of type factor

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

Factors can be modified with the `modify_hyper_parameter_levels` function. For example, to exclude the `sigmoid` kernel from the tuning, the `kernel` hyperparameter of the `SVC` model can be modified as follows:

```
fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["linear",
"rbf"])
```

The new setting can be controlled via:

```
fun_control["core_model_hyper_dict"]["kernel"]
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
# XGBoost:
# fun_control = modify_hyper_parameter_levels(fun_control, "loss", ["log_loss"])
```

> **Note: RandomForestClassifier and Out-of-bag Estimation**
>
> Since `oob_score` requires the `bootstrap` hyperparameter to `True`, we set the `oob_score` parameter to `False`. The `oob_score` is later discussed in Section 15.7.3.

```
fun_control = modify_hyper_parameter_bounds(fun_control, "bootstrap", bounds=[0, 1])
fun_control = modify_hyper_parameter_bounds(fun_control, "oob_score", bounds=[0, 0])
```

15.6.3 Optimizers

Optimizers are described in Section 14.6.1.

15.6.4 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

15.7 Step 7: Selection of the Objective (Loss) Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

15.7.1 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

15.7.1.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

15.7.1.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
                "weights": -1,
                "metric_sklearn": mapk_score,
                "predict_proba": True,
                "metric_params": {"k": 3},
                })
```

15.7.2 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
})
```

15.7.3 OOB Score

Using the OOB-Score is a very efficient way to estimate the performance of a random forest classifier. The OOB-Score is calculated on the training data and does not require a hold-out test set. If the OOB-Score is used, the key "eval" in the `fun_control` dictionary should be set to `"oob_score"` as shown below.

> **OOB-Score**
>
> In addition to setting the key `"eval"` in the `fun_control` dictionary to `"oob_score"`, the keys `"oob_score"` and `"bootstrap"` have to be set to `True`, because the OOB-Score requires the bootstrap method.

- Uncomment the following lines to use the OOB-Score:

```
fun_control.update({
    "eval": "eval_oob_score",
})
fun_control = modify_hyper_parameter_bounds(fun_control, "bootstrap", bounds=[1, 1])
fun_control = modify_hyper_parameter_bounds(fun_control, "oob_score", bounds=[1, 1])
```

15.7.3.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key `"k_folds"`. For example, to use 5-fold cross validation, the key `"k_folds"` is set to `5`. Uncomment the following line to use cross validation:

```
# fun_control.update({
#      "eval": "train_cv",
#      "k_folds": 10,
# })
```

15.8 Step 8: Calling the SPOT Function

15.8.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name                      | type   | default   |   lower |   upper | transform
|---------------------------|--------|-----------|---------|---------|----------------------
| n_estimators              | int    | 7         |       5 |   10    | transform_power_2_int
| criterion                 | factor | gini      |       0 |    2    | None
| max_depth                 | int    | 10        |       1 |   20    | transform_power_2_int
| min_samples_split         | int    | 2         |       2 |  100    | None
| min_samples_leaf          | int    | 1         |       1 |   25    | None
| min_weight_fraction_leaf  | float  | 0.0       |       0 |    0.01 | None
| max_features              | factor | sqrt      |       0 |    1    | transform_none_to_None
| max_leaf_nodes            | int    | 10        |       7 |   12    | transform_power_2_int
| min_impurity_decrease     | float  | 0.0       |       0 |    0.01 | None
| bootstrap                 | factor | 1         |       1 |    1    | None
| oob_score                 | factor | 0         |       1 |    1    | None
```

15.8.2 The Objective Function

The objective function is selected next. It implements an interface from `sklearn`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

15.8.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=SklearnHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
array([[ 7.,  0., 10.,  2.,  1.,  0.,  0., 10.,  0.,  1.,  0.]])
```

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
```

```
                                    "min_theta": -4,
                                    "max_theta": 3,
                                    "n_theta": len(var_name),
                                    "model_fun_evals": 10_000,
                                    "log_level": 50
                                    })
spot_tuner.run(X_start=X_start)
```

```
spotPython tuning: -0.3361635220125786 [----------] 1.39%

spotPython tuning: -0.33962264150943394 [----------] 2.82%

spotPython tuning: -0.33962264150943394 [----------] 4.50%

spotPython tuning: -0.33962264150943394 [#---------] 5.84%

spotPython tuning: -0.33962264150943394 [#---------] 7.50%

spotPython tuning: -0.33962264150943394 [#---------] 9.59%

spotPython tuning: -0.33962264150943394 [#---------] 11.08%

spotPython tuning: -0.35094339622641507 [#---------] 13.59%

spotPython tuning: -0.35094339622641507 [#---------] 14.87%

spotPython tuning: -0.35094339622641507 [##--------] 15.84%

spotPython tuning: -0.3641509433962264 [##--------] 18.40%

spotPython tuning: -0.3641509433962264 [##--------] 20.81%

spotPython tuning: -0.3641509433962264 [###-------] 25.00%

spotPython tuning: -0.3641509433962264 [###-------] 29.38%

spotPython tuning: -0.3641509433962264 [###-------] 34.01%
```

```
spotPython tuning: -0.3641509433962264 [####------] 39.17%

spotPython tuning: -0.3641509433962264 [####------] 43.64%

spotPython tuning: -0.3694968553459119 [#####-----] 47.48%

spotPython tuning: -0.3694968553459119 [#####-----] 51.84%

spotPython tuning: -0.3694968553459119 [######----] 57.05%

spotPython tuning: -0.3694968553459119 [######----] 61.60%

spotPython tuning: -0.3694968553459119 [#######---] 65.70%

spotPython tuning: -0.3694968553459119 [#######---] 69.71%

spotPython tuning: -0.3694968553459119 [#######---] 73.86%

spotPython tuning: -0.3694968553459119 [########--] 77.96%

spotPython tuning: -0.3694968553459119 [########--] 82.20%

spotPython tuning: -0.3694968553459119 [#########-] 86.53%

spotPython tuning: -0.3694968553459119 [#########-] 92.21%

spotPython tuning: -0.3694968553459119 [##########] 98.87%

spotPython tuning: -0.3694968553459119 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2b9d75f60>
```

15.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

15.10 Step 10: Results

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

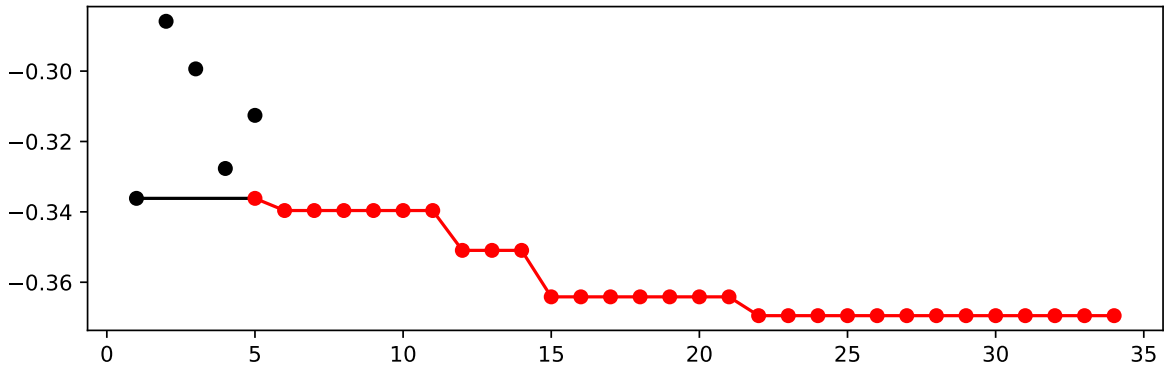


Figure 15.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

```
print(gen_design_table(fun_control=fun_control,
    spot=spot_tuner))
```

name	type	default	lower	upper	tuned
n_estimators	int	7	5.0	10.0	10.0
criterion	factor	gini	0.0	2.0	1.0
max_depth	int	10	1.0	20.0	8.0
min_samples_split	int	2	2.0	100.0	15.0
min_samples_leaf	int	1	1.0	25.0	1.0
min_weight_fraction_leaf	float	0.0	0.0	0.01	0.009298535461845475
max_features	factor	sqrt	0.0	1.0	0.0
max_leaf_nodes	int	10	7.0	12.0	10.0
min_impurity_decrease	float	0.0	0.0	0.01	0.0
bootstrap	factor	1	1.0	1.0	1.0
oob_score	factor	0	1.0	1.0	1.0

15.10.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

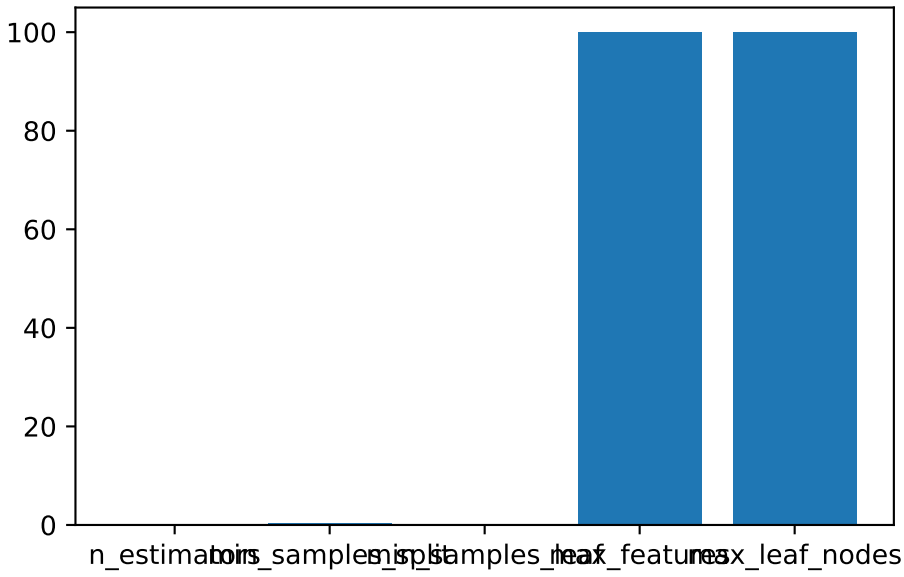


Figure 15.2: Variable importance plot, threshold 0.025.

15.10.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'n_estimators': 128,
 'criterion': 'gini',
 'max_depth': 1024,
 'min_samples_split': 2,
 'min_samples_leaf': 1,
 'min_weight_fraction_leaf': 0.0,
 'max_features': 'sqrt',
 'max_leaf_nodes': 1024,
 'min_impurity_decrease': 0.0,
```

```
 'bootstrap': 1,
 'oob_score': 0}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('randomforestclassifier',
                 RandomForestClassifier(bootstrap=1, max_depth=1024,
                                        max_leaf_nodes=1024, n_estimators=128,
                                        oob_score=0))])
```

15.10.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[1.00000000e+01 1.00000000e+00 8.00000000e+00 1.50000000e+01
  1.00000000e+00 9.29853546e-03 0.00000000e+00 1.00000000e+01
  0.00000000e+00 1.00000000e+00 1.00000000e+00]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'n_estimators': 1024,
  'criterion': 'entropy',
  'max_depth': 256,
  'min_samples_split': 15,
  'min_samples_leaf': 1,
  'min_weight_fraction_leaf': 0.009298535461845475,
  'max_features': 'sqrt',
  'max_leaf_nodes': 1024,
  'min_impurity_decrease': 0.0,
  'bootstrap': 1,
  'oob_score': 1}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
RandomForestClassifier(bootstrap=1, criterion='entropy', max_depth=256,
                       max_leaf_nodes=1024, min_samples_split=15,
                       min_weight_fraction_leaf=0.009298535461845475,
                       n_estimators=1024, oob_score=1)
```

15.10.4 Evaluate SPOT Results

- Fetch the data.

```
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.35404896421845566
```

```
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
```

```
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

15.10.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.3603578154425611
std_res: 0.005587383690827419
min_res: 0.3483992467043315
max_res: 0.37099811676082867
median_res: 0.3615819209039548
```

15.10.6 Evalution of the Default Hyperparameters

```
model_default.fit(X_train, y_train)["randomforestclassifier"]
```

```
RandomForestClassifier(bootstrap=1, max_depth=1024, max_leaf_nodes=1024,
                       n_estimators=128, oob_score=0)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.3295668549905838
```

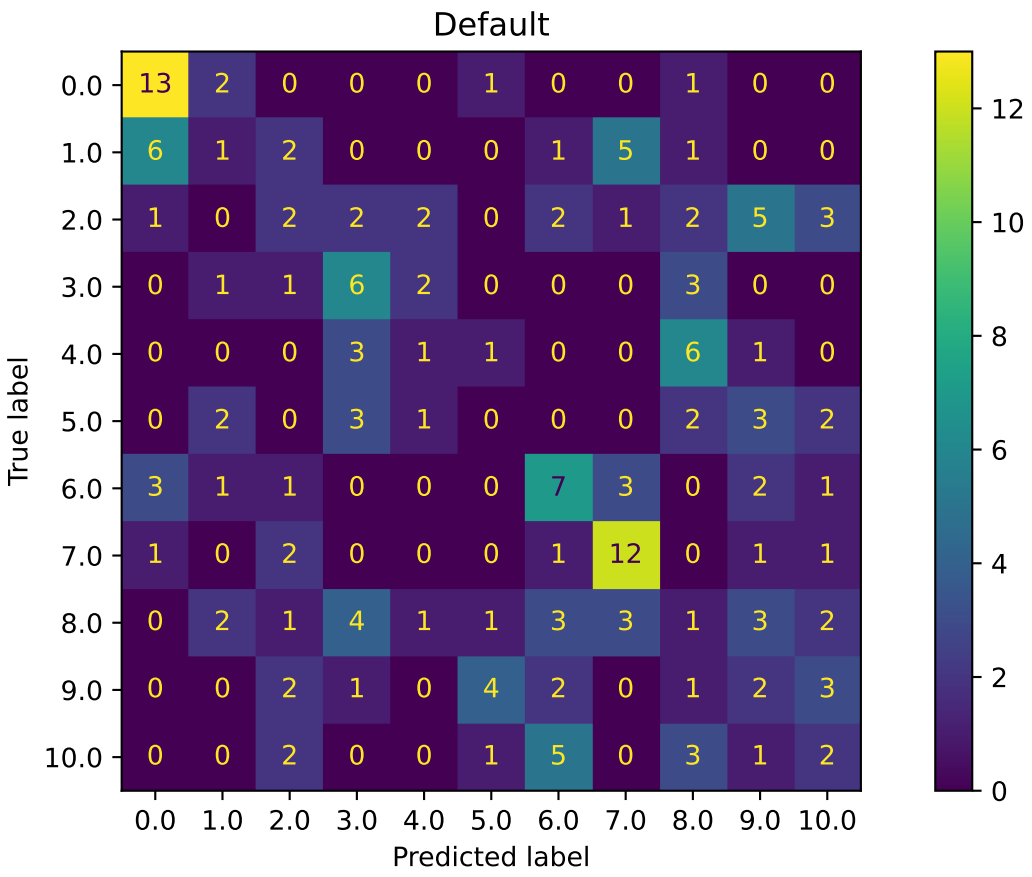
Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_default)
```

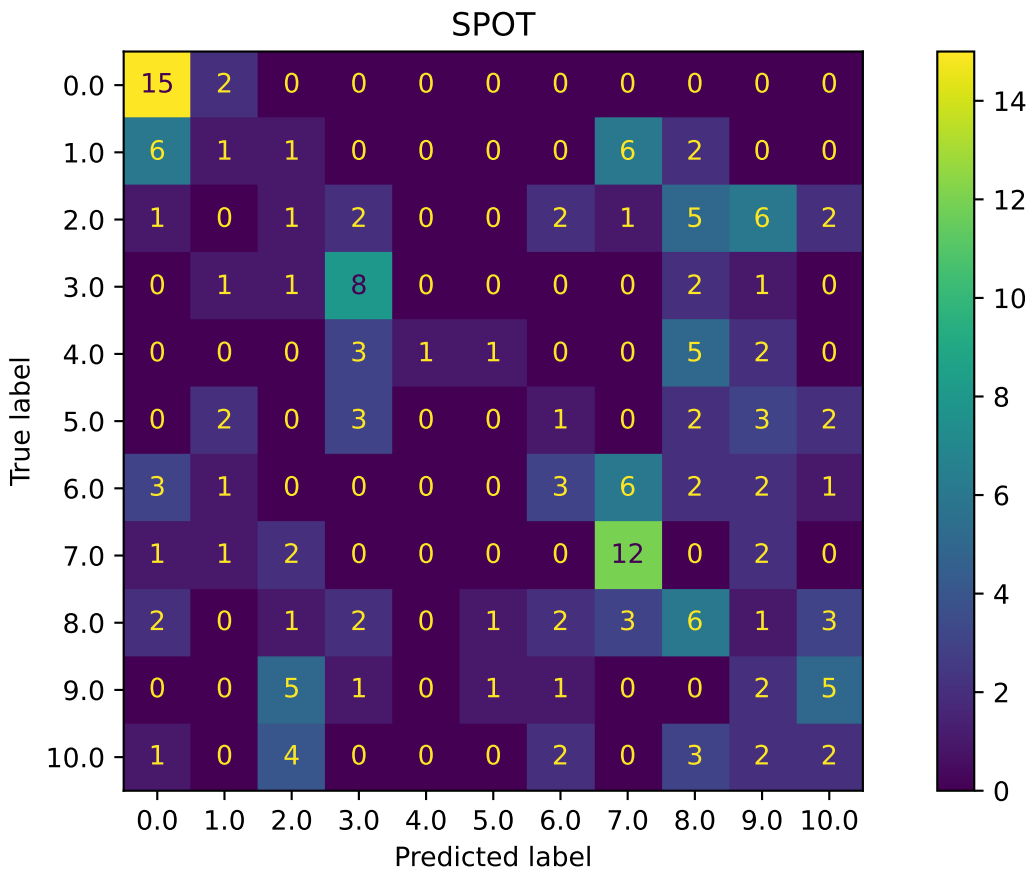
```
mean_res: 0.338480853735091
std_res: 0.013688038473151918
min_res: 0.31544256120527303
max_res: 0.3681732580037665
median_res: 0.3366290018832392
```

15.10.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```




```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```




```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.3694968553459119, -0.2858490566037736)
```

15.10.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3660377358490566, None)
```

```
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.29793028322440085, None)
```

- This is the evaluation that will be used in the comparison:

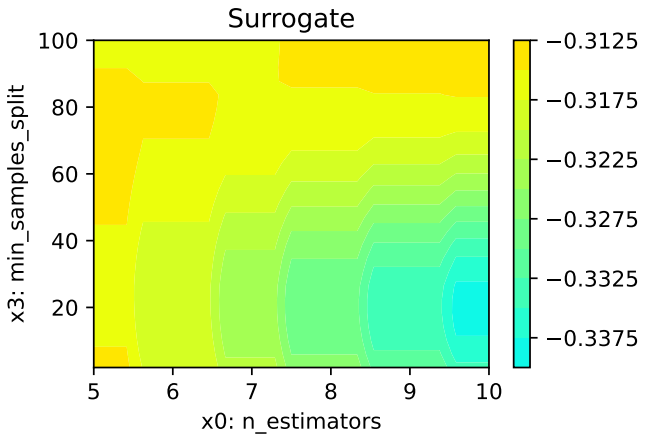
```
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

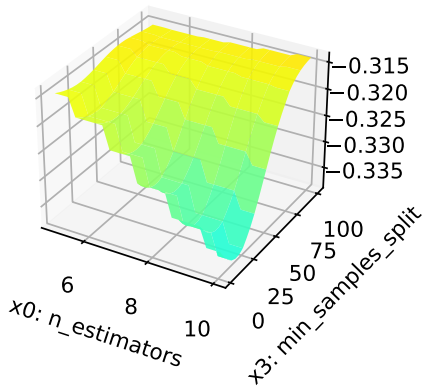
```
(0.3598859825620389, None)
```

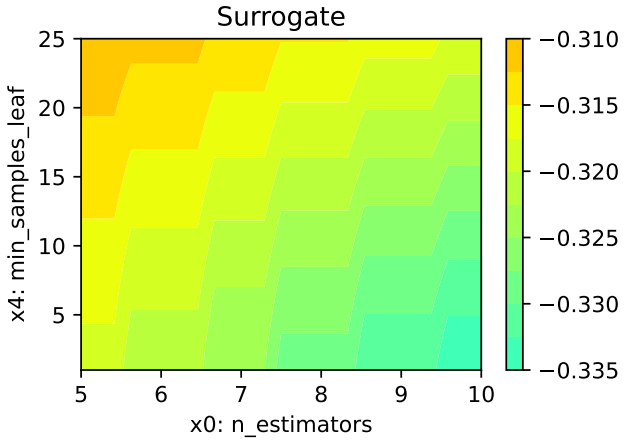
15.10.9 Detailed Hyperparameter Plots

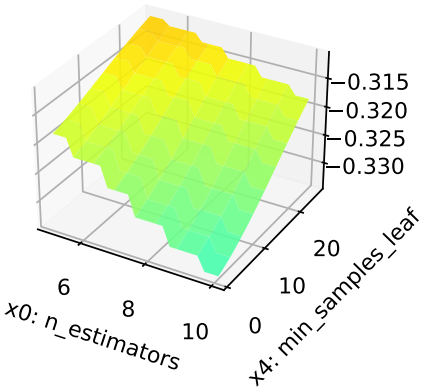
```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

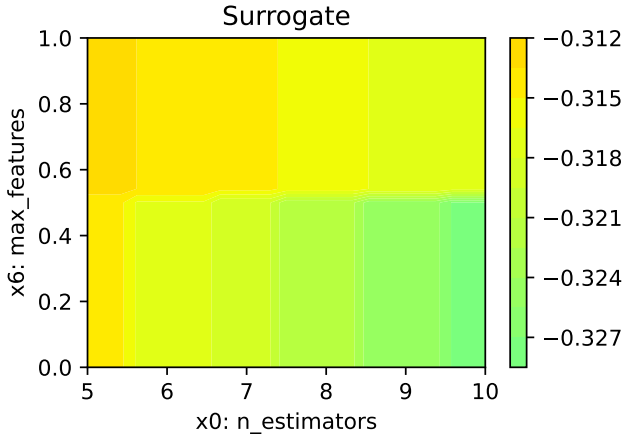
```
n_estimators:  0.06242752772054072
min_samples_split:  0.36314083309831824
min_samples_leaf:  0.04240927390389511
max_features:  100.0
max_leaf_nodes:  100.0
```

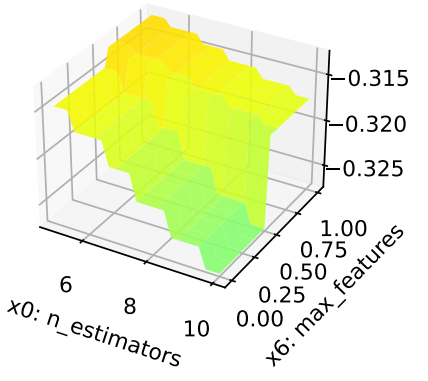

Surrogate
x3: min_samples_split
x0: n_estimators
100
80
60
40
20
5
6
7
8
9
10
−0.3125
−0.3175
−0.3225
−0.3275
−0.3325
−0.3375

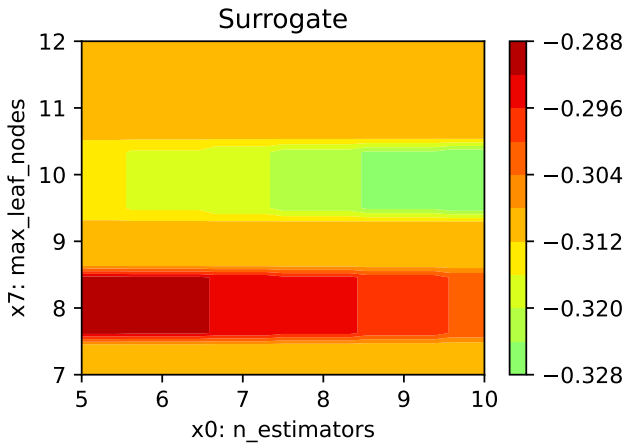

x0: n_estimators
x3: min_samples_split
6
8
10
0
25
50
75
100
−0.315
−0.320
−0.325
−0.330
−0.335

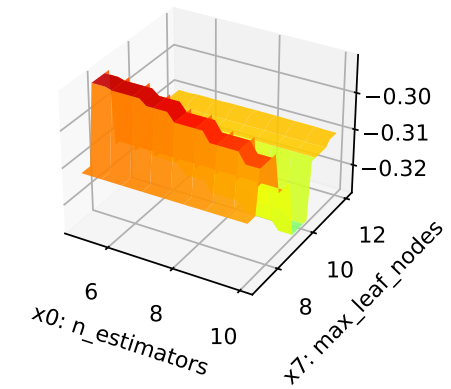

Surrogate
x4: min_samples_leaf
x0: n_estimators
25
20
15
10
5
5
6
7
8
9
10
−0.310
−0.315
−0.320
−0.325
−0.330
−0.335

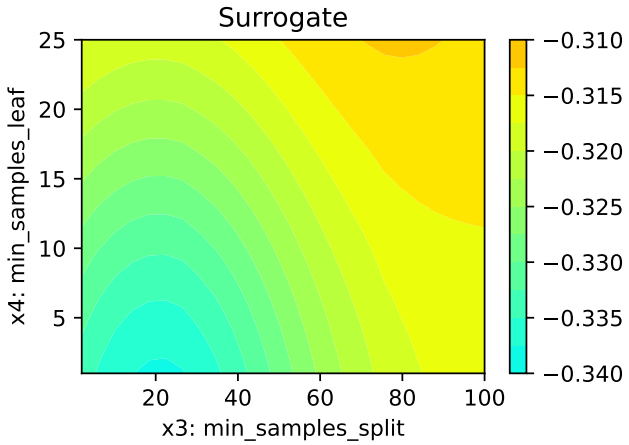

x0: n_estimators
x4: min_samples_leaf
6
8
10
0
10
20
−0.315
−0.320
−0.325
−0.330

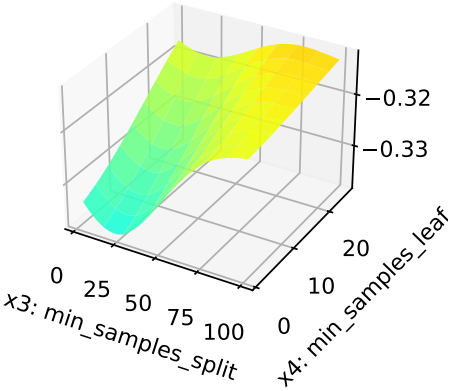

Surrogate
x6: max_features
x0: n_estimators
1.0
0.8
0.6
0.4
0.2
0.0
5
6
7
8
9
10
−0.312
−0.315
−0.318
−0.321
−0.324
−0.327

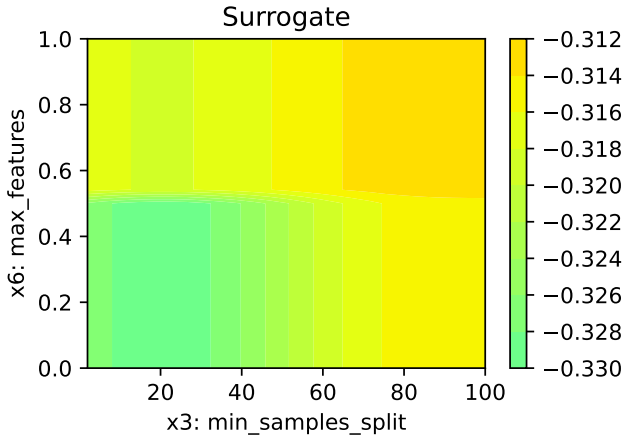

x0: n_estimators
x6: max_features
6
8
10
0.00
0.25
0.50
0.75
1.00
−0.315
−0.320
−0.325

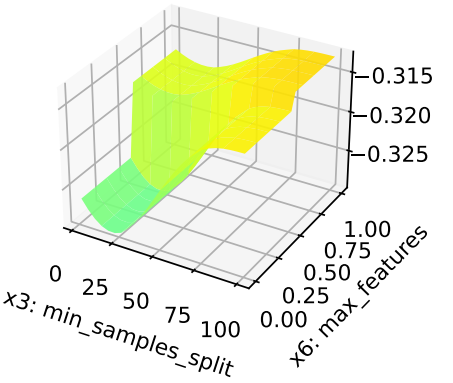

Surrogate
x7: max_leaf_nodes
x0: n_estimators
12
11
10
9
8
7
5
6
7
8
9
10
−0.288
−0.296
−0.304
−0.312
−0.320
−0.328

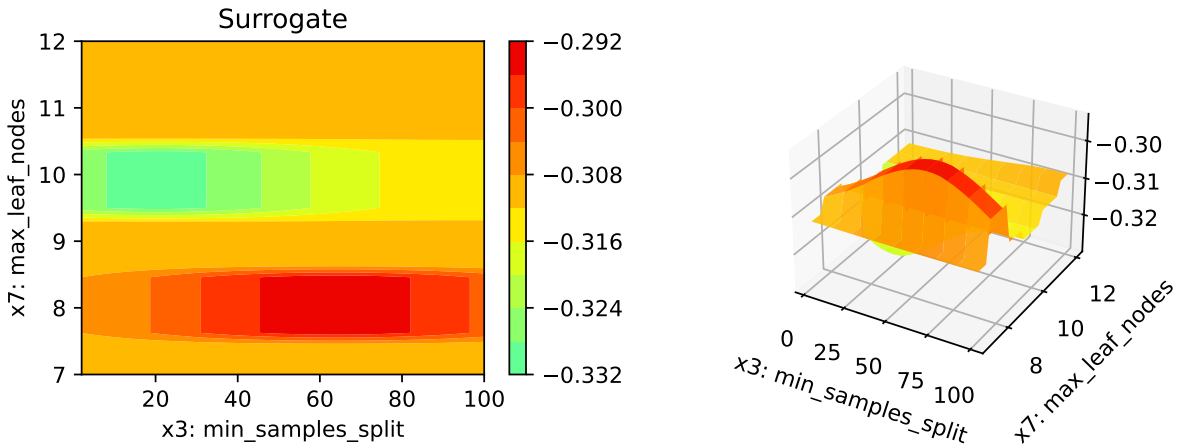

x0: n_estimators
x7: max_leaf_nodes
6
8
10
8
10
12
−0.30
−0.31
−0.32

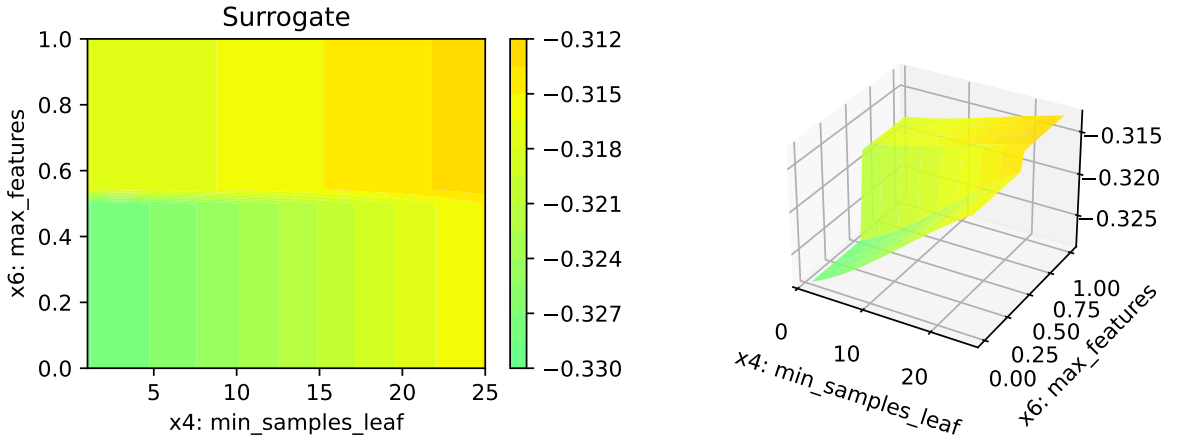

Surrogate
x4: min_samples_leaf
x3: min_samples_split
25
20
15
10
5
20
40
60
80
100
−0.310
−0.315
−0.320
−0.325
−0.330
−0.335
−0.340

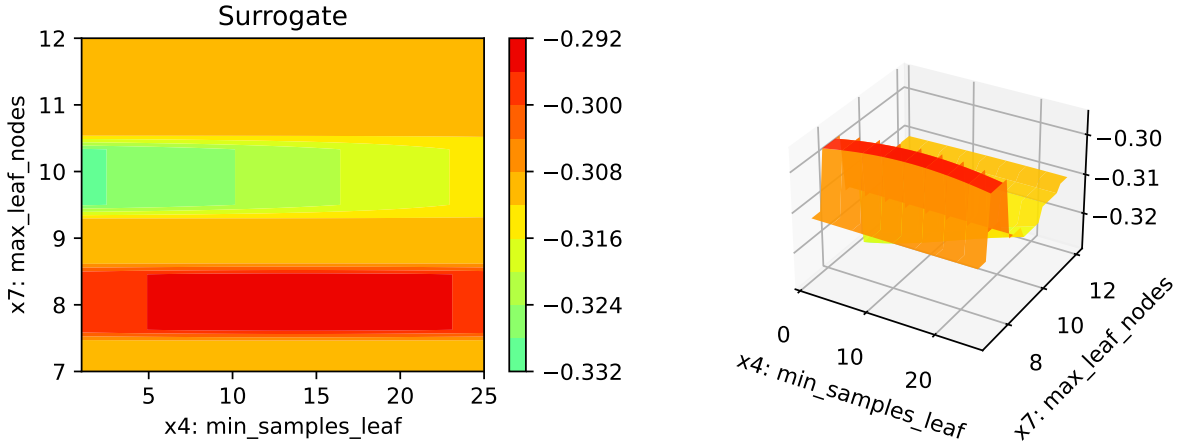

x3: min_samples_split
x4: min_samples_leaf
0
25
50
75
100
0
10
20
−0.32
−0.33

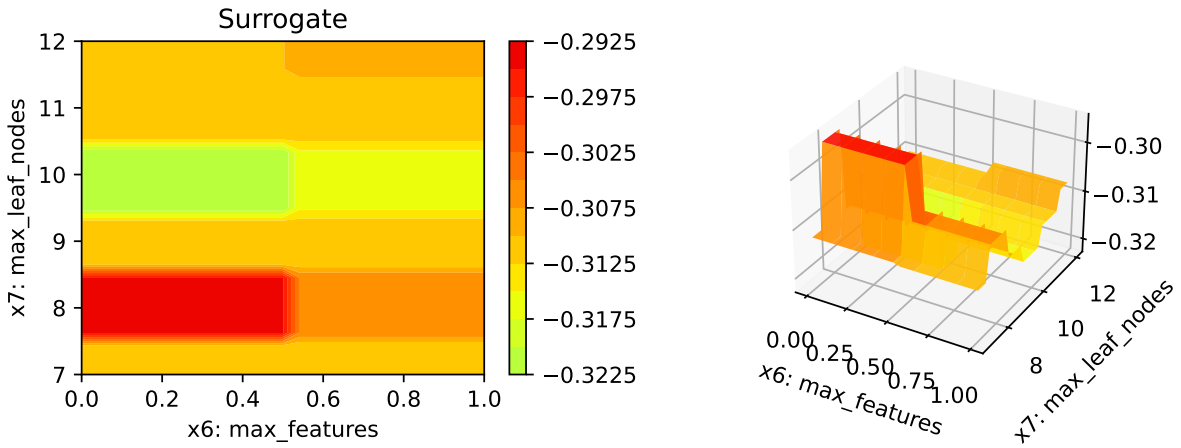

Surrogate
x6: max_features
x3: min_samples_split
1.0
0.8
0.6
0.4
0.2
0.0
20
40
60
80
100
−0.312
−0.314
−0.316
−0.318
−0.320
−0.322
−0.324
−0.326
−0.328
−0.330


x3: min_samples_split
x6: max_features
0
25
50
75
100
0.00
0.25
0.50
0.75
1.00
−0.315
−0.320
−0.325


Surrogate
x7: max_leaf_nodes
x3: min_samples_split
x3: min_samples_split
x7: max_leaf_nodes


Surrogate
x6: max_features
x4: min_samples_leaf
x4: min_samples_leaf
x6: max_features


Surrogate
x7: max_leaf_nodes
x4: min_samples_leaf
x4: min_samples_leaf
x7: max_leaf_nodes



15.10.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

15.10.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

16 HPT: sklearn XGB Classifier VBDP Data

This document refers to the following software versions:

- python: 3.10.10

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

spotPython can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of spotPython from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

16.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time and the initial design size.

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '17-xgb-sklearn' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(I
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
17-xgb-sklearn_bartz09_1min_5init_2023-06-19_04-09-05
```

```
import warnings
warnings.filterwarnings("ignore")
```

16.2 Step 2: Initialization of the Empty `fun_control` Dictionary

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/16_spot_hpt_sklearn_classification")
```

16.3 Step 3: PyTorch Data Loading

16.3.1 1. Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

16.3.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
# add the dataset to the fun_control
fun_control.update({"data": train_df, # full dataset,
                    "train": train,
                    "test": test,
                    "n_samples": n_samples,
                    "target_column": target_column})
```

16.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

```
prep_model = None
fun_control.update({"prep_model": prep_model})
```

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

```
# categorical_columns = []
# one_hot_encoder = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
# prep_model = ColumnTransformer(
#         transformers=[
#             ("categorical", one_hot_encoder, categorical_columns),
#         ],
#         remainder=StandardScaler(),
#     )
```

16.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

`fun_control = add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)`

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
core_model = RandomForestClassifier
# core_model = SVC
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
core_model = HistGradientBoostingClassifier
fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=SklearnHyperDict,
                                filename=None)
```

Now `fun_control` has the information from the JSON file. The available hyperparameters are:

```
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
loss
learning_rate
max_iter
max_leaf_nodes
max_depth
min_samples_leaf
l2_regularization
max_bins
early_stopping
```

```
n_iter_no_change
tol
```

16.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

16.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the `modify_hyper_parameter_bounds` method. For example, to change the `tol` hyperparameter of the `SVC` model to the interval [1e-3, 1e-2], the following code can be used:

```
fun_control = modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3,
1e-2])
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
# fun_control = modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])
# fun_control = modify_hyper_parameter_bounds(fun_control, "min_samples_split", bounds=[3,
# fun_control = modify_hyper_parameter_bounds(fun_control, "dual", bounds=[0, 0])
# fun_control = modify_hyper_parameter_bounds(fun_control, "probability", bounds=[1, 1])
# fun_control["core_model_hyper_dict"]["tol"]
# fun_control = modify_hyper_parameter_bounds(fun_control, "min_samples_leaf", bounds=[1,
# fun_control = modify_hyper_parameter_bounds(fun_control, "n_estimators", bounds=[5, 10])
```

16.6.2 Modify hyperparameter of type factor

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

Factors can be modified with the `modify_hyper_parameter_levels` function. For example, to exclude the `sigmoid` kernel from the tuning, the `kernel` hyperparameter of the `SVC` model can be modified as follows:

```
fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["linear",
"rbf"])
```

The new setting can be controlled via:

```
fun_control["core_model_hyper_dict"]["kernel"]
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
# XGBoost:
fun_control = modify_hyper_parameter_levels(fun_control, "loss", ["log_loss"])
```

16.6.3 Optimizers

Optimizers are described in Section 14.6.1.

16.7 Step 7: Selection of the Objective (Loss) Function

16.7.1 Evaluation

The evaluation procedure requires the specification of two elements:

1. the way how the data is split into a train and a test set and
2. the loss function (and a metric).

16.7.2 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

16.7.3 Loss Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

16.7.4 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

16.7.4.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

16.7.4.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
                "weights": -1,
                "metric_sklearn": mapk_score,
                "predict_proba": True,
                "metric_params": {"k": 3},
                })
```

16.7.5 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
})
```

16.7.5.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key `"k_folds"`. For example, to use 5-fold cross validation, the key `"k_folds"` is set to `5`. Uncomment the following line to use cross validation:

```
# fun_control.update({
#      "eval": "train_cv",
#      "k_folds": 10,
# })
```

16.8 Step 8: Calling the SPOT Function

16.8.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name              | type   | default   |   lower |   upper | transform             |
|-------------------|--------|-----------|---------|---------|-----------------------|
| loss              | factor | log_loss  |   0     |   0     | None                  |
| learning_rate     | float  | -1.0      |  -5     |   0     | transform_power_10    |
| max_iter          | int    | 7         |   3     |  10     | transform_power_2_int |
| max_leaf_nodes    | int    | 5         |   1     |  12     | transform_power_2_int |
| max_depth         | int    | 2         |   1     |  20     | transform_power_2_int |
| min_samples_leaf  | int    | 4         |   2     |  10     | transform_power_2_int |
| l2_regularization | float  | 0.0       |   0     |  10     | None                  |
| max_bins          | int    | 255       | 127     | 255     | None                  |
| early_stopping    | factor | 1         |   0     |   1     | None                  |
| n_iter_no_change  | int    | 10        |   5     |  20     | None                  |
| tol               | float  | 0.0001    |   1e-05 |   0.001 | None                  |
```

16.8.2 The Objective Function

The objective function is selected next. It implements an interface from `sklearn`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

16.8.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=SklearnHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
array([[ 0.00e+00, -1.00e+00,  7.00e+00,  5.00e+00,  2.00e+00,  4.00e+00,
         0.00e+00,  2.55e+02,  1.00e+00,  1.00e+01,  1.00e-04]])
```

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
spotPython tuning: -0.3082706766917293 [----------] 4.50%

spotPython tuning: -0.32832080200501257 [##--------] 16.24%

spotPython tuning: -0.3446115288220551 [##--------] 22.25%

spotPython tuning: -0.3446115288220551 [##--------] 24.49%

spotPython tuning: -0.3446115288220551 [###-------] 26.75%
```

```
spotPython tuning: -0.3609022556390977 [####------] 36.44%

spotPython tuning: -0.3609022556390977 [####------] 44.05%

spotPython tuning: -0.3609022556390977 [########--] 84.16%

spotPython tuning: -0.3609022556390977 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x28d365300>
```

16.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

16.10 Step 10: Results

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

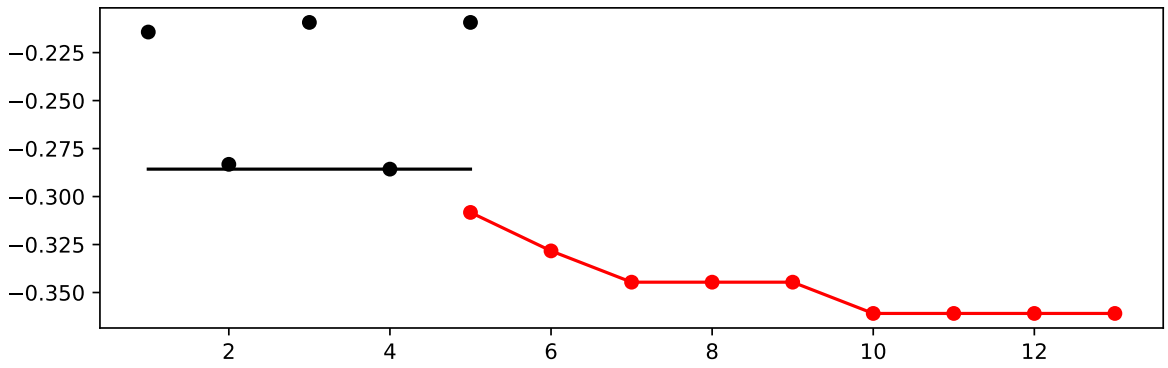


Figure 16.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

```
print(gen_design_table(fun_control=fun_control,
    spot=spot_tuner))
```

name	type	default	lower	upper	tuned	transi
loss	factor	log_loss	0.0	0.0	0.0	None
learning_rate	float	-1.0	-5.0	0.0	-1.8860361379529507	transi
max_iter	int	7	3.0	10.0	8.0	transi
max_leaf_nodes	int	5	1.0	12.0	2.0	transi
max_depth	int	2	1.0	20.0	20.0	transi
min_samples_leaf	int	4	2.0	10.0	2.0	transi
l2_regularization	float	0.0	0.0	10.0	5.0648633125794476	None
max_bins	int	255	127.0	255.0	130.0	None
early_stopping	factor	1	0.0	1.0	0.0	None
n_iter_no_change	int	10	5.0	20.0	12.0	None
tol	float	0.0001	1e-05	0.001	0.0009999411112607051	None

16.10.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

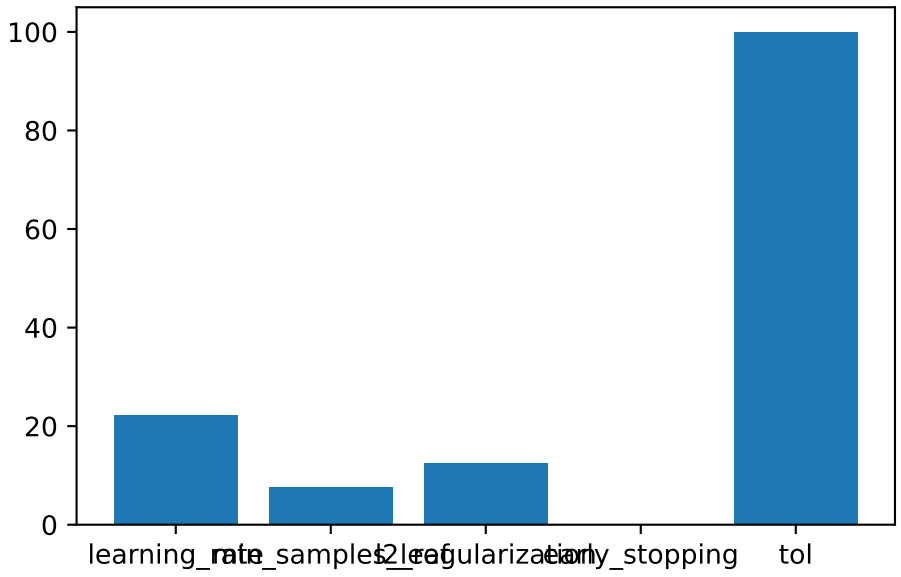


Figure 16.2: Variable importance plot, threshold 0.025.

16.10.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'loss': 'log_loss',
 'learning_rate': 0.1,
 'max_iter': 128,
 'max_leaf_nodes': 32,
 'max_depth': 4,
 'min_samples_leaf': 16,
 'l2_regularization': 0.0,
 'max_bins': 255,
 'early_stopping': 1,
 'n_iter_no_change': 10,
 'tol': 0.0001}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('histgradientboostingclassifier',
                 HistGradientBoostingClassifier(early_stopping=1, max_depth=4,
                                                max_iter=128, max_leaf_nodes=32,
                                                min_samples_leaf=16,
                                                tol=0.0001))])
```

16.10.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[ 0.00000000e+00 -1.88603614e+00  8.00000000e+00  2.00000000e+00
   2.00000000e+01  2.00000000e+00  5.06486331e+00  1.30000000e+02
   0.00000000e+00  1.20000000e+01  9.99941111e-04]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'loss': 'log_loss',
  'learning_rate': 0.013000613944983763,
  'max_iter': 256,
  'max_leaf_nodes': 4,
  'max_depth': 1048576,
  'min_samples_leaf': 4,
  'l2_regularization': 5.0648633125794476,
  'max_bins': 130,
  'early_stopping': 0,
  'n_iter_no_change': 12,
  'tol': 0.00099994111112607051}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
HistGradientBoostingClassifier(early_stopping=0,
                               l2_regularization=5.0648633125794476,
                               learning_rate=0.013000613944983763, max_bins=130,
                               max_depth=1048576, max_iter=256,
                               max_leaf_nodes=4, min_samples_leaf=4,
                               n_iter_no_change=12, tol=0.0009999411112607051)
```

16.10.4 Evaluate SPOT Results

- Fetch the data.

```
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.3295668549905838
```

```
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

16.10.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.3295668549905837
std_res: 1.1102230246251565e-16
min_res: 0.3295668549905838
max_res: 0.3295668549905838
median_res: 0.3295668549905838
```

16.10.6 Evalution of the Default Hyperparameters

```
model_default.fit(X_train, y_train)["histgradientboostingclassifier"]
```

```
HistGradientBoostingClassifier(early_stopping=1, max_depth=4, max_iter=128,
                               max_leaf_nodes=32, min_samples_leaf=16,
                               tol=0.0001)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.3389830508474576
```

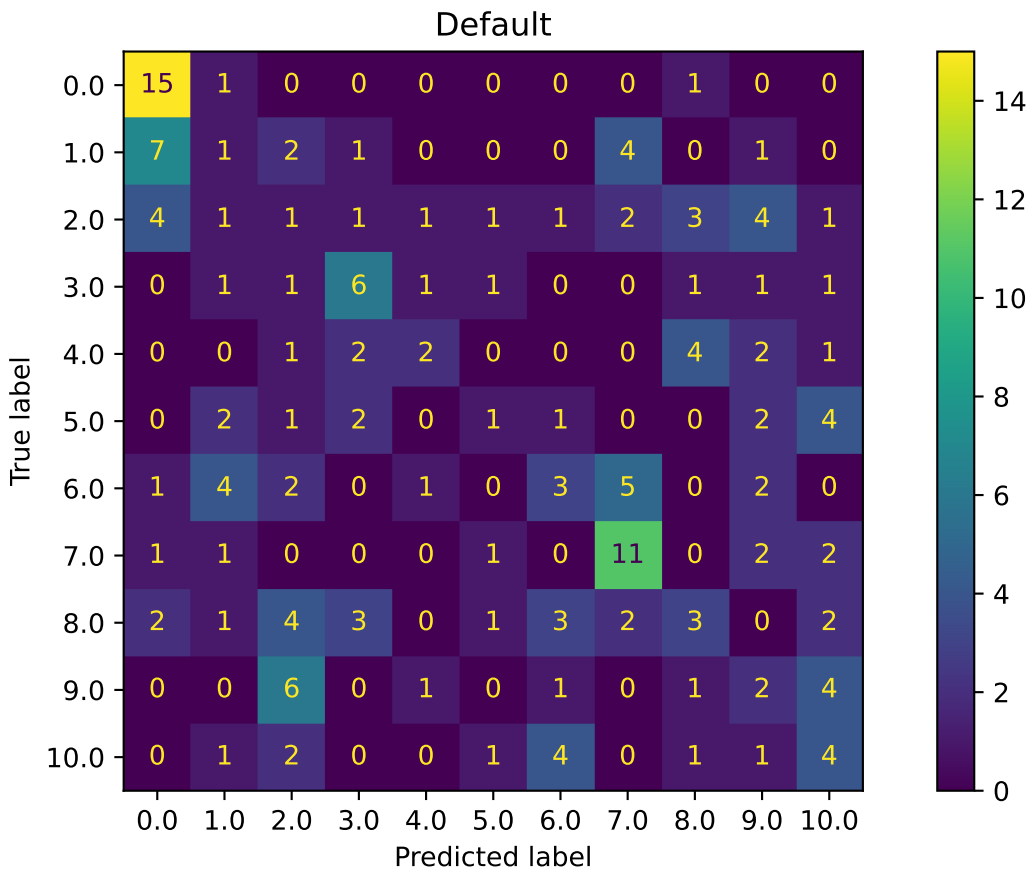
Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_default)
```

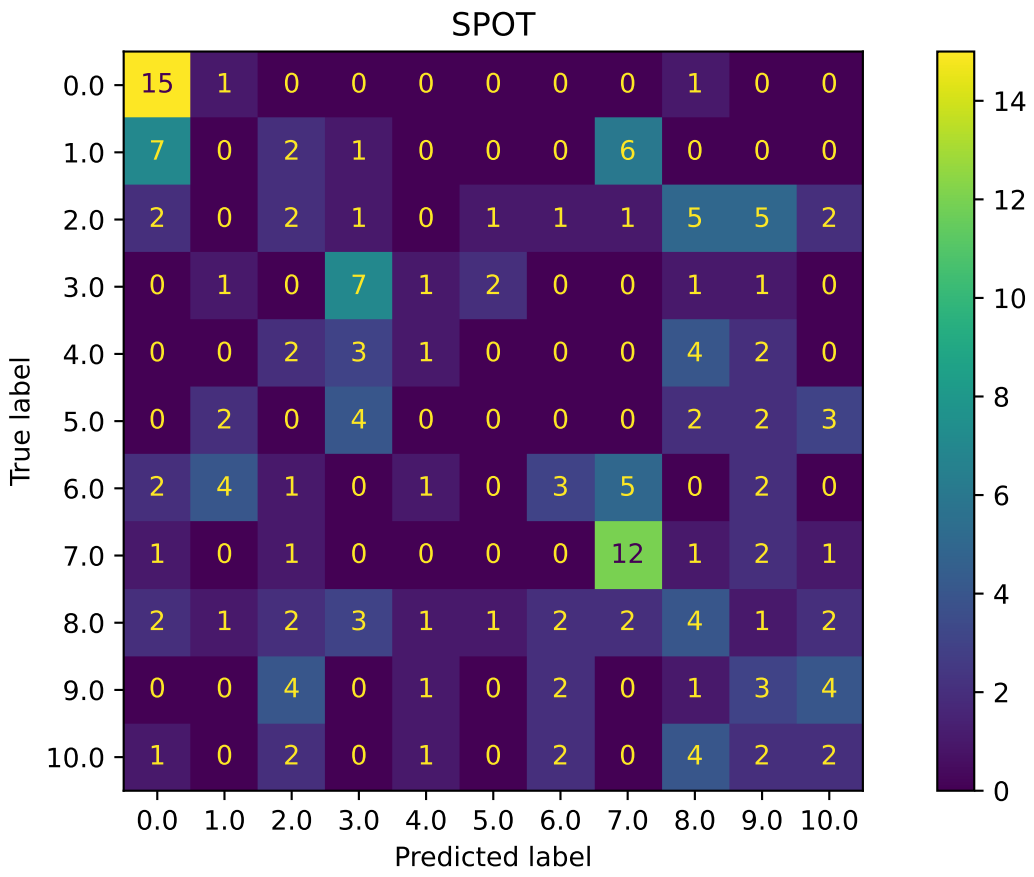
```
mean_res: 0.3375706214689266
std_res: 0.012500864451367001
min_res: 0.3107344632768362
max_res: 0.3615819209039548
median_res: 0.3408662900188324
```

16.10.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```




```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```




```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.3609022556390977, -0.20927318295739344)
```

16.10.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.35062893081761004, None)
```

```
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.30468409586056644, None)
```

- This is the evaluation that will be used in the comparison:

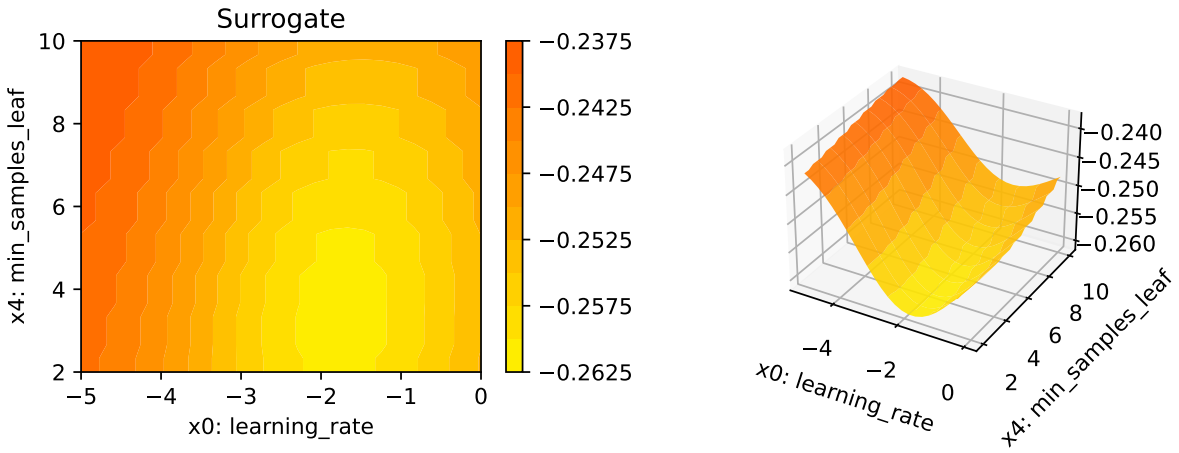
```
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

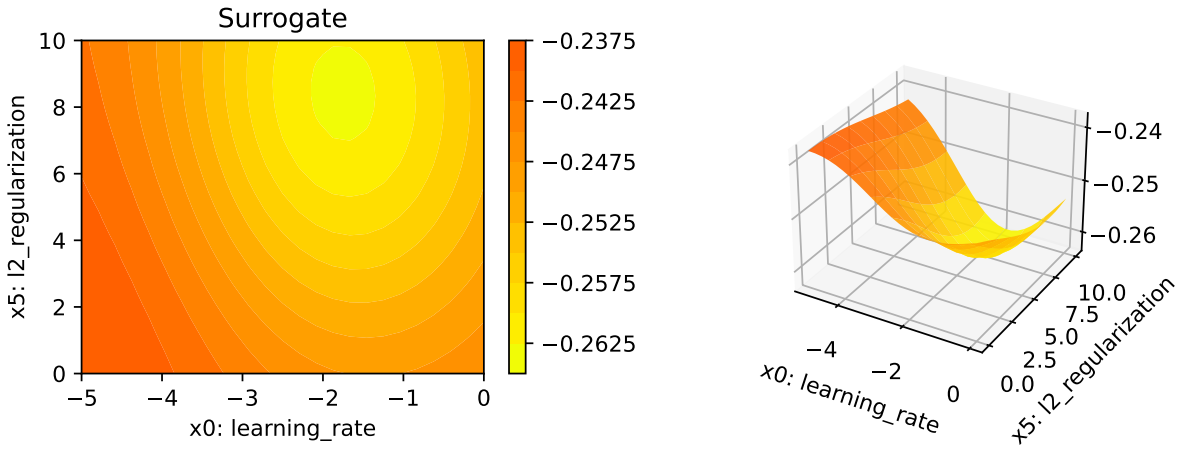
```
(0.3542924211938296, None)
```

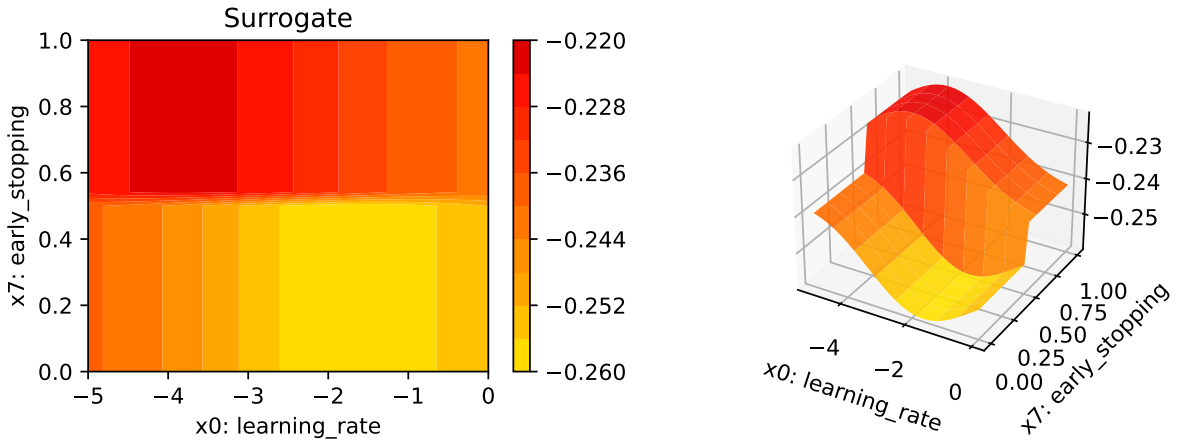
16.10.9 Detailed Hyperparameter Plots

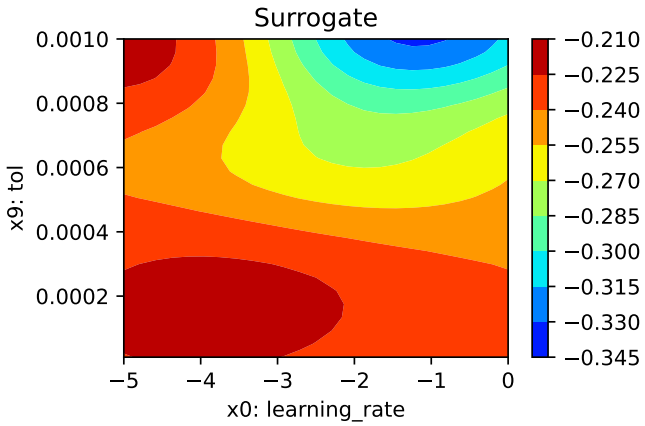
```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

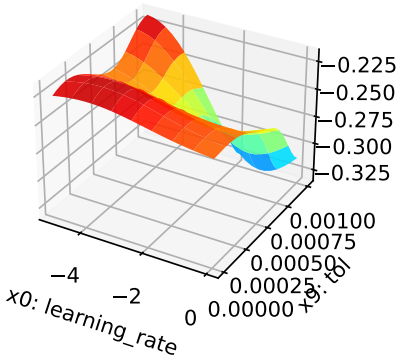
```
learning_rate:  22.139137766465417
min_samples_leaf:  7.571463764452644
l2_regularization:  12.511775110768742
early_stopping:  0.10772129685854573
tol:  100.0
```

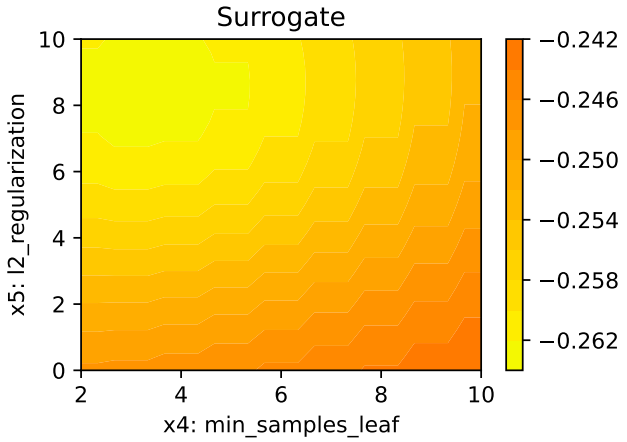

Surrogate
x4: min_samples_leaf
x0: learning_rate
x0: learning_rate
x4: min_samples_leaf

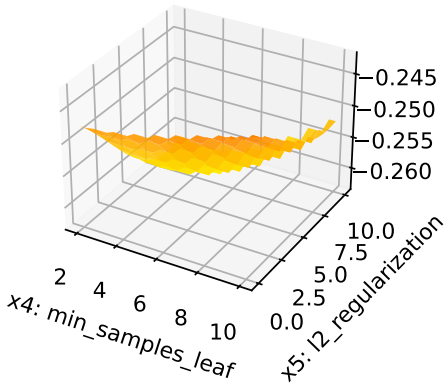

Surrogate
x5: l2_regularization
x0: learning_rate
x0: learning_rate
x5: l2_regularization

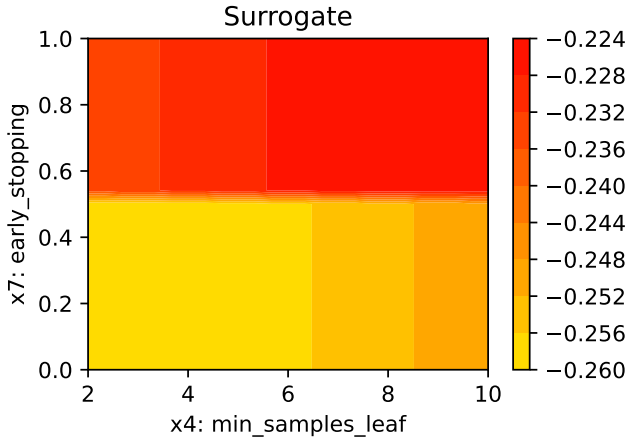

Surrogate
x7: early_stopping
x0: learning_rate
x0: learning_rate
x7: early_stopping

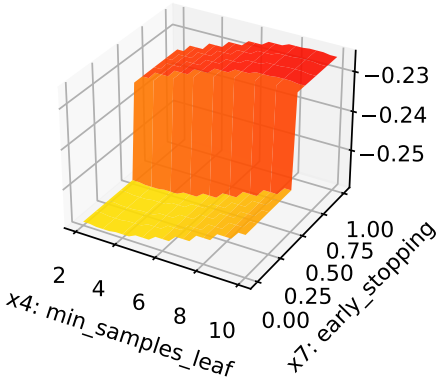

Surrogate
x9: tol
x0: learning_rate
0.0010
0.0008
0.0006
0.0004
0.0002
−5
−4
−3
−2
−1
0
−0.210
−0.225
−0.240
−0.255
−0.270
−0.285
−0.300
−0.315
−0.330
−0.345

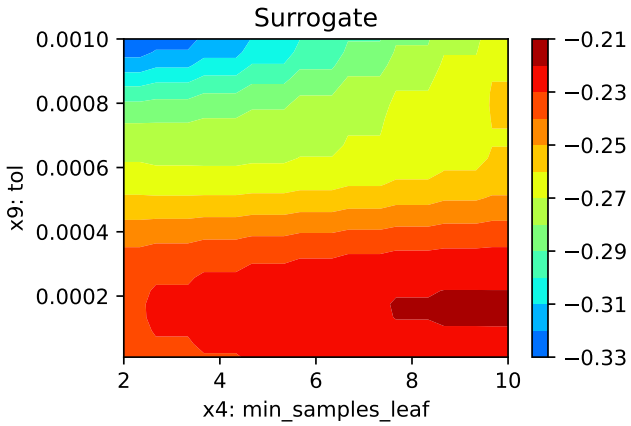

x0: learning_rate
x9: tol
−4
−2
0
0.00100
0.00075
0.00050
0.00025
0.00000
−0.225
−0.250
−0.275
−0.300
−0.325

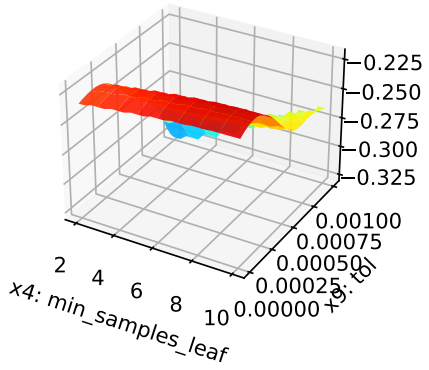

Surrogate
x5: l2_regularization
x4: min_samples_leaf
10
8
6
4
2
0
2
4
6
8
10
−0.242
−0.246
−0.250
−0.254
−0.258
−0.262

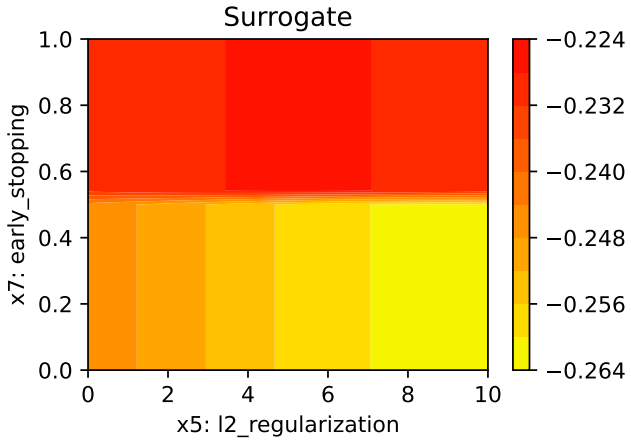

x4: min_samples_leaf
x5: l2_regularization
2
4
6
8
10
10.0
7.5
5.0
2.5
0.0
−0.245
−0.250
−0.255
−0.260

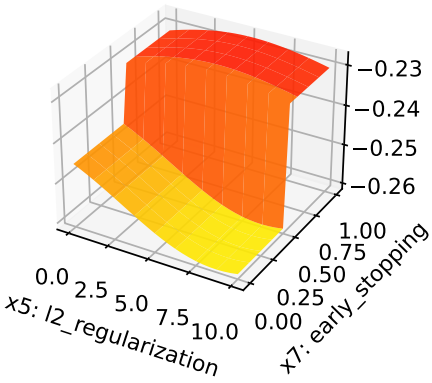

Surrogate
x7: early_stopping
x4: min_samples_leaf
1.0
0.8
0.6
0.4
0.2
0.0
2
4
6
8
10
−0.224
−0.228
−0.232
−0.236
−0.240
−0.244
−0.248
−0.252
−0.256
−0.260

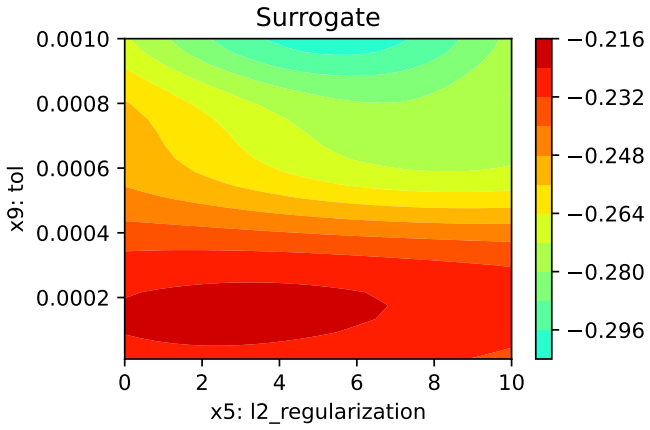

x4: min_samples_leaf
x7: early_stopping
2
4
6
8
10
1.00
0.75
0.50
0.25
0.00
−0.23
−0.24
−0.25

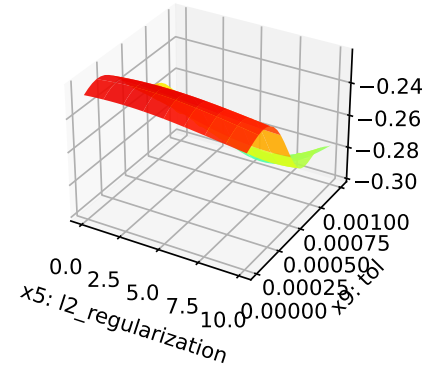

Surrogate
x9: tol
x4: min_samples_leaf
0.0010
0.0008
0.0006
0.0004
0.0002
2
4
6
8
10
−0.21
−0.23
−0.25
−0.27
−0.29
−0.31
−0.33

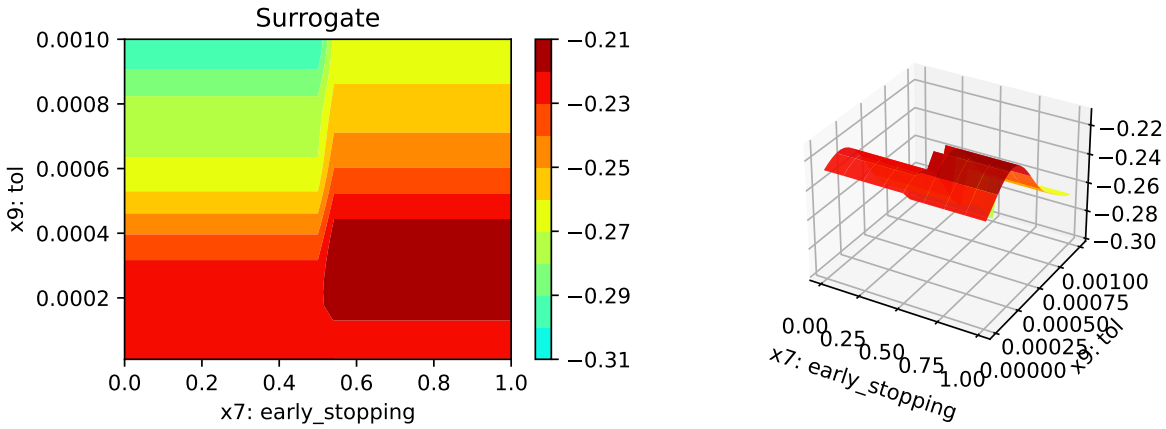

x4: min_samples_leaf
x9: tol
2
4
6
8
10
0.00000
0.00025
0.00050
0.00075
0.00100
−0.225
−0.250
−0.275
−0.300
−0.325


Surrogate
x7: early_stopping
x5: l2_regularization
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
−0.224
−0.232
−0.240
−0.248
−0.256
−0.264


x5: l2_regularization
x7: early_stopping
0.0
2.5
5.0
7.5
10.0
0.00
0.25
0.50
0.75
1.00
−0.23
−0.24
−0.25
−0.26


Surrogate
x9: tol
x5: l2_regularization
0.0010
0.0008
0.0006
0.0004
0.0002
0
2
4
6
8
10
−0.216
−0.232
−0.248
−0.264
−0.280
−0.296


x5: l2_regularization
x9: tol
0.0
2.5
5.0
7.5
10.0
0.00000
0.00025
0.00050
0.00075
0.00100
−0.24
−0.26
−0.28
−0.30



16.10.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

16.10.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

17 HPT: sklearn SVC VBDP Data

This document refers to the following software versions:

- python: 3.10.10

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

spotPython can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of spotPython from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

17.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time and the initial design size.

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '18-svc-sklearn' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(I
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
18-svc-sklearn_bartz09_1min_5init_2023-06-19_04-16-46
```

```
import warnings
warnings.filterwarnings("ignore")
```

17.2 Step 2: Initialization of the Empty `fun_control` Dictionary

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/16_spot_hpt_sklearn_classification")
```

17.3 Step 3: PyTorch Data Loading

17.3.1 1. Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

17.3.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
# add the dataset to the fun_control
fun_control.update({"data": train_df, # full dataset,
                    "train": train,
                    "test": test,
                    "n_samples": n_samples,
                    "target_column": target_column})
```

17.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

```
prep_model = None
fun_control.update({"prep_model": prep_model})
```

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

```
# categorical_columns = []
# one_hot_encoder = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
# prep_model = ColumnTransformer(
#         transformers=[
#             ("categorical", one_hot_encoder, categorical_columns),
#         ],
#         remainder=StandardScaler(),
#     )
```

17.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

```
fun_control = add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)
```

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
# core_model = RandomForestClassifier
core_model = SVC
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
# core_model = HistGradientBoostingClassifier
fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=SklearnHyperDict,
                                filename=None)
```

Now `fun_control` has the information from the JSON file. The available hyperparameters are:

```
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
C
kernel
degree
gamma
coef0
shrinking
probability
tol
cache_size
```

break_ties

17.6 Step 6: Modify hyper_dict Hyperparameters for the Selected Algorithm aka core_model

17.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the modify_hyper_parameter_bounds method. For example, to change the tol hyperparameter of the SVC model to the interval [1e-3, 1e-2], the following code can be used:

```
fun_control = modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3,
1e-2])
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
fun_control = modify_hyper_parameter_bounds(fun_control, "probability", bounds=[1, 1])
```

17.6.2 Modify hyperparameter of type factor

spotPython provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

Factors can be modified with the modify_hyper_parameter_levels function. For example, to exclude the sigmoid kernel from the tuning, the kernel hyperparameter of the SVC model can be modified as follows:

```
fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["linear",
"rbf"])
```

The new setting can be controlled via:

```
fun_control["core_model_hyper_dict"]["kernel"]
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["rbf"])
```

17.6.3 Optimizers

Optimizers are described in Section 14.6.1.

17.6.4 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

17.7 Step 7: Selection of the Objective (Loss) Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

17.7.1 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

17.7.1.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

17.7.1.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
               "weights": -1,
               "metric_sklearn": mapk_score,
               "predict_proba": True,
               "metric_params": {"k": 3},
               })
```

17.7.2 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
})
```

17.7.2.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key `"k_folds"`. For example, to use 5-fold cross validation, the key `"k_folds"` is set to `5`. Uncomment the following line to use cross validation:

```
# fun_control.update({
#      "eval": "train_cv",
#      "k_folds": 10,
# })
```

17.8 Step 8: Calling the SPOT Function

17.8.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name        | type   | default   |    lower |   upper | transform   |
|-------------|--------|-----------|----------|---------|-------------|
| C           | float  | 1.0       |   0.1    |   10    | None        |
| kernel      | factor | rbf       |   0      |    0    | None        |
| degree      | int    | 3         |   3      |    3    | None        |
| gamma       | factor | scale     |   0      |    1    | None        |
| coef0       | float  | 0.0       |   0      |    0    | None        |
| shrinking   | factor | 0         |   0      |    1    | None        |
| probability | factor | 0         |   1      |    1    | None        |
| tol         | float  | 0.001     |   0.0001 |    0.01 | None        |
| cache_size  | float  | 200.0     | 100      |  400    | None        |
| break_ties  | factor | 0         |   0      |    1    | None        |
```

17.8.2 The Objective Function

The objective function is selected next. It implements an interface from `sklearn`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

17.8.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=SklearnHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
array([[1.e+00, 2.e+00, 3.e+00, 0.e+00, 0.e+00, 0.e+00, 0.e+00, 1.e-03,
        2.e+02, 0.e+00]])
```

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
```

```
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
spotPython tuning: -0.3646616541353383 [----------] 0.33%

spotPython tuning: -0.3646616541353383 [----------] 0.79%

spotPython tuning: -0.3646616541353383 [----------] 1.38%

spotPython tuning: -0.3646616541353383 [----------] 1.90%

spotPython tuning: -0.3646616541353383 [----------] 2.52%

spotPython tuning: -0.3646616541353383 [----------] 3.03%

spotPython tuning: -0.3646616541353383 [----------] 3.51%

spotPython tuning: -0.3646616541353383 [----------] 3.94%

spotPython tuning: -0.3646616541353383 [----------] 4.36%

spotPython tuning: -0.3734335839598997 [----------] 4.73%

spotPython tuning: -0.3734335839598997 [#---------] 5.23%

spotPython tuning: -0.37844611528822053 [#---------] 5.69%
```

```
spotPython tuning: -0.3847117794486215 [#---------] 7.44%

spotPython tuning: -0.3847117794486215 [#---------] 8.99%

spotPython tuning: -0.3847117794486215 [#---------] 10.67%

spotPython tuning: -0.3847117794486215 [#---------] 12.53%

spotPython tuning: -0.3847117794486215 [#---------] 14.16%

spotPython tuning: -0.3847117794486215 [##--------] 15.51%

spotPython tuning: -0.3847117794486215 [##--------] 16.90%

spotPython tuning: -0.3847117794486215 [##--------] 18.88%

spotPython tuning: -0.3847117794486215 [##--------] 20.54%

spotPython tuning: -0.3847117794486215 [##--------] 21.79%

spotPython tuning: -0.3847117794486215 [##--------] 23.10%

spotPython tuning: -0.38596491228070173 [##--------] 24.48%

spotPython tuning: -0.38596491228070173 [###-------] 25.91%

spotPython tuning: -0.38596491228070173 [###-------] 27.08%

spotPython tuning: -0.38596491228070173 [###-------] 28.13%

spotPython tuning: -0.38721804511278196 [###-------] 29.35%

spotPython tuning: -0.3922305764411027 [###-------] 30.74%

spotPython tuning: -0.3922305764411027 [###-------] 32.61%

spotPython tuning: -0.3922305764411027 [###-------] 34.94%
```

```
spotPython tuning: -0.3922305764411027 [####------] 37.51%

spotPython tuning: -0.3922305764411027 [####------] 40.38%

spotPython tuning: -0.3922305764411027 [####------] 43.00%

spotPython tuning: -0.3922305764411027 [#####-----] 45.57%

spotPython tuning: -0.3922305764411027 [#####-----] 48.59%

spotPython tuning: -0.3922305764411027 [#####-----] 51.19%

spotPython tuning: -0.3922305764411027 [#####-----] 53.60%

spotPython tuning: -0.3922305764411027 [######----] 56.12%

spotPython tuning: -0.3922305764411027 [######----] 58.45%

spotPython tuning: -0.3922305764411027 [######----] 61.00%

spotPython tuning: -0.3922305764411027 [######----] 63.76%

spotPython tuning: -0.3922305764411027 [#######---] 66.76%

spotPython tuning: -0.3922305764411027 [#######---] 70.26%

spotPython tuning: -0.3922305764411027 [#######---] 73.44%

spotPython tuning: -0.3922305764411027 [########--] 76.50%

spotPython tuning: -0.3922305764411027 [########--] 78.98%

spotPython tuning: -0.3922305764411027 [########--] 82.50%

spotPython tuning: -0.3922305764411027 [#########-] 85.12%

spotPython tuning: -0.3922305764411027 [#########-] 87.79%
```

```
spotPython tuning: -0.39348370927318294 [#########-] 90.18%

spotPython tuning: -0.39348370927318294 [#########-] 93.68%

spotPython tuning: -0.39348370927318294 [##########] 97.03%

spotPython tuning: -0.39348370927318294 [##########] 99.79%

spotPython tuning: -0.39348370927318294 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x28f2ec580>
```

17.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

17.10 Step 10: Results

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

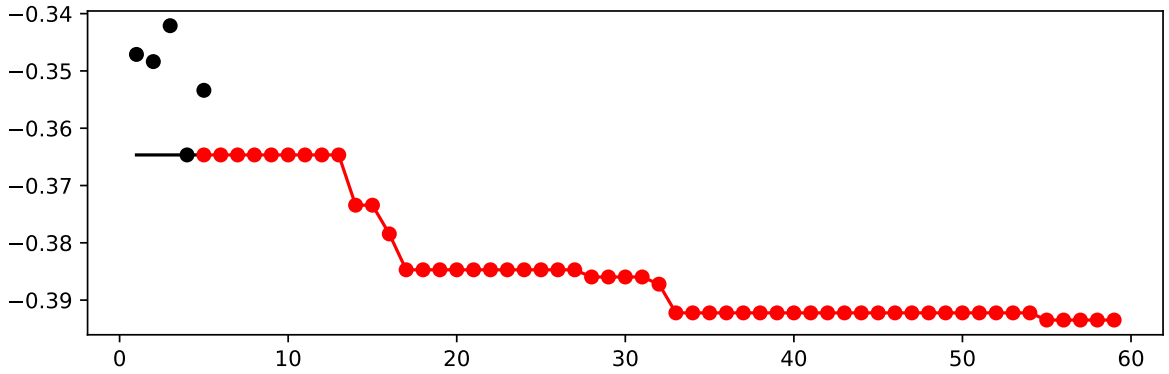


Figure 17.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

```
print(gen_design_table(fun_control=fun_control,
    spot=spot_tuner))
```

name	type	default	lower	upper	tuned	transform
C	float	1.0	0.1	10.0	4.016160671342672	None
kernel	factor	rbf	0.0	0.0	0.0	None
degree	int	3	3.0	3.0	3.0	None
gamma	factor	scale	0.0	1.0	1.0	None
coef0	float	0.0	0.0	0.0	0.0	None
shrinking	factor	0	0.0	1.0	1.0	None
probability	factor	0	1.0	1.0	1.0	None
tol	float	0.001	0.0001	0.01	0.002210461951108952	None
cache_size	float	200.0	100.0	400.0	156.83495628776507	None
break_ties	factor	0	0.0	1.0	0.0	None

17.10.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

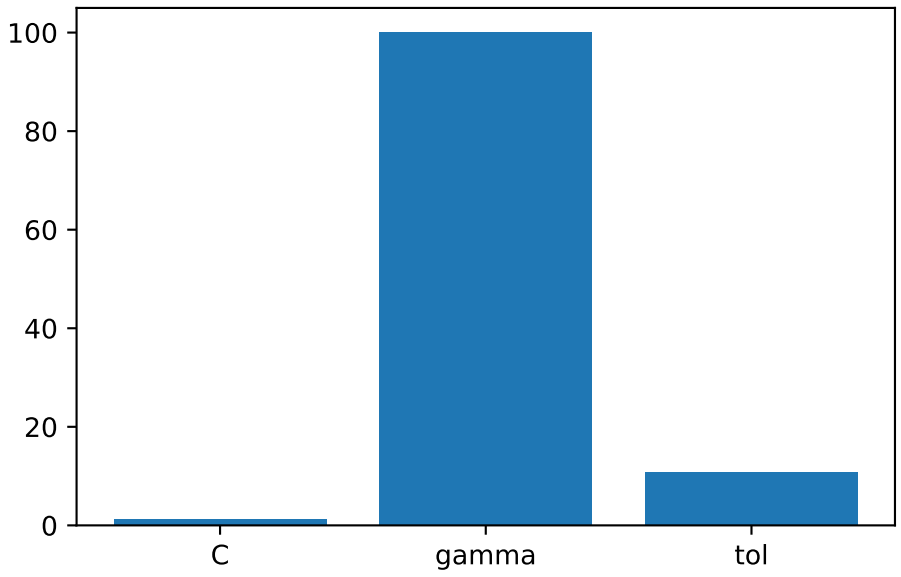


Figure 17.2: Variable importance plot, threshold 0.025.

17.10.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'C': 1.0,
 'kernel': 'rbf',
 'degree': 3,
 'gamma': 'scale',
 'coef0': 0.0,
 'shrinking': 0,
 'probability': 0,
 'tol': 0.001,
 'cache_size': 200.0,
 'break_ties': 0}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('svc',
                 SVC(break_ties=0, cache_size=200.0, probability=0,
                     shrinking=0))])
```

> **Note**
>
> - Default value for “probability” is False, but we need it to be True for the metric “mapk_score”.
>
> ```
> values_default.update({"probability": 1})
> ```

17.10.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[4.01616067e+00 0.00000000e+00 3.00000000e+00 1.00000000e+00
  0.00000000e+00 1.00000000e+00 1.00000000e+00 2.21046195e-03
  1.56834956e+02 0.00000000e+00]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'C': 4.016160671342672,
  'kernel': 'rbf',
  'degree': 3,
  'gamma': 'auto',
  'coef0': 0.0,
  'shrinking': 1,
  'probability': 1,
  'tol': 0.002210461951108952,
  'cache_size': 156.83495628776507,
  'break_ties': 0}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
SVC(C=4.016160671342672, break_ties=0, cache_size=156.83495628776507,
    gamma='auto', probability=1, shrinking=1, tol=0.002210461951108952)
```

17.10.4 Evaluate SPOT Results

- Fetch the data.

```
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
```

```
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.37947269303201503
```

```
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

17.10.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.37790332705586943
std_res: 0.003721747359141646
min_res: 0.3700564971751412
max_res: 0.3851224105461393
median_res: 0.378060263653484
```

17.10.6 Evalution of the Default Hyperparameters

```
model_default["svc"].probability = True
model_default.fit(X_train, y_train)["svc"]
```

```
SVC(break_ties=0, cache_size=200.0, probability=True, shrinking=0)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.3794726930320151
```

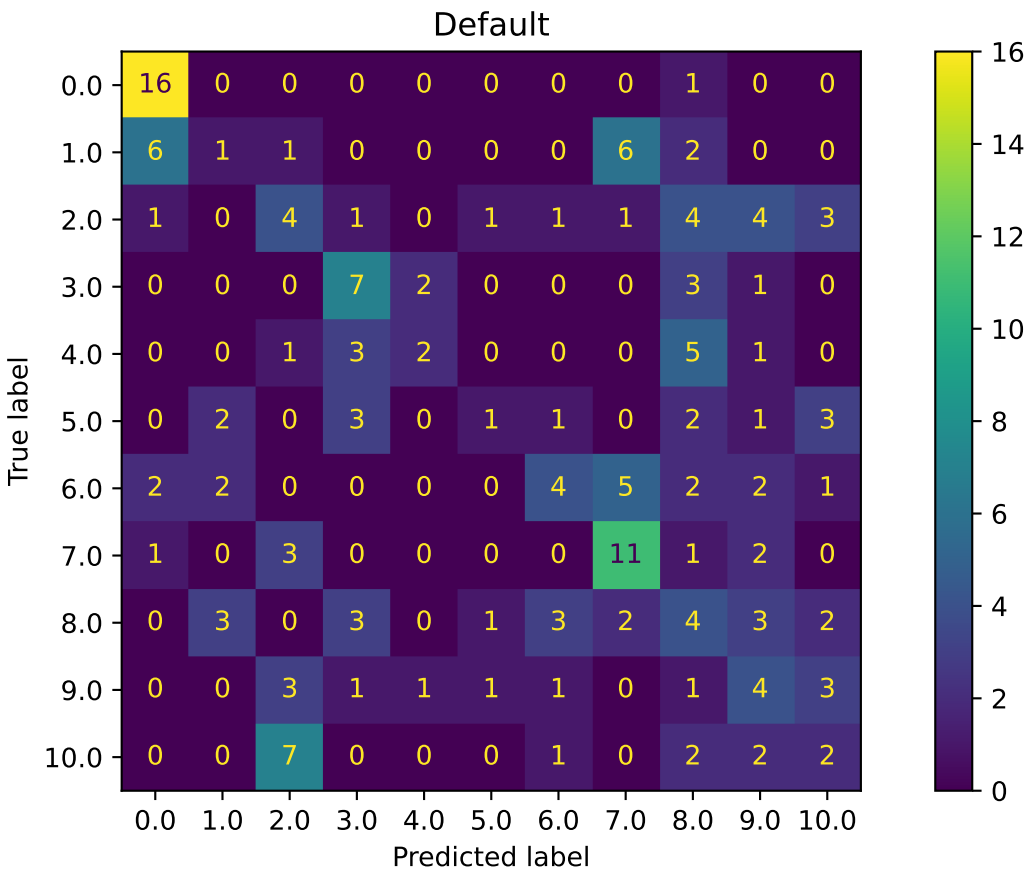
Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_default)
```

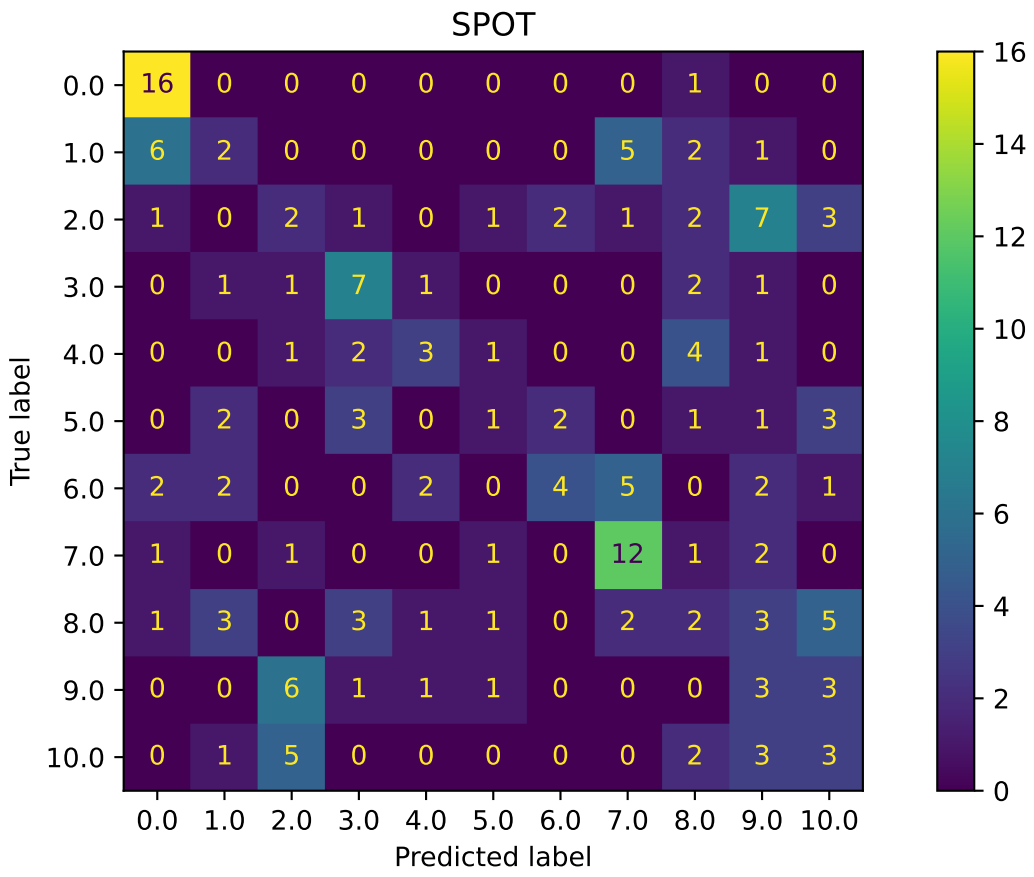
```
mean_res: 0.3841180163214062
std_res: 0.004389289668904793
min_res: 0.37664783427495285
max_res: 0.39453860640301314
median_res: 0.38465160075329563
```

17.10.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```




```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```




```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.39348370927318294, -0.3345864661654135)
```

17.10.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.35188679245283017, None)
```

```
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.34008714596949885, None)
```

- This is the evaluation that will be used in the comparison:

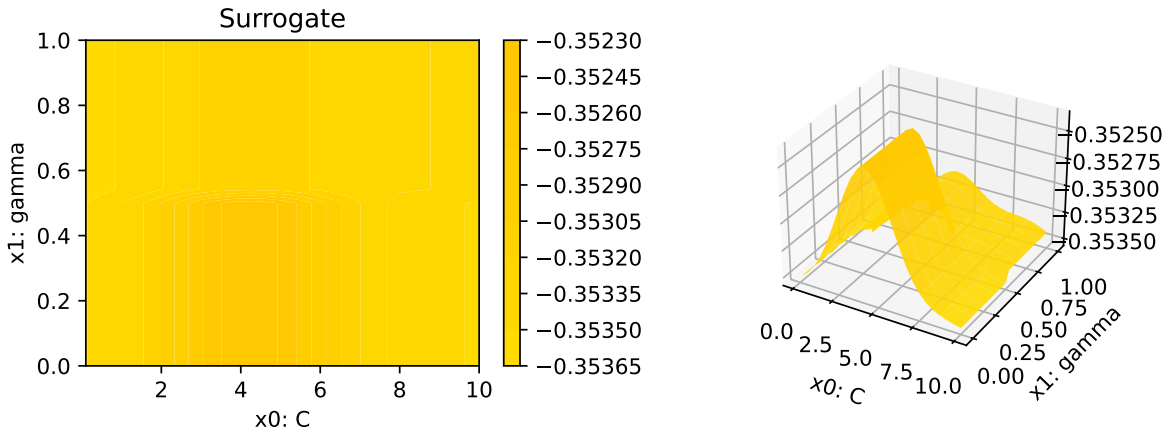
```
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

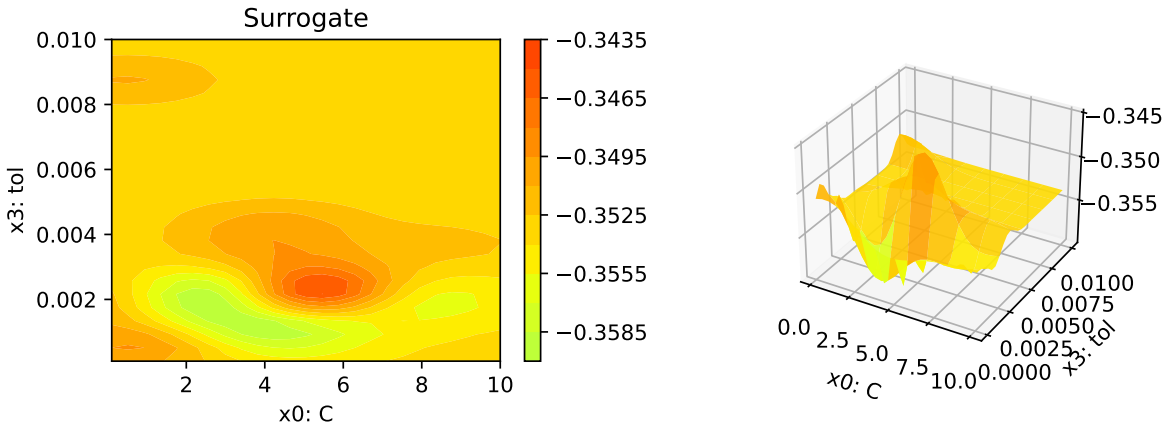
```
(0.3612709590878605, None)
```

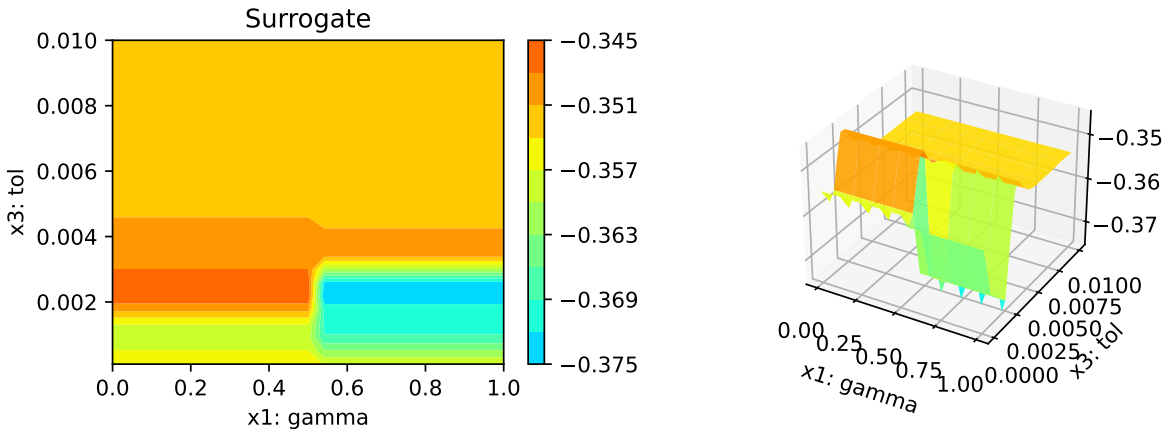
17.10.9 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
C:  1.1840993181254122
gamma:  100.0
tol:  10.866921286853268
```







17.10.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

17.10.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

18 HPT: sklearn KNN Classifier VBDP Data

This document refers to the following software versions:

- python: 3.10.10

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

spotPython can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of spotPython from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

18.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time and the initial design size.

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '19-knn-sklearn' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(I
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
19-knn-sklearn_bartz09_1min_5init_2023-06-19_04-19-17
```

```
import warnings
warnings.filterwarnings("ignore")
```

18.2 Step 2: Initialization of the Empty `fun_control` Dictionary

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/16_spot_hpt_sklearn_classification")
```

18.2.1 Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
```

```
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

18.2.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
```

```
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
# add the dataset to the fun_control
fun_control.update({"data": train_df, # full dataset,
                "train": train,
                "test": test,
                "n_samples": n_samples,
                "target_column": target_column})
```

18.3 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

```
prep_model = None
fun_control.update({"prep_model": prep_model})
```

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

```
# categorical_columns = []
# one_hot_encoder = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
# prep_model = ColumnTransformer(
#         transformers=[
#             ("categorical", one_hot_encoder, categorical_columns),
#         ],
#         remainder=StandardScaler(),
#     )
```

18.4 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

```
fun_control = add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)
```

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.linear_model import ElasticNet
```

```
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
# core_model = RandomForestClassifier
core_model = KNeighborsClassifier
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
# core_model = HistGradientBoostingClassifier
fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=SklearnHyperDict,
                                filename=None)
```

Now `fun_control` has the information from the JSON file. The available hyperparameters are:

```
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
n_neighbors
weights
algorithm
leaf_size
p
```

18.5 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

18.5.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the `modify_hyper_parameter_bounds` method. For example, to change the `tol` hyperparameter of the `SVC` model to the interval [1e-3, 1e-2], the following code can be used:

```
fun_control = modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3,
1e-2])
```

```
# from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
# fun_control = modify_hyper_parameter_bounds(fun_control, "probability", bounds=[1, 1])
```

18.5.2 Modify hyperparameter of type factor

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

Factors can be modified with the `modify_hyper_parameter_levels` function. For example, to exclude the `sigmoid` kernel from the tuning, the `kernel` hyperparameter of the `SVC` model can be modified as follows:

```
fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["linear",
"rbf"])
```

The new setting can be controlled via:

```
fun_control["core_model_hyper_dict"]["kernel"]
```

```
# from spotPython.hyperparameters.values import modify_hyper_parameter_levels
# fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["rbf"])
```

18.5.3 Optimizers

Optimizers are described in Section 14.6.1.

18.5.4 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

18.6 Step 7: Selection of the Objective (Loss) Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

18.6.1 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

18.6.1.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

18.6.1.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
               "weights": -1,
               "metric_sklearn": mapk_score,
               "predict_proba": True,
               "metric_params": {"k": 3},
               })
```

18.6.2 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
})
```

18.6.2.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key `"k_folds"`. For example, to use 5-fold cross validation, the key `"k_folds"` is set to `5`. Uncomment the following line to use cross validation:

```
# fun_control.update({
#      "eval": "train_cv",
#      "k_folds": 10,
# })
```

18.7 Step 8: Calling the SPOT Function

18.7.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
```

```
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name        | type   | default   |   lower |   upper | transform             |
|-------------|--------|-----------|---------|---------|-----------------------|
| n_neighbors | int    | 2         |       1 |       7 | transform_power_2_int |
| weights     | factor | uniform   |       0 |       1 | None                  |
| algorithm   | factor | auto      |       0 |       3 | None                  |
| leaf_size   | int    | 5         |       2 |       7 | transform_power_2_int |
| p           | int    | 2         |       1 |       2 | None                  |
```

18.7.2 The Objective Function

The objective function is selected next. It implements an interface from `sklearn`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

18.7.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=SklearnHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
array([[2, 0, 0, 5, 2]])
```

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
spotPython tuning: -0.3107769423558897 [----------] 0.24%

spotPython tuning: -0.3107769423558897 [----------] 0.51%

spotPython tuning: -0.3107769423558897 [----------] 0.77%

spotPython tuning: -0.3107769423558897 [----------] 1.02%

spotPython tuning: -0.3107769423558897 [----------] 1.27%
```

```
spotPython tuning: -0.3107769423558897 [----------] 1.59%

spotPython tuning: -0.3107769423558897 [----------] 1.97%

spotPython tuning: -0.3107769423558897 [----------] 2.30%

spotPython tuning: -0.3107769423558897 [----------] 2.62%

spotPython tuning: -0.3107769423558897 [----------] 2.91%

spotPython tuning: -0.3107769423558897 [----------] 3.20%

spotPython tuning: -0.3107769423558897 [----------] 4.18%

spotPython tuning: -0.3107769423558897 [#---------] 5.15%

spotPython tuning: -0.3107769423558897 [#---------] 6.33%

spotPython tuning: -0.3107769423558897 [#---------] 7.52%

spotPython tuning: -0.3107769423558897 [#---------] 8.76%

spotPython tuning: -0.3107769423558897 [#---------] 10.20%

spotPython tuning: -0.3107769423558897 [#---------] 11.32%

spotPython tuning: -0.3107769423558897 [#---------] 13.27%

spotPython tuning: -0.3107769423558897 [#---------] 14.52%

spotPython tuning: -0.3107769423558897 [##--------] 15.56%

spotPython tuning: -0.3107769423558897 [##--------] 16.43%

spotPython tuning: -0.3107769423558897 [##--------] 17.43%

spotPython tuning: -0.3107769423558897 [##--------] 18.65%
```

```
spotPython tuning: -0.3107769423558897 [##--------] 19.76%

spotPython tuning: -0.3107769423558897 [##--------] 20.98%

spotPython tuning: -0.3107769423558897 [##--------] 22.40%

spotPython tuning: -0.3107769423558897 [##--------] 23.99%

spotPython tuning: -0.3107769423558897 [###-------] 25.74%

spotPython tuning: -0.3107769423558897 [###-------] 27.68%

spotPython tuning: -0.3107769423558897 [###-------] 29.34%

spotPython tuning: -0.3107769423558897 [###-------] 31.78%

spotPython tuning: -0.3107769423558897 [###-------] 33.87%

spotPython tuning: -0.3107769423558897 [####------] 36.42%

spotPython tuning: -0.3107769423558897 [####------] 40.27%

spotPython tuning: -0.3107769423558897 [####------] 43.10%

spotPython tuning: -0.3107769423558897 [#####-----] 45.80%

spotPython tuning: -0.3107769423558897 [#####-----] 48.82%

spotPython tuning: -0.3107769423558897 [#####-----] 51.67%

spotPython tuning: -0.3107769423558897 [#####-----] 54.63%

spotPython tuning: -0.3107769423558897 [######----] 57.81%

spotPython tuning: -0.3107769423558897 [######----] 60.86%

spotPython tuning: -0.3107769423558897 [######----] 64.07%
```

```
spotPython tuning: -0.3107769423558897 [#######---] 67.24%

spotPython tuning: -0.3107769423558897 [#######---] 70.04%

spotPython tuning: -0.3107769423558897 [#######---] 73.05%

spotPython tuning: -0.3107769423558897 [########--] 77.21%

spotPython tuning: -0.3107769423558897 [########--] 80.49%

spotPython tuning: -0.3107769423558897 [########--] 84.07%

spotPython tuning: -0.3107769423558897 [#########-] 87.87%

spotPython tuning: -0.3107769423558897 [#########-] 91.85%

spotPython tuning: -0.3107769423558897 [##########] 95.14%

spotPython tuning: -0.3107769423558897 [##########] 97.58%

spotPython tuning: -0.3107769423558897 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x14f8e8790>
```

18.8 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

18.9 Step 10: Results

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from **?@fig-progress**.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

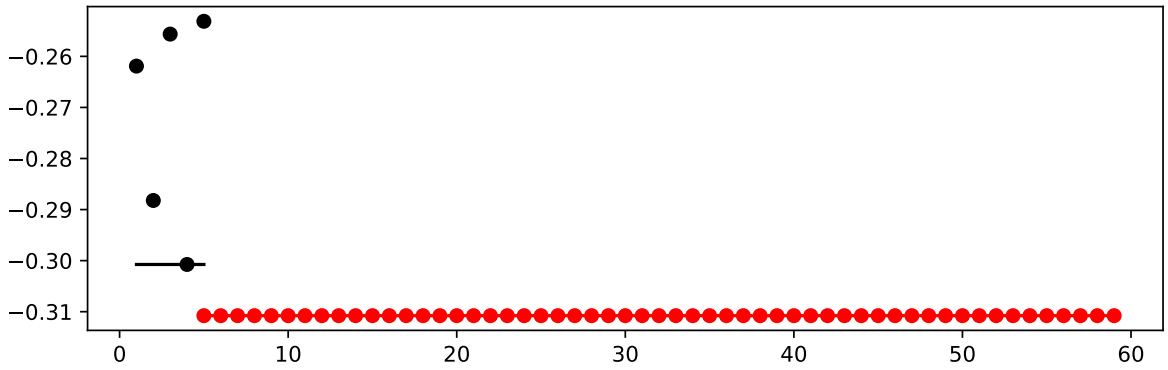


Figure 18.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

```
print(gen_design_table(fun_control=fun_control,
    spot=spot_tuner))
```

name	type	default	lower	upper	tuned	transform	
n_neighbors	int	2	1	7	4.0	transform_power_2_int	
weights	factor	uniform	0	1	1.0	None	
algorithm	factor	auto	0	3	2.0	None	
leaf_size	int	5	2	7	6.0	transform_power_2_int	
p	int	2	1	2	1.0	None	

18.9.1 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

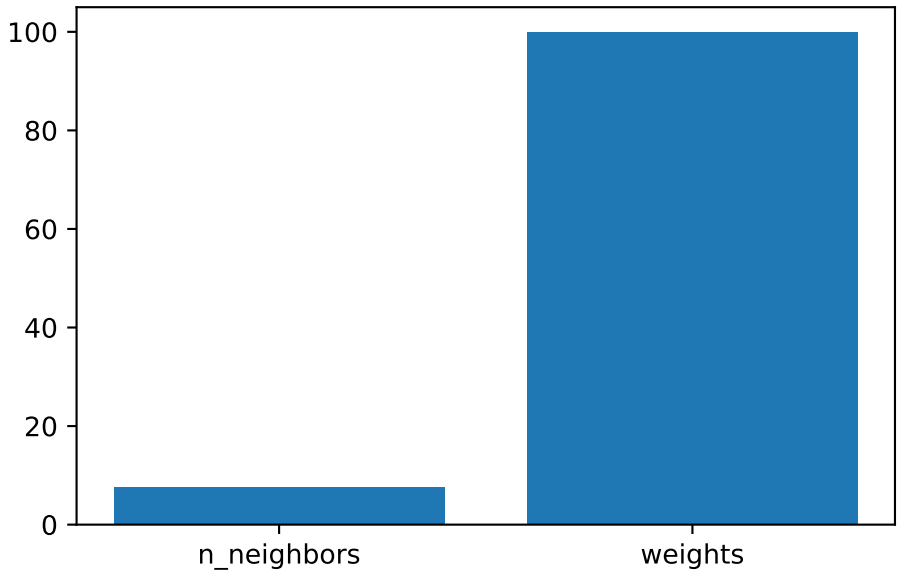


Figure 18.2: Variable importance plot, threshold 0.025.

18.9.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'n_neighbors': 4,
 'weights': 'uniform',
 'algorithm': 'auto',
 'leaf_size': 32,
 'p': 2}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('kneighborsclassifier',
                 KNeighborsClassifier(leaf_size=32, n_neighbors=4))])
```

18.9.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[4. 1. 2. 6. 1.]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'n_neighbors': 16,
  'weights': 'distance',
  'algorithm': 'kd_tree',
  'leaf_size': 64,
  'p': 1}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
KNeighborsClassifier(algorithm='kd_tree', leaf_size=64, n_neighbors=16, p=1,
                     weights='distance')
```

18.9.4 Evaluate SPOT Results

- Fetch the data.

```
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.3267419962335216
```

```
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

18.9.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.3267419962335218
std_res: 1.6653345369377348e-16
min_res: 0.3267419962335216
max_res: 0.3267419962335216
median_res: 0.3267419962335216
```

18.9.6 Evalution of the Default Hyperparameters

```
model_default.fit(X_train, y_train)["kneighborsclassifier"]
```

```
KNeighborsClassifier(leaf_size=32, n_neighbors=4)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.2768361581920904
```

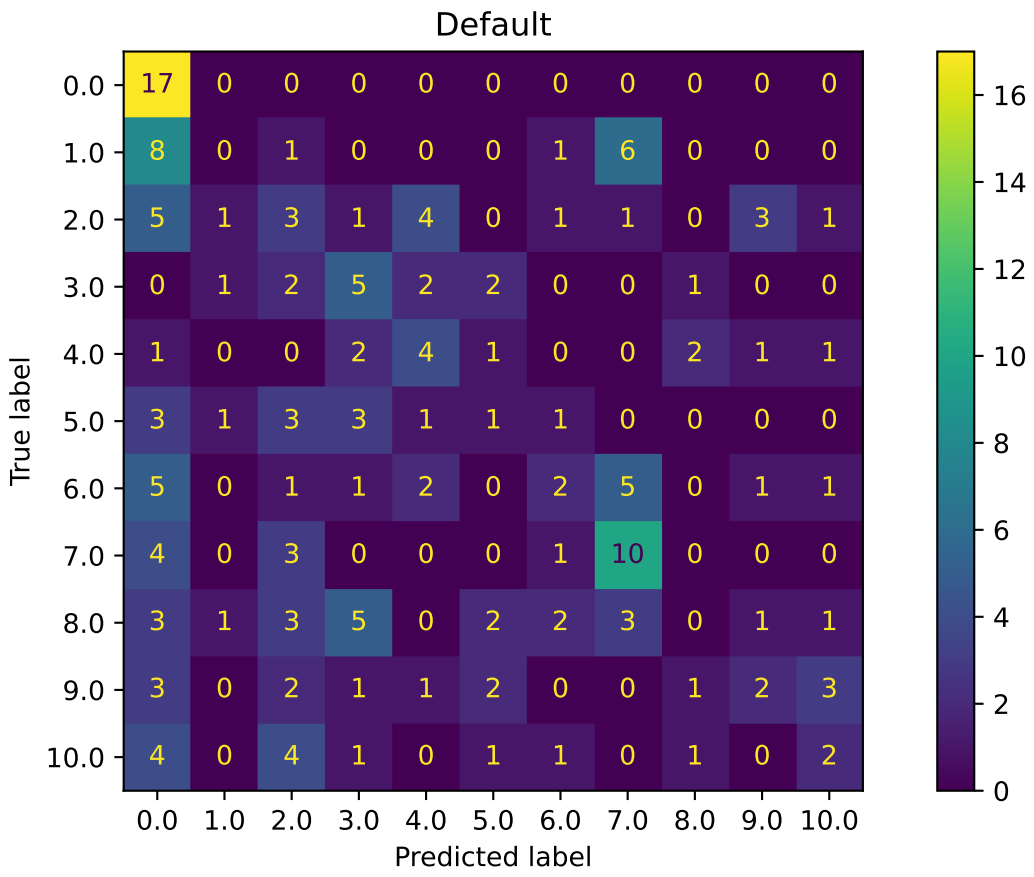
Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_default)
```

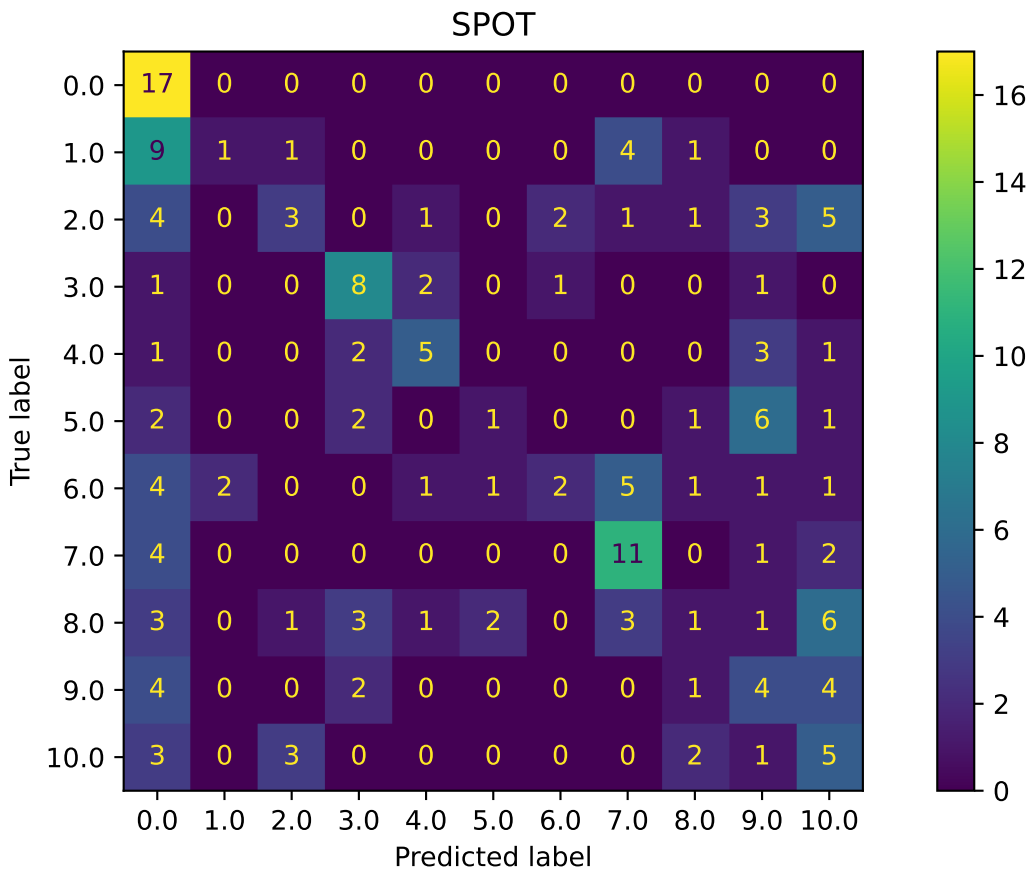
```
mean_res: 0.2768361581920903
std_res: 1.1102230246251565e-16
min_res: 0.2768361581920904
max_res: 0.2768361581920904
median_res: 0.2768361581920904
```

18.9.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```




```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```




```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.3107769423558897, -0.23558897243107768)
```

18.9.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3157232704402516, None)
```

```
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.2832788671023965, None)
```

- This is the evaluation that will be used in the comparison:

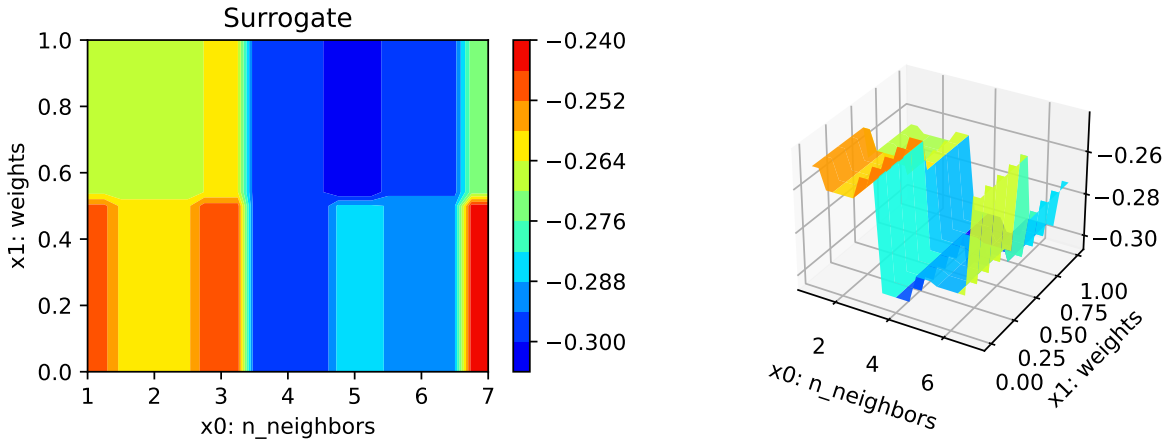
```
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3061904761904762, None)
```

18.9.9 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
n_neighbors:  7.659298853276286
weights:  100.0
```



18.9.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

18.9.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

19 HPT PyTorch: Regression

In this tutorial, we will show how `spotPython` can be integrated into the `PyTorch` training workflow for regreession tasks.

This document refers to the following software versions:

- `python`: 3.10.10
- `torch`: 2.0.1
- `torchvision`: 0.15.0

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93

Note: you may need to restart the kernel to use updated packages.
```

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

19.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size and the device that is used.

Caution: Run time and initial design size should be increased for real experiments

- MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
- INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.

Note: Device selection

- The device can be selected by setting the variable `DEVICE`.
- Since we are using a simple neural net, the setting `"cpu"` is preferred (on Mac).
- If you have a GPU, you can use `"cuda:0"` instead.
- If DEVICE is set to `None`, `spotPython` will automatically select the device.
  - This might result in `"mps"` on Macs, which is not the best choice for simple neural nets.

```
MAX_TIME = 1
INIT_SIZE = 5
DEVICE = "cpu" # "cuda:0"
```

```
from spotPython.utils.device import getDevice
DEVICE = getDevice(DEVICE)
print(DEVICE)
```

```
cpu
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '24-torch' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(INIT_SI
experiment_name = experiment_name.replace(':', '-')
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
24-torch_bartz09_1min_5init_2023-06-19_04-24-41
```

19.2 Step 2: Initialization of the `fun_control` Dictionary

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

`spotPython` uses a Python dictionary for storing the information required for the hyperparameter tuning process, which was described in Section 14.2.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="regression",
 tensorboard_path="runs/24_spot_torch_regression",
 device=DEVICE)
```

19.3 Step 3: PyTorch Data Loading

```
# Create dataset
import pandas as pd
import numpy as np
from sklearn import datasets as sklearn_datasets
from sklearn.preprocessing import MinMaxScaler
from sklearn.model_selection import train_test_split
X, y = sklearn_datasets.make_regression(
    n_samples=1000, n_features=10, noise=1, random_state=123)
y = y.reshape(-1, 1)

# Normalize the data
X_scaler = MinMaxScaler()
X_scaled = X_scaler.fit_transform(X)
y_scaler = MinMaxScaler()
y_scaled = y_scaler.fit_transform(y)

# combine the features and target into a single dataframe named train_df
train_df = pd.DataFrame(np.hstack((X_scaled, y_scaled)))

target_column = "y"
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
```

```
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column,
    axis=1),
    train_df[target_column],
    random_state=42,
    test_size=0.25)
trainset = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
testset = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
trainset.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
testset.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
print(trainset.shape)
print(testset.shape)
```

```
(1000, 11)
(750, 11)
(250, 11)
```

```
import torch
from spotPython.torch.dataframedataset import DataFrameDataset
dtype_x = torch.float32
dtype_y = torch.float32
train_df = DataFrameDataset(train_df, target_column=target_column,
    dtype_x=dtype_x, dtype_y=dtype_y)
train = DataFrameDataset(trainset, target_column=target_column,
    dtype_x=dtype_x, dtype_y=dtype_y)
test = DataFrameDataset(testset, target_column=target_column,
    dtype_x=dtype_x, dtype_y=dtype_y)
n_samples = len(train)
```

- Now we can test the data loading:

```
from spotPython.torch.traintest import create_train_val_data_loaders
trainloader, testloader = create_train_val_data_loaders(train, 2, True, 0)
for i, data in enumerate(trainloader, 0):
    inputs, labels = data
    print(inputs.shape)
    print(labels.shape)
    print(inputs)
    print(labels)
    break
```

```
torch.Size([2, 10])
torch.Size([2])
tensor([[0.2893, 0.2240, 0.6973, 0.5556, 0.5022, 0.3423, 0.4093, 0.6143, 0.3057,
         0.6452],
        [0.4557, 0.3300, 0.7537, 0.6591, 0.2341, 0.3079, 0.6961, 0.1191, 0.5170,
         0.4020]])
tensor([0.2696, 0.1006])
```

- Since this works fine, we can add the data loading to the `fun_control` dictionary:

```
# add the dataset to the fun_control
fun_control.update({"data": train_df, # full dataset,
                "train": train,
                "test": test,
                "n_samples": n_samples,
                "target_column": target_column,})
```

19.4 Step 4: Specification of the Preprocessing Model

After the training and test data are specified and added to the `fun_control` dictionary, `spotPython` allows the specification of a data preprocessing pipeline, e.g., for the scaling of the data or for the one-hot encoding of categorical variables, see Section 14.4. This feature is not used here, so we do not change the default value (which is `None`).

19.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

19.5.1 Implementing a Configurable Neural Network With spotPython

`spotPython` includes the `Net_lin_reg` class which is implemented in the file `netregression.py`.

This class inherits from the class `Net_Core` which is implemented in the file `netcore.py`, see Section 14.5.1.

```
from torch import nn
import spotPython.torch.netcore as netcore


class Net_lin_reg(netcore.Net_Core):
    def __init__(
```

```
        self, _L_in, _L_out, l1, dropout_prob, lr_mult,
        batch_size, epochs, k_folds, patience, optimizer,
        sgd_momentum
    ):
        super(Net_lin_reg, self).__init__(
            lr_mult=lr_mult,
            batch_size=batch_size,
            epochs=epochs,
            k_folds=k_folds,
            patience=patience,
            optimizer=optimizer,
            sgd_momentum=sgd_momentum,
        )
        l2 = max(l1 // 2, 4)
        self.fc1 = nn.Linear(_L_in, l1)
        self.fc2 = nn.Linear(l1, l2)
        self.fc3 = nn.Linear(l2, _L_out)
        self.relu = nn.ReLU()
        self.softmax = nn.Softmax(dim=1)
        self.dropout1 = nn.Dropout(p=dropout_prob)
        self.dropout2 = nn.Dropout(p=dropout_prob / 2)

    def forward(self, x):
        x = self.fc1(x)
        x = self.relu(x)
        x = self.dropout1(x)
        x = self.fc2(x)
        x = self.relu(x)
        x = self.dropout2(x)
        x = self.fc3(x)
        return x
```

19.5.1.1 The `Net_Core` class

`Net_lin_reg` inherits from the class `Net_Core` which is implemented in the file `netcore.py`. This class was described in Section 14.5.1.

```
from spotPython.torch.netregression import Net_lin_reg
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
fun_control = add_core_model_to_fun_control(core_model=Net_lin_reg,
```

```
                                fun_control=fun_control,
                                hyper_dict=TorchHyperDict,
                                filename=None)
```

19.5.2 The Search Space

19.5.3 Configuring the Search Space With spotPython

19.5.3.1 The `hyper_dict` Hyperparameters for the Selected Algorithm

`spotPython` uses `JSON` files for the specification of the hyperparameters, which were described in Section 14.5.5.

The corresponding entries for the `core_model` class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'_L_in': {'type': 'int',
  'default': 10,
  'transform': 'None',
  'lower': 10,
  'upper': 10},
 '_L_out': {'type': 'int',
  'default': 1,
  'transform': 'None',
  'lower': 1,
  'upper': 1},
 'l1': {'type': 'int',
  'default': 3,
  'transform': 'transform_power_2_int',
  'lower': 3,
  'upper': 8},
 'dropout_prob': {'type': 'float',
  'default': 0.01,
  'transform': 'None',
  'lower': 0.0,
  'upper': 0.9},
 'lr_mult': {'type': 'float',
  'default': 1.0,
  'transform': 'None',
  'lower': 0.1,
```

```
 'upper': 10.0},
'batch_size': {'type': 'int',
 'default': 4,
 'transform': 'transform_power_2_int',
 'lower': 1,
 'upper': 4},
'epochs': {'type': 'int',
 'default': 4,
 'transform': 'transform_power_2_int',
 'lower': 4,
 'upper': 9},
'k_folds': {'type': 'int',
 'default': 1,
 'transform': 'None',
 'lower': 1,
 'upper': 1},
'patience': {'type': 'int',
 'default': 2,
 'transform': 'transform_power_2_int',
 'lower': 1,
 'upper': 5},
'optimizer': {'levels': ['Adadelta',
  'Adagrad',
  'Adam',
  'AdamW',
  'SparseAdam',
  'Adamax',
  'ASGD',
  'NAdam',
  'RAdam',
  'RMSprop',
  'Rprop',
  'SGD'],
 'type': 'factor',
 'default': 'SGD',
 'transform': 'None',
 'class_name': 'torch.optim',
 'core_model_parameter_type': 'str',
 'lower': 0,
 'upper': 12},
'sgd_momentum': {'type': 'float',
 'default': 0.0,
 'transform': 'None',
```

```
'lower': 0.0,
'upper': 1.0}}
```

19.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

19.6.1 Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

19.6.1.1 Modify Hyperparameters of Type numeric and integer (boolean)

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds

fun_control = modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[2, 16])
fun_control = modify_hyper_parameter_bounds(fun_control, "patience", bounds=[3, 7])
```

19.6.1.2 Modify Hyperparameter of Type factor

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer",
    ["Adadelta", "Adagrad", "Adam", "AdamW", "Adamax", "ASGD", "NAdam"])


fun_control.update({
               "_L_in": n_features,
               "_L_out": 1,})
```

19.6.2 Optimizers

Optimizers are described in Section 14.6.1.

19.7 Step 7: Selection of the Objective (Loss) Function

19.7.1 Evaluation

The evaluation procedure requires the specification of two elements:

1. the way how the data is split into a train and a test set (see Section 14.7.1)
2. the loss function (and a metric).

19.7.2 Loss Functions and Metrics

The key `"loss_function"` specifies the loss function which is used during the optimization, see Section 14.7.5.

We will use MSE loss for the regression task.

```
from torch.nn import MSELoss
loss_torch = MSELoss()
fun_control.update({"loss_function": loss_torch})
```

19.7.3 Metric

```
from torchmetrics import MeanAbsoluteError
metric_torch = MeanAbsoluteError().to(fun_control["device"])
fun_control.update({"metric_torch": metric_torch})
```

19.8 Step 8: Calling the SPOT Function

19.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
fun_control.update({"var_type": var_type,
```

```
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name         | type   | default   |   lower |   upper | transform             |
|--------------|--------|-----------|---------|---------|-----------------------|
| _L_in        | int    | 10        |    10   |    10   | None                  |
| _L_out       | int    | 1         |     1   |     1   | None                  |
| l1           | int    | 3         |     3   |     8   | transform_power_2_int |
| dropout_prob | float  | 0.01      |     0   |     0.9 | None                  |
| lr_mult      | float  | 1.0       |     0.1 |    10   | None                  |
| batch_size   | int    | 4         |     1   |     4   | transform_power_2_int |
| epochs       | int    | 4         |     2   |    16   | transform_power_2_int |
| k_folds      | int    | 1         |     1   |     1   | None                  |
| patience     | int    | 2         |     3   |     7   | transform_power_2_int |
| optimizer    | factor | SGD       |     0   |     6   | None                  |
| sgd_momentum | float  | 0.0       |     0   |     1   | None                  |
```

19.8.2 The Objective Function `fun_torch`

The objective function `fun_torch` is selected next. It implements an interface from `PyTorch`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypertorch import HyperTorch
fun = HyperTorch().fun_torch
```

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=TorchHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
```

19.8.3 Starting the Hyperparameter Tuning

The `spotPython` hyperparameter tuning is started by calling the `Spot` function as described in Section 14.8.4.

```
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
config: {'_L_in': 10, '_L_out': 1, 'l1': 64, 'dropout_prob': 0.7103122166156, 'lr_mult': 3.6
Epoch: 1 |

MeanAbsoluteError: 0.1601102948188782 | Loss: 0.0404565179548962 | Epoch: 2 | MeanAbsoluteEr

MeanAbsoluteError: 0.1188025027513504 | Loss: 0.0226461006156904 | Epoch: 10 |

MeanAbsoluteError: 0.1162779778242111 | Loss: 0.0218368963902130 | Epoch: 11 | MeanAbsoluteE
```

```
MeanAbsoluteError: 0.1110387668013573 | Loss: 0.0201997655002694 | Epoch: 13 | MeanAbsoluteEr

MeanAbsoluteError: 0.0965183302760124 | Loss: 0.0158265021592869 | Epoch: 21 |

MeanAbsoluteError: 0.0922852382063866 | Loss: 0.0147978182220341 | Epoch: 22 | MeanAbsoluteEr

MeanAbsoluteError: 0.0933773964643478 | Loss: 0.0145014572128850 | Epoch: 24 | MeanAbsoluteEr

MeanAbsoluteError: 0.0840223059058189 | Loss: 0.0132114910459342 | Epoch: 32 |

MeanAbsoluteError: 0.0798487067222595 | Loss: 0.0115149722550996 | Epoch: 33 | MeanAbsoluteEr

MeanAbsoluteError: 0.0771048516035080 | Loss: 0.0100658434354333 | Epoch: 35 | MeanAbsoluteEr

MeanAbsoluteError: 0.0751999095082283 | Loss: 0.0100256902668135 | Epoch: 43 |

MeanAbsoluteError: 0.0762479156255722 | Loss: 0.0095815105167659 | Epoch: 44 | MeanAbsoluteEr

MeanAbsoluteError: 0.0837002620100975 | Loss: 0.0120471901701469 | Epoch: 46 | MeanAbsoluteEr

MeanAbsoluteError: 0.0691955089569092 | Loss: 0.0084583916131554 | Epoch: 54 |

MeanAbsoluteError: 0.0699153617024422 | Loss: 0.0088047922227385 | Epoch: 55 | MeanAbsoluteEr

MeanAbsoluteError: 0.0690940245985985 | Loss: 0.0087129603060404 | Epoch: 57 | MeanAbsoluteEr

MeanAbsoluteError: 0.0657618269324303 | Loss: 0.0092513991525936 | Epoch: 65 |

MeanAbsoluteError: 0.0739136412739754 | Loss: 0.0103740964366711 | Epoch: 66 | MeanAbsoluteEr

MeanAbsoluteError: 0.0754689499735832 | Loss: 0.0108573954295073 | Epoch: 68 | MeanAbsoluteEr

MeanAbsoluteError: 0.0825603902339935 | Loss: 0.0114418036292160 | Early stopping at epoch 74
Returned to Spot: Validation loss: 0.011441803629216003

config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.19981931523998656, 'lr_mult':
Epoch: 1 |
```

```
MeanAbsoluteError: 0.1285235434770584 | Loss: 0.0255406690075209 | Epoch: 2 | MeanAbsoluteErr
MeanAbsoluteError: 0.1041038855910301 | Loss: 0.0166600543613497 | Epoch: 6 | MeanAbsoluteErr
MeanAbsoluteError: 0.0694405138492584 | Loss: 0.0078225458334935 | Epoch: 21 |
MeanAbsoluteError: 0.0613898709416389 | Loss: 0.0064352994392577 | Epoch: 22 | MeanAbsoluteE
MeanAbsoluteError: 0.0749706923961639 | Loss: 0.0081256309793772 | Epoch: 26 | MeanAbsoluteE
MeanAbsoluteError: 0.1428901404142380 | Loss: 0.0232064912193700 | Epoch: 41 |
MeanAbsoluteError: 0.0527426935732365 | Loss: 0.0045689562102780 | Epoch: 42 | MeanAbsoluteE
MeanAbsoluteError: 0.0561683401465416 | Loss: 0.0051905093101883 | Epoch: 46 | MeanAbsoluteE
MeanAbsoluteError: 0.1025368124246597 | Loss: 0.0124958825150603 | Epoch: 61 |
MeanAbsoluteError: 0.0518786795437336 | Loss: 0.0044410075061023 | Epoch: 62 | MeanAbsoluteE
MeanAbsoluteError: 0.0467758290469646 | Loss: 0.0036402315783658 | Epoch: 66 | MeanAbsoluteE
MeanAbsoluteError: 0.0589869506657124 | Loss: 0.0048729497571721 | Epoch: 81 |
MeanAbsoluteError: 0.0840588286519051 | Loss: 0.0111870647800204 | Epoch: 82 | MeanAbsoluteE
MeanAbsoluteError: 0.0776453688740730 | Loss: 0.0082958192368479 | Epoch: 86 | MeanAbsoluteE
MeanAbsoluteError: 0.0356966890394688 | Loss: 0.0028338138516502 | Epoch: 101 |
MeanAbsoluteError: 0.0442608445882797 | Loss: 0.0031996979776427 | Epoch: 102 | MeanAbsolute
MeanAbsoluteError: 0.0576076693832874 | Loss: 0.0049367160107450 | Epoch: 106 | MeanAbsolute
MeanAbsoluteError: 0.0624696351587772 | Loss: 0.0056513458073727 | Epoch: 121 |
MeanAbsoluteError: 0.0531211905181408 | Loss: 0.0037555727237639 | Epoch: 122 | MeanAbsolute
```

```
MeanAbsoluteError: 0.0679961740970612 | Loss: 0.0081456070030598 | Epoch: 126 | MeanAbsoluteE
Returned to Spot: Validation loss: 0.002616552669726508

config: {'_L_in': 10, '_L_out': 1, 'l1': 128, 'dropout_prob': 0.8582565260508446, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.2388423383235931 | Loss: 0.0856057045635922 | Epoch: 2 |

MeanAbsoluteError: 0.1964479535818100 | Loss: 0.0599899871575569 | Epoch: 3 |

MeanAbsoluteError: 0.1779501587152481 | Loss: 0.0507678757516745 | Epoch: 4 | MeanAbsoluteErr

MeanAbsoluteError: 0.1731915920972824 | Loss: 0.0485286914499011 | Epoch: 6 |

MeanAbsoluteError: 0.1680796444416046 | Loss: 0.0449270305226188 | Epoch: 7 | MeanAbsoluteErr

MeanAbsoluteError: 0.1564714312553406 | Loss: 0.0406929800090923 | Epoch: 9 |

MeanAbsoluteError: 0.1478200256824493 | Loss: 0.0351595105797363 | Epoch: 10 | MeanAbsoluteEr

MeanAbsoluteError: 0.1448971778154373 | Loss: 0.0332233455942090 | Epoch: 12 |

MeanAbsoluteError: 0.1484622061252594 | Loss: 0.0344434601031389 | Epoch: 13 | MeanAbsoluteEr

MeanAbsoluteError: 0.1478764712810516 | Loss: 0.0351434745641503 | Epoch: 15 |

MeanAbsoluteError: 0.1444035619497299 | Loss: 0.0332980251424768 | Epoch: 16 | MeanAbsoluteEr

MeanAbsoluteError: 0.1424248069524765 | Loss: 0.0324452003145901 | Epoch: 18 |

MeanAbsoluteError: 0.1394856125116348 | Loss: 0.0322075113552880 | Epoch: 19 | MeanAbsoluteEr

MeanAbsoluteError: 0.1452996879816055 | Loss: 0.0335653647920117 | Epoch: 21 |

MeanAbsoluteError: 0.1441339701414108 | Loss: 0.0327896479222303 | Epoch: 22 | MeanAbsoluteEr

MeanAbsoluteError: 0.1386503279209137 | Loss: 0.0318827000080879 | Epoch: 24 |

MeanAbsoluteError: 0.1428792923688889 | Loss: 0.0326077520717323 | Epoch: 25 | MeanAbsoluteEr
```

MeanAbsoluteError: 0.1433090120553970 | Loss: 0.0322113928193054 | Epoch: 27 |

MeanAbsoluteError: 0.1434110254049301 | Loss: 0.0326007635802186 | Epoch: 28 | MeanAbsoluteE

MeanAbsoluteError: 0.1439524888992310 | Loss: 0.0322994961411071 | Epoch: 30 |

MeanAbsoluteError: 0.1396969556808472 | Loss: 0.0315996324743173 | Epoch: 31 | MeanAbsoluteE

MeanAbsoluteError: 0.1406234800815582 | Loss: 0.0324784485347724 | Epoch: 33 |

MeanAbsoluteError: 0.1395697146654129 | Loss: 0.0311478909936947 | Epoch: 34 | MeanAbsoluteE

MeanAbsoluteError: 0.1376837790012360 | Loss: 0.0306010694957513 | Epoch: 36 |

MeanAbsoluteError: 0.1391707360744476 | Loss: 0.0314540806531052 | Epoch: 37 | MeanAbsoluteE

MeanAbsoluteError: 0.1370310485363007 | Loss: 0.0316148921005273 | Epoch: 39 |

MeanAbsoluteError: 0.1375934034585953 | Loss: 0.0306637983043523 | Epoch: 40 | MeanAbsoluteE

MeanAbsoluteError: 0.1430599540472031 | Loss: 0.0326819322009881 | Epoch: 42 |

MeanAbsoluteError: 0.1441847681999207 | Loss: 0.0320939676389874 | Epoch: 43 | MeanAbsoluteE

MeanAbsoluteError: 0.1366764158010483 | Loss: 0.0301272337008656 | Epoch: 45 |

MeanAbsoluteError: 0.1420582085847855 | Loss: 0.0311487587107695 | Epoch: 46 | MeanAbsoluteE

MeanAbsoluteError: 0.1374262273311615 | Loss: 0.0302541757219781 | Epoch: 48 |

MeanAbsoluteError: 0.1379495412111282 | Loss: 0.0314791454951046 | Epoch: 49 | MeanAbsoluteE

MeanAbsoluteError: 0.1411153525114059 | Loss: 0.0321870837764194 | Epoch: 51 |

MeanAbsoluteError: 0.1407373547554016 | Loss: 0.0313053134295236 | Epoch: 52 | MeanAbsoluteE

MeanAbsoluteError: 0.1387081593275070 | Loss: 0.0312055863823237 | Epoch: 54 |

MeanAbsoluteError: 0.1368575096130371 | Loss: 0.0310989914258759 | Epoch: 55 | MeanAbsoluteEr

MeanAbsoluteError: 0.1411862522363663 | Loss: 0.0317030826597572 | Epoch: 57 |

MeanAbsoluteError: 0.1407575458288193 | Loss: 0.0315680355561199 | Epoch: 58 | MeanAbsoluteEr

MeanAbsoluteError: 0.1384860724210739 | Loss: 0.0312285285633940 | Epoch: 60 |

MeanAbsoluteError: 0.1383236199617386 | Loss: 0.0306956717501938 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.1386741548776627 | Loss: 0.0310652788671238 | Epoch: 63 |

MeanAbsoluteError: 0.1377692073583603 | Loss: 0.0299367827040260 | Epoch: 64 | MeanAbsoluteEr

MeanAbsoluteError: 0.1375640481710434 | Loss: 0.0307705067817005 | Epoch: 66 |

MeanAbsoluteError: 0.1389013975858688 | Loss: 0.0303686141961953 | Epoch: 67 | MeanAbsoluteEr

MeanAbsoluteError: 0.1394073814153671 | Loss: 0.0311817009362130 | Epoch: 69 |

MeanAbsoluteError: 0.1403766572475433 | Loss: 0.0321219426812604 | Epoch: 70 | MeanAbsoluteEr

MeanAbsoluteError: 0.1426118165254593 | Loss: 0.0326408725848887 | Epoch: 72 |

MeanAbsoluteError: 0.1407147198915482 | Loss: 0.0313990318420110 | Epoch: 73 | MeanAbsoluteEr

MeanAbsoluteError: 0.1356390565633774 | Loss: 0.0296504653904897 | Epoch: 75 |

MeanAbsoluteError: 0.1393146961927414 | Loss: 0.0309464088677972 | Epoch: 76 | MeanAbsoluteEr

MeanAbsoluteError: 0.1393281817436218 | Loss: 0.0310093173607796 | Epoch: 78 |

MeanAbsoluteError: 0.1332419961690903 | Loss: 0.0280423711391631 | Epoch: 79 | MeanAbsoluteEr

MeanAbsoluteError: 0.1365984827280045 | Loss: 0.0307244451430840 | Epoch: 81 |

MeanAbsoluteError: 0.1341423243284225 | Loss: 0.0293213327607373 | Epoch: 82 | MeanAbsoluteEr

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MeanAbsoluteError: 0.1411965787410736 | Loss: 0.0325048757477877 | Epoch: 84 |

MeanAbsoluteError: 0.1401728242635727 | Loss: 0.0313650476891780 | Epoch: 85 | MeanAbsoluteE

MeanAbsoluteError: 0.1399764865636826 | Loss: 0.0314035333051773 | Epoch: 87 |

MeanAbsoluteError: 0.1397745758295059 | Loss: 0.0307054841263744 | Epoch: 88 | MeanAbsoluteE

MeanAbsoluteError: 0.1414524018764496 | Loss: 0.0313294751920330 | Epoch: 90 |

MeanAbsoluteError: 0.1355191171169281 | Loss: 0.0299577264483863 | Epoch: 91 | MeanAbsoluteE

MeanAbsoluteError: 0.1376853883266449 | Loss: 0.0305649406720477 | Epoch: 93 |

MeanAbsoluteError: 0.1361009925603867 | Loss: 0.0306828916974579 | Epoch: 94 | MeanAbsoluteE

MeanAbsoluteError: 0.1377325505018234 | Loss: 0.0293978021023213 | Epoch: 96 |

MeanAbsoluteError: 0.1370553672313690 | Loss: 0.0297081933851587 | Epoch: 97 | MeanAbsoluteE

MeanAbsoluteError: 0.1370528787374496 | Loss: 0.0302792378686718 | Epoch: 99 |

MeanAbsoluteError: 0.1371410638093948 | Loss: 0.0295009834085795 | Epoch: 100 | MeanAbsolute

MeanAbsoluteError: 0.1330109089612961 | Loss: 0.0282311750476947 | Epoch: 102 |

MeanAbsoluteError: 0.1352411508560181 | Loss: 0.0298016918178958 | Epoch: 103 | MeanAbsolute

MeanAbsoluteError: 0.1395914554595947 | Loss: 0.0307571879188375 | Epoch: 105 |

MeanAbsoluteError: 0.1355815231800079 | Loss: 0.0294904962637277 | Epoch: 106 | MeanAbsolute

MeanAbsoluteError: 0.1371858566999435 | Loss: 0.0304561324491321 | Epoch: 108 |

MeanAbsoluteError: 0.1363332420587540 | Loss: 0.0303062791479169 | Epoch: 109 | MeanAbsolute

MeanAbsoluteError: 0.1385216712951660 | Loss: 0.0310823449473052 | Epoch: 111 |
```

MeanAbsoluteError: 0.1362326741218567 | Loss: 0.0302719425225708 | Epoch: 112 | MeanAbsolutel

MeanAbsoluteError: 0.1368238180875778 | Loss: 0.0293952258579278 | Epoch: 114 |

MeanAbsoluteError: 0.1396768838167191 | Loss: 0.0309487396001350 | Epoch: 115 | MeanAbsolutel

MeanAbsoluteError: 0.1398329287767410 | Loss: 0.0309237475347860 | Epoch: 117 |

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MeanAbsoluteError: 0.1408552229404449 | Loss: 0.0312702649897741 | Epoch: 123 |

MeanAbsoluteError: 0.1401572227478027 | Loss: 0.0317785010307853 | Epoch: 124 | MeanAbsolutel

MeanAbsoluteError: 0.1363142728805542 | Loss: 0.0303039754342171 | Epoch: 126 |

MeanAbsoluteError: 0.1360335350036621 | Loss: 0.0296516883795266 | Epoch: 127 | MeanAbsolutel

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MeanAbsoluteError: 0.1372626274824142 | Loss: 0.0304680362900884 | Epoch: 145 | MeanAbsolutel

MeanAbsoluteError: 0.1382762640714645 | Loss: 0.0313304909632037 | Epoch: 147 |

MeanAbsoluteError: 0.1380169540643692 | Loss: 0.0306622618690017 | Epoch: 148 | MeanAbsolutel

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MeanAbsoluteError: 0.1318342536687851 | Loss: 0.0287973995880263 | Epoch: 153 |

MeanAbsoluteError: 0.1358292549848557 | Loss: 0.0293529462134272 | Epoch: 154 | MeanAbsolutel

MeanAbsoluteError: 0.1403776556253433 | Loss: 0.0321658388456854 | Epoch: 156 |

MeanAbsoluteError: 0.1334628164768219 | Loss: 0.0289739706391507 | Epoch: 157 | MeanAbsolutel

MeanAbsoluteError: 0.1343490183353424 | Loss: 0.0297320331781521 | Epoch: 159 |

MeanAbsoluteError: 0.1348469704389572 | Loss: 0.0298085070737094 | Epoch: 160 | MeanAbsolutel

MeanAbsoluteError: 0.1361219733953476 | Loss: 0.0294330167223234 | Epoch: 162 |

MeanAbsoluteError: 0.1370345205068588 | Loss: 0.0296588205251707 | Epoch: 163 | MeanAbsolutel

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MeanAbsoluteError: 0.1362742930650711 | Loss: 0.0291855764850334 | Epoch: 166 | MeanAbsolutel

MeanAbsoluteError: 0.1375095993280411 | Loss: 0.0288208475947613 | Epoch: 168 |

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MeanAbsoluteError: 0.1379045397043228 | Loss: 0.0297404186014319 | Epoch: 171 |

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MeanAbsoluteError: 0.1361813247203827 | Loss: 0.0293832107112636 | Epoch: 174 |

MeanAbsoluteError: 0.1341451704502106 | Loss: 0.0299626988438346 | Epoch: 175 | MeanAbsolutel

MeanAbsoluteError: 0.1327986866235733 | Loss: 0.0284976897125792 | Epoch: 177 |

MeanAbsoluteError: 0.1338888406753540 | Loss: 0.0286528620581764 | Epoch: 178 | MeanAbsolutel

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MeanAbsoluteError: 0.1341343075037003 | Loss: 0.0293422745988937 | Epoch: 186 |

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MeanAbsoluteError: 0.1282214671373367 | Loss: 0.0258546913651905 | Epoch: 189 |

MeanAbsoluteError: 0.1370003819465637 | Loss: 0.0295187026314670 | Epoch: 190 | MeanAbsolutel

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MeanAbsoluteError: 0.1376602351665497 | Loss: 0.0295546540190602 | Epoch: 201 |

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MeanAbsoluteError: 0.1380791813135147 | Loss: 0.0296551289246903 | Epoch: 207 |

MeanAbsoluteError: 0.1341572552919388 | Loss: 0.0288272898017021 | Epoch: 208 | MeanAbsolute

MeanAbsoluteError: 0.1288682073354721 | Loss: 0.0261408846603202 | Epoch: 210 |

MeanAbsoluteError: 0.1330207437276840 | Loss: 0.0291963440484930 | Epoch: 211 | MeanAbsolute

MeanAbsoluteError: 0.1394057422876358 | Loss: 0.0313721590387286 | Epoch: 213 |

MeanAbsoluteError: 0.1295985132455826 | Loss: 0.0271830963300999 | Epoch: 214 | MeanAbsolute

MeanAbsoluteError: 0.1319358348846436 | Loss: 0.0280005775883910 | Epoch: 216 |

MeanAbsoluteError: 0.1315614879131317 | Loss: 0.0290409765935813 | Epoch: 217 | MeanAbsolute

MeanAbsoluteError: 0.1287194788455963 | Loss: 0.0277105604157744 | Epoch: 219 |

MeanAbsoluteError: 0.1299667060375214 | Loss: 0.0268688624852120 | Epoch: 220 | MeanAbsolute

MeanAbsoluteError: 0.1351269334554672 | Loss: 0.0291309571649375 | Epoch: 222 |

MeanAbsoluteError: 0.1320157051086426 | Loss: 0.0274007470364450 | Epoch: 223 | MeanAbsolute

MeanAbsoluteError: 0.1311803758144379 | Loss: 0.0286482639482711 | Epoch: 225 |

MeanAbsoluteError: 0.1284197419881821 | Loss: 0.0267033961167908 | Epoch: 226 | MeanAbsolutel

MeanAbsoluteError: 0.1331575810909271 | Loss: 0.0281832760368646 | Epoch: 228 |

MeanAbsoluteError: 0.1317401081323624 | Loss: 0.0278004055438214 | Epoch: 229 | MeanAbsolutel

MeanAbsoluteError: 0.1264787614345551 | Loss: 0.0263003176310061 | Epoch: 231 |

MeanAbsoluteError: 0.1327133178710938 | Loss: 0.0279882648245984 | Epoch: 232 | MeanAbsolutel

MeanAbsoluteError: 0.1247668489813805 | Loss: 0.0255998719922460 | Epoch: 234 |

MeanAbsoluteError: 0.1317458748817444 | Loss: 0.0284127798808671 | Epoch: 235 | MeanAbsolutel

MeanAbsoluteError: 0.1320269107818604 | Loss: 0.0269779763697685 | Epoch: 237 |

MeanAbsoluteError: 0.1312605887651443 | Loss: 0.0283686165447580 | Epoch: 238 | MeanAbsolutel

MeanAbsoluteError: 0.1300470530986786 | Loss: 0.0276701137912460 | Epoch: 240 |

MeanAbsoluteError: 0.1293242573738098 | Loss: 0.0271862335960032 | Epoch: 241 | MeanAbsolutel

MeanAbsoluteError: 0.1370288133621216 | Loss: 0.0287656490059696 | Epoch: 243 |

MeanAbsoluteError: 0.1325301378965378 | Loss: 0.0284183841207899 | Epoch: 244 | MeanAbsolutel

MeanAbsoluteError: 0.1318372040987015 | Loss: 0.0267326949748288 | Epoch: 246 |

MeanAbsoluteError: 0.1242349147796631 | Loss: 0.0255774877105917 | Epoch: 247 | MeanAbsolutel

MeanAbsoluteError: 0.1317847222089767 | Loss: 0.0285940568777490 | Epoch: 249 |

MeanAbsoluteError: 0.1310194581747055 | Loss: 0.0276943076968503 | Epoch: 250 | MeanAbsolutel

MeanAbsoluteError: 0.1320689320564270 | Loss: 0.0278794523216735 | Epoch: 252 |

MeanAbsoluteError: 0.1313036680221558 | Loss: 0.0276235040654338 | Epoch: 253 | MeanAbsolutel

MeanAbsoluteError: 0.1318035423755646 | Loss: 0.0271831327560358 | Epoch: 255 |

MeanAbsoluteError: 0.1255322843790054 | Loss: 0.0255165518723273 | Epoch: 256 | MeanAbsolute

MeanAbsoluteError: 0.1328963041305542 | Loss: 0.0274179629157637 | Epoch: 258 |

MeanAbsoluteError: 0.1299600154161453 | Loss: 0.0273879893561631 | Epoch: 259 | MeanAbsolute

MeanAbsoluteError: 0.1256195157766342 | Loss: 0.0258862118818797 | Epoch: 261 |

MeanAbsoluteError: 0.1267097890377045 | Loss: 0.0265098322766426 | Epoch: 262 | MeanAbsolute

MeanAbsoluteError: 0.1292830854654312 | Loss: 0.0275549091245436 | Epoch: 264 |

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MeanAbsoluteError: 0.1284626722335815 | Loss: 0.0269588652646780 | Epoch: 268 | MeanAbsolute

MeanAbsoluteError: 0.1312844902276993 | Loss: 0.0270620739020039 | Epoch: 270 |

MeanAbsoluteError: 0.1317726969718933 | Loss: 0.0271841016062535 | Epoch: 271 | MeanAbsolute

MeanAbsoluteError: 0.1309649348258972 | Loss: 0.0267362869348532 | Epoch: 273 |

MeanAbsoluteError: 0.1332586705684662 | Loss: 0.0282610271194911 | Epoch: 274 | MeanAbsolute

MeanAbsoluteError: 0.1304628401994705 | Loss: 0.0270747860043775 | Epoch: 276 |

MeanAbsoluteError: 0.1254433989524841 | Loss: 0.0260165572548431 | Epoch: 277 | MeanAbsolute

MeanAbsoluteError: 0.1350724697113037 | Loss: 0.0293320919935165 | Epoch: 279 |

MeanAbsoluteError: 0.1309100687503815 | Loss: 0.0262592869275250 | Epoch: 280 | MeanAbsolute

MeanAbsoluteError: 0.1316926330327988 | Loss: 0.0276744631583279 | Epoch: 282 |

MeanAbsoluteError: 0.1315719336271286 | Loss: 0.0277478296079789 | Epoch: 283 | MeanAbsolutel

MeanAbsoluteError: 0.1280479878187180 | Loss: 0.0267350972954349 | Epoch: 285 |

MeanAbsoluteError: 0.1314600408077240 | Loss: 0.0274624155480221 | Epoch: 286 | MeanAbsolutel

MeanAbsoluteError: 0.1300276815891266 | Loss: 0.0263229235740922 | Epoch: 288 |

MeanAbsoluteError: 0.1381802111864090 | Loss: 0.0299661014220328 | Epoch: 289 | MeanAbsolutel

MeanAbsoluteError: 0.1249421164393425 | Loss: 0.0250683379721401 | Epoch: 291 |

MeanAbsoluteError: 0.1254620999097824 | Loss: 0.0254232222107445 | Epoch: 292 | MeanAbsolutel

MeanAbsoluteError: 0.1251504570245743 | Loss: 0.0258731536175280 | Epoch: 294 |

MeanAbsoluteError: 0.1259124428033829 | Loss: 0.0254536174224146 | Epoch: 295 | MeanAbsolutel

MeanAbsoluteError: 0.1232094839215279 | Loss: 0.0242145087626219 | Epoch: 297 |

MeanAbsoluteError: 0.1261363178491592 | Loss: 0.0256611447573232 | Epoch: 298 | MeanAbsolutel

MeanAbsoluteError: 0.1285180002450943 | Loss: 0.0257367642097718 | Epoch: 300 |

MeanAbsoluteError: 0.1268004775047302 | Loss: 0.0258037206227891 | Epoch: 301 | MeanAbsolutel

MeanAbsoluteError: 0.1314958930015564 | Loss: 0.0274887814225319 | Epoch: 303 |

MeanAbsoluteError: 0.1253576278686523 | Loss: 0.0249695983647446 | Epoch: 304 | MeanAbsolutel

MeanAbsoluteError: 0.1239471212029457 | Loss: 0.0253455219474078 | Epoch: 306 |

MeanAbsoluteError: 0.1211020424962044 | Loss: 0.0245878614609440 | Epoch: 307 | MeanAbsolutel

MeanAbsoluteError: 0.1241138577461243 | Loss: 0.0248863854034183 | Epoch: 309 |

MeanAbsoluteError: 0.1298381537199020 | Loss: 0.0276404545996532 | Epoch: 310 | MeanAbsolutel

MeanAbsoluteError: 0.1256634593009949 | Loss: 0.0256056599076692 | Epoch: 312 |

MeanAbsoluteError: 0.1284182965755463 | Loss: 0.0264935907151084 | Epoch: 313 | MeanAbsolutel

MeanAbsoluteError: 0.1286122053861618 | Loss: 0.0274394082310270 | Epoch: 315 |

MeanAbsoluteError: 0.1247081086039543 | Loss: 0.0254868176849171 | Epoch: 316 | MeanAbsolutel

MeanAbsoluteError: 0.1299386918544769 | Loss: 0.0270193143154029 | Epoch: 318 |

MeanAbsoluteError: 0.1267980188131332 | Loss: 0.0251817280432927 | Epoch: 319 | MeanAbsolutel

MeanAbsoluteError: 0.1229846850037575 | Loss: 0.0253037055706939 | Epoch: 321 |

MeanAbsoluteError: 0.1249031946063042 | Loss: 0.0253790452082952 | Epoch: 322 | MeanAbsolutel

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MeanAbsoluteError: 0.1033967807888985 | Loss: 0.0179931668935751 | Epoch: 652 | MeanAbsoluteE

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MeanAbsoluteError: 0.1011879220604897 | Loss: 0.0177575510546255 | Epoch: 672 |
MeanAbsoluteError: 0.1066883876919746 | Loss: 0.0187175919121364 | Epoch: 673 | MeanAbsolutel
MeanAbsoluteError: 0.1027997061610222 | Loss: 0.0176676001956306 | Epoch: 675 |
MeanAbsoluteError: 0.0996896773576736 | Loss: 0.0164347479746599 | Epoch: 676 | MeanAbsolutel
MeanAbsoluteError: 0.1013355106115341 | Loss: 0.0174178135933835 | Epoch: 678 |
MeanAbsoluteError: 0.1007369384169579 | Loss: 0.0176884642694980 | Epoch: 679 | MeanAbsolutel
MeanAbsoluteError: 0.1016495674848557 | Loss: 0.0171614808255981 | Epoch: 681 |
```

MeanAbsoluteError: 0.0929012671113014 | Loss: 0.0146624048944432 | Epoch: 682 | MeanAbsolutel

MeanAbsoluteError: 0.1011923104524612 | Loss: 0.0166313008878812 | Epoch: 684 |

MeanAbsoluteError: 0.1013982892036438 | Loss: 0.0170682395592545 | Epoch: 685 | MeanAbsolutel

MeanAbsoluteError: 0.1005206629633904 | Loss: 0.0171257663330762 | Epoch: 687 |

MeanAbsoluteError: 0.1045465990900993 | Loss: 0.0180903734318296 | Epoch: 688 | MeanAbsolutel

MeanAbsoluteError: 0.0999929606914520 | Loss: 0.0171453575682244 | Epoch: 690 |

MeanAbsoluteError: 0.1009135767817497 | Loss: 0.0165136124051423 | Epoch: 691 | MeanAbsolutel

MeanAbsoluteError: 0.1021961793303490 | Loss: 0.0173513565485094 | Epoch: 693 |

MeanAbsoluteError: 0.1006621271371841 | Loss: 0.0164082185812974 | Epoch: 694 | MeanAbsolutel

MeanAbsoluteError: 0.1020176410675049 | Loss: 0.0175668680061669 | Epoch: 696 |

MeanAbsoluteError: 0.0994136482477188 | Loss: 0.0171662637109572 | Epoch: 697 | MeanAbsolutel

MeanAbsoluteError: 0.1057325899600983 | Loss: 0.0187269466000362 | Epoch: 699 |

MeanAbsoluteError: 0.1001793891191483 | Loss: 0.0166507516397784 | Epoch: 700 | MeanAbsolutel

MeanAbsoluteError: 0.1007820144295692 | Loss: 0.0172408050282199 | Epoch: 702 |

MeanAbsoluteError: 0.1031623482704163 | Loss: 0.0170707658373673 | Epoch: 703 | MeanAbsolutel

MeanAbsoluteError: 0.0962612628936768 | Loss: 0.0159240856503796 | Epoch: 705 |

MeanAbsoluteError: 0.1036509498953819 | Loss: 0.0183847641063524 | Epoch: 706 | MeanAbsolutel

MeanAbsoluteError: 0.0988019183278084 | Loss: 0.0172447313053514 | Epoch: 708 |

MeanAbsoluteError: 0.0970178917050362 | Loss: 0.0157342836867610 | Epoch: 709 | MeanAbsolutel

MeanAbsoluteError: 0.0981377288699150 | Loss: 0.0164491149381502 | Epoch: 711 |

MeanAbsoluteError: 0.0985470041632652 | Loss: 0.0160858718905365 | Epoch: 712 | MeanAbsoluteE

MeanAbsoluteError: 0.0981759205460548 | Loss: 0.0161107653316382 | Epoch: 714 |

MeanAbsoluteError: 0.0983947291970253 | Loss: 0.0158231249045881 | Epoch: 715 | MeanAbsoluteE

MeanAbsoluteError: 0.1015727892518044 | Loss: 0.0179424921590059 | Epoch: 717 |

MeanAbsoluteError: 0.1003616675734520 | Loss: 0.0173221626306380 | Epoch: 718 | MeanAbsoluteE

MeanAbsoluteError: 0.0986120998859406 | Loss: 0.0167913342037355 | Epoch: 720 |

MeanAbsoluteError: 0.1007067710161209 | Loss: 0.0163432166783605 | Epoch: 721 | MeanAbsoluteE

MeanAbsoluteError: 0.0973814800381660 | Loss: 0.0161536684884535 | Epoch: 723 |

MeanAbsoluteError: 0.0959409549832344 | Loss: 0.0150623327889965 | Epoch: 724 | MeanAbsoluteE

MeanAbsoluteError: 0.1061602383852005 | Loss: 0.0184779917397585 | Epoch: 726 |

MeanAbsoluteError: 0.0928905904293060 | Loss: 0.0144650431418268 | Epoch: 727 | MeanAbsoluteE

MeanAbsoluteError: 0.0985680371522903 | Loss: 0.0157471253839321 | Epoch: 729 |

MeanAbsoluteError: 0.0994159728288651 | Loss: 0.0165386747511608 | Epoch: 730 | MeanAbsoluteE

MeanAbsoluteError: 0.1083010360598564 | Loss: 0.0195118837318538 | Epoch: 732 |

MeanAbsoluteError: 0.0970344915986061 | Loss: 0.0157529007344662 | Epoch: 733 | MeanAbsoluteE

MeanAbsoluteError: 0.1006526723504066 | Loss: 0.0173769718848598 | Epoch: 735 |

MeanAbsoluteError: 0.1050557345151901 | Loss: 0.0182304356609772 | Epoch: 736 | MeanAbsoluteE

MeanAbsoluteError: 0.0997761338949203 | Loss: 0.0160831342991150 | Epoch: 738 |

MeanAbsoluteError: 0.0982650220394135 | Loss: 0.0164411953450084 | Epoch: 739 | MeanAbsolutel

MeanAbsoluteError: 0.1020341664552689 | Loss: 0.0169301671040497 | Epoch: 741 |

MeanAbsoluteError: 0.0951727777719498 | Loss: 0.0152098842764584 | Epoch: 742 | MeanAbsolutel

MeanAbsoluteError: 0.0960153639316559 | Loss: 0.0165982580734029 | Epoch: 744 |

MeanAbsoluteError: 0.0971679612994194 | Loss: 0.0156964519294464 | Epoch: 745 | MeanAbsolutel

MeanAbsoluteError: 0.0981511995196342 | Loss: 0.0162253226322355 | Epoch: 747 |

MeanAbsoluteError: 0.0955171436071396 | Loss: 0.0157643125692509 | Epoch: 748 | MeanAbsolutel

MeanAbsoluteError: 0.0994499549269676 | Loss: 0.0168575408682227 | Epoch: 750 |

MeanAbsoluteError: 0.0963399708271027 | Loss: 0.0164820031750423 | Epoch: 751 | MeanAbsolutel

MeanAbsoluteError: 0.0995475798845291 | Loss: 0.0163898703745023 | Epoch: 753 |

MeanAbsoluteError: 0.0950276181101799 | Loss: 0.0161137710275458 | Epoch: 754 | MeanAbsolutel

MeanAbsoluteError: 0.1021111235022545 | Loss: 0.0183456548606046 | Epoch: 756 |

MeanAbsoluteError: 0.1004953086376190 | Loss: 0.0162740312981380 | Epoch: 757 | MeanAbsolutel

MeanAbsoluteError: 0.0982325151562691 | Loss: 0.0163922074744672 | Epoch: 759 |

MeanAbsoluteError: 0.0981122329831123 | Loss: 0.0164642730100604 | Epoch: 760 | MeanAbsolutel

MeanAbsoluteError: 0.1019392237067223 | Loss: 0.0171489957990222 | Epoch: 762 |

MeanAbsoluteError: 0.0953502207994461 | Loss: 0.0152001790058906 | Epoch: 763 | MeanAbsolutel

MeanAbsoluteError: 0.0907617881894112 | Loss: 0.0141405998285336 | Epoch: 765 |

MeanAbsoluteError: 0.0962938815355301 | Loss: 0.0157706608519948 | Epoch: 766 | MeanAbsolutel

MeanAbsoluteError: 0.0992054119706154 | Loss: 0.0159764312126208 | Epoch: 768 |

MeanAbsoluteError: 0.1011943370103836 | Loss: 0.0162104140326846 | Epoch: 769 | MeanAbsolute

MeanAbsoluteError: 0.1000064015388489 | Loss: 0.0168411061903741 | Epoch: 771 |

MeanAbsoluteError: 0.0942044034600258 | Loss: 0.0152744118848386 | Epoch: 772 | MeanAbsolute

MeanAbsoluteError: 0.0910591483116150 | Loss: 0.0145060059351575 | Epoch: 774 |

MeanAbsoluteError: 0.0967089906334877 | Loss: 0.0158893699822026 | Epoch: 775 | MeanAbsolute

MeanAbsoluteError: 0.0923384875059128 | Loss: 0.0140206549184101 | Epoch: 777 |

MeanAbsoluteError: 0.0971237048506737 | Loss: 0.0152784394326348 | Epoch: 778 | MeanAbsolute

MeanAbsoluteError: 0.0973426476120949 | Loss: 0.0159019126486965 | Epoch: 780 |

MeanAbsoluteError: 0.0956884622573853 | Loss: 0.0150283993591438 | Epoch: 781 | MeanAbsolute

MeanAbsoluteError: 0.0971700102090836 | Loss: 0.0152078277585739 | Epoch: 783 |

MeanAbsoluteError: 0.0984471291303635 | Loss: 0.0167226721541192 | Epoch: 784 | MeanAbsolute

MeanAbsoluteError: 0.0923895761370659 | Loss: 0.0136245046240704 | Epoch: 786 |

MeanAbsoluteError: 0.0922588482499123 | Loss: 0.0141494800593258 | Epoch: 787 | MeanAbsolute

MeanAbsoluteError: 0.0932257175445557 | Loss: 0.0157888659615370 | Epoch: 789 |

MeanAbsoluteError: 0.0932410731911659 | Loss: 0.0146960425603902 | Epoch: 790 | MeanAbsolute

MeanAbsoluteError: 0.0923603475093842 | Loss: 0.0141003478299050 | Epoch: 792 |

MeanAbsoluteError: 0.0985226184129715 | Loss: 0.0166834699600198 | Epoch: 793 | MeanAbsolute

MeanAbsoluteError: 0.0943809673190117 | Loss: 0.0158968969879788 | Epoch: 795 |

MeanAbsoluteError: 0.0966450199484825 | Loss: 0.0161618629592704 | Epoch: 796 | MeanAbsolutel

MeanAbsoluteError: 0.0943591445684433 | Loss: 0.0158760314639342 | Epoch: 798 |

MeanAbsoluteError: 0.0979014858603477 | Loss: 0.0161095741969499 | Epoch: 799 | MeanAbsolutel

MeanAbsoluteError: 0.1020555198192596 | Loss: 0.0169399424697137 | Epoch: 801 |

MeanAbsoluteError: 0.0947271734476089 | Loss: 0.0154431627095134 | Epoch: 802 | MeanAbsolutel

MeanAbsoluteError: 0.0932342037558556 | Loss: 0.0144883562927862 | Epoch: 804 |

MeanAbsoluteError: 0.0969276055693626 | Loss: 0.0155108447787158 | Epoch: 805 | MeanAbsolutel

MeanAbsoluteError: 0.0960832461714745 | Loss: 0.0158011959169865 | Epoch: 807 |

MeanAbsoluteError: 0.0977315232157707 | Loss: 0.0165770321927024 | Epoch: 808 | MeanAbsolutel

MeanAbsoluteError: 0.0928321778774261 | Loss: 0.0146101860308408 | Epoch: 810 |

MeanAbsoluteError: 0.0971784368157387 | Loss: 0.0161171178775840 | Epoch: 811 | MeanAbsolutel

MeanAbsoluteError: 0.0842342004179955 | Loss: 0.0119925857175258 | Epoch: 813 |

MeanAbsoluteError: 0.0890534147620201 | Loss: 0.0140876651603806 | Epoch: 814 | MeanAbsolutel

MeanAbsoluteError: 0.0906349718570709 | Loss: 0.0142340297237388 | Epoch: 816 |

MeanAbsoluteError: 0.0975719615817070 | Loss: 0.0161067189776804 | Epoch: 817 | MeanAbsolutel

MeanAbsoluteError: 0.0919321179389954 | Loss: 0.0150429678906221 | Epoch: 819 |

MeanAbsoluteError: 0.0970854386687279 | Loss: 0.0163618652737205 | Epoch: 820 | MeanAbsolutel

MeanAbsoluteError: 0.0943026915192604 | Loss: 0.0158372606959074 | Epoch: 822 |

MeanAbsoluteError: 0.0933899208903313 | Loss: 0.0152412532761567 | Epoch: 823 | MeanAbsolutel

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MeanAbsoluteError: 0.0955378711223602 | Loss: 0.0154935410584480 | Epoch: 825 |

MeanAbsoluteError: 0.0931416898965836 | Loss: 0.0146562517306302 | Epoch: 826 | MeanAbsolutel

MeanAbsoluteError: 0.0925639942288399 | Loss: 0.0142314712998874 | Epoch: 828 |

MeanAbsoluteError: 0.0947838127613068 | Loss: 0.0153073989096144 | Epoch: 829 | MeanAbsolutel

MeanAbsoluteError: 0.0949512645602226 | Loss: 0.0151505220945789 | Epoch: 831 |

MeanAbsoluteError: 0.0945107862353325 | Loss: 0.0157217176605870 | Epoch: 832 | MeanAbsolutel

MeanAbsoluteError: 0.0943966805934906 | Loss: 0.0143498473948299 | Epoch: 834 |

MeanAbsoluteError: 0.0950543656945229 | Loss: 0.0149650085644680 | Epoch: 835 | MeanAbsolutel

MeanAbsoluteError: 0.0919704139232635 | Loss: 0.0146635710523030 | Epoch: 837 |

MeanAbsoluteError: 0.0866925716400146 | Loss: 0.0137410020935446 | Epoch: 838 | MeanAbsolutel

MeanAbsoluteError: 0.0888545066118240 | Loss: 0.0134990676906940 | Epoch: 840 |

MeanAbsoluteError: 0.0897268876433372 | Loss: 0.0138668577935702 | Epoch: 841 | MeanAbsolutel

MeanAbsoluteError: 0.0967288091778755 | Loss: 0.0149478258004334 | Epoch: 843 |

MeanAbsoluteError: 0.0940672084689140 | Loss: 0.0148848106863928 | Epoch: 844 | MeanAbsolutel

MeanAbsoluteError: 0.0923726409673691 | Loss: 0.0149564693983605 | Epoch: 846 |

MeanAbsoluteError: 0.0972796082496643 | Loss: 0.0154710923142072 | Epoch: 847 | MeanAbsolutel

MeanAbsoluteError: 0.0898391231894493 | Loss: 0.0137364220361633 | Epoch: 849 |

MeanAbsoluteError: 0.0972773209214211 | Loss: 0.0157828888055277 | Epoch: 850 | MeanAbsolutel

MeanAbsoluteError: 0.0885674580931664 | Loss: 0.0137219115074864 | Epoch: 852 |
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MeanAbsoluteError: 0.0889675170183182 | Loss: 0.0136165656675136 | Epoch: 853 | MeanAbsolutel

MeanAbsoluteError: 0.0938826724886894 | Loss: 0.0148640208718765 | Epoch: 855 |

MeanAbsoluteError: 0.0902736037969589 | Loss: 0.0140396268186547 | Epoch: 856 | MeanAbsolutel

MeanAbsoluteError: 0.0956207215785980 | Loss: 0.0154243684133689 | Epoch: 858 |

MeanAbsoluteError: 0.0923597812652588 | Loss: 0.0149355275224176 | Epoch: 859 | MeanAbsolutel

MeanAbsoluteError: 0.0895022079348564 | Loss: 0.0133875974431066 | Epoch: 861 |

MeanAbsoluteError: 0.0902871042490005 | Loss: 0.0139294442514741 | Epoch: 862 | MeanAbsolutel

MeanAbsoluteError: 0.0952467843890190 | Loss: 0.0151088429598137 | Epoch: 864 |

MeanAbsoluteError: 0.0949311107397079 | Loss: 0.0155106873012119 | Epoch: 865 | MeanAbsolutel

MeanAbsoluteError: 0.0972053185105324 | Loss: 0.0163018087010035 | Epoch: 867 |

MeanAbsoluteError: 0.0929144918918610 | Loss: 0.0149304286260788 | Epoch: 868 | MeanAbsolutel

MeanAbsoluteError: 0.0888573080301285 | Loss: 0.0148441093856673 | Epoch: 870 |

MeanAbsoluteError: 0.0945555716753006 | Loss: 0.0150047322203197 | Epoch: 871 | MeanAbsolutel

MeanAbsoluteError: 0.0914585143327713 | Loss: 0.0138689494968215 | Epoch: 873 |

MeanAbsoluteError: 0.0908390581607819 | Loss: 0.0147230571905675 | Epoch: 874 | MeanAbsolutel

MeanAbsoluteError: 0.0912820249795914 | Loss: 0.0138751871580325 | Epoch: 876 |

MeanAbsoluteError: 0.0882806926965714 | Loss: 0.0135034842674456 | Epoch: 877 | MeanAbsolutel

MeanAbsoluteError: 0.0918176248669624 | Loss: 0.0151763588309647 | Epoch: 879 |

MeanAbsoluteError: 0.0955032035708427 | Loss: 0.0154270013005104 | Epoch: 880 | MeanAbsolutel

MeanAbsoluteError: 0.0922941491007805 | Loss: 0.0145518563371540 | Epoch: 882 |

MeanAbsoluteError: 0.0920543670654297 | Loss: 0.0157285554742460 | Epoch: 883 | MeanAbsolute

MeanAbsoluteError: 0.0938300266861916 | Loss: 0.0155638820174499 | Epoch: 885 |

MeanAbsoluteError: 0.0908783748745918 | Loss: 0.0139381371456655 | Epoch: 886 | MeanAbsolute

MeanAbsoluteError: 0.0919426381587982 | Loss: 0.0154362994761323 | Epoch: 888 |

MeanAbsoluteError: 0.0883331522345543 | Loss: 0.0148875595483211 | Epoch: 889 | MeanAbsolute

MeanAbsoluteError: 0.0919242650270462 | Loss: 0.0148638810523456 | Epoch: 891 |

MeanAbsoluteError: 0.0907325893640518 | Loss: 0.0146195812678222 | Epoch: 892 | MeanAbsolute

MeanAbsoluteError: 0.0907133892178535 | Loss: 0.0141848694054352 | Epoch: 894 |

MeanAbsoluteError: 0.0898244380950928 | Loss: 0.0141555894480067 | Epoch: 895 | MeanAbsolute

MeanAbsoluteError: 0.0918782129883766 | Loss: 0.0144951475769631 | Epoch: 897 |

MeanAbsoluteError: 0.0886125043034554 | Loss: 0.0137304951814197 | Epoch: 898 | MeanAbsolute

MeanAbsoluteError: 0.0889383032917976 | Loss: 0.0141911212831231 | Epoch: 900 |

MeanAbsoluteError: 0.0896413102746010 | Loss: 0.0141183183339551 | Epoch: 901 | MeanAbsolute

MeanAbsoluteError: 0.0889725089073181 | Loss: 0.0144346220001413 | Epoch: 903 |

MeanAbsoluteError: 0.0853799879550934 | Loss: 0.0132699511687436 | Epoch: 904 | MeanAbsolute

MeanAbsoluteError: 0.0912100449204445 | Loss: 0.0145358693122398 | Epoch: 906 |

MeanAbsoluteError: 0.0913767591118813 | Loss: 0.0137612145014767 | Epoch: 907 | MeanAbsolute

MeanAbsoluteError: 0.0873437002301216 | Loss: 0.0127499121374103 | Epoch: 909 |

MeanAbsoluteError: 0.0873957797884941 | Loss: 0.0138823560483676 | Epoch: 910 | MeanAbsolutel

MeanAbsoluteError: 0.0936939492821693 | Loss: 0.0148624464014817 | Epoch: 912 |

MeanAbsoluteError: 0.0912870615720749 | Loss: 0.0147408133824138 | Epoch: 913 | MeanAbsolutel

MeanAbsoluteError: 0.0881325155496597 | Loss: 0.0128277834166996 | Epoch: 915 |

MeanAbsoluteError: 0.0897951945662498 | Loss: 0.0140411837648814 | Epoch: 916 | MeanAbsolutel

MeanAbsoluteError: 0.0874848365783691 | Loss: 0.0127232413450838 | Epoch: 918 |

MeanAbsoluteError: 0.0938879698514938 | Loss: 0.0144801068743982 | Epoch: 919 | MeanAbsolutel

MeanAbsoluteError: 0.0942796990275383 | Loss: 0.0151419906209291 | Epoch: 921 |

MeanAbsoluteError: 0.0845179408788681 | Loss: 0.0131081483804640 | Epoch: 922 | MeanAbsolutel

MeanAbsoluteError: 0.0890274718403816 | Loss: 0.0135296544342418 | Epoch: 924 |

MeanAbsoluteError: 0.0864583775401115 | Loss: 0.0131860420468486 | Epoch: 925 | MeanAbsolutel

MeanAbsoluteError: 0.0871563553810120 | Loss: 0.0136100280903823 | Epoch: 927 |

MeanAbsoluteError: 0.0900646299123764 | Loss: 0.0136893373083634 | Epoch: 928 | MeanAbsolutel

MeanAbsoluteError: 0.0903374180197716 | Loss: 0.0140126019508655 | Epoch: 930 |

MeanAbsoluteError: 0.0928129479289055 | Loss: 0.0151121907373211 | Epoch: 931 | MeanAbsolutel

MeanAbsoluteError: 0.0892394483089447 | Loss: 0.0143038608552464 | Epoch: 933 |

MeanAbsoluteError: 0.0916456282138824 | Loss: 0.0143451999868315 | Epoch: 934 | MeanAbsolutel

MeanAbsoluteError: 0.0889278277754784 | Loss: 0.0140302458469159 | Epoch: 936 |

MeanAbsoluteError: 0.0849668085575104 | Loss: 0.0128195640394673 | Epoch: 937 | MeanAbsolutel

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MeanAbsoluteError: 0.0961063355207443 | Loss: 0.0165980820448992 | Epoch: 939 |

MeanAbsoluteError: 0.0928683057427406 | Loss: 0.0141827037453671 | Epoch: 940 | MeanAbsolutel
Returned to Spot: Validation loss: 0.015143395054760731

config: {'_L_in': 10, '_L_out': 1, 'l1': 16, 'dropout_prob': 0.1773189149831582, 'lr_mult': 9
Epoch: 1 | MeanAbsoluteError: 0.1589266955852509 | Loss: 0.0396107463864610 | Epoch: 2 |

MeanAbsoluteError: 0.1385613828897476 | Loss: 0.0305150567926466 | Epoch: 3 | MeanAbsoluteErr

MeanAbsoluteError: 0.1253505945205688 | Loss: 0.0253665243213375 | Returned to Spot: Validati

config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.3840970624671163, 'lr_mult': 4
Epoch: 1 | MeanAbsoluteError: 0.1594958007335663 | Loss: 0.0378252000694996 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1188225299119949 | Loss: 0.0216705332338614 | Epoch: 9 | MeanAbsoluteErr

MeanAbsoluteError: 0.0922567695379257 | Loss: 0.0130999888673327 | Epoch: 12 | MeanAbsoluteEr

MeanAbsoluteError: 0.0632167607545853 | Loss: 0.0072452452180809 | Epoch: 20 | MeanAbsoluteEr

MeanAbsoluteError: 0.0552488006651402 | Loss: 0.0051966664246529 | Epoch: 23 | MeanAbsoluteEr

MeanAbsoluteError: 0.0509727448225021 | Loss: 0.0046219598949201 | Epoch: 31 | MeanAbsoluteEr

MeanAbsoluteError: 0.0481102131307125 | Loss: 0.0042923886442287 | Epoch: 34 | MeanAbsoluteEr

MeanAbsoluteError: 0.0462850928306580 | Loss: 0.0041914032343285 | Epoch: 42 | MeanAbsoluteEr

MeanAbsoluteError: 0.0526083037257195 | Loss: 0.0052131456537417 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.0546875186264515 | Loss: 0.0051224719178495 | Epoch: 53 | MeanAbsoluteEr

MeanAbsoluteError: 0.0587547682225704 | Loss: 0.0052781668154670 | Epoch: 56 | MeanAbsoluteEr

MeanAbsoluteError: 0.0486871413886547 | Loss: 0.0048688383172511 | Epoch: 64 | MeanAbsoluteEr

MeanAbsoluteError: 0.0678964033722878 | Loss: 0.0065304376246212 | Epoch: 67 | MeanAbsoluteEr
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MeanAbsoluteError: 0.0430374108254910 | Loss: 0.0036049185276313 | Epoch: 75 | MeanAbsoluteE

MeanAbsoluteError: 0.0412441343069077 | Loss: 0.0035073819009612 | Epoch: 78 | MeanAbsoluteE

MeanAbsoluteError: 0.0375385470688343 | Loss: 0.0025915994100567 | Epoch: 86 | MeanAbsoluteE

MeanAbsoluteError: 0.0486825928092003 | Loss: 0.0046143816863677 | Epoch: 89 | MeanAbsoluteE

Epoch: 97 | MeanAbsoluteError: 0.0512637495994568 | Loss: 0.0048938488731724 | Epoch: 98 | M

MeanAbsoluteError: 0.0390989370644093 | Loss: 0.0029917780300725 | Epoch: 100 | MeanAbsolute

MeanAbsoluteError: 0.0464583635330200 | Loss: 0.0047108315185668 | Epoch: 108 | MeanAbsolute

MeanAbsoluteError: 0.0462678819894791 | Loss: 0.0040446847928443 | Epoch: 111 | MeanAbsolute

MeanAbsoluteError: 0.0449468269944191 | Loss: 0.0037452920690779 | Epoch: 119 | MeanAbsolute

MeanAbsoluteError: 0.0385937988758087 | Loss: 0.0031782205945714 | Epoch: 122 | MeanAbsolute

MeanAbsoluteError: 0.0397592559456825 | Loss: 0.0027568183768859 | Epoch: 130 | MeanAbsolute

MeanAbsoluteError: 0.0441173948347569 | Loss: 0.0040700652645778 | Epoch: 133 | MeanAbsolute

Epoch: 141 | MeanAbsoluteError: 0.0624889247119427 | Loss: 0.0069354968038265 | Epoch: 142 |

Epoch: 144 | MeanAbsoluteError: 0.0457574538886547 | Loss: 0.0038846386477847 | Epoch: 145 |
Returned to Spot: Validation loss: 0.0036308488557360284

config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.24580168789011042, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1775597184896469 | Loss: 0.0445753564371874 | Epoch: 2 | Mea

MeanAbsoluteError: 0.1454614251852036 | Loss: 0.0260739028453827 | Epoch: 21 | MeanAbsoluteE

MeanAbsoluteError: 0.1459318995475769 | Loss: 0.0252722677235541 | Epoch: 41 | MeanAbsoluteE

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MeanAbsoluteError: 0.1268258541822433 | Loss: 0.0187740137212371 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.0641660168766975 | Loss: 0.0054286807211802 | Epoch: 81 | MeanAbsoluteEr

MeanAbsoluteError: 0.0529515109956264 | Loss: 0.0046637564542164 | Epoch: 101 | MeanAbsolutel

MeanAbsoluteError: 0.0443784222006798 | Loss: 0.0040601667500787 | Epoch: 121 | MeanAbsolutel
Returned to Spot: Validation loss: 0.01517733024727357
spotPython tuning: 0.002616552669726508 [----------] 2.71%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.22837518654402147, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1308252066373825 | Loss: 0.0265597031990948 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1069270074367523 | Loss: 0.0178842768563252 | Epoch: 21 | MeanAbsoluteEr

MeanAbsoluteError: 0.0597703754901886 | Loss: 0.0062055303592627 | Epoch: 41 | MeanAbsoluteEr

MeanAbsoluteError: 0.1089378520846367 | Loss: 0.0150901309067481 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.0719462558627129 | Loss: 0.0067318116902913 | Epoch: 81 | MeanAbsoluteEr

MeanAbsoluteError: 0.0696906223893166 | Loss: 0.0081204373487516 | Epoch: 101 | MeanAbsolutel

MeanAbsoluteError: 0.0611213296651840 | Loss: 0.0048668051849266 | Epoch: 121 | MeanAbsolutel

MeanAbsoluteError: 0.0380189679563046 | Loss: 0.0024404489300459 | Epoch: 141 | MeanAbsolutel
Returned to Spot: Validation loss: 0.005170660289494615

spotPython tuning: 0.002616552669726508 [#---------] 5.96%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.19678865158046985, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1275790929794312 | Loss: 0.0253350573778152 | Epoch: 2 | Mean

MeanAbsoluteError: 0.0661873370409012 | Loss: 0.0069111135570953 | Epoch: 7 | MeanAbsoluteErr

MeanAbsoluteError: 0.0467432662844658 | Loss: 0.0043522030753472 | Epoch: 13 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.0466980598866940 | Loss: 0.0039003083331045 | Epoch: 19 | MeanAbsoluteEr

MeanAbsoluteError: 0.0457979887723923 | Loss: 0.0040228050011986 | Epoch: 25 | MeanAbsoluteEr

MeanAbsoluteError: 0.0347631834447384 | Loss: 0.0025733338040300 | Epoch: 31 | MeanAbsoluteEr

MeanAbsoluteError: 0.0444794781506062 | Loss: 0.0032055134675466 | Epoch: 37 | MeanAbsoluteEr

MeanAbsoluteError: 0.0444412045180798 | Loss: 0.0046647486839599 | Epoch: 43 | MeanAbsoluteEr

MeanAbsoluteError: 0.0509976670145988 | Loss: 0.0046998962290430 | Epoch: 49 | MeanAbsoluteEr

MeanAbsoluteError: 0.0509128123521805 | Loss: 0.0050164787824421 | Epoch: 55 | MeanAbsoluteEr

MeanAbsoluteError: 0.0405981652438641 | Loss: 0.0033934029686498 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.0533174723386765 | Loss: 0.0074600999536536 | Epoch: 67 | MeanAbsoluteEr

MeanAbsoluteError: 0.0753298401832581 | Loss: 0.0079268644641464 | Epoch: 73 | MeanAbsoluteEr

MeanAbsoluteError: 0.0492283552885056 | Loss: 0.0050330607480525 | Epoch: 79 | MeanAbsoluteEr

MeanAbsoluteError: 0.0493206232786179 | Loss: 0.0053274197876453 | Epoch: 85 | MeanAbsoluteEr

MeanAbsoluteError: 0.0561037883162498 | Loss: 0.0059418327745516 | Epoch: 91 | MeanAbsoluteEr

MeanAbsoluteError: 0.0489932931959629 | Loss: 0.0058350499216855 | Epoch: 97 | MeanAbsoluteEr

MeanAbsoluteError: 0.0501342155039310 | Loss: 0.0051888407611599 | Epoch: 103 | MeanAbsolutel
Returned to Spot: Validation loss: 0.005212400178036963

spotPython tuning: 0.002616552669726508 [#---------] 12.69%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.30307433204932804, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1706100106239319 | Loss: 0.0451106128135794 | Epoch: 2 | Mean
```

```
MeanAbsoluteError: 0.1653519570827484 | Loss: 0.0355563676474910 | Epoch: 13 | MeanAbsoluteE

MeanAbsoluteError: 0.0747667104005814 | Loss: 0.0089444822974895 | Epoch: 25 | MeanAbsoluteE
Returned to Spot: Validation loss: 0.016290426266526704

spotPython tuning: 0.002616552669726508 [#---------] 14.32%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.8628392823470216, 'lr_mult': 1
Epoch: 1 | MeanAbsoluteError: 0.2146806865930557 | Loss: 0.0723293547175432 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1322571486234665 | Loss: 0.0282383693480178 | Epoch: 20 | MeanAbsoluteE

MeanAbsoluteError: 0.1324374079704285 | Loss: 0.0281580863030333 | Epoch: 39 | MeanAbsoluteE

MeanAbsoluteError: 0.1271349340677261 | Loss: 0.0275305566426955 | Epoch: 59 | MeanAbsoluteE

MeanAbsoluteError: 0.1154948696494102 | Loss: 0.0212981859222054 | Epoch: 78 | MeanAbsoluteE

MeanAbsoluteError: 0.1144222542643547 | Loss: 0.0212672250345349 | Epoch: 97 | MeanAbsoluteE

MeanAbsoluteError: 0.1010147854685783 | Loss: 0.0171388577130672 | Epoch: 117 | MeanAbsolutel

MeanAbsoluteError: 0.0958815738558769 | Loss: 0.0176301640703490 | Epoch: 136 | MeanAbsolutel

MeanAbsoluteError: 0.0934851467609406 | Loss: 0.0156441889703274 | Epoch: 155 | MeanAbsolutel

MeanAbsoluteError: 0.0991537570953369 | Loss: 0.0176874779066757 | Epoch: 175 | MeanAbsolutel

MeanAbsoluteError: 0.1081068441271782 | Loss: 0.0213530002848098 | Epoch: 194 | MeanAbsolutel
Returned to Spot: Validation loss: 0.018607519567012787

spotPython tuning: 0.002616552669726508 [##--------] 18.60%


config: {'_L_in': 10, '_L_out': 1, 'l1': 64, 'dropout_prob': 0.7103107631285819, 'lr_mult': 9
Epoch: 1 | MeanAbsoluteError: 0.1484457105398178 | Loss: 0.0354797716128329 | Epoch: 2 | Mean
```

```
MeanAbsoluteError: 0.1385626494884491 | Loss: 0.0296473820817967 | Epoch: 6 |

MeanAbsoluteError: 0.1356103718280792 | Loss: 0.0286731227394193 | Epoch: 7 | MeanAbsoluteErr

MeanAbsoluteError: 0.1379132717847824 | Loss: 0.0301302732372036 | Epoch: 12 |

MeanAbsoluteError: 0.1361361891031265 | Loss: 0.0297206921176985 | Epoch: 13 | MeanAbsoluteE

MeanAbsoluteError: 0.1287064403295517 | Loss: 0.0272098044585437 | Epoch: 18 |

MeanAbsoluteError: 0.1286418288946152 | Loss: 0.0275937212367232 | Epoch: 19 | MeanAbsoluteE

MeanAbsoluteError: 0.1244635879993439 | Loss: 0.0267346769458770 | Epoch: 24 |

MeanAbsoluteError: 0.1428149044513702 | Loss: 0.0322177020693198 | Epoch: 25 | MeanAbsoluteE

MeanAbsoluteError: 0.1264004707336426 | Loss: 0.0267952924503091 | Epoch: 30 |

MeanAbsoluteError: 0.1339374482631683 | Loss: 0.0290738498543700 | Epoch: 31 | MeanAbsoluteE
Returned to Spot: Validation loss: 0.03217077505231525
spotPython tuning: 0.002616552669726508 [##--------] 20.64%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.1890993228956366, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1773824244737625 | Loss: 0.0453626172813146 | Epoch: 2 | Mean

MeanAbsoluteError: 0.0970599725842476 | Loss: 0.0139431930637281 | Epoch: 13 | MeanAbsoluteE

MeanAbsoluteError: 0.0822291150689125 | Loss: 0.0091155101422613 | Epoch: 25 | MeanAbsoluteE
Returned to Spot: Validation loss: 0.018819046893010016

spotPython tuning: 0.002616552669726508 [##--------] 22.45%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.3835145831979707, 'lr_mult':


Epoch: 1 | MeanAbsoluteError: 0.1489920169115067 | Loss: 0.0356704042244114 | Epoch: 2 | Mean
```

```
MeanAbsoluteError: 0.0820037648081779 | Loss: 0.0115389609035399 | Epoch: 12 | MeanAbsoluteE

MeanAbsoluteError: 0.0596814677119255 | Loss: 0.0058988091094713 | Epoch: 23 | MeanAbsoluteE

MeanAbsoluteError: 0.0582116134464741 | Loss: 0.0058222524974936 | Epoch: 34 | MeanAbsoluteE

MeanAbsoluteError: 0.0492109656333923 | Loss: 0.0048178747268761 | Epoch: 45 | MeanAbsoluteE

MeanAbsoluteError: 0.0504262782633305 | Loss: 0.0045588772550936 | Epoch: 56 | MeanAbsoluteE

MeanAbsoluteError: 0.0598067790269852 | Loss: 0.0063105148606394 | Epoch: 67 | MeanAbsoluteE

MeanAbsoluteError: 0.0794244483113289 | Loss: 0.0094187081619901 | Epoch: 78 | MeanAbsoluteE

MeanAbsoluteError: 0.0437474623322487 | Loss: 0.0036801710972979 | Epoch: 89 | MeanAbsoluteE

Epoch: 100 | MeanAbsoluteError: 0.0562689900398254 | Loss: 0.0059406774388136 | Epoch: 101 |

MeanAbsoluteError: 0.0607690699398518 | Loss: 0.0068627441865637 | Epoch: 111 | MeanAbsolute

Epoch: 122 | MeanAbsoluteError: 0.0598649866878986 | Loss: 0.0066692082266519 | Epoch: 123 |

MeanAbsoluteError: 0.0535027496516705 | Loss: 0.0052996922596848 | Epoch: 133 | MeanAbsolute

Epoch: 144 | MeanAbsoluteError: 0.0468924976885319 | Loss: 0.0040765977326756 | Epoch: 145 |

MeanAbsoluteError: 0.0695816949009895 | Loss: 0.0074796419235339 | Epoch: 155 | MeanAbsolute
Returned to Spot: Validation loss: 0.004756120258733924

spotPython tuning: 0.002616552669726508 [###-------] 28.08%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.40135685211463074, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1695955097675323 | Loss: 0.0437562819815388 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1079661324620247 | Loss: 0.0187867664683022 | Epoch: 12 | MeanAbsoluteE
```

```
MeanAbsoluteError: 0.0875907763838768 | Loss: 0.0126785195898265 | Epoch: 23 | MeanAbsoluteE

MeanAbsoluteError: 0.0613874047994614 | Loss: 0.0065921421199547 | Epoch: 34 | MeanAbsoluteE

MeanAbsoluteError: 0.0597726888954639 | Loss: 0.0061596736042319 | Epoch: 46 | MeanAbsoluteE

MeanAbsoluteError: 0.0547145195305347 | Loss: 0.0053882033113807 | Epoch: 57 | MeanAbsoluteE

MeanAbsoluteError: 0.0495417602360249 | Loss: 0.0046079174897290 | Epoch: 68 | MeanAbsoluteE

Epoch: 79 | MeanAbsoluteError: 0.0474483631551266 | Loss: 0.0038625205098039 | Epoch: 80 | Me

MeanAbsoluteError: 0.0476360954344273 | Loss: 0.0038943909457885 | Epoch: 90 | MeanAbsoluteE

MeanAbsoluteError: 0.0600732751190662 | Loss: 0.0066696898092663 | Epoch: 101 | MeanAbsolutel

MeanAbsoluteError: 0.0483831837773323 | Loss: 0.0044231331220975 | Epoch: 112 | MeanAbsolutel

MeanAbsoluteError: 0.0410999022424221 | Loss: 0.0030726504728112 | Epoch: 123 | MeanAbsolutel

MeanAbsoluteError: 0.0428813584148884 | Loss: 0.0037233148445682 | Epoch: 134 | MeanAbsolutel

MeanAbsoluteError: 0.0580237768590450 | Loss: 0.0047887946956938 | Epoch: 145 | MeanAbsolutel

MeanAbsoluteError: 0.0470833890140057 | Loss: 0.0042149910219259 | Epoch: 156 | MeanAbsolutel
Returned to Spot: Validation loss: 0.0032871504985163675

spotPython tuning: 0.002616552669726508 [###-------] 34.18%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.5036868011192788, 'lr_mult': 0
Epoch: 1 | MeanAbsoluteError: 0.5931276679039001 | Loss: 0.3876352882698962 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1885185986757278 | Loss: 0.0561530161894074 | Epoch: 12 | MeanAbsoluteE

MeanAbsoluteError: 0.1695781201124191 | Loss: 0.0453501213587036 | Epoch: 23 | MeanAbsoluteE
```

MeanAbsoluteError: 0.1609495580196381 | Loss: 0.0389755930457460 | Epoch: 34 | MeanAbsoluteEr

MeanAbsoluteError: 0.1499064862728119 | Loss: 0.0370555248748707 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.1495599895715714 | Loss: 0.0351669098691721 | Epoch: 56 | MeanAbsoluteEr

MeanAbsoluteError: 0.1450883597135544 | Loss: 0.0322472212934180 | Epoch: 67 | MeanAbsoluteEr

MeanAbsoluteError: 0.1369211524724960 | Loss: 0.0286052595995563 | Epoch: 78 | MeanAbsoluteEr

MeanAbsoluteError: 0.1317282915115356 | Loss: 0.0284721241700218 | Epoch: 89 | MeanAbsoluteEr

MeanAbsoluteError: 0.1357117295265198 | Loss: 0.0278955287986288 | Epoch: 100 | MeanAbsoluteE

MeanAbsoluteError: 0.1209888681769371 | Loss: 0.0217036396436589 | Epoch: 111 | MeanAbsoluteE

MeanAbsoluteError: 0.1195110455155373 | Loss: 0.0221455399388153 | Epoch: 122 | MeanAbsoluteE

MeanAbsoluteError: 0.1228398233652115 | Loss: 0.0228623643296918 | Epoch: 133 | MeanAbsoluteE

MeanAbsoluteError: 0.1220626831054688 | Loss: 0.0222875854417093 | Epoch: 144 | MeanAbsoluteE

MeanAbsoluteError: 0.1157317608594894 | Loss: 0.0212904203585104 | Epoch: 155 | MeanAbsoluteE

MeanAbsoluteError: 0.1132365539669991 | Loss: 0.0207484713265378 | Epoch: 166 | MeanAbsoluteE

MeanAbsoluteError: 0.1124493032693863 | Loss: 0.0203929552195692 | Epoch: 177 | MeanAbsoluteE

MeanAbsoluteError: 0.1103010177612305 | Loss: 0.0189801586032110 | Epoch: 188 | MeanAbsoluteE

MeanAbsoluteError: 0.1113350316882133 | Loss: 0.0202908302461238 | Epoch: 199 | MeanAbsoluteE

MeanAbsoluteError: 0.0997997745871544 | Loss: 0.0160152249920525 | Epoch: 210 | MeanAbsoluteE

MeanAbsoluteError: 0.1015908494591713 | Loss: 0.0158760220939784 | Epoch: 221 | MeanAbsoluteE

MeanAbsoluteError: 0.1028972342610359 | Loss: 0.0177104644060723 | Epoch: 232 | MeanAbsoluteE

MeanAbsoluteError: 0.1048801988363266 | Loss: 0.0177423135855382 | Epoch: 243 | MeanAbsolutel

MeanAbsoluteError: 0.0999438613653183 | Loss: 0.0160156120852518 | Epoch: 254 | MeanAbsolutel

MeanAbsoluteError: 0.0991988480091095 | Loss: 0.0153858663857375 | Epoch: 265 | MeanAbsolutel

MeanAbsoluteError: 0.0945722088217735 | Loss: 0.0142707333495644 | Epoch: 276 | MeanAbsolutel

MeanAbsoluteError: 0.0918072834610939 | Loss: 0.0137357267085463 | Epoch: 287 | MeanAbsolutel

MeanAbsoluteError: 0.0955623611807823 | Loss: 0.0142148323602190 | Epoch: 298 | MeanAbsolutel

MeanAbsoluteError: 0.0892868787050247 | Loss: 0.0129434747841993 | Epoch: 310 | MeanAbsolutel

MeanAbsoluteError: 0.0869562178850174 | Loss: 0.0121787094302770 | Epoch: 322 | MeanAbsolutel

MeanAbsoluteError: 0.0888782516121864 | Loss: 0.0126225851954108 | Epoch: 334 | MeanAbsolutel

MeanAbsoluteError: 0.0883611589670181 | Loss: 0.0131018353491335 | Epoch: 346 | MeanAbsolutel

MeanAbsoluteError: 0.0844801813364029 | Loss: 0.0114552778633017 | Epoch: 358 | MeanAbsolutel

MeanAbsoluteError: 0.0824109315872192 | Loss: 0.0119312813591310 | Epoch: 369 | MeanAbsolutel

MeanAbsoluteError: 0.0785521864891052 | Loss: 0.0100318926852196 | Epoch: 381 | MeanAbsolutel

MeanAbsoluteError: 0.0789810717105865 | Loss: 0.0102680172207520 | Epoch: 393 | MeanAbsolutel

MeanAbsoluteError: 0.0823595449328423 | Loss: 0.0114889626550537 | Epoch: 405 | MeanAbsolutel

MeanAbsoluteError: 0.0808084309101105 | Loss: 0.0106043945569055 | Epoch: 417 | MeanAbsolutel

MeanAbsoluteError: 0.0810906141996384 | Loss: 0.0110518900358951 | Epoch: 429 | MeanAbsolutel

MeanAbsoluteError: 0.0793781057000160 | Loss: 0.0104996873169990 | Epoch: 441 | MeanAbsolutel

MeanAbsoluteError: 0.0808492004871368 | Loss: 0.0106817211735209 | Epoch: 453 | MeanAbsolutel

MeanAbsoluteError: 0.0750740021467209 | Loss: 0.0096362217047595 | Epoch: 465 | MeanAbsolute

MeanAbsoluteError: 0.0725083500146866 | Loss: 0.0085721278109735 | Epoch: 477 | MeanAbsolute

Epoch: 488 | MeanAbsoluteError: 0.0678060725331306 | Loss: 0.0083882487562828 | Epoch: 489 |

MeanAbsoluteError: 0.0699660703539848 | Loss: 0.0089004616066201 | Epoch: 499 | MeanAbsolute

MeanAbsoluteError: 0.0733854323625565 | Loss: 0.0098794503811453 | Epoch: 511 | MeanAbsolute

MeanAbsoluteError: 0.0714439451694489 | Loss: 0.0090278598761774 | Epoch: 522 | MeanAbsolute

MeanAbsoluteError: 0.0712707936763763 | Loss: 0.0085624547209591 | Epoch: 533 | MeanAbsolute

MeanAbsoluteError: 0.0639542937278748 | Loss: 0.0072774823669246 | Epoch: 544 | MeanAbsolute

MeanAbsoluteError: 0.0670913979411125 | Loss: 0.0074517531351088 | Epoch: 555 | MeanAbsolute

MeanAbsoluteError: 0.0666804909706116 | Loss: 0.0075022669411019 | Epoch: 566 | MeanAbsolute

MeanAbsoluteError: 0.0680078119039536 | Loss: 0.0079325616580287 | Epoch: 577 | MeanAbsolute

MeanAbsoluteError: 0.0702364295721054 | Loss: 0.0081321073812433 | Epoch: 588 | MeanAbsolute

MeanAbsoluteError: 0.0662970840930939 | Loss: 0.0070339055780910 | Epoch: 600 | MeanAbsolute

MeanAbsoluteError: 0.0642794594168663 | Loss: 0.0069190201772328 | Epoch: 611 | MeanAbsolute

MeanAbsoluteError: 0.0650640577077866 | Loss: 0.0070021160890495 | Epoch: 623 | MeanAbsolute

MeanAbsoluteError: 0.0673015266656876 | Loss: 0.0077777473733907 | Epoch: 634 | MeanAbsolute

MeanAbsoluteError: 0.0663975998759270 | Loss: 0.0075232183995755 | Epoch: 645 | MeanAbsolute

MeanAbsoluteError: 0.0646947175264359 | Loss: 0.0073831045179089 | Epoch: 656 | MeanAbsolute

MeanAbsoluteError: 0.0656514614820480 | Loss: 0.0076107638979968 | Epoch: 667 | MeanAbsolute

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MeanAbsoluteError: 0.0643883422017097 | Loss: 0.0074537023013507 | Epoch: 678 | MeanAbsoluteE

MeanAbsoluteError: 0.0644911453127861 | Loss: 0.0073796604809008 | Epoch: 689 | MeanAbsoluteE

MeanAbsoluteError: 0.0619570910930634 | Loss: 0.0067619482808942 | Epoch: 700 | MeanAbsoluteE

MeanAbsoluteError: 0.0587562359869480 | Loss: 0.0058638014383369 | Epoch: 711 | MeanAbsoluteE

MeanAbsoluteError: 0.0647131130099297 | Loss: 0.0075051490045888 | Epoch: 722 | MeanAbsoluteE

MeanAbsoluteError: 0.0617118403315544 | Loss: 0.0064530393788836 | Epoch: 733 | MeanAbsoluteE

MeanAbsoluteError: 0.0623588673770428 | Loss: 0.0071821224624536 | Epoch: 744 | MeanAbsoluteE

MeanAbsoluteError: 0.0620541460812092 | Loss: 0.0067342705013672 | Epoch: 755 | MeanAbsoluteE

MeanAbsoluteError: 0.0631132647395134 | Loss: 0.0070466536984129 | Epoch: 766 | MeanAbsoluteE

MeanAbsoluteError: 0.0617800280451775 | Loss: 0.0067000734668813 | Epoch: 777 | MeanAbsoluteE

MeanAbsoluteError: 0.0600574575364590 | Loss: 0.0064638236592720 | Epoch: 788 | MeanAbsoluteE
Returned to Spot: Validation loss: 0.005667992542791916

spotPython tuning: 0.002616552669726508 [######----] 59.85%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.09812795088415356, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1330081373453140 | Loss: 0.0283971591117351 | Epoch: 2 | Mean

spotPython tuning: 0.002616552669726508 [######----] 61.10%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.4146353558497759, 'lr_mult': 0
Epoch: 1 | MeanAbsoluteError: 0.2809319198131561 | Loss: 0.1010542855058846 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1353554725646973 | Loss: 0.0296399691387227 | Epoch: 12 | MeanAbsoluteEr

MeanAbsoluteError: 0.1395519971847534 | Loss: 0.0302981980831215 | Epoch: 23 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.1406530439853668 | Loss: 0.0303019578323552 | Epoch: 34 | MeanAbsoluteEr

MeanAbsoluteError: 0.1315870732069016 | Loss: 0.0265682202420737 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.1241538971662521 | Loss: 0.0252094543416445 | Epoch: 56 | MeanAbsoluteEr

spotPython tuning: 0.002616552669726508 [######----] 64.24%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.3454297531343123, 'lr_mult': 0
Epoch: 1 | MeanAbsoluteError: 0.6466159820556641 | Loss: 0.4571257570856496 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1758672595024109 | Loss: 0.0480883218544094 | Epoch: 12 | MeanAbsoluteEr

MeanAbsoluteError: 0.1591475009918213 | Loss: 0.0419428259330361 | Epoch: 23 | MeanAbsoluteEr

MeanAbsoluteError: 0.1576700657606125 | Loss: 0.0406377203885074 | Epoch: 34 | MeanAbsoluteEr

MeanAbsoluteError: 0.1424781084060669 | Loss: 0.0305439145549348 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.1321230381727219 | Loss: 0.0265958934017506 | Epoch: 56 | MeanAbsoluteEr

MeanAbsoluteError: 0.1463057100772858 | Loss: 0.0328241545878547 | Epoch: 67 | MeanAbsoluteEr

MeanAbsoluteError: 0.1292199343442917 | Loss: 0.0262561885909619 | Epoch: 78 | MeanAbsoluteEr

MeanAbsoluteError: 0.1244555935263634 | Loss: 0.0262714760059393 | Epoch: 89 | MeanAbsoluteEr

MeanAbsoluteError: 0.1233636364340782 | Loss: 0.0243618843684855 | Epoch: 100 | MeanAbsolutel

MeanAbsoluteError: 0.1175804659724236 | Loss: 0.0216915724112799 | Epoch: 111 | MeanAbsolutel

MeanAbsoluteError: 0.1088113263249397 | Loss: 0.0199027889604239 | Epoch: 122 | MeanAbsolutel

MeanAbsoluteError: 0.1119735315442085 | Loss: 0.0208020176076771 | Epoch: 133 | MeanAbsolutel

MeanAbsoluteError: 0.1104564443230629 | Loss: 0.0185120579124869 | Epoch: 144 | MeanAbsolutel
```

```
MeanAbsoluteError: 0.1189845651388168 | Loss: 0.0220712307031806 | Epoch: 155 | MeanAbsoluteE

MeanAbsoluteError: 0.1003573536872864 | Loss: 0.0169107798229609 | Epoch: 166 | MeanAbsoluteE

Epoch: 177 | MeanAbsoluteError: 0.1114745214581490 | Loss: 0.0201589544181173 | Epoch: 178 |

Epoch: 188 | MeanAbsoluteError: 0.1045009270310402 | Loss: 0.0177273846194638 | Epoch: 189 |

MeanAbsoluteError: 0.1064056679606438 | Loss: 0.0175288841986146 | Epoch: 199 | MeanAbsoluteE

MeanAbsoluteError: 0.1007914319634438 | Loss: 0.0168243052781020 | Epoch: 210 | MeanAbsoluteE

MeanAbsoluteError: 0.0967372134327888 | Loss: 0.0157573309322623 | Epoch: 221 | MeanAbsoluteE

MeanAbsoluteError: 0.0981932431459427 | Loss: 0.0157681055869417 | Epoch: 232 | MeanAbsoluteE

MeanAbsoluteError: 0.0960341989994049 | Loss: 0.0143786190678120 | Epoch: 243 | MeanAbsoluteE

MeanAbsoluteError: 0.0889477655291557 | Loss: 0.0125491731450893 | Epoch: 254 | MeanAbsoluteE

spotPython tuning: 0.002616552669726508 [#######---] 74.36%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.41921602704146355, 'lr_mult':
Epoch: 1 | MeanAbsoluteError: 0.1587115973234177 | Loss: 0.0406297259522896 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1002310812473297 | Loss: 0.0160988827701658 | Epoch: 12 | MeanAbsoluteEr

MeanAbsoluteError: 0.0714611187577248 | Loss: 0.0088827022731206 | Epoch: 23 | MeanAbsoluteEr

MeanAbsoluteError: 0.0660282298922539 | Loss: 0.0076956648661412 | Epoch: 34 | MeanAbsoluteEr

MeanAbsoluteError: 0.0575409904122353 | Loss: 0.0057987174613548 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.0513945743441582 | Loss: 0.0045919121353348 | Epoch: 56 | MeanAbsoluteEr

MeanAbsoluteError: 0.0492617227137089 | Loss: 0.0046260678806759 | Epoch: 67 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.0454136766493320 | Loss: 0.0040135599694239 | Epoch: 78 | MeanAbsoluteEr

MeanAbsoluteError: 0.0513865798711777 | Loss: 0.0046360343388331 | Epoch: 89 | MeanAbsoluteEr

MeanAbsoluteError: 0.0492322705686092 | Loss: 0.0037936542097381 | Epoch: 100 | MeanAbsoluteE

MeanAbsoluteError: 0.0501753203570843 | Loss: 0.0052436442163430 | Epoch: 111 | MeanAbsoluteE

MeanAbsoluteError: 0.0505392812192440 | Loss: 0.0045989126037488 | Epoch: 122 | MeanAbsoluteE

MeanAbsoluteError: 0.0535916015505791 | Loss: 0.0052973073049399 | Epoch: 133 | MeanAbsoluteE

MeanAbsoluteError: 0.0531311333179474 | Loss: 0.0049514193639257 | Epoch: 144 | MeanAbsoluteE

MeanAbsoluteError: 0.0517830625176430 | Loss: 0.0054072680619643 | Epoch: 155 | MeanAbsoluteE
Returned to Spot: Validation loss: 0.005373125329099007

spotPython tuning: 0.002616552669726508 [#########-] 85.14%


config: {'_L_in': 10, '_L_out': 1, 'l1': 32, 'dropout_prob': 0.2329665337331769, 'lr_mult': 3
Epoch: 1 | MeanAbsoluteError: 0.1418680101633072 | Loss: 0.0329092004833122 | Epoch: 2 | Mean

MeanAbsoluteError: 0.0834220647811890 | Loss: 0.0114520774843792 | Epoch: 7 | MeanAbsoluteErr

MeanAbsoluteError: 0.0723373442888260 | Loss: 0.0077882206925036 | Epoch: 13 | MeanAbsoluteEr

MeanAbsoluteError: 0.0544917099177837 | Loss: 0.0051272296251652 | Epoch: 19 | MeanAbsoluteEr

MeanAbsoluteError: 0.0469007901847363 | Loss: 0.0038455050912065 | Epoch: 25 | MeanAbsoluteEr

MeanAbsoluteError: 0.0423949733376503 | Loss: 0.0040610903109579 | Epoch: 31 | MeanAbsoluteEr

MeanAbsoluteError: 0.0397197604179382 | Loss: 0.0029869433181011 | Epoch: 37 | MeanAbsoluteEr

MeanAbsoluteError: 0.0434052832424641 | Loss: 0.0038018397973307 | Epoch: 43 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.0580024980008602 | Loss: 0.0054147510211139 | Epoch: 49 | MeanAbsoluteEr
MeanAbsoluteError: 0.0366057083010674 | Loss: 0.0026266111431566 | Epoch: 55 | MeanAbsoluteEr
MeanAbsoluteError: 0.0440691933035851 | Loss: 0.0033013638947159 | Epoch: 61 | MeanAbsoluteEr
MeanAbsoluteError: 0.0355960801243782 | Loss: 0.0024697162634887 | Epoch: 67 | MeanAbsoluteEr
MeanAbsoluteError: 0.0441784635186195 | Loss: 0.0032939165762218 | Epoch: 73 | MeanAbsoluteEr
MeanAbsoluteError: 0.0371045731008053 | Loss: 0.0029758054268314 | Epoch: 79 | MeanAbsoluteEr
MeanAbsoluteError: 0.0345577895641327 | Loss: 0.0023971278136984 | Epoch: 85 | MeanAbsoluteEr
MeanAbsoluteError: 0.0387997254729271 | Loss: 0.0026114425817893 | Epoch: 91 | MeanAbsoluteEr
MeanAbsoluteError: 0.0357546694576740 | Loss: 0.0025868095501210 | Epoch: 97 | MeanAbsoluteEr
MeanAbsoluteError: 0.0376084260642529 | Loss: 0.0025542132544797 | Epoch: 103 | MeanAbsoluteE
MeanAbsoluteError: 0.0363630689680576 | Loss: 0.0025113605616692 | Epoch: 109 | MeanAbsoluteE
MeanAbsoluteError: 0.0347551181912422 | Loss: 0.0022541738994914 | Epoch: 115 | MeanAbsoluteE
MeanAbsoluteError: 0.0326102934777737 | Loss: 0.0018003056561186 | Epoch: 121 | MeanAbsoluteE
MeanAbsoluteError: 0.0354748331010342 | Loss: 0.0028137335800178 | Epoch: 127 | MeanAbsoluteE
MeanAbsoluteError: 0.0365852825343609 | Loss: 0.0028655014280230 | Epoch: 133 | MeanAbsoluteE
MeanAbsoluteError: 0.0372179709374905 | Loss: 0.0028832547731387 | Epoch: 139 | MeanAbsoluteE
MeanAbsoluteError: 0.0375973507761955 | Loss: 0.0025292277737753 | Epoch: 145 | MeanAbsoluteE
MeanAbsoluteError: 0.0362293124198914 | Loss: 0.0024698337898008 | Epoch: 151 | MeanAbsoluteE
MeanAbsoluteError: 0.0353367440402508 | Loss: 0.0027586833432239 | Epoch: 157 | MeanAbsoluteE
```

```
MeanAbsoluteError: 0.0425825566053391 | Loss: 0.0031510238716146 | Epoch: 163 | MeanAbsolutel

MeanAbsoluteError: 0.0416178405284882 | Loss: 0.0033716384705622 | Epoch: 169 | MeanAbsolutel

MeanAbsoluteError: 0.0401275977492332 | Loss: 0.0026937047006019 | Epoch: 175 | MeanAbsolutel

MeanAbsoluteError: 0.0397470891475677 | Loss: 0.0028817041835282 | Epoch: 181 | MeanAbsolutel

MeanAbsoluteError: 0.0399562604725361 | Loss: 0.0032089473323625 | Epoch: 187 | MeanAbsolutel

MeanAbsoluteError: 0.0476062931120396 | Loss: 0.0038837005950821 | Epoch: 193 | MeanAbsolutel

MeanAbsoluteError: 0.0438828840851784 | Loss: 0.0034048447804525 | Epoch: 199 | MeanAbsolutel

MeanAbsoluteError: 0.0338208228349686 | Loss: 0.0022729066933971 | Epoch: 205 | MeanAbsolutel

MeanAbsoluteError: 0.0490919128060341 | Loss: 0.0046230089369540 | Epoch: 211 | MeanAbsolutel
Returned to Spot: Validation loss: 0.003087497500043052

spotPython tuning: 0.002616552669726508 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x17fccbc40>
```

19.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

19.10 Step 10: Results

After the hyperparameter tuning run is finished, the results can be analyzed as described in Section 14.10.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

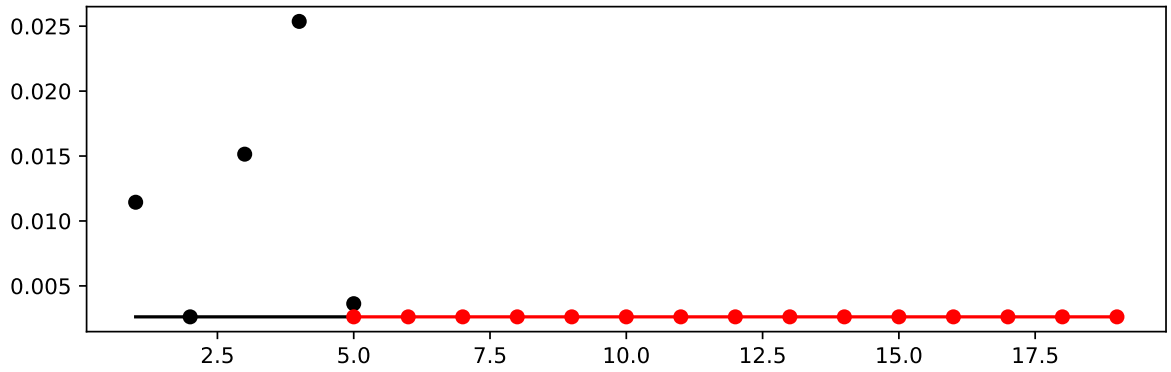


Figure 19.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

```
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

name	type	default	lower	upper	tuned	transform
_L_in	int	10	10.0	10.0	10.0	None
_L_out	int	1	1.0	1.0	1.0	None
l1	int	3	3.0	8.0	5.0	transform_pow
dropout_prob	float	0.01	0.0	0.9	0.19981931523998656	None
lr_mult	float	1.0	0.1	10.0	7.004318498645526	None
batch_size	int	4	1.0	4.0	4.0	transform_pow
epochs	int	4	2.0	16.0	11.0	transform_pow
k_folds	int	1	1.0	1.0	1.0	None
patience	int	2	3.0	7.0	5.0	transform_pow
optimizer	factor	SGD	0.0	6.0	0.0	None
sgd_momentum	float	0.0	0.0	1.0	0.07401195908206384	None

```
spot_tuner.plot_importance(threshold=0.025,
    filename="./figures/" + experiment_name+"_importance.png")
```

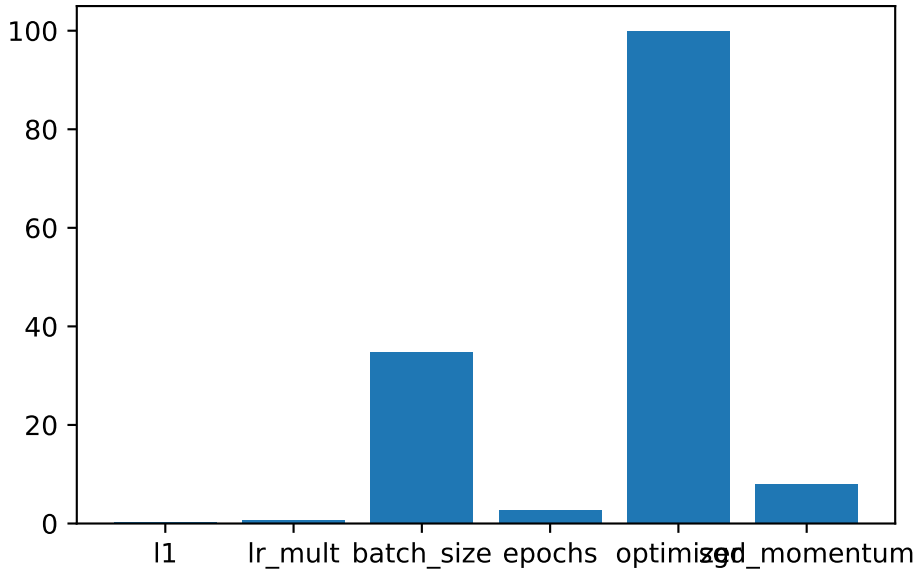


Figure 19.2: Variable importance plot, threshold 0.025.

19.10.1 Get the Tuned Architecture (SPOT Results)

```
from spotPython.hyperparameters.values import get_one_core_model_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
model_spot = get_one_core_model_from_X(X, fun_control)
model_spot
```

```
Net_lin_reg(
  (fc1): Linear(in_features=10, out_features=32, bias=True)
  (fc2): Linear(in_features=32, out_features=16, bias=True)
  (fc3): Linear(in_features=16, out_features=1, bias=True)
  (relu): ReLU()
  (softmax): Softmax(dim=1)
  (dropout1): Dropout(p=0.19981931523998656, inplace=False)
  (dropout2): Dropout(p=0.09990965761999328, inplace=False)
)
```

19.10.2 Evaluation of the Tuned Architecture

```
from spotPython.torch.traintest import (
    train_tuned,
    test_tuned,
    )
```

```
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=True,
        device = fun_control["device"],
        path=None,
        task=fun_control["task"],)
```

```
Epoch: 1 | MeanAbsoluteError: 0.1370587348937988 | Loss: 0.0296040675357768 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1273256391286850 | Loss: 0.0254505154137549 | Epoch: 6 | MeanAbsoluteErr

MeanAbsoluteError: 0.1084648370742798 | Loss: 0.0162495498692519 | Epoch: 21 | MeanAbsoluteEr

MeanAbsoluteError: 0.0921800211071968 | Loss: 0.0120782979862078 | Epoch: 26 | MeanAbsoluteEr

MeanAbsoluteError: 0.0608531460165977 | Loss: 0.0063501899130642 | Epoch: 41 | MeanAbsoluteEr

MeanAbsoluteError: 0.0506178848445415 | Loss: 0.0047787399411103 | Epoch: 46 | MeanAbsoluteEr

MeanAbsoluteError: 0.0487709417939186 | Loss: 0.0039907744901843 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.1488473564386368 | Loss: 0.0273869378786338 | Epoch: 66 | MeanAbsoluteEr

MeanAbsoluteError: 0.0829284191131592 | Loss: 0.0092043102424788 | Epoch: 81 | MeanAbsoluteEr

MeanAbsoluteError: 0.0774341747164726 | Loss: 0.0094372643108823 | Epoch: 86 | MeanAbsoluteEr

MeanAbsoluteError: 0.0726040303707123 | Loss: 0.0073204866708501 | Epoch: 101 | MeanAbsolutel

MeanAbsoluteError: 0.0559390708804131 | Loss: 0.0048706169289194 | Epoch: 106 | MeanAbsolutel
```

```
MeanAbsoluteError: 0.0840886309742928 | Loss: 0.0093243038281798 | Epoch: 121 | MeanAbsolutel

MeanAbsoluteError: 0.0962029844522476 | Loss: 0.0123873427755346 | Epoch: 126 | MeanAbsolutel

MeanAbsoluteError: 0.0664651840925217 | Loss: 0.0069836770723525 | Epoch: 142 | MeanAbsolutel

MeanAbsoluteError: 0.0932655557990074 | Loss: 0.0104182182419065 | Epoch: 147 | MeanAbsolutel

MeanAbsoluteError: 0.1201086938381195 | Loss: 0.0178982440480276 | Epoch: 162 | MeanAbsolutel

MeanAbsoluteError: 0.0302110612392426 | Loss: 0.0021190302918273 | Epoch: 167 | MeanAbsolutel

MeanAbsoluteError: 0.0590001121163368 | Loss: 0.0049689801556892 | Epoch: 182 | MeanAbsolutel
Returned to Spot: Validation loss: 0.008977211006966076
```

If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be loaded from this file.

```
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = fun_control["device"],
            task=fun_control["task"],)
```

```
MeanAbsoluteError: 0.0897793695330620 | Loss: 0.0096923084929585 | Final evaluation: Validati
Final evaluation: Validation metric: 0.08977936953306198
---------------------------------------------
```

```
(0.009692308492958546, nan, tensor(0.0898))
```

19.10.3 Cross-validated Evaluations

- This is the evaluation that will be used in the comparison (evaluatecv has to be updated before, to get metric vlaues!):

```
from spotPython.torch.traintest import evaluate_cv
# modify k-kolds:
```

```
setattr(model_spot, "k_folds",  10)
df_eval, df_preds, df_metrics = evaluate_cv(net=model_spot,
            dataset=fun_control["data"],
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            task=fun_control["task"],
            writer=fun_control["writer"],
            writerId="model_spot_cv",
            device = fun_control["device"])
```

```
Fold: 1
Epoch: 1 | MeanAbsoluteError: 0.2074535191059113 | Loss: 0.0568870306015015 | Epoch: 2 |

MeanAbsoluteError: 0.1662064939737320 | Loss: 0.0420318836612361 | Epoch: 3 | MeanAbsoluteEr

MeanAbsoluteError: 0.1947877258062363 | Loss: 0.0447941528899329 | Epoch: 11 | MeanAbsoluteE

MeanAbsoluteError: 0.0690206214785576 | Loss: 0.0081713101826608 | Epoch: 13 | MeanAbsoluteE

MeanAbsoluteError: 0.0666046813130379 | Loss: 0.0085620973591826 | Epoch: 15 | MeanAbsoluteE

MeanAbsoluteError: 0.0844514369964600 | Loss: 0.0123406526898699 | Epoch: 23 | MeanAbsoluteE

MeanAbsoluteError: 0.1196470633149147 | Loss: 0.0246764271120940 | Epoch: 25 | MeanAbsoluteE

MeanAbsoluteError: 0.0736473277211189 | Loss: 0.0080379972766553 | Epoch: 27 | MeanAbsoluteE

MeanAbsoluteError: 0.1055080518126488 | Loss: 0.0147056539676019 | Epoch: 35 | MeanAbsoluteE

MeanAbsoluteError: 0.0430901236832142 | Loss: 0.0027375899787460 | Epoch: 37 | MeanAbsoluteE

MeanAbsoluteError: 0.0461486764252186 | Loss: 0.0035476277282994 | Epoch: 39 | MeanAbsoluteE

MeanAbsoluteError: 0.0895985960960388 | Loss: 0.0097864660035287 | Epoch: 47 | MeanAbsoluteE

MeanAbsoluteError: 0.0772603824734688 | Loss: 0.0082105003031237 | Epoch: 49 | MeanAbsoluteE
```

```
MeanAbsoluteError: 0.0968873798847198 | Loss: 0.0150861990238939 | Epoch: 51 | MeanAbsoluteEr

MeanAbsoluteError: 0.0677198693156242 | Loss: 0.0054549230096330 | Epoch: 59 | MeanAbsoluteEr

MeanAbsoluteError: 0.0576495490968227 | Loss: 0.0059405884905053 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.1951318234205246 | Loss: 0.0425204416470868 | Epoch: 63 | MeanAbsoluteEr
Fold: 2
Epoch: 1 | MeanAbsoluteError: 0.1407433450222015 | Loss: 0.0319495682737657 | Epoch: 2 |

MeanAbsoluteError: 0.1173545867204666 | Loss: 0.0225886432453990 | Epoch: 3 | MeanAbsoluteErr

MeanAbsoluteError: 0.1336389482021332 | Loss: 0.0250639971345663 | Epoch: 5 | MeanAbsoluteErr

MeanAbsoluteError: 0.0849720537662506 | Loss: 0.0144682430795261 | Epoch: 7 | MeanAbsoluteErr

MeanAbsoluteError: 0.1487204581499100 | Loss: 0.0257674178906849 | Epoch: 15 | MeanAbsoluteEr

MeanAbsoluteError: 0.1087015941739082 | Loss: 0.0154955834150314 | Epoch: 17 | MeanAbsoluteEr

MeanAbsoluteError: 0.0714541226625443 | Loss: 0.0098788006497281 | Epoch: 19 | MeanAbsoluteEr

MeanAbsoluteError: 0.0678072720766068 | Loss: 0.0083405432690467 | Epoch: 27 | MeanAbsoluteEr

MeanAbsoluteError: 0.0489613041281700 | Loss: 0.0036614821209306 | Epoch: 29 | MeanAbsoluteEr

MeanAbsoluteError: 0.1330788582563400 | Loss: 0.0210440454206296 | Epoch: 31 | MeanAbsoluteEr

MeanAbsoluteError: 0.1064446046948433 | Loss: 0.0138260341648545 | Epoch: 39 | MeanAbsoluteEr

MeanAbsoluteError: 0.0998014062643051 | Loss: 0.0132981617269771 | Epoch: 41 | MeanAbsoluteEr

MeanAbsoluteError: 0.0924433320760727 | Loss: 0.0098646959689047 | Epoch: 43 | MeanAbsoluteEr

MeanAbsoluteError: 0.0478178709745407 | Loss: 0.0043848697595032 | Epoch: 51 | MeanAbsoluteEr

MeanAbsoluteError: 0.0798176750540733 | Loss: 0.0078416550864599 | Epoch: 53 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.1274478882551193 | Loss: 0.0178430314574923 | Epoch: 55 | MeanAbsoluteEr
Fold: 3
Epoch: 1 | MeanAbsoluteError: 0.1542282402515411 | Loss: 0.0357009462480034 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1568806767463684 | Loss: 0.0341383319880281 | Epoch: 4 | MeanAbsoluteErr

MeanAbsoluteError: 0.0843581855297089 | Loss: 0.0103826552762517 | Epoch: 6 | MeanAbsoluteErr

MeanAbsoluteError: 0.0806842967867851 | Loss: 0.0114095261586564 | Epoch: 8 | MeanAbsoluteErr

MeanAbsoluteError: 0.1074833422899246 | Loss: 0.0158243976267321 | Epoch: 16 | MeanAbsoluteEr

MeanAbsoluteError: 0.0929571092128754 | Loss: 0.0125159719692809 | Epoch: 18 | MeanAbsoluteEr

MeanAbsoluteError: 0.0965605676174164 | Loss: 0.0125609539848353 | Epoch: 20 | MeanAbsoluteEr

MeanAbsoluteError: 0.0376981422305107 | Loss: 0.0028690162414153 | Epoch: 28 | MeanAbsoluteEr

MeanAbsoluteError: 0.0609404407441616 | Loss: 0.0055710257230593 | Epoch: 30 | MeanAbsoluteEr

MeanAbsoluteError: 0.0602562539279461 | Loss: 0.0060453641760562 | Epoch: 32 | MeanAbsoluteEr

MeanAbsoluteError: 0.0512497462332249 | Loss: 0.0037724909405889 | Epoch: 40 | MeanAbsoluteEr

MeanAbsoluteError: 0.0368779525160789 | Loss: 0.0019391310717245 | Epoch: 42 | MeanAbsoluteEr

MeanAbsoluteError: 0.0317623168230057 | Loss: 0.0021358685251991 | Epoch: 44 | MeanAbsoluteEr

MeanAbsoluteError: 0.0690457001328468 | Loss: 0.0065441590268165 | Epoch: 52 | MeanAbsoluteEr

MeanAbsoluteError: 0.0768565386533737 | Loss: 0.0075964066865189 | Epoch: 54 | MeanAbsoluteEr

MeanAbsoluteError: 0.0286490153521299 | Loss: 0.0016000884019637 | Epoch: 56 | MeanAbsoluteEr

MeanAbsoluteError: 0.0854295268654823 | Loss: 0.0092990450960185 | Epoch: 64 | MeanAbsoluteEr

MeanAbsoluteError: 0.0591040328145027 | Loss: 0.0047485152525561 | Epoch: 66 | MeanAbsoluteEr
```

MeanAbsoluteError: 0.0399408563971519 | Loss: 0.0022265247368653 | Epoch: 68 | MeanAbsoluteEr

MeanAbsoluteError: 0.0321230478584766 | Loss: 0.0018570320348122 | Epoch: 76 | MeanAbsoluteEr

MeanAbsoluteError: 0.0608917176723480 | Loss: 0.0044224276207387 | Epoch: 78 | MeanAbsoluteEr

MeanAbsoluteError: 0.0570819079875946 | Loss: 0.0038611046371183 | Epoch: 80 | MeanAbsoluteEr

MeanAbsoluteError: 0.0795265883207321 | Loss: 0.0078631915551211 | Epoch: 88 | MeanAbsoluteEr

MeanAbsoluteError: 0.0495218485593796 | Loss: 0.0045100579570447 | Epoch: 90 | MeanAbsoluteEr

MeanAbsoluteError: 0.0427144579589367 | Loss: 0.0032473812046062 | Epoch: 92 | MeanAbsoluteEr

MeanAbsoluteError: 0.0529210604727268 | Loss: 0.0037669243922989 | Epoch: 100 | MeanAbsoluteE

MeanAbsoluteError: 0.0308412592858076 | Loss: 0.0016081157872187 | Epoch: 102 | MeanAbsoluteE

MeanAbsoluteError: 0.1251624524593353 | Loss: 0.0226234257487314 | Epoch: 104 | MeanAbsoluteE

MeanAbsoluteError: 0.0232830904424191 | Loss: 0.0011768913037875 | Epoch: 112 | MeanAbsoluteE

MeanAbsoluteError: 0.0373995900154114 | Loss: 0.0022113513467567 | Epoch: 114 | MeanAbsoluteE

MeanAbsoluteError: 0.1019664257764816 | Loss: 0.0121278472776924 | Epoch: 116 | MeanAbsoluteE

MeanAbsoluteError: 0.1250427663326263 | Loss: 0.0195915512740612 | Epoch: 124 | MeanAbsoluteE

MeanAbsoluteError: 0.0343714617192745 | Loss: 0.0019450686273298 | Epoch: 126 | MeanAbsoluteE

MeanAbsoluteError: 0.0393057651817799 | Loss: 0.0027623526818518 | Epoch: 128 | MeanAbsoluteE

MeanAbsoluteError: 0.0860252305865288 | Loss: 0.0084457891727132 | Epoch: 136 | MeanAbsoluteE

MeanAbsoluteError: 0.0419947430491447 | Loss: 0.0028372788801789 | Epoch: 138 | MeanAbsoluteE

```
MeanAbsoluteError: 0.0427188687026501 | Loss: 0.0033188502670133 | Epoch: 140 | MeanAbsolutel
Fold: 4
Epoch: 1 | MeanAbsoluteError: 0.1893421709537506 | Loss: 0.0510192444281919 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1292681694030762 | Loss: 0.0248842381739191 | Epoch: 7 | MeanAbsoluteErr

MeanAbsoluteError: 0.0929643735289574 | Loss: 0.0152713307844741 | Epoch: 9 | MeanAbsoluteErr

MeanAbsoluteError: 0.0643733963370323 | Loss: 0.0068193971112903 | Epoch: 11 | MeanAbsoluteEr

MeanAbsoluteError: 0.0857416316866875 | Loss: 0.0136293342470058 | Epoch: 19 | MeanAbsoluteEr

MeanAbsoluteError: 0.0747352689504623 | Loss: 0.0087248173409275 | Epoch: 21 | MeanAbsoluteEr

MeanAbsoluteError: 0.1132913082838058 | Loss: 0.0166570484372122 | Epoch: 23 | MeanAbsoluteEr

MeanAbsoluteError: 0.0616661831736565 | Loss: 0.0063082840892353 | Epoch: 31 | MeanAbsoluteEr

MeanAbsoluteError: 0.0950428172945976 | Loss: 0.0138609357444303 | Epoch: 33 | MeanAbsoluteEr

MeanAbsoluteError: 0.0501921176910400 | Loss: 0.0036914133732872 | Epoch: 35 | MeanAbsoluteEr

MeanAbsoluteError: 0.0495618358254433 | Loss: 0.0041083113236320 | Epoch: 43 | MeanAbsoluteEr

MeanAbsoluteError: 0.1223235502839088 | Loss: 0.0239439808896610 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.0705046057701111 | Loss: 0.0067208765207657 | Epoch: 47 | MeanAbsoluteEr

MeanAbsoluteError: 0.0528327189385891 | Loss: 0.0038923427595624 | Epoch: 55 | MeanAbsoluteEr

MeanAbsoluteError: 0.0676848292350769 | Loss: 0.0061007653961756 | Epoch: 57 | MeanAbsoluteEr

MeanAbsoluteError: 0.0665725842118263 | Loss: 0.0063063667954079 | Epoch: 59 | MeanAbsoluteEr

MeanAbsoluteError: 0.0520522259175777 | Loss: 0.0046127661730030 | Epoch: 67 | MeanAbsoluteEr

MeanAbsoluteError: 0.0436571128666401 | Loss: 0.0031189851496103 | Epoch: 69 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.0890257805585861 | Loss: 0.0109283778417323 | Epoch: 71 | MeanAbsoluteEr

MeanAbsoluteError: 0.0636503174901009 | Loss: 0.0062934905290604 | Epoch: 79 | MeanAbsoluteEr

MeanAbsoluteError: 0.1296603381633759 | Loss: 0.0189358596024769 | Epoch: 81 | MeanAbsoluteEr

MeanAbsoluteError: 0.0400524809956551 | Loss: 0.0027643695274102 | Epoch: 83 | MeanAbsoluteEr

MeanAbsoluteError: 0.0320393815636635 | Loss: 0.0021322620949442 | Epoch: 91 | MeanAbsoluteEr

MeanAbsoluteError: 0.0714936405420303 | Loss: 0.0094864719680377 | Epoch: 93 | MeanAbsoluteEr

MeanAbsoluteError: 0.0424944646656513 | Loss: 0.0035145867482892 | Epoch: 95 | MeanAbsoluteEr
Fold: 5
Epoch: 1 | MeanAbsoluteError: 0.2128690779209137 | Loss: 0.0633987880178860 | Epoch: 2 | Mean

MeanAbsoluteError: 0.0684989914298058 | Loss: 0.0069009853926088 | Epoch: 8 | MeanAbsoluteErr

MeanAbsoluteError: 0.2181337475776672 | Loss: 0.0560905140425478 | Epoch: 10 | MeanAbsoluteEr

MeanAbsoluteError: 0.1143022254109383 | Loss: 0.0160619865304657 | Epoch: 12 | MeanAbsoluteEr

MeanAbsoluteError: 0.0461497195065022 | Loss: 0.0038473213623677 | Epoch: 20 | MeanAbsoluteEr

MeanAbsoluteError: 0.1638076454401016 | Loss: 0.0321640063609396 | Epoch: 22 | MeanAbsoluteEr

MeanAbsoluteError: 0.0675982013344765 | Loss: 0.0071500979496964 | Epoch: 24 | MeanAbsoluteEr

MeanAbsoluteError: 0.0577786304056644 | Loss: 0.0046593038007684 | Epoch: 32 | MeanAbsoluteEr

MeanAbsoluteError: 0.1285535097122192 | Loss: 0.0190455727279186 | Epoch: 34 | MeanAbsoluteEr

MeanAbsoluteError: 0.0576459839940071 | Loss: 0.0054684286005795 | Epoch: 36 | MeanAbsoluteEr

MeanAbsoluteError: 0.0375327728688717 | Loss: 0.0020682091791449 | Epoch: 44 | MeanAbsoluteEr

MeanAbsoluteError: 0.0545713864266872 | Loss: 0.0041839025049870 | Epoch: 46 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.1498713642358780 | Loss: 0.0254791323095560 | Epoch: 48 | MeanAbsoluteEr
MeanAbsoluteError: 0.0420306362211704 | Loss: 0.0034979840607515 | Epoch: 56 | MeanAbsoluteEr
MeanAbsoluteError: 0.0767666995525360 | Loss: 0.0081599744568978 | Epoch: 58 | MeanAbsoluteEr
MeanAbsoluteError: 0.0704204365611076 | Loss: 0.0058203193558646 | Epoch: 60 | MeanAbsoluteEr
MeanAbsoluteError: 0.1394743323326111 | Loss: 0.0206028744578362 | Epoch: 68 | MeanAbsoluteEr
MeanAbsoluteError: 0.0397067368030548 | Loss: 0.0021038191709002 | Epoch: 70 | MeanAbsoluteEr
MeanAbsoluteError: 0.0537646487355232 | Loss: 0.0036111596772181 | Epoch: 72 | MeanAbsoluteEr
MeanAbsoluteError: 0.0320966355502605 | Loss: 0.0016343049480513 | Epoch: 80 | MeanAbsoluteEr
MeanAbsoluteError: 0.0689565166831017 | Loss: 0.0061769180798105 | Epoch: 82 | MeanAbsoluteEr
MeanAbsoluteError: 0.0466229729354382 | Loss: 0.0033827678167394 | Epoch: 84 | MeanAbsoluteEr
MeanAbsoluteError: 0.0465262047946453 | Loss: 0.0033745758534808 | Epoch: 92 | MeanAbsoluteEr
MeanAbsoluteError: 0.0667791366577148 | Loss: 0.0059603773988783 | Epoch: 94 | MeanAbsoluteEr
MeanAbsoluteError: 0.0571188181638718 | Loss: 0.0051670750336988 | Epoch: 96 | MeanAbsoluteEr
MeanAbsoluteError: 0.0317107960581779 | Loss: 0.0027027608427618 | Epoch: 104 | MeanAbsoluteE
MeanAbsoluteError: 0.0347635187208652 | Loss: 0.0020779435290024 | Epoch: 106 | MeanAbsoluteE
MeanAbsoluteError: 0.0503709279000759 | Loss: 0.0032750917931220 | Epoch: 108 | MeanAbsoluteE
MeanAbsoluteError: 0.0508828833699226 | Loss: 0.0033752926059866 | Epoch: 116 | MeanAbsoluteE
MeanAbsoluteError: 0.0345439016819000 | Loss: 0.0019689274985077 | Epoch: 118 | MeanAbsoluteE
MeanAbsoluteError: 0.0860725715756416 | Loss: 0.0104001417223896 | Epoch: 120 | MeanAbsoluteE
```

```
MeanAbsoluteError: 0.0812200754880905 | Loss: 0.0081478301435709 | Epoch: 128 | MeanAbsoluteE
MeanAbsoluteError: 0.0806282982230186 | Loss: 0.0078249687461981 | Epoch: 130 | MeanAbsoluteE
MeanAbsoluteError: 0.0302772950381041 | Loss: 0.0022701361033666 | Epoch: 132 | MeanAbsoluteE
MeanAbsoluteError: 0.0256523862481117 | Loss: 0.0013573030841404 | Epoch: 140 | MeanAbsoluteE
MeanAbsoluteError: 0.0347516462206841 | Loss: 0.0016345145995729 | Epoch: 142 | MeanAbsoluteE
MeanAbsoluteError: 0.0347325317561626 | Loss: 0.0024909455927887 | Epoch: 144 | MeanAbsoluteE
MeanAbsoluteError: 0.0282910186797380 | Loss: 0.0013988183428799 | Epoch: 152 | MeanAbsoluteE
MeanAbsoluteError: 0.0252205897122622 | Loss: 0.0012151143746451 | Epoch: 154 | MeanAbsoluteE
MeanAbsoluteError: 0.0320511125028133 | Loss: 0.0017143444191398 | Epoch: 156 | MeanAbsoluteE
MeanAbsoluteError: 0.0337777845561504 | Loss: 0.0019601409689390 | Epoch: 164 | MeanAbsoluteE
MeanAbsoluteError: 0.0698640421032906 | Loss: 0.0067616530161883 | Epoch: 166 | MeanAbsoluteE
MeanAbsoluteError: 0.0356783755123615 | Loss: 0.0027172199334018 | Epoch: 168 | MeanAbsoluteE
MeanAbsoluteError: 0.0265904758125544 | Loss: 0.0011159265330727 | Epoch: 176 | MeanAbsoluteE
MeanAbsoluteError: 0.0211132168769836 | Loss: 0.0010845178704975 | Epoch: 178 | MeanAbsoluteE
MeanAbsoluteError: 0.0411709435284138 | Loss: 0.0026702611607366 | Epoch: 180 | MeanAbsoluteE
MeanAbsoluteError: 0.0295281745493412 | Loss: 0.0014181847551039 | Epoch: 188 | MeanAbsoluteE
MeanAbsoluteError: 0.0560182668268681 | Loss: 0.0069649208204022 | Epoch: 190 | MeanAbsoluteE
MeanAbsoluteError: 0.0836994946002960 | Loss: 0.0084086195565760 | Epoch: 192 | MeanAbsoluteE
MeanAbsoluteError: 0.0370085351169109 | Loss: 0.0024428167047777 | Epoch: 200 | MeanAbsoluteE
```

```
MeanAbsoluteError: 0.0323572680354118 | Loss: 0.0020049366285093 | Epoch: 202 | MeanAbsolutel

MeanAbsoluteError: 0.0428925938904285 | Loss: 0.0027718404307961 | Epoch: 204 | MeanAbsolutel

MeanAbsoluteError: 0.0526868999004364 | Loss: 0.0038620602406029 | Epoch: 212 | MeanAbsolutel

MeanAbsoluteError: 0.0451387614011765 | Loss: 0.0031499898593341 | Epoch: 214 | MeanAbsolutel

MeanAbsoluteError: 0.0730337798595428 | Loss: 0.0086456406196313 | Early stopping at epoch 21
Fold: 6
Epoch: 1 | MeanAbsoluteError: 0.1346546709537506 | Loss: 0.0265847138528313 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1069301888346672 | Loss: 0.0194445913657546 | Epoch: 9 | MeanAbsoluteErr

MeanAbsoluteError: 0.0662481710314751 | Loss: 0.0090369447134435 | Epoch: 11 | MeanAbsoluteEr

MeanAbsoluteError: 0.1175867468118668 | Loss: 0.0196409462285893 | Epoch: 13 | MeanAbsoluteEr

MeanAbsoluteError: 0.0909956544637680 | Loss: 0.0127026022944067 | Epoch: 21 | MeanAbsoluteEr

MeanAbsoluteError: 0.0799708142876625 | Loss: 0.0094593444040843 | Epoch: 23 | MeanAbsoluteEr

MeanAbsoluteError: 0.0353655815124512 | Loss: 0.0036776750348508 | Epoch: 25 | MeanAbsoluteEr

MeanAbsoluteError: 0.0815592184662819 | Loss: 0.0082514008307563 | Epoch: 33 | MeanAbsoluteEr

MeanAbsoluteError: 0.0964762121438980 | Loss: 0.0129564121099455 | Epoch: 35 | MeanAbsoluteEr

MeanAbsoluteError: 0.0364330038428307 | Loss: 0.0029340277459206 | Epoch: 37 | MeanAbsoluteEr

MeanAbsoluteError: 0.0900591835379601 | Loss: 0.0100917171553842 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.0435834266245365 | Loss: 0.0032434092967638 | Epoch: 47 | MeanAbsoluteEr

MeanAbsoluteError: 0.1061887815594673 | Loss: 0.0131645092208471 | Epoch: 49 | MeanAbsoluteEr

MeanAbsoluteError: 0.0745141804218292 | Loss: 0.0083165096917323 | Epoch: 57 | MeanAbsoluteEr
```

MeanAbsoluteError: 0.0690166875720024 | Loss: 0.0071214307099581 | Epoch: 59 | MeanAbsoluteEr

MeanAbsoluteError: 0.0411369353532791 | Loss: 0.0031270795568292 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.0516226813197136 | Loss: 0.0051458943302610 | Epoch: 69 | MeanAbsoluteEr

MeanAbsoluteError: 0.0294028241187334 | Loss: 0.0014659352933190 | Epoch: 71 | MeanAbsoluteEr

MeanAbsoluteError: 0.0610737465322018 | Loss: 0.0053998500620115 | Epoch: 73 | MeanAbsoluteEr

MeanAbsoluteError: 0.0842074230313301 | Loss: 0.0095718503663582 | Epoch: 81 | MeanAbsoluteEr

MeanAbsoluteError: 0.0511040054261684 | Loss: 0.0035406228354467 | Epoch: 83 | MeanAbsoluteEr

MeanAbsoluteError: 0.0933254882693291 | Loss: 0.0120574829966894 | Epoch: 85 | MeanAbsoluteEr

MeanAbsoluteError: 0.0678454786539078 | Loss: 0.0066296332515776 | Epoch: 93 | MeanAbsoluteEr

MeanAbsoluteError: 0.0902836546301842 | Loss: 0.0094881671081696 | Epoch: 95 | MeanAbsoluteEr

MeanAbsoluteError: 0.0424184240400791 | Loss: 0.0026035617338493 | Epoch: 97 | MeanAbsoluteEr

MeanAbsoluteError: 0.0281500890851021 | Loss: 0.0020000811782666 | Epoch: 105 | MeanAbsolutel

MeanAbsoluteError: 0.0628974288702011 | Loss: 0.0056362181369747 | Epoch: 107 | MeanAbsolutel

MeanAbsoluteError: 0.0326974205672741 | Loss: 0.0022886837416861 | Epoch: 109 | MeanAbsolutel

MeanAbsoluteError: 0.0559377782046795 | Loss: 0.0044457019373242 | Epoch: 117 | MeanAbsolutel

MeanAbsoluteError: 0.0769031122326851 | Loss: 0.0100162563446377 | Epoch: 119 | MeanAbsolutel

MeanAbsoluteError: 0.0841882005333900 | Loss: 0.0088208856593285 | Epoch: 121 | MeanAbsolutel

MeanAbsoluteError: 0.0594875141978264 | Loss: 0.0048883236345968 | Epoch: 129 | MeanAbsolutel

MeanAbsoluteError: 0.0620157159864902 | Loss: 0.0051237943116575 | Epoch: 131 | MeanAbsolutel

```
MeanAbsoluteError: 0.0375395901501179 | Loss: 0.0022825206812870 | Epoch: 133 | MeanAbsoluteE
Fold: 7
Epoch: 1 | MeanAbsoluteError: 0.1370203495025635 | Loss: 0.0265946356313569 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1833667308092117 | Loss: 0.0450882837176323 | Epoch: 6 | MeanAbsoluteErr

MeanAbsoluteError: 0.1242559701204300 | Loss: 0.0212752933480910 | Epoch: 8 | MeanAbsoluteErr

MeanAbsoluteError: 0.0525866411626339 | Loss: 0.0041564054720636 | Epoch: 10 | MeanAbsoluteEr

MeanAbsoluteError: 0.0534257404506207 | Loss: 0.0048628899468375 | Epoch: 15 | MeanAbsoluteEr

MeanAbsoluteError: 0.1047440469264984 | Loss: 0.0162744330508368 | Epoch: 17 | MeanAbsoluteEr

MeanAbsoluteError: 0.0418944582343102 | Loss: 0.0027184267694663 | Epoch: 19 | MeanAbsoluteEr

MeanAbsoluteError: 0.0397686921060085 | Loss: 0.0028525824059865 | Epoch: 27 | MeanAbsoluteEr

MeanAbsoluteError: 0.0424597114324570 | Loss: 0.0042379681253806 | Epoch: 29 | MeanAbsoluteEr

MeanAbsoluteError: 0.0620200969278812 | Loss: 0.0068909312997546 | Epoch: 31 | MeanAbsoluteEr

MeanAbsoluteError: 0.0569294206798077 | Loss: 0.0046856240868302 | Epoch: 39 | MeanAbsoluteEr

MeanAbsoluteError: 0.0848564803600311 | Loss: 0.0081963027561350 | Epoch: 41 | MeanAbsoluteEr

MeanAbsoluteError: 0.0896770954132080 | Loss: 0.0122174087113568 | Epoch: 43 | MeanAbsoluteEr

MeanAbsoluteError: 0.1014292985200882 | Loss: 0.0147084523258465 | Epoch: 51 | MeanAbsoluteEr

MeanAbsoluteError: 0.0467028841376305 | Loss: 0.0029742699781699 | Epoch: 53 | MeanAbsoluteEr

MeanAbsoluteError: 0.1093698963522911 | Loss: 0.0146242777949997 | Epoch: 55 | MeanAbsoluteEr

MeanAbsoluteError: 0.1652097254991531 | Loss: 0.0298585662884372 | Epoch: 63 | MeanAbsoluteEr

MeanAbsoluteError: 0.0438104756176472 | Loss: 0.0027028415684721 | Epoch: 65 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.1364165395498276 | Loss: 0.0202788484415838 | Epoch: 67 | MeanAbsoluteEr

MeanAbsoluteError: 0.0703717917203903 | Loss: 0.0059199528768659 | Epoch: 75 | MeanAbsoluteEr

MeanAbsoluteError: 0.0518786236643791 | Loss: 0.0032977144832590 | Epoch: 77 | MeanAbsoluteEr

MeanAbsoluteError: 0.0350730717182159 | Loss: 0.0019058479145834 | Epoch: 79 | MeanAbsoluteEr

MeanAbsoluteError: 0.0621104389429092 | Loss: 0.0048273009514170 | Epoch: 87 | MeanAbsoluteEr

MeanAbsoluteError: 0.0394702777266502 | Loss: 0.0020904428924301 | Epoch: 89 | MeanAbsoluteEr

MeanAbsoluteError: 0.0333004631102085 | Loss: 0.0018569822090545 | Epoch: 91 | MeanAbsoluteEr

MeanAbsoluteError: 0.0443581156432629 | Loss: 0.0025392353002514 | Epoch: 99 | MeanAbsoluteEr

MeanAbsoluteError: 0.0754874646663666 | Loss: 0.0071894304294671 | Epoch: 101 | MeanAbsolutel

MeanAbsoluteError: 0.0630412325263023 | Loss: 0.0054307399384145 | Early stopping at epoch 10
Fold: 8
Epoch: 1 | MeanAbsoluteError: 0.1156925112009048 | Loss: 0.0179215836396907 | Epoch: 2 | Mean

MeanAbsoluteError: 0.0813768282532692 | Loss: 0.0098236128687859 | Epoch: 9 | MeanAbsoluteErr

MeanAbsoluteError: 0.0755551755428314 | Loss: 0.0088962934179498 | Epoch: 11 | MeanAbsoluteEr

MeanAbsoluteError: 0.0575885027647018 | Loss: 0.0055108191445470 | Epoch: 13 | MeanAbsoluteEr

MeanAbsoluteError: 0.1062692478299141 | Loss: 0.0163583468113627 | Epoch: 21 | MeanAbsoluteEr

MeanAbsoluteError: 0.1012537702918053 | Loss: 0.0134234594048134 | Epoch: 23 | MeanAbsoluteEr

MeanAbsoluteError: 0.0791864097118378 | Loss: 0.0082532927127821 | Epoch: 25 | MeanAbsoluteEr

MeanAbsoluteError: 0.0822725072503090 | Loss: 0.0087978024967015 | Epoch: 33 | MeanAbsoluteEr

MeanAbsoluteError: 0.0484629012644291 | Loss: 0.0041886536803629 | Epoch: 35 | MeanAbsoluteEr
```

MeanAbsoluteError: 0.0359791368246078 | Loss: 0.0024832545812907 | Epoch: 37 | MeanAbsoluteEr

MeanAbsoluteError: 0.0768731981515884 | Loss: 0.0075377783505246 | Epoch: 45 | MeanAbsoluteEr

MeanAbsoluteError: 0.1013431772589684 | Loss: 0.0154116731137037 | Epoch: 47 | MeanAbsoluteEr

MeanAbsoluteError: 0.0352274924516678 | Loss: 0.0021427150474795 | Epoch: 49 | MeanAbsoluteEr

MeanAbsoluteError: 0.0375023409724236 | Loss: 0.0027384013270161 | Epoch: 57 | MeanAbsoluteEr

MeanAbsoluteError: 0.0589179769158363 | Loss: 0.0046783224679530 | Epoch: 59 | MeanAbsoluteEr

MeanAbsoluteError: 0.0746714621782303 | Loss: 0.0067318119441292 | Epoch: 61 | MeanAbsoluteEr

MeanAbsoluteError: 0.0765606537461281 | Loss: 0.0071533454715141 | Epoch: 69 | MeanAbsoluteEr

MeanAbsoluteError: 0.0550800897181034 | Loss: 0.0044759520928242 | Epoch: 71 | MeanAbsoluteEr

MeanAbsoluteError: 0.0353555269539356 | Loss: 0.0019493311909693 | Epoch: 73 | MeanAbsoluteEr

MeanAbsoluteError: 0.0814784616231918 | Loss: 0.0109383894928864 | Epoch: 81 | MeanAbsoluteEr

MeanAbsoluteError: 0.0487115867435932 | Loss: 0.0037295889508511 | Epoch: 83 | MeanAbsoluteEr

MeanAbsoluteError: 0.0370934158563614 | Loss: 0.0033076892557022 | Epoch: 85 | MeanAbsoluteEr

MeanAbsoluteError: 0.0440841279923916 | Loss: 0.0033477660202022 | Epoch: 93 | MeanAbsoluteEr

MeanAbsoluteError: 0.0456829071044922 | Loss: 0.0033408167738734 | Epoch: 95 | MeanAbsoluteEr

MeanAbsoluteError: 0.0472746230661869 | Loss: 0.0032127811407138 | Epoch: 97 | MeanAbsoluteEr

MeanAbsoluteError: 0.0784432366490364 | Loss: 0.0079786722947444 | Epoch: 105 | MeanAbsoluteE

MeanAbsoluteError: 0.0534877106547356 | Loss: 0.0046265995728650 | Epoch: 107 | MeanAbsoluteE

MeanAbsoluteError: 0.0656893104314804 | Loss: 0.0067169601264011 | Epoch: 109 | MeanAbsoluteE

```
MeanAbsoluteError: 0.0355729162693024 | Loss: 0.0017865368863568 | Epoch: 117 | MeanAbsolutel

MeanAbsoluteError: 0.0813054293394089 | Loss: 0.0084872172613229 | Epoch: 119 | MeanAbsolutel

MeanAbsoluteError: 0.0420827306807041 | Loss: 0.0024862750267078 | Epoch: 121 | MeanAbsolutel
Fold: 9
Epoch: 1 | MeanAbsoluteError: 0.1093776300549507 | Loss: 0.0196784185245633 | Epoch: 2 | Mean

MeanAbsoluteError: 0.1098095476627350 | Loss: 0.0195106019132904 | Epoch: 6 | MeanAbsoluteErr

MeanAbsoluteError: 0.0761941969394684 | Loss: 0.0088079256072108 | Epoch: 8 | MeanAbsoluteErr

MeanAbsoluteError: 0.1320157945156097 | Loss: 0.0246795844286680 | Epoch: 10 | MeanAbsoluteEr

MeanAbsoluteError: 0.0661281719803810 | Loss: 0.0060716712780829 | Epoch: 18 | MeanAbsoluteEr

MeanAbsoluteError: 0.0418697111308575 | Loss: 0.0036924471080835 | Epoch: 20 | MeanAbsoluteEr

MeanAbsoluteError: 0.0816631689667702 | Loss: 0.0083304268441030 | Epoch: 22 | MeanAbsoluteEr

MeanAbsoluteError: 0.1652997136116028 | Loss: 0.0298960868801389 | Epoch: 30 | MeanAbsoluteEr

MeanAbsoluteError: 0.0700830295681953 | Loss: 0.0068491678019719 | Epoch: 32 | MeanAbsoluteEr

MeanAbsoluteError: 0.0707055032253265 | Loss: 0.0068638981319964 | Epoch: 34 | MeanAbsoluteEr

MeanAbsoluteError: 0.0482214652001858 | Loss: 0.0042268679244444 | Epoch: 42 | MeanAbsoluteEr

MeanAbsoluteError: 0.0625448971986771 | Loss: 0.0051882348821631 | Epoch: 44 | MeanAbsoluteEr

MeanAbsoluteError: 0.0471100807189941 | Loss: 0.0037728795515639 | Epoch: 46 | MeanAbsoluteEr

MeanAbsoluteError: 0.0636444464325905 | Loss: 0.0060236525189664 | Epoch: 54 | MeanAbsoluteEr

MeanAbsoluteError: 0.0831866934895515 | Loss: 0.0082947955732899 | Epoch: 56 | MeanAbsoluteEr

MeanAbsoluteError: 0.0364131815731525 | Loss: 0.0022351121962337 | Epoch: 58 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.0285384468734264 | Loss: 0.0015082774417741 | Epoch: 66 | MeanAbsoluteEr
MeanAbsoluteError: 0.0687597841024399 | Loss: 0.0066980745510331 | Epoch: 68 | MeanAbsoluteEr
MeanAbsoluteError: 0.0706854835152626 | Loss: 0.0068893689396126 | Epoch: 70 | MeanAbsoluteEr
MeanAbsoluteError: 0.0938337594270706 | Loss: 0.0121193771649684 | Epoch: 78 | MeanAbsoluteEr
MeanAbsoluteError: 0.0341943055391312 | Loss: 0.0020393597660586 | Epoch: 80 | MeanAbsoluteEr
MeanAbsoluteError: 0.0933109447360039 | Loss: 0.0129981432110071 | Epoch: 82 | MeanAbsoluteEr
MeanAbsoluteError: 0.0552825257182121 | Loss: 0.0039910430620824 | Epoch: 90 | MeanAbsoluteEr
MeanAbsoluteError: 0.0472887232899666 | Loss: 0.0034648361511894 | Epoch: 92 | MeanAbsoluteEr
MeanAbsoluteError: 0.0608188360929489 | Loss: 0.0055414781173957 | Epoch: 94 | MeanAbsoluteEr
MeanAbsoluteError: 0.0519650690257549 | Loss: 0.0040370161046407 | Epoch: 102 | MeanAbsoluteE
MeanAbsoluteError: 0.0224034544080496 | Loss: 0.0009628019179218 | Epoch: 104 | MeanAbsoluteE
MeanAbsoluteError: 0.0482478886842728 | Loss: 0.0041446289978921 | Epoch: 106 | MeanAbsoluteE
MeanAbsoluteError: 0.0872446447610855 | Loss: 0.0096452876127192 | Epoch: 114 | MeanAbsoluteE
MeanAbsoluteError: 0.0839137732982635 | Loss: 0.0099963785282203 | Epoch: 116 | MeanAbsoluteE
MeanAbsoluteError: 0.0356399789452553 | Loss: 0.0019720518695457 | Epoch: 118 | MeanAbsoluteE
MeanAbsoluteError: 0.0637345165014267 | Loss: 0.0061902959631490 | Epoch: 126 | MeanAbsoluteE
MeanAbsoluteError: 0.0816340520977974 | Loss: 0.0085473517870664 | Epoch: 128 | MeanAbsoluteE
MeanAbsoluteError: 0.0555757433176041 | Loss: 0.0072591837628611 | Epoch: 130 | MeanAbsoluteE
Fold: 10
Epoch: 1 | MeanAbsoluteError: 0.2425923943519592 | Loss: 0.0862785130739212 | Epoch: 2 |
```

```
MeanAbsoluteError: 0.1260890960693359 | Loss: 0.0240717508963176 | Epoch: 3 | MeanAbsoluteErr
MeanAbsoluteError: 0.1558067649602890 | Loss: 0.0343957982425179 | Epoch: 5 | MeanAbsoluteErr
MeanAbsoluteError: 0.0965519025921822 | Loss: 0.0152133787716074 | Epoch: 7 | MeanAbsoluteErr
MeanAbsoluteError: 0.1063379794359207 | Loss: 0.0162980662924903 | Epoch: 15 | MeanAbsoluteEr
MeanAbsoluteError: 0.0575015991926193 | Loss: 0.0062753236852586 | Epoch: 17 | MeanAbsoluteEr
MeanAbsoluteError: 0.1054733544588089 | Loss: 0.0141306991821953 | Epoch: 19 | MeanAbsoluteEr
MeanAbsoluteError: 0.1045430004596710 | Loss: 0.0134495752863586 | Epoch: 27 | MeanAbsoluteEr
MeanAbsoluteError: 0.0635204911231995 | Loss: 0.0054292434693447 | Epoch: 29 | MeanAbsoluteEr
MeanAbsoluteError: 0.0875741764903069 | Loss: 0.0113198063336313 | Epoch: 31 | MeanAbsoluteEr
MeanAbsoluteError: 0.0738276168704033 | Loss: 0.0078694924512612 | Epoch: 39 | MeanAbsoluteEr
MeanAbsoluteError: 0.0944607555866241 | Loss: 0.0128695347479412 | Epoch: 41 | MeanAbsoluteEr
MeanAbsoluteError: 0.0417012497782707 | Loss: 0.0023812707929340 | Epoch: 43 | MeanAbsoluteEr
MeanAbsoluteError: 0.0399968698620796 | Loss: 0.0027412603542741 | Epoch: 51 | MeanAbsoluteEr
MeanAbsoluteError: 0.0432002581655979 | Loss: 0.0030508547788486 | Epoch: 53 | MeanAbsoluteEr
MeanAbsoluteError: 0.0538352727890015 | Loss: 0.0057469435435321 | Epoch: 55 | MeanAbsoluteEr
MeanAbsoluteError: 0.0729368403553963 | Loss: 0.0067361936505352 | Epoch: 63 | MeanAbsoluteEr
MeanAbsoluteError: 0.0649194270372391 | Loss: 0.0062978419342211 | Epoch: 65 | MeanAbsoluteEr
MeanAbsoluteError: 0.0487823672592640 | Loss: 0.0033901842377548 | Epoch: 67 | MeanAbsoluteEr
MeanAbsoluteError: 0.0701905265450478 | Loss: 0.0065975417383015 | Epoch: 75 | MeanAbsoluteEr
```

```
MeanAbsoluteError: 0.0331846438348293 | Loss: 0.0024428384245506 | Epoch: 77 | MeanAbsoluteE
MeanAbsoluteError: 0.0703106746077538 | Loss: 0.0066594999682690 | Epoch: 79 | MeanAbsoluteE
MeanAbsoluteError: 0.0261448640376329 | Loss: 0.0012291404834416 | Epoch: 87 | MeanAbsoluteE
MeanAbsoluteError: 0.0571299977600574 | Loss: 0.0044869496154466 | Epoch: 89 | MeanAbsoluteE
MeanAbsoluteError: 0.0373268276453018 | Loss: 0.0019920719246979 | Epoch: 91 | MeanAbsoluteE
MeanAbsoluteError: 0.0308549497276545 | Loss: 0.0028105406839001 | Epoch: 99 | MeanAbsoluteE
MeanAbsoluteError: 0.0313827544450760 | Loss: 0.0021055158078005 | Epoch: 101 | MeanAbsolutel
MeanAbsoluteError: 0.0933097377419472 | Loss: 0.0116164674982429 | Epoch: 103 | MeanAbsolutel
MeanAbsoluteError: 0.0642709657549858 | Loss: 0.0066170622594655 | Epoch: 111 | MeanAbsolutel
MeanAbsoluteError: 0.0863091275095940 | Loss: 0.0098497354691582 | Epoch: 113 | MeanAbsolutel
MeanAbsoluteError: 0.0325586535036564 | Loss: 0.0021816564673957 | Epoch: 115 | MeanAbsolutel
```

```
metric_name = type(fun_control["metric_torch"]).__name__
print(f"loss: {df_eval}, Cross-validated {metric_name}: {df_metrics}")
```

```
loss: 0.005902799277100713, Cross-validated MeanAbsoluteError: 0.06115343049168587
```

19.10.4 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
l1:  0.3845829890028423
lr_mult:  0.6700872031230476
batch_size:  34.88391531114552
epochs:  2.81430669035911
optimizer:  99.99999999999999
sgd_momentum:  7.9175041709670655
```

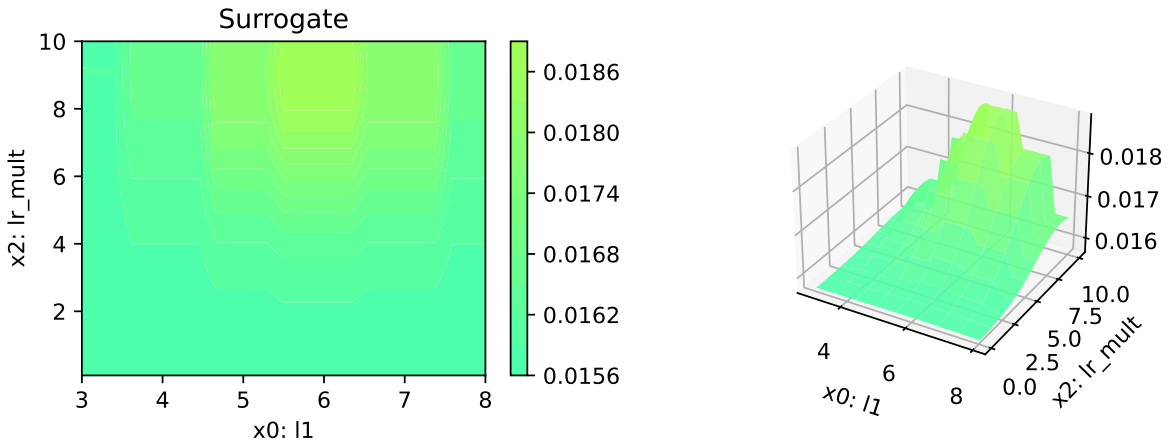
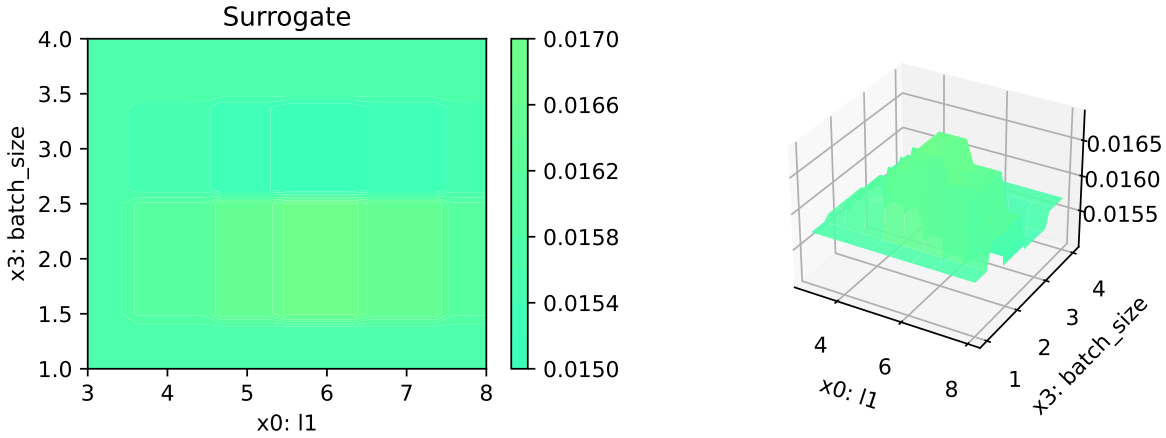
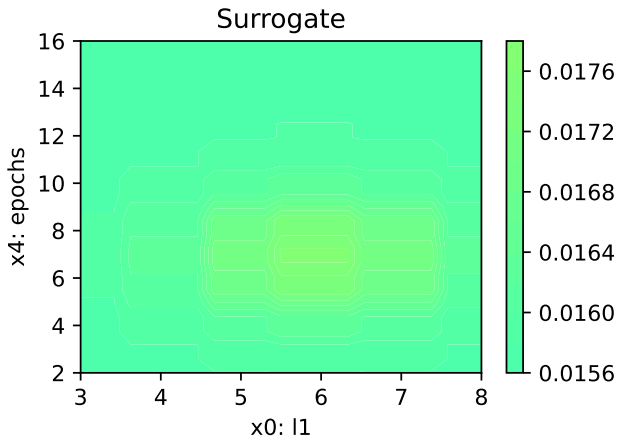
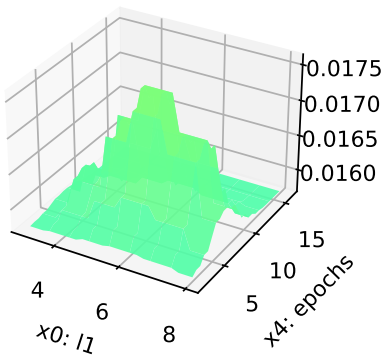
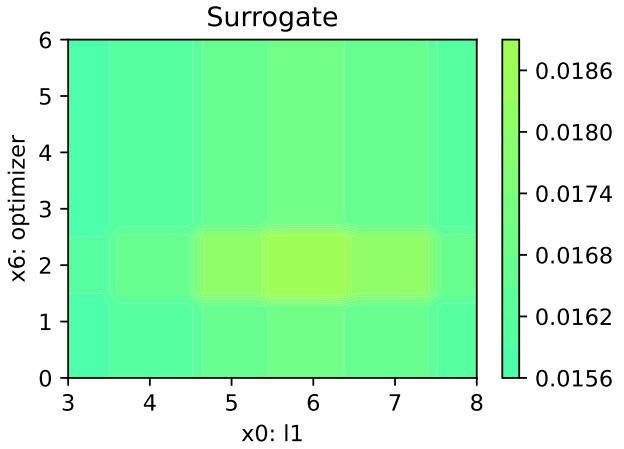


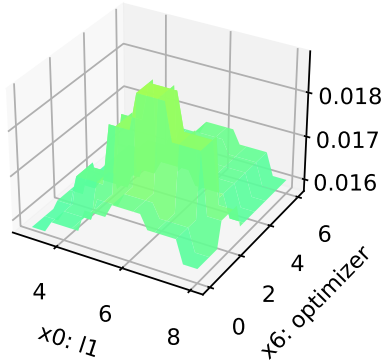
Figure 19.3: Contour plots.

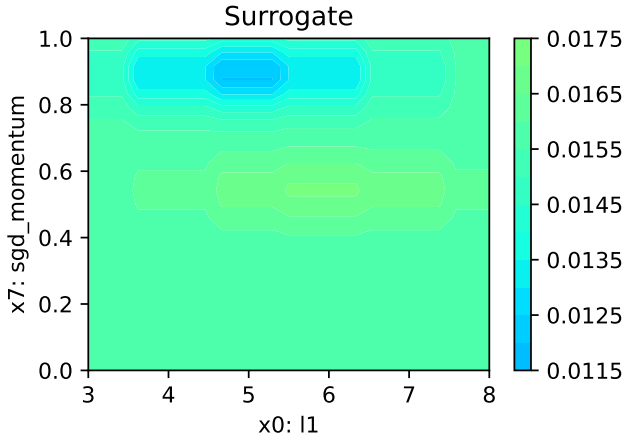


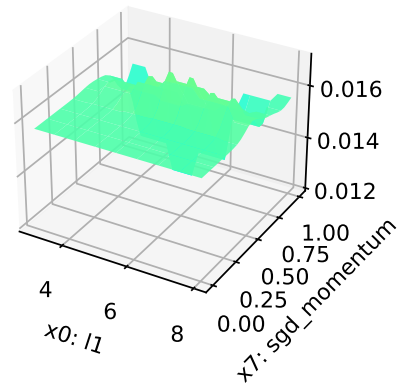

Surrogate
x4: epochs
x0: l1
0.0176
0.0172
0.0168
0.0164
0.0160
0.0156

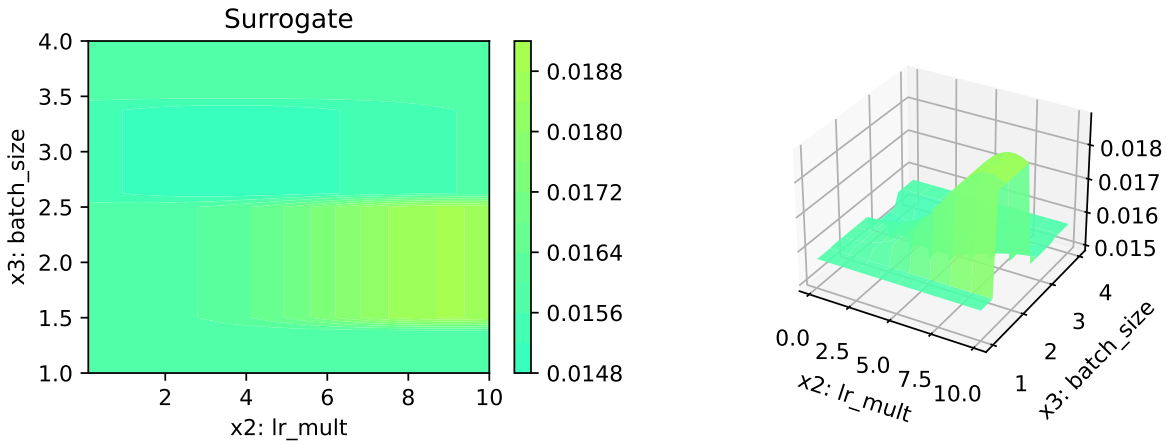

0.0175
0.0170
0.0165
0.0160
x0: l1
x4: epochs

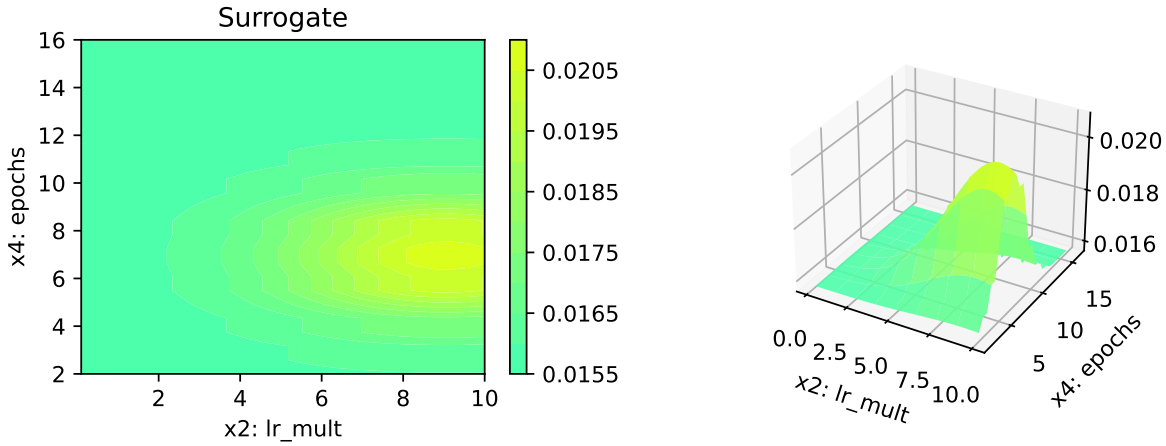

Surrogate
x6: optimizer
x0: l1
0.0186
0.0180
0.0174
0.0168
0.0162
0.0156

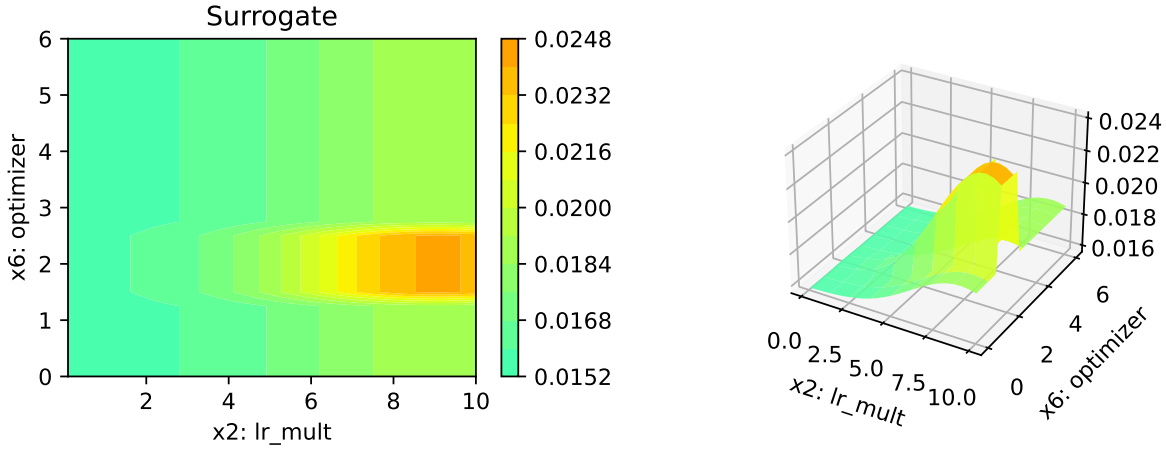

0.018
0.017
0.016
x0: l1
x6: optimizer

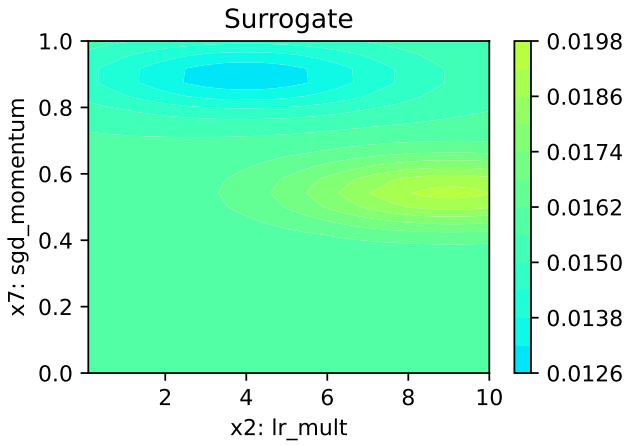

Surrogate
x7: sgd_momentum
x0: l1
0.0175
0.0165
0.0155
0.0145
0.0135
0.0125
0.0115

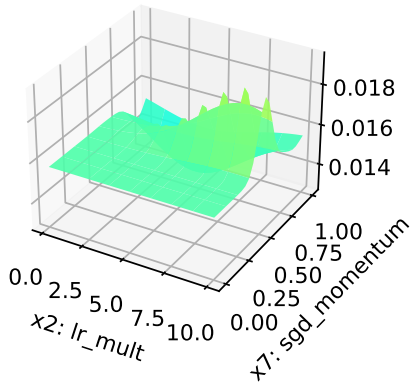

0.016
0.014
0.012
x0: l1
x7: sgd_momentum

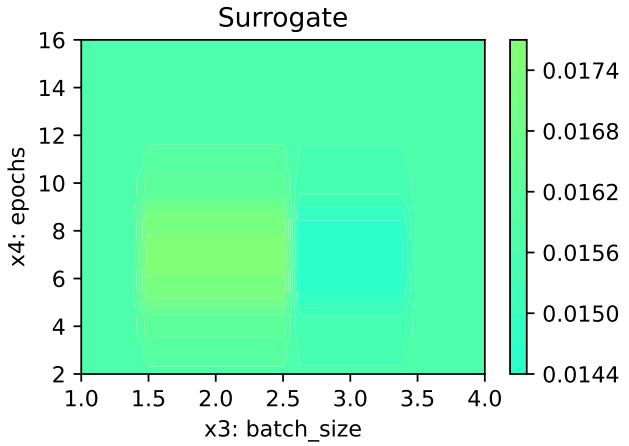

Surrogate
x3: batch_size
x2: lr_mult
x2: lr_mult
x3: batch_size

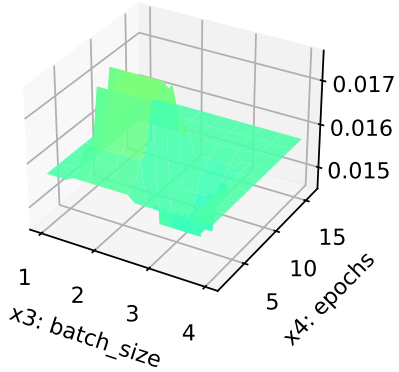

Surrogate
x4: epochs
x2: lr_mult
x2: lr_mult
x4: epochs

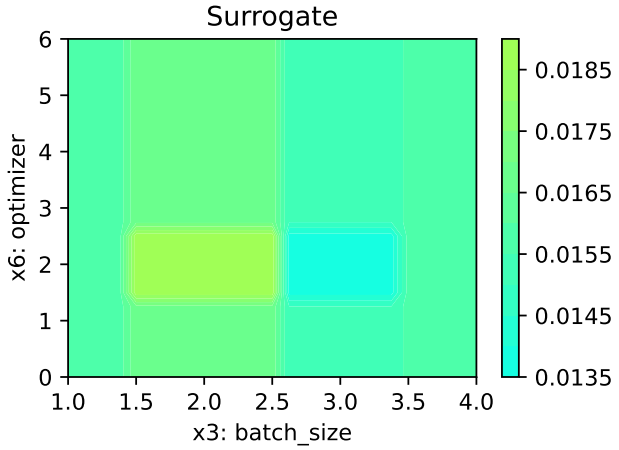

Surrogate
x6: optimizer
x2: lr_mult
x2: lr_mult
x6: optimizer

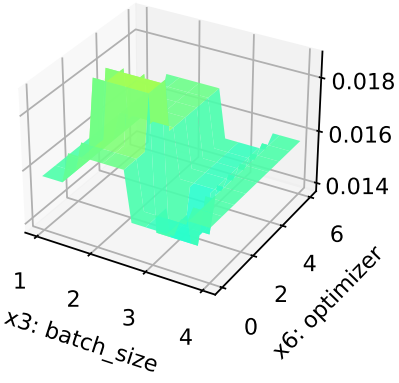

Surrogate
x7: sgd_momentum
x2: lr_mult
1.0
0.8
0.6
0.4
0.2
0.0
2
4
6
8
10
0.0198
0.0186
0.0174
0.0162
0.0150
0.0138
0.0126

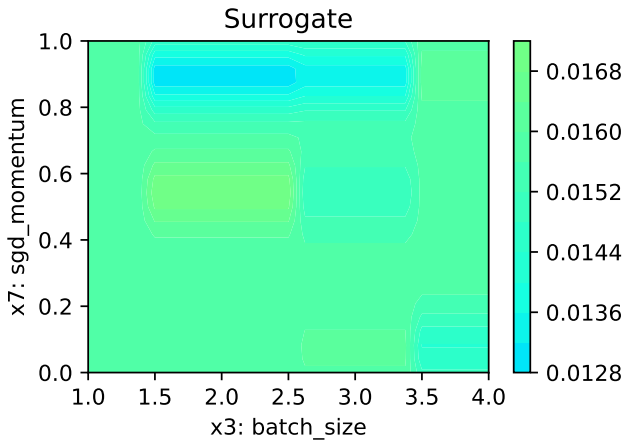

0.018
0.016
0.014
0.0
2.5
5.0
7.5
10.0
x2: lr_mult
1.00
0.75
0.50
0.25
0.00
x7: sgd_momentum

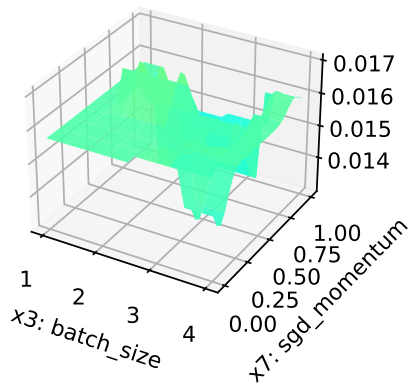

Surrogate
x4: epochs
x3: batch_size
16
14
12
10
8
6
4
2
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0.0174
0.0168
0.0162
0.0156
0.0150
0.0144

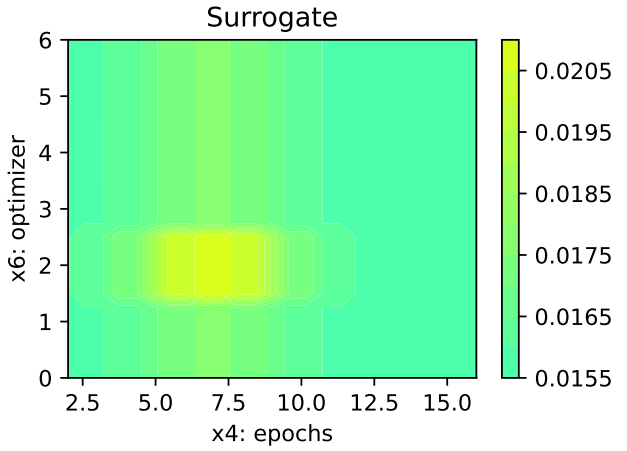

0.017
0.016
0.015
1
2
3
4
x3: batch_size
15
10
5
x4: epochs

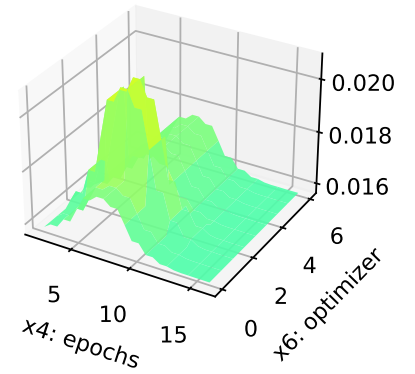

Surrogate
x6: optimizer
x3: batch_size
6
5
4
3
2
1
0
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0.0185
0.0175
0.0165
0.0155
0.0145
0.0135

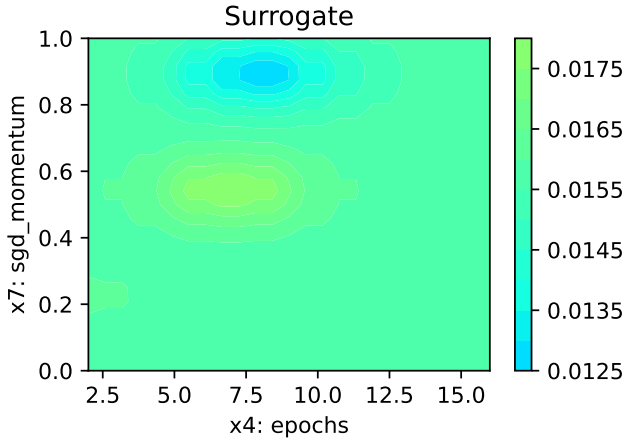

0.018
0.016
0.014
1
2
3
4
x3: batch_size
6
4
2
0
x6: optimizer

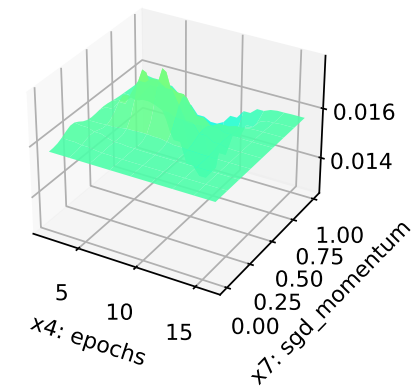

Surrogate
x7: sgd_momentum
x3: batch_size
1.0
0.8
0.6
0.4
0.2
0.0
1.0 1.5 2.0 2.5 3.0 3.5 4.0
0.0168
0.0160
0.0152
0.0144
0.0136
0.0128

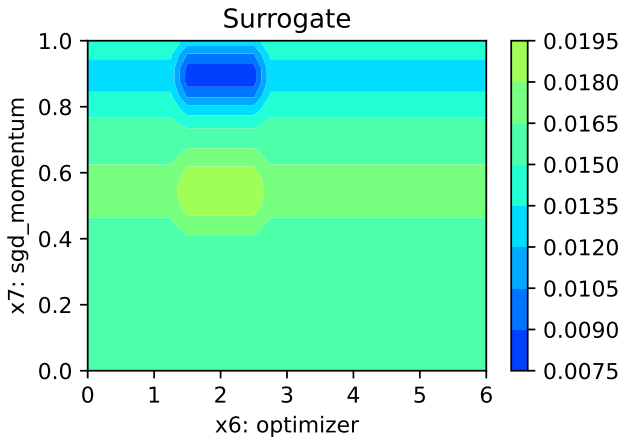

0.017
0.016
0.015
0.014
1 2 3 4
x3: batch_size
1.00
0.75
0.50
0.25
0.00
x7: sgd_momentum

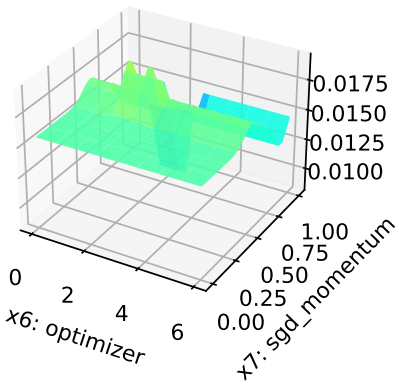

Surrogate
x6: optimizer
x4: epochs
6
5
4
3
2
1
0
2.5 5.0 7.5 10.0 12.5 15.0
0.0205
0.0195
0.0185
0.0175
0.0165
0.0155


0.020
0.018
0.016
5 10 15
x4: epochs
6
4
2
0
x6: optimizer


Surrogate
x7: sgd_momentum
x4: epochs
1.0
0.8
0.6
0.4
0.2
0.0
2.5 5.0 7.5 10.0 12.5 15.0
0.0175
0.0165
0.0155
0.0145
0.0135
0.0125


0.016
0.014
5 10 15
x4: epochs
1.00
0.75
0.50
0.25
0.00
x7: sgd_momentum





19.10.5 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

Parallel coordinates plots

```
Unable to display output for mime type(s): text/html
```

19.11 Summary and Outlook

This tutorial presents the hyperparameter tuning open source software `spotPython` for `PyTorch`. Some of the advantages of `spotPython` are:

- Numerical and categorical hyperparameters.
- Powerful surrogate models.
- Flexible approach and easy to use.
- Simple JSON files for the specification of the hyperparameters.
- Extension of default and user specified network classes.
- Noise handling techniques.
- Online visualization of the hyperparameter tuning process with `tensorboard`.

Currently, only rudimentary parallel and distributed neural network training is possible, but these capabilities will be extended in the future. The next version of `spotPython` will also include a more detailed documentation and more examples.

> **Important**
>
> Important: This tutorial does not present a complete benchmarking study (Bartz-Beielstein et al. 2020). The results are only preliminary and highly dependent on the local configuration (hard- and software). Our goal is to provide a first impression of the performance of the hyperparameter tuning package `spotPython`. The results should be interpreted with care.

20 HPT: PyTorch With VBDP

In this tutorial, we will show how `spotPython` can be integrated into the `PyTorch` training workflow for a classifiaction task.

> Caution: Data must be downloaded manually
>
> - Ensure that the correspondiing data is available as `./data/VBDP/train.csv`.

This document refers to the following software versions:

- `python`: 3.10.10
- `torch`: 2.0.1
- `torchvision`: 0.15.0

```
pip list | grep  "spot[RiverPython]"
```

```
spotPython                0.2.38
spotRiver                 0.0.93
```

```
Note: you may need to restart the kernel to use updated packages.
```

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

20.1 Step 1: Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size and the device that is used.

> Caution: Run time and initial design size should be increased for real experiments
>
> - MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
> - INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.

> Note: Device selection
>
> - The device can be selected by setting the variable `DEVICE`.
> - Since we are using a simple neural net, the setting `"cpu"` is preferred (on Mac).
> - If you have a GPU, you can use `"cuda:0"` instead.
> - If DEVICE is set to `None`, `spotPython` will automatically select the device.
>
> – This might result in `"mps"` on Macs, which is not the best choice for simple neural nets.

```
MAX_TIME = 1
INIT_SIZE = 5
DEVICE = None # "cpu" # "cuda:0"
```

```
from spotPython.utils.device import getDevice
DEVICE = getDevice(DEVICE)
print(DEVICE)
```

```
mps
```

```
import os
import copy
import socket
from datetime import datetime
from dateutil.tz import tzlocal
start_time = datetime.now(tzlocal())
HOSTNAME = socket.gethostname().split(".")[0]
experiment_name = '25-torch' + "_" + HOSTNAME + "_" + str(MAX_TIME) + "min_" + str(INIT_SI
experiment_name = experiment_name.replace(':', '-')
```

```
print(experiment_name)
if not os.path.exists('./figures'):
    os.makedirs('./figures')
```

```
25-torch_bartz09_1min_5init_2023-06-19_04-32-01
```

20.2 Step 2: Initialization of the `fun_control` Dictionary

> Caution: Tensorboard does not work under Windows
>
> - Since tensorboard does not work under Windows, we recommend setting the parameter `tensorboard_path` to `None` if you are working under Windows.

`spotPython` uses a Python dictionary for storing the information required for the hyperparameter tuning process, which was described in Section 14.2, see Initialization of the fun_control Dictionary in the documentation.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/25_spot_torch_vbdp",
    device=DEVICE)
```

20.3 Step 3: PyTorch Data Loading

20.3.1 1. Load VBDP Data

```
import pandas as pd
from sklearn.preprocessing import OrdinalEncoder
train_df = pd.read_csv('./data/VBDP/train.csv')
# remove the id column
train_df = train_df.drop(columns=['id'])
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# # Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.head()
```

```
# convert all entries to int for faster processing
train_df = train_df.astype(int)
```

- Add logical combinations (AND, OR, XOR) of the features to the data set:

```
from spotPython.utils.convert import add_logical_columns
df_new = train_df.copy()
# save the target column using "target_column" as the column name
target = train_df[target_column]
# remove the target column
df_new = df_new.drop(columns=[target_column])
train_df = add_logical_columns(df_new)
# add the target column back
train_df[target_column] = target
train_df = train_df.astype(int)
train_df.head()
```

	sudden_fever	headache	mouth_bleed	nose_bleed	muscle_pain	joint_pain	vomiting	rash	dia
0	1	1	0	1	1	1	1	0	1
1	0	0	0	0	0	0	1	0	1
2	0	1	1	1	0	1	1	1	1
3	0	0	1	1	1	1	0	1	0
4	0	0	0	0	0	0	0	0	1

```
from sklearn.model_selection import train_test_split
import numpy as np

n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
train_df.head()
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x6104	x6105	x6106	x6107	x6108	x6109	x61
0	1	1	0	1	1	1	1	0	1	1	...	0	0	0	0	0	0	0
1	0	0	0	0	0	0	1	0	1	0	...	0	0	0	0	0	0	0
2	0	1	1	1	0	1	1	1	1	1	...	1	1	0	1	1	0	1
3	0	0	1	1	1	1	0	1	0	1	...	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	1	0	...	0	1	1	0	1	1	0

20.3.2 Check content of the target column

```
train_df[target_column].head()
```

```
0     3
1     7
2     3
3    10
4     6
Name: prognosis, dtype: int64
```

```
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
trainset = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
testset = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
trainset.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
testset.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
print(trainset.shape)
print(testset.shape)
```

```
(707, 6113)
(530, 6113)
(177, 6113)
```

```
import torch
from sklearn.model_selection import train_test_split
from spotPython.torch.dataframedataset import DataFrameDataset
dtype_x = torch.float32
dtype_y = torch.long
train_df = DataFrameDataset(train_df, target_column=target_column, dtype_x=dtype_x, dtype_
train = DataFrameDataset(trainset, target_column=target_column, dtype_x=dtype_x, dtype_y=d
test = DataFrameDataset(testset, target_column=target_column, dtype_x=dtype_x, dtype_y=dty
n_samples = len(train)
```

```
# add the dataset to the fun_control
fun_control.update({"data": train_df, # full dataset,
                "train": train,
                "test": test,
                "n_samples": n_samples,
                "target_column": target_column})
```

20.4 Step 4: Specification of the Preprocessing Model

After the training and test data are specified and added to the `fun_control` dictionary, `spotPython` allows the specification of a data preprocessing pipeline, e.g., for the scaling of the data or for the one-hot encoding of categorical variables, see Section 14.4. This feature is not used here, so we do not change the default value (which is `None`).

20.5 Step 5: Select `algorithm` and `core_model_hyper_dict`

20.5.1 Implementing a Configurable Neural Network With spotPython

`spotPython` includes the `Net_vbdp` class which is implemented in the file `netvbdp.py`. The class is imported here.

This class inherits from the class `Net_Core` which is implemented in the file `netcore.py`, see Section 14.5.1.

20.5.2 Add the NN Model to the fun_control Dictionary

```
from spotPython.torch.netvbdp import Net_vbdp
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
fun_control = add_core_model_to_fun_control(core_model=Net_vbdp,
                                fun_control=fun_control,
                                hyper_dict=TorchHyperDict)
```

The corresponding entries for the `core_model` class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'_L0': {'type': 'int',
  'default': 64,
  'transform': 'None',
  'lower': 64,
  'upper': 64},
 'l1': {'type': 'int',
  'default': 8,
  'transform': 'transform_power_2_int',
  'lower': 8,
  'upper': 16},
 'dropout_prob': {'type': 'float',
  'default': 0.01,
  'transform': 'None',
  'lower': 0.0,
  'upper': 0.9},
 'lr_mult': {'type': 'float',
  'default': 1.0,
  'transform': 'None',
  'lower': 0.1,
  'upper': 10.0},
 'batch_size': {'type': 'int',
  'default': 4,
  'transform': 'transform_power_2_int',
  'lower': 1,
  'upper': 4},
 'epochs': {'type': 'int',
  'default': 4,
  'transform': 'transform_power_2_int',
  'lower': 4,
  'upper': 9},
 'k_folds': {'type': 'int',
  'default': 1,
  'transform': 'None',
  'lower': 1,
  'upper': 1},
 'patience': {'type': 'int',
  'default': 2,
  'transform': 'transform_power_2_int',
  'lower': 1,
  'upper': 5},
 'optimizer': {'levels': ['Adadelta',
   'Adagrad',
   'Adam',
```

```
   'AdamW',
   'SparseAdam',
   'Adamax',
   'ASGD',
   'NAdam',
   'RAdam',
   'RMSprop',
   'Rprop',
   'SGD'],
  'type': 'factor',
  'default': 'SGD',
  'transform': 'None',
  'class_name': 'torch.optim',
  'core_model_parameter_type': 'str',
  'lower': 0,
  'upper': 12},
 'sgd_momentum': {'type': 'float',
  'default': 0.0,
  'transform': 'None',
  'lower': 0.0,
  'upper': 1.0}}
```

20.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions were described in Section 14.6.

> Caution: Small number of epochs for demonstration purposes
>
> - `epochs` and `patience` are set to small values for demonstration purposes. These values are too small for a real application.
> - More resonable values are, e.g.:
>   - `fun_control = modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[7, 9])` and
>   - `fun_control = modify_hyper_parameter_bounds(fun_control, "patience", bounds=[2, 7])`

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds

fun_control = modify_hyper_parameter_bounds(fun_control, "_L0", bounds=[n_features, n_feat
fun_control = modify_hyper_parameter_bounds(fun_control, "l1", bounds=[6, 13])
fun_control = modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[2, 3])
fun_control = modify_hyper_parameter_bounds(fun_control, "patience", bounds=[2, 2])
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer",["Adam", "AdamW", "Ad
# fun_control = modify_hyper_parameter_levels(fun_control, "optimizer", ["Adam"])
# fun_control["core_model_hyper_dict"]
```

20.6.1 Optimizers

Optimizers are described in Section 14.6.1.

```
fun_control = modify_hyper_parameter_bounds(fun_control,
    "lr_mult", bounds=[1e-3, 1e-3])
fun_control = modify_hyper_parameter_bounds(fun_control,
    "sgd_momentum", bounds=[0.9, 0.9])
```

20.7 Step 7: Selection of the Objective (Loss) Function

20.7.1 Evaluation

The evaluation procedure requires the specification of two elements:

1. the way how the data is split into a train and a test set (see Section 14.7.1)
2. the loss function (and a metric).

20.7.2 Loss Functions and Metrics

The loss function is specified by the key `"loss_function"`. We will use CrossEntropy loss for the multiclass-classification task.

```
from torch.nn import CrossEntropyLoss
loss_function = CrossEntropyLoss()
fun_control.update({"loss_function": loss_function})
```

20.7.3 Metric

- We will use the MAP@k metric for the evaluation of the model. Here is an example how this metric is calculated.

```
from spotPython.torch.mapk import MAPK
import torch
mapk = MAPK(k=2)
target = torch.tensor([0, 1, 2, 2])
preds = torch.tensor(
    [
        [0.5, 0.2, 0.2],  # 0 is in top 2
        [0.3, 0.4, 0.2],  # 1 is in top 2
        [0.2, 0.4, 0.3],  # 2 is in top 2
        [0.7, 0.2, 0.1],  # 2 isn't in top 2
    ]
)
mapk.update(preds, target)
print(mapk.compute()) # tensor(0.6250)
```

```
tensor(0.6250)
```

```
from spotPython.torch.mapk import MAPK
import torchmetrics
metric_torch = MAPK(k=3)
fun_control.update({"metric_torch": metric_torch})
```

20.8 Step 8: Calling the SPOT Function

20.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
```

```
fun_control.update({"var_type": var_type,
                    "var_name": var_name})
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

Now, the dictionary `fun_control` contains all information needed for the hyperparameter tuning. Before the hyperparameter tuning is started, it is recommended to take a look at the experimental design. The method `gen_design_table` generates a design table as follows:

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

```
| name          | type   | default   |    lower |    upper | transform             |
|---------------|--------|-----------|----------|----------|-----------------------|
| _L0           | int    | 64        | 6112     | 6112     | None                  |
| l1            | int    | 8         |    6     |   13     | transform_power_2_int |
| dropout_prob  | float  | 0.01      |    0     |    0.9   | None                  |
| lr_mult       | float  | 1.0       |    0.001 |    0.001 | None                  |
| batch_size    | int    | 4         |    1     |    4     | transform_power_2_int |
| epochs        | int    | 4         |    2     |    3     | transform_power_2_int |
| k_folds       | int    | 1         |    1     |    1     | None                  |
| patience      | int    | 2         |    2     |    2     | transform_power_2_int |
| optimizer     | factor | SGD       |    0     |    3     | None                  |
| sgd_momentum  | float  | 0.0       |    0.9   |    0.9   | None                  |
```

This allows to check if all information is available and if the information is correct.

20.8.2 The Objective Function `fun_torch`

The objective function `fun_torch` is selected next. It implements an interface from `PyTorch`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypertorch import HyperTorch
fun = HyperTorch().fun_torch
```

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
hyper_dict=TorchHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
```

20.8.3 Starting the Hyperparameter Tuning

The `spotPython` hyperparameter tuning is started by calling the `Spot` function as described in Section 14.8.4.

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                    lower = lower,
                    upper = upper,
                    fun_evals = inf,
                    fun_repeats = 1,
                    max_time = MAX_TIME,
                    noise = False,
                    tolerance_x = np.sqrt(np.spacing(1)),
                    var_type = var_type,
                    var_name = var_name,
                    infill_criterion = "y",
                    n_points = 1,
                    seed=123,
                    log_level = 50,
                    show_models= False,
                    show_progress= True,
                    fun_control = fun_control,
                    design_control={"init_size": INIT_SIZE,
                                    "repeats": 1},
                    surrogate_control={"noise": True,
                                       "cod_type": "norm",
                                       "min_theta": -4,
                                       "max_theta": 3,
                                       "n_theta": len(var_name),
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

```
config: {'_L0': 6112, 'l1': 2048, 'dropout_prob': 0.17031221661559992, 'lr_mult': 0.001, 'ba
Epoch: 1 |

MAPK: 0.1778273731470108 | Loss: 2.3978227717535838 | Acc: 0.1132075471698113.
```

```
Epoch: 2 |

MAPK: 0.1755952388048172 | Loss: 2.3978894608361379 | Acc: 0.1084905660377359.
Epoch: 3 |

MAPK: 0.1845238059759140 | Loss: 2.3977681398391724 | Acc: 0.1273584905660377.
Epoch: 4 |

MAPK: 0.1889880895614624 | Loss: 2.3977671180452620 | Acc: 0.1367924528301887.
Epoch: 5 | MAPK: 0.1956845223903656 | Loss: 2.3977283069065640 | Acc: 0.1650943396226415.
Epoch: 6 |

MAPK: 0.1934523731470108 | Loss: 2.3976699795041765 | Acc: 0.1320754716981132.
Epoch: 7 |

MAPK: 0.1867559403181076 | Loss: 2.3975695712225780 | Acc: 0.1320754716981132.
Epoch: 8 |

MAPK: 0.1912202388048172 | Loss: 2.3975362437111989 | Acc: 0.1273584905660377.
Returned to Spot: Validation loss: 2.397536243711199

config: {'_L0': 6112, 'l1': 256, 'dropout_prob': 0.193797900355129 87, 'lr_mult': 0.001, 'bat
Epoch: 1 |

MAPK: 0.1589506417512894 | Loss: 2.3977898138540761 | Acc: 0.0801886792452830.
Epoch: 2 |

MAPK: 0.1635802537202835 | Loss: 2.3977428807152643 | Acc: 0.0801886792452830.
Epoch: 3 |

MAPK: 0.1620370596647263 | Loss: 2.3977394987035683 | Acc: 0.0707547169811321.
Epoch: 4 |

MAPK: 0.1658950746059418 | Loss: 2.3977184383957475 | Acc: 0.0801886792452830.
Returned to Spot: Validation loss: 2.3977184383957475

config: {'_L0': 6112, 'l1': 4096, 'dropout_prob': 0.6759063718076167, 'lr_mult': 0.001, 'bat
Epoch: 1 |
```

```
MAPK: 0.1871068924665451 | Loss: 2.3979439443012454 | Acc: 0.1179245283018868.
Epoch: 2 |

MAPK: 0.2421383112668991 | Loss: 2.3975673734017140 | Acc: 0.1415094339622641.
Epoch: 3 |

MAPK: 0.2531446516513824 | Loss: 2.3974374240299441 | Acc: 0.1462264150943396.
Epoch: 4 |

MAPK: 0.2303458899259567 | Loss: 2.3974605888690590 | Acc: 0.1320754716981132.
Epoch: 5 |

MAPK: 0.2287735193967819 | Loss: 2.3970276544678888 | Acc: 0.1226415094339623.
Epoch: 6 |

MAPK: 0.2264150828123093 | Loss: 2.3968495602877633 | Acc: 0.1320754716981132.
Epoch: 7 |

MAPK: 0.2091194838285446 | Loss: 2.3965910470710612 | Acc: 0.1084905660377359.
Epoch: 8 |

MAPK: 0.2224842458963394 | Loss: 2.3959322245615833 | Acc: 0.1320754716981132.
Returned to Spot: Validation loss: 2.3959322245615833

config: {'_L0': 6112, 'l1': 128, 'dropout_prob': 0.37306669346546995, 'lr_mult': 0.001, 'bat
Epoch: 1 |

MAPK: 0.1588050574064255 | Loss: 2.3982574624835320 | Acc: 0.0896226415094340.
Epoch: 2 |

MAPK: 0.1588050574064255 | Loss: 2.3983343322322055 | Acc: 0.0849056603773585.
Epoch: 3 |

MAPK: 0.1588050425052643 | Loss: 2.3981994233041442 | Acc: 0.0849056603773585.
Epoch: 4 |

MAPK: 0.1572327017784119 | Loss: 2.3983834644533553 | Acc: 0.0801886792452830.
Returned to Spot: Validation loss: 2.3983834644533553

config: {'_L0': 6112, 'l1': 1024, 'dropout_prob': 0.870137281216666, 'lr_mult': 0.001, 'batc
Epoch: 1 |
```

```
MAPK: 0.1766975373029709 | Loss: 2.3976071499012135 | Acc: 0.0990566037735849.
Epoch: 2 |

MAPK: 0.1929012537002563 | Loss: 2.3974499084331371 | Acc: 0.1084905660377359.
Epoch: 3 |

MAPK: 0.2060185223817825 | Loss: 2.3974460937358715 | Acc: 0.1367924528301887.
Epoch: 4 |

MAPK: 0.2183642238378525 | Loss: 2.3971893434171325 | Acc: 0.1084905660377359.
Epoch: 5 |

MAPK: 0.2052469253540039 | Loss: 2.3975013008824102 | Acc: 0.1084905660377359.
Epoch: 6 |

MAPK: 0.1867283880710602 | Loss: 2.3977151093659579 | Acc: 0.1320754716981132.
Epoch: 7 |

MAPK: 0.2160493582487106 | Loss: 2.3974010591153747 | Acc: 0.1320754716981132.
Epoch: 8 |

MAPK: 0.2083333283662796 | Loss: 2.3972757657368979 | Acc: 0.1226415094339623.
Early stopping at epoch 7
Returned to Spot: Validation loss: 2.397275765736898

config: {'_L0': 6112, 'l1': 4096, 'dropout_prob': 0.4132005099912892, 'lr_mult': 0.001, 'bat
Epoch: 1 |

MAPK: 0.1800314486026764 | Loss: 2.3976828557140424 | Acc: 0.0943396226415094.
Epoch: 2 |

MAPK: 0.2114779800176620 | Loss: 2.3973630531778873 | Acc: 0.1132075471698113.
Epoch: 3 |

MAPK: 0.2311320602893829 | Loss: 2.3970617730662509 | Acc: 0.1320754716981132.
Epoch: 4 |

MAPK: 0.2295597791671753 | Loss: 2.3964778162398428 | Acc: 0.1320754716981132.
Epoch: 5 |
```

```
MAPK: 0.2507861554622650 | Loss: 2.3957185700254620 | Acc: 0.1745283018867924.
Epoch: 6 |

MAPK: 0.2421383261680603 | Loss: 2.3945849076756893 | Acc: 0.1792452830188679.
Epoch: 7 |

MAPK: 0.2319181859493256 | Loss: 2.3930445887007803 | Acc: 0.1650943396226415.
Epoch: 8 |

MAPK: 0.2405660003423691 | Loss: 2.3900625323349574 | Acc: 0.1792452830188679.
Returned to Spot: Validation loss: 2.3900625323349574
spotPython tuning: 2.3900625323349574 [####------] 35.87%


config: {'_L0': 6112, 'l1': 512, 'dropout_prob': 0.41307021636436325, 'lr_mult': 0.001, 'bat
Epoch: 1 |

MAPK: 0.2106918543577194 | Loss: 2.3969543834902205 | Acc: 0.1273584905660377.
Epoch: 2 |

MAPK: 0.2209119200706482 | Loss: 2.3968141033964336 | Acc: 0.1320754716981132.
Epoch: 3 |

MAPK: 0.2264150977134705 | Loss: 2.3968117731922076 | Acc: 0.1462264150943396.
Epoch: 4 |

MAPK: 0.2382074892520905 | Loss: 2.3967072468883588 | Acc: 0.1603773584905660.
Epoch: 5 |

MAPK: 0.2499999403953552 | Loss: 2.3965636019436820 | Acc: 0.1745283018867924.
Epoch: 6 |

MAPK: 0.2460691630840302 | Loss: 2.3965558735829480 | Acc: 0.1698113207547170.
Epoch: 7 |

MAPK: 0.2555030882358551 | Loss: 2.3965241774073185 | Acc: 0.1745283018867924.
Epoch: 8 |
```

```
MAPK: 0.2555031180381775 | Loss: 2.3964265607437998 | Acc: 0.1886792452830189.
Returned to Spot: Validation loss: 2.3964265607438
spotPython tuning: 2.3900625323349574 [#####-----] 46.13%


config: {'_L0': 6112, 'l1': 128, 'dropout_prob': 0.41300574671604434, 'lr_mult': 0.001, 'bat
Epoch: 1 |

MAPK: 0.1462264358997345 | Loss: 2.3985383555574238 | Acc: 0.0613207547169811.
Epoch: 2 |

MAPK: 0.1525157392024994 | Loss: 2.3986691416434520 | Acc: 0.0613207547169811.
Epoch: 3 |

MAPK: 0.1477987617254257 | Loss: 2.3986250297078548 | Acc: 0.0613207547169811.
Epoch: 4 |

MAPK: 0.1477987766265869 | Loss: 2.3985712978075133 | Acc: 0.0613207547169811.
Epoch: 5 |

MAPK: 0.1509434133768082 | Loss: 2.3984091821706519 | Acc: 0.0613207547169811.
Epoch: 6 |

MAPK: 0.1525157392024994 | Loss: 2.3983121615535810 | Acc: 0.0613207547169811.
Epoch: 7 |

MAPK: 0.1556603908538818 | Loss: 2.3983128160800575 | Acc: 0.0613207547169811.
Epoch: 8 |

MAPK: 0.1509434282779694 | Loss: 2.3983534754447215 | Acc: 0.0613207547169811.
Returned to Spot: Validation loss: 2.3983534754447215
spotPython tuning: 2.3900625323349574 [######----] 63.56%


config: {'_L0': 6112, 'l1': 8192, 'dropout_prob': 0.41444870177080323, 'lr_mult': 0.001, 'ba

Epoch: 1 |
```

```
MAPK: 0.1973270177841187 | Loss: 2.3975810734730847 | Acc: 0.1132075471698113.
Epoch: 2 |

MAPK: 0.2287735342979431 | Loss: 2.3971492974263318 | Acc: 0.1415094339622641.
Epoch: 3 |

MAPK: 0.1973270773887634 | Loss: 2.3966462432213551 | Acc: 0.1179245283018868.
Epoch: 4 |

MAPK: 0.1918238997459412 | Loss: 2.3957121237268986 | Acc: 0.1132075471698113.
Returned to Spot: Validation loss: 2.3957121237268986
spotPython tuning: 2.3900625323349574 [########--] 83.85%


config: {'_L0': 6112, 'l1': 4096, 'dropout_prob': 0.41474501146092996, 'lr_mult': 0.001, 'ba

Epoch: 1 |

MAPK: 0.1604938507080078 | Loss: 2.3979456159803600 | Acc: 0.0801886792452830.
Epoch: 2 |

MAPK: 0.2060185074806213 | Loss: 2.3978245876453541 | Acc: 0.1179245283018868.
Epoch: 3 |

MAPK: 0.2037036716938019 | Loss: 2.3978362613254123 | Acc: 0.1320754716981132.
Epoch: 4 |

MAPK: 0.1844135522842407 | Loss: 2.3978672910619667 | Acc: 0.1084905660377359.
Epoch: 5 |

MAPK: 0.1944444328546524 | Loss: 2.3977656982563160 | Acc: 0.1132075471698113.
Epoch: 6 |

MAPK: 0.2322530597448349 | Loss: 2.3975858246838606 | Acc: 0.1603773584905660.
Epoch: 7 |

MAPK: 0.2075617164373398 | Loss: 2.3976335437209517 | Acc: 0.1179245283018868.
Epoch: 8 |
```

```
MAPK: 0.2060184776782990 | Loss: 2.3975747161441379 | Acc: 0.1226415094339623.
Returned to Spot: Validation loss: 2.397574716144138
spotPython tuning: 2.3900625323349574 [##########-] 92.60%


config: {'_L0': 6112, 'l1': 4096, 'dropout_prob': 0.41094634811682174, 'lr_mult': 0.001, 'ba
Epoch: 1 |

MAPK: 0.2044025063514709 | Loss: 2.3975967506192766 | Acc: 0.1462264150943396.
Epoch: 2 |

MAPK: 0.1926100701093674 | Loss: 2.3974419134967730 | Acc: 0.1084905660377359.
Epoch: 3 |

MAPK: 0.1957547366619110 | Loss: 2.3972251460237324 | Acc: 0.0943396226415094.
Epoch: 4 |

MAPK: 0.2106918096542358 | Loss: 2.3968959259537033 | Acc: 0.0943396226415094.
Epoch: 5 |

MAPK: 0.2059748619794846 | Loss: 2.3968038244067498 | Acc: 0.0896226415094340.
Epoch: 6 |

MAPK: 0.1933962404727936 | Loss: 2.3964082070116728 | Acc: 0.0896226415094340.
Epoch: 7 |

MAPK: 0.1926100403070450 | Loss: 2.3958087822176375 | Acc: 0.0896226415094340.
Epoch: 8 |

MAPK: 0.1745283007621765 | Loss: 2.3954800929663316 | Acc: 0.0896226415094340.
Returned to Spot: Validation loss: 2.3954800929663316
spotPython tuning: 2.3900625323349574 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2c97937f0>
```

20.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section 14.9, see also the description in the documentation: Tensorboard.

20.10 Step 10: Results

After the hyperparameter tuning run is finished, the results can be analyzed as described in Section 14.10.

```
spot_tuner.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

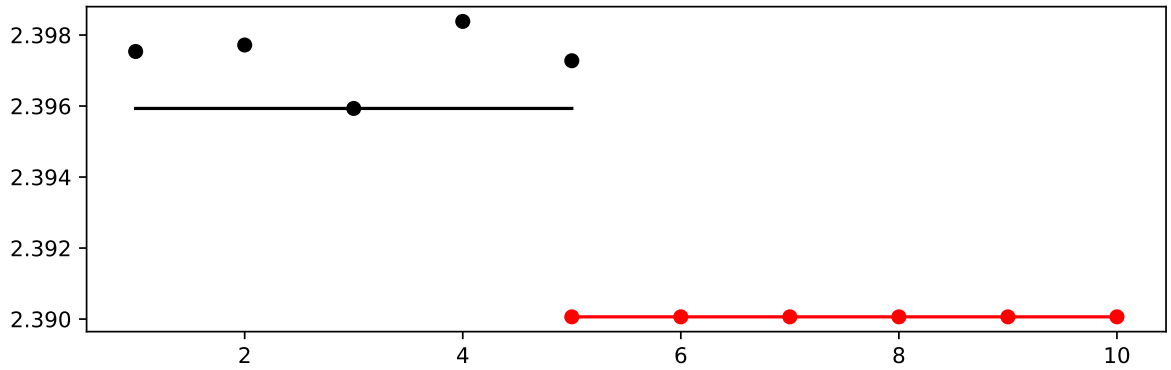


Figure 20.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

name	type	default	lower	upper	tuned	transform
_L0	int	64	6112.0	6112.0	6112.0	None
l1	int	8	6.0	13.0	12.0	transform_powe
dropout_prob	float	0.01	0.0	0.9	0.4132005099912892	None
lr_mult	float	1.0	0.001	0.001	0.001	None
batch_size	int	4	1.0	4.0	1.0	transform_powe
epochs	int	4	2.0	3.0	3.0	transform_powe
k_folds	int	1	1.0	1.0	1.0	None
patience	int	2	2.0	2.0	2.0	transform_powe
optimizer	factor	SGD	0.0	3.0	3.0	None
sgd_momentum	float	0.0	0.9	0.9	0.9	None

```
spot_tuner.plot_importance(threshold=0.025,
    filename="./figures/" + experiment_name+"_importance.png")
```

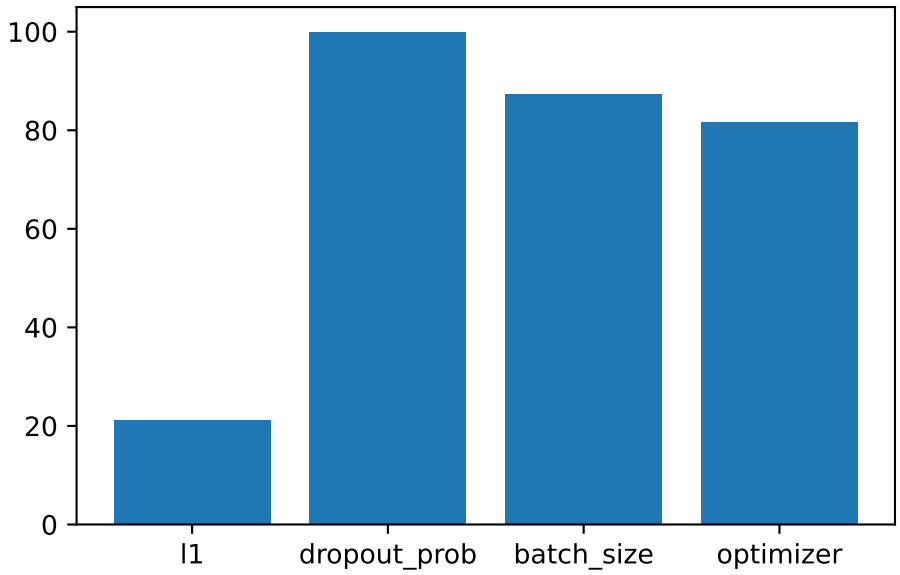


Figure 20.2: Variable importance plot, threshold 0.025.

20.10.1 Get the Tuned Architecture

```
from spotPython.hyperparameters.values import get_one_core_model_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
model_spot = get_one_core_model_from_X(X, fun_control)
model_spot
```

```
Net_vbdp(
  (fc1): Linear(in_features=6112, out_features=4096, bias=True)
  (fc2): Linear(in_features=4096, out_features=2048, bias=True)
  (fc3): Linear(in_features=2048, out_features=1024, bias=True)
  (fc4): Linear(in_features=1024, out_features=512, bias=True)
  (fc5): Linear(in_features=512, out_features=11, bias=True)
  (relu): ReLU()
  (softmax): Softmax(dim=1)
  (dropout1): Dropout(p=0.4132005099912892, inplace=False)
  (dropout2): Dropout(p=0.2066002549956446, inplace=False)
)
```

20.10.2 Evaluation of the Tuned Architecture

```
from spotPython.torch.traintest import (
    train_tuned,
    test_tuned,
    )
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=True,
        device = fun_control["device"],
        path=None,
        task=fun_control["task"],)
```

```
Epoch: 1 |

MAPK: 0.1753144711256027 | Loss: 2.3976820324951746 | Acc: 0.1084905660377359.
Epoch: 2 |

MAPK: 0.1753144562244415 | Loss: 2.3973140176737084 | Acc: 0.1132075471698113.
Epoch: 3 |

MAPK: 0.1816037595272064 | Loss: 2.3969395947906205 | Acc: 0.1179245283018868.
Epoch: 4 |

MAPK: 0.1816037744283676 | Loss: 2.3961891678144349 | Acc: 0.1179245283018868.
Epoch: 5 |

MAPK: 0.1823899447917938 | Loss: 2.3951856910057789 | Acc: 0.1179245283018868.
Epoch: 6 |

MAPK: 0.1784591376781464 | Loss: 2.3940786213245033 | Acc: 0.1179245283018868.
Epoch: 7 |

MAPK: 0.1800314337015152 | Loss: 2.3925867305611663 | Acc: 0.1179245283018868.
Epoch: 8 |

MAPK: 0.1816037744283676 | Loss: 2.3907402348968216 | Acc: 0.1179245283018868.
Returned to Spot: Validation loss: 2.3907402348968216
```

If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be loaded from this file.

```
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = fun_control["device"],
            task=fun_control["task"],)
```

```
MAPK: 0.1910112500190735 | Loss: 2.3872228097379877 | Acc: 0.1186440677966102.
Final evaluation: Validation loss: 2.3872228097379877
Final evaluation: Validation metric: 0.1910112500190735
---------------------------------------------
```

```
(2.3872228097379877, nan, tensor(0.1910))
```

20.10.3 Cross-validated Evaluations

- This is the evaluation that will be used in the comparison.

> Caution: Cross-validated Evaluations
>
> - The number of folds is set to 1 by default.
> - Here it was changed to 3 for demonstration purposes.
> - Set the number of folds to a reasonable value, e.g., 10.
> - This can be done by setting the `k_folds` attribute of the model as follows:
> - `setattr(model_spot, "k_folds", 10)`

```
from spotPython.torch.traintest import evaluate_cv
# modify k-kolds:
setattr(model_spot, "k_folds", 3)
df_eval, df_preds, df_metrics = evaluate_cv(net=model_spot,
    dataset=fun_control["data"],
    loss_function=fun_control["loss_function"],
    metric=fun_control["metric_torch"],
    task=fun_control["task"],
    writer=fun_control["writer"],
    writerId="model_spot_cv",
    device = fun_control["device"])
```

```
Fold: 1
Epoch: 1 |

MAPK: 0.1744349896907806 | Loss: 2.3973758847026501 | Acc: 0.0805084745762712.
Epoch: 2 |

MAPK: 0.2146892547607422 | Loss: 2.3967134689880631 | Acc: 0.1483050847457627.
Epoch: 3 |

MAPK: 0.2161016911268234 | Loss: 2.3958126387353671 | Acc: 0.1271186440677966.
Epoch: 4 |

MAPK: 0.2266948670148849 | Loss: 2.3945004879418068 | Acc: 0.1271186440677966.
Epoch: 5 |

MAPK: 0.2457626760005951 | Loss: 2.3925800707380649 | Acc: 0.1271186440677966.
Epoch: 6 |

MAPK: 0.2598869800567627 | Loss: 2.3892519857923862 | Acc: 0.1271186440677966.
Epoch: 7 |

MAPK: 0.2853107452392578 | Loss: 2.3845437946966137 | Acc: 0.1313559322033898.
Epoch: 8 |

MAPK: 0.3227401077747345 | Loss: 2.3799093315156838 | Acc: 0.1949152542372881.
Fold: 2
Epoch: 1 |

MAPK: 0.1871468871831894 | Loss: 2.3975351159855469 | Acc: 0.0889830508474576.
Epoch: 2 |

MAPK: 0.2281073182821274 | Loss: 2.3968891127634855 | Acc: 0.1186440677966102.
Epoch: 3 |

MAPK: 0.2358756810426712 | Loss: 2.3959750260336925 | Acc: 0.1186440677966102.
Epoch: 4 |

MAPK: 0.2337570190429688 | Loss: 2.3945896524493979 | Acc: 0.1186440677966102.
Epoch: 5 |
```

```
MAPK: 0.2337570339441299 | Loss: 2.3920788482084112 | Acc: 0.1228813559322034.
Epoch: 6 |

MAPK: 0.2302259504795074 | Loss: 2.3886764635473994 | Acc: 0.1186440677966102.
Epoch: 7 |

MAPK: 0.2422316074371338 | Loss: 2.3847005751173374 | Acc: 0.1228813559322034.
Epoch: 8 |

MAPK: 0.2824858725070953 | Loss: 2.3816417132393788 | Acc: 0.1737288135593220.
Fold: 3
Epoch: 1 |

MAPK: 0.1829096078872681 | Loss: 2.3976690526735984 | Acc: 0.0978723404255319.
Epoch: 2 |

MAPK: 0.1956214606761932 | Loss: 2.3971529390852329 | Acc: 0.1234042553191489.
Epoch: 3 |

MAPK: 0.2026835680007935 | Loss: 2.3964017508393627 | Acc: 0.1191489361702128.
Epoch: 4 |

MAPK: 0.1991525441408157 | Loss: 2.3954021526595293 | Acc: 0.1148936170212766.
Epoch: 5 |

MAPK: 0.2083333134651184 | Loss: 2.3936718278012035 | Acc: 0.1148936170212766.
Epoch: 6 |

MAPK: 0.2111581861972809 | Loss: 2.3913376068664811 | Acc: 0.1148936170212766.
Epoch: 7 |

MAPK: 0.2139830440282822 | Loss: 2.3877145233800854 | Acc: 0.1148936170212766.
Epoch: 8 |

MAPK: 0.2351694703102112 | Loss: 2.3849314491627580 | Acc: 0.1148936170212766.
```

```
metric_name = type(fun_control["metric_torch"]).__name__
print(f"loss: {df_eval}, Cross-validated {metric_name}: {df_metrics}")
```

```
loss: 2.3821608313059404, Cross-validated MAPK: 0.28013181686401367
```

20.10.4 Detailed Hyperparameter Plots

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

```
l1:  21.13433159251595
dropout_prob:  100.0
batch_size:  87.40863288608274
optimizer:  81.7067553304582
```

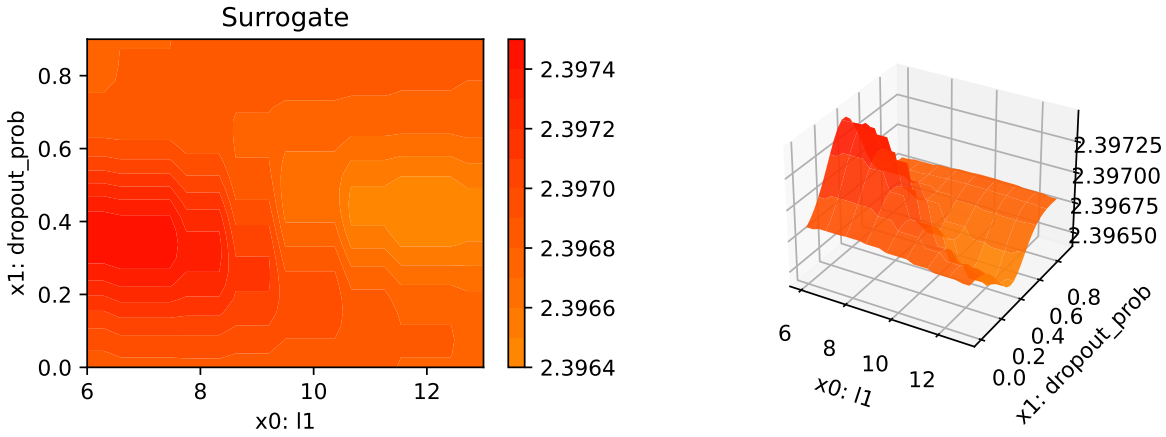
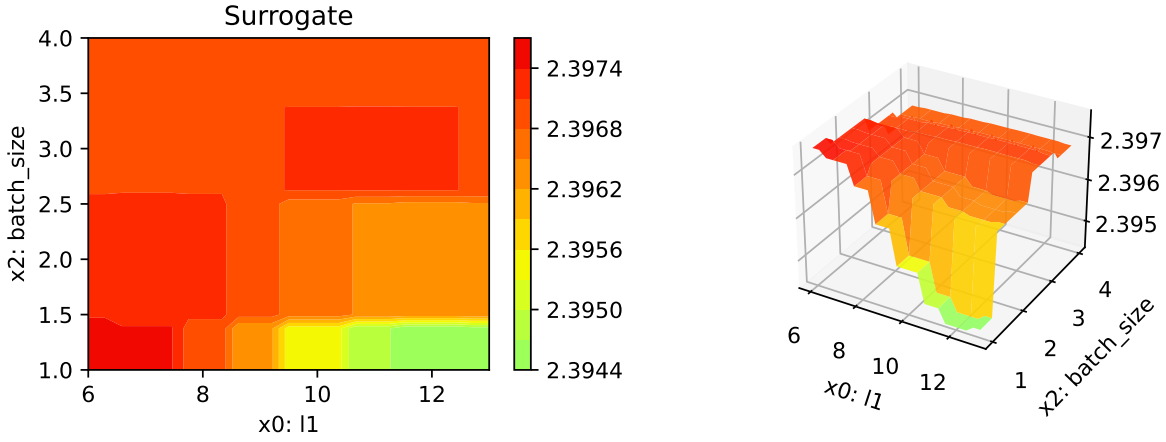
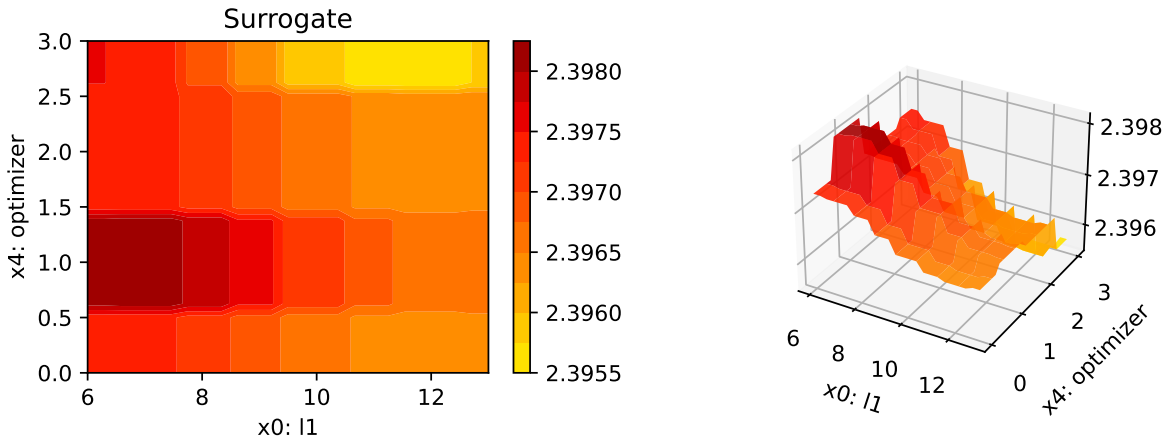
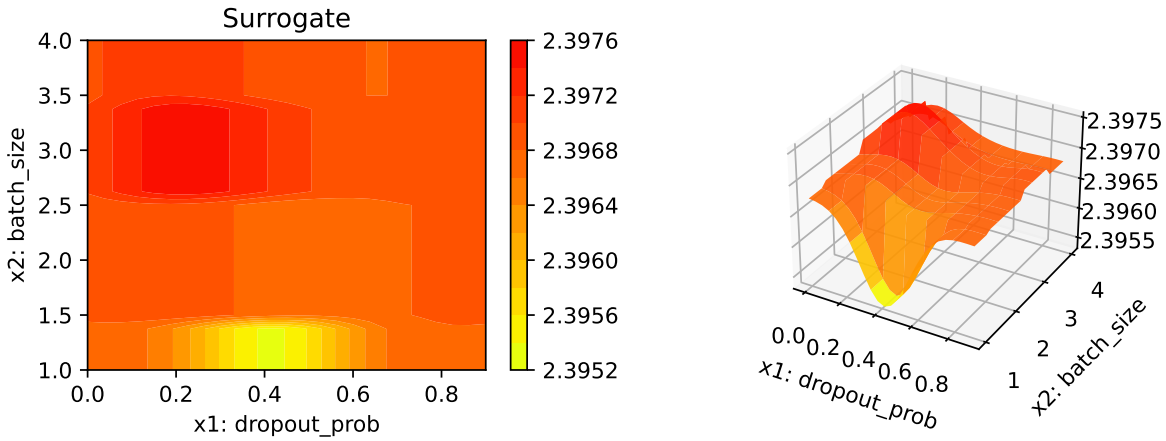
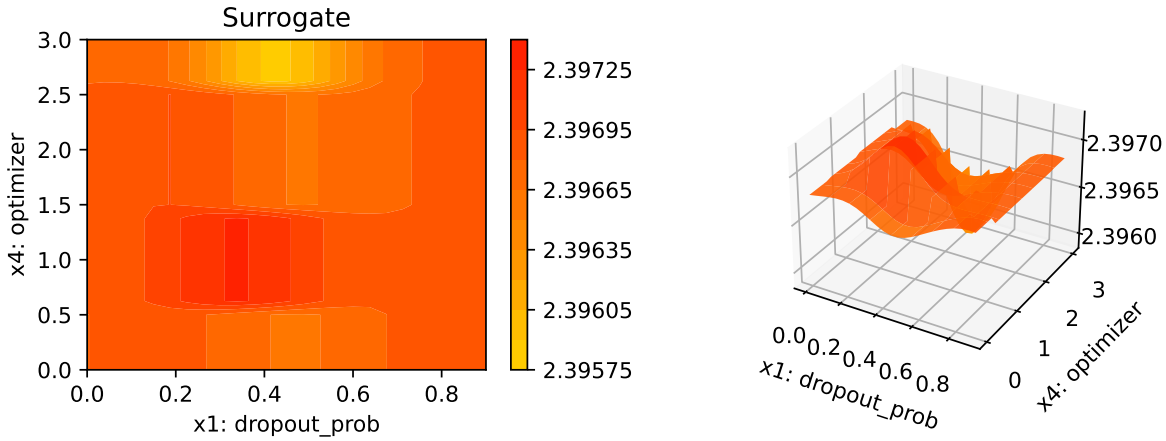


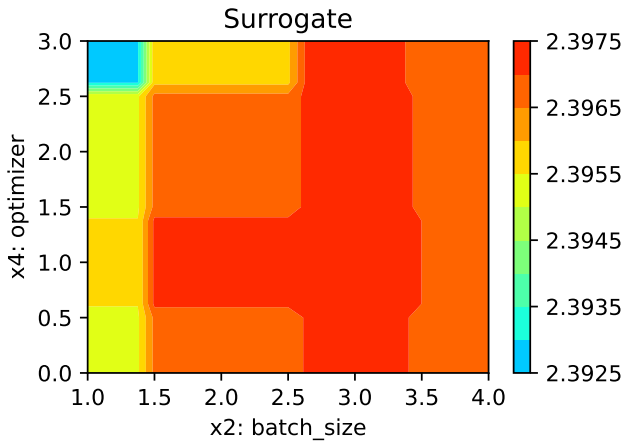
Figure 20.3: Contour plots.

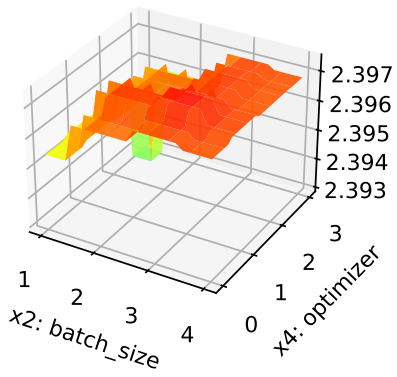



Surrogate
x4: optimizer
x0: l1
2.3980
2.3975
2.3970
2.3965
2.3960
2.3955
x0: l1
x4: optimizer
2.398
2.397
2.396


Surrogate
x2: batch_size
x1: dropout_prob
2.3976
2.3972
2.3968
2.3964
2.3960
2.3956
2.3952
x1: dropout_prob
x2: batch_size
2.3975
2.3970
2.3965
2.3960
2.3955


Surrogate
x4: optimizer
x1: dropout_prob
2.39725
2.39695
2.39665
2.39635
2.39605
2.39575
x1: dropout_prob
x4: optimizer
2.3970
2.3965
2.3960





20.10.5 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

Parallel coordinates plots

```
Unable to display output for mime type(s): text/html
```

```
# close tensorbaoard writer
if fun_control["writer"] is not None:
    fun_control["writer"].close()
```

20.10.6 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

21 Documentation of the Sequential Parameter Optimization

This document describes the `Spot` features.

21.1 Example: spot

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

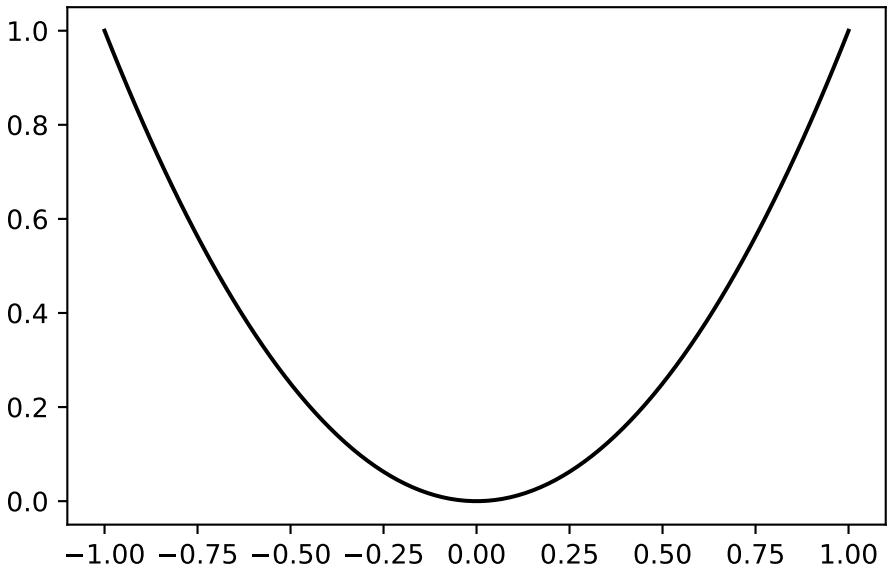
21.1.1 The Objective Function

The `spotPython` package provides several classes of objective functions. We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = x^2$$

```
fun = analytical().fun_sphere
```

```
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x)
plt.figure()
plt.plot(x,y, "k")
plt.show()
```




```
spot_1 = spot.Spot(fun=fun,
                   lower = np.array([-10]),
                   upper = np.array([100]),
                   fun_evals = 7,
                   fun_repeats = 1,
                   max_time = inf,
                   noise = False,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   var_type=["num"],
                   infill_criterion = "y",
                   n_points = 1,
                   seed=123,
                   log_level = 50,
                   show_models=True,
                   fun_control = {},
                   design_control={"init_size": 5,
                                   "repeats": 1},
                   surrogate_control={"noise": False,
                                      "cod_type": "norm",
                                      "min_theta": -4,
                                      "max_theta": 3,
                                      "n_theta": 1,
                                      "model_optimizer": differential_evolution,
                                      "model_fun_evals": 1000,
```

```
                                                    })
```

`spot`'s `__init__` method sets the control parameters. There are two parameter groups:

1. external parameters can be specified by the user
2. internal parameters, which are handled by `spot`.

21.1.2 External Parameters

external parameter	type	description	default	mandatory
`fun`	object	objective function		yes
`lower`	array	lower bound		yes
`upper`	array	upper bound		yes
`fun_evals`	int	number of function evaluations	15	no
`fun_evals`	int	number of function evaluations	15	no
`fun_control`	dict	noise etc.	{}	n
`max_time`	int	max run time budget	`inf`	no
`noise`	bool	if repeated evaluations of `fun` results in different values, then `noise` should be set to `True`.	`False`	no

external parameter	type	description	default	mandatory
`tolerance_x`	float	tolerance for new x solutions. Minimum distance of new solutions, generated by `suggest_new_X`, to already existing solutions. If zero (which is the default), every new solution is accepted.	`0`	no
`var_type`	list	list of type information, can be either `"num"` or `"factor"`	`["num"]`	no
`infill_criterion`	string	Can be `"y"`, `"s"`, `"ei"` (negative expected improvement), or `"all"`	`"y"`	no
`n_points`	int	number of infill points	1	no
`seed`	int	initial seed. If `Spot.run()` is called twice, different results will be generated. To reproduce results, the `seed` can be used.	`123`	no

external parameter	type	description	default	mandatory
`log_level`	int	log level with the following settings: `NOTSET` (`0`), `DEBUG` (`10`: Detailed information, typically of interest only when diagnosing problems.), `INFO` (`20`: Confirmation that things are working as expected.), `WARNING` (`30`: An indication that something unexpected happened, or indicative of some problem in the near future (e.g. 'disk space low'). The software is still working as expected.), `ERROR` (`40`: Due to a more serious problem, the software has not been able to perform some function.), and `CRITICAL` (`50`: A serious error, indicating that the program itself may be unable to continue running.)	`50`	no

external parameter	type	description	default	mandatory
`show_models`	bool	Plot model. Currently only 1-dim functions are supported	`False`	no
`design`	object	experimental design	`None`	no
`design_control`	dict	control parameters	see below	no
`surrogate`		surrogate model	`kriging`	no
`surrogate_control`	dict	control parameters	see below	no
`optimizer`	object	optimizer	see below	no
`optimizer_control`	dict	control parameters	see below	no

- Besides these single parameters, the following parameter dictionaries can be specified by the user:
  - `fun_control`
  - `design_control`
  - `surrogate_control`
  - `optimizer_control`

21.2 The `fun_control` Dictionary

external parameter	type	description	default	mandatory
`sigma`	float	noise: standard deviation	`0`	yes
`seed`	int	seed for rng	`124`	yes

21.3 The `design_control` Dictionary

external parameter	type	description	default	mandatory
`init_size`	int	initial sample size	`10`	yes

external parameter	type	description	default	mandatory
`repeats`	int	number of repeats of the initial sammples	`1`	yes

21.4 The `surrogate_control` Dictionary

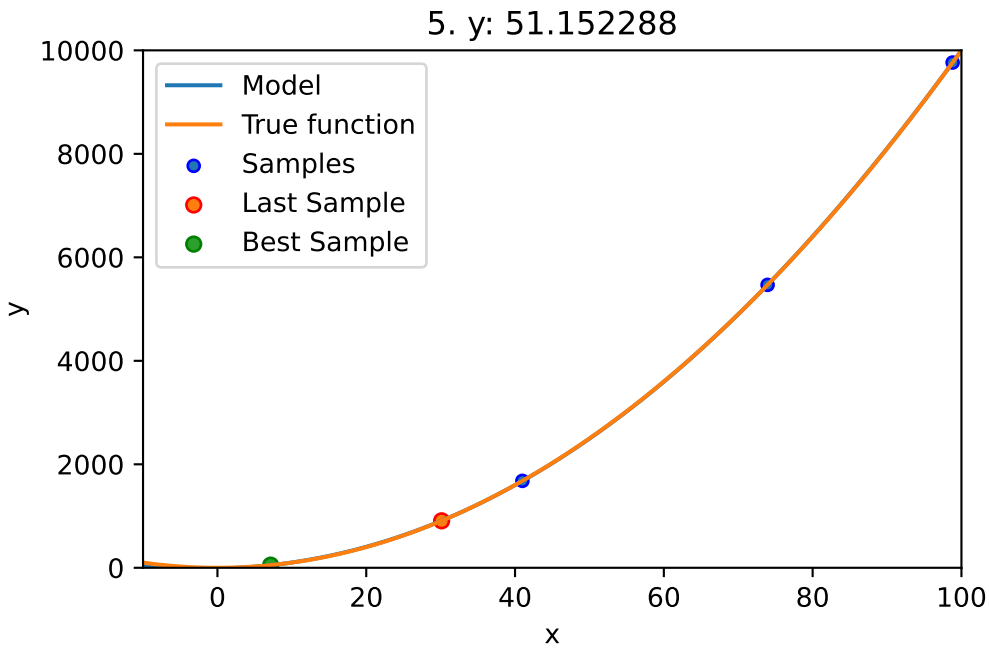
external parameter	type	description	default	mandatory
`noise_model_optimizer`	object	optimizer	`differential_evolution`	no
`model_fun_evals`				
`min_theta`			`-3.`	
`max_theta`			`3.`	
`n_theta`			`1`	
`n_p`			`1`	
`optim_p`			`False`	
`cod_type`			`"norm"`	
`var_type`				
`use_cod_y`	bool		`False`	

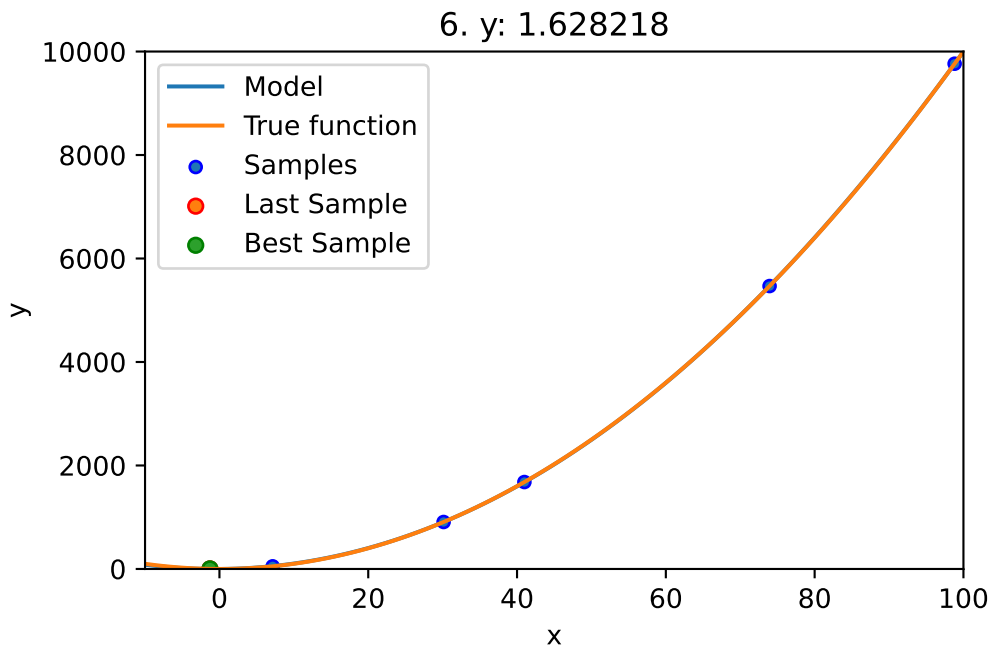
21.5 The `optimizer_control` Dictionary

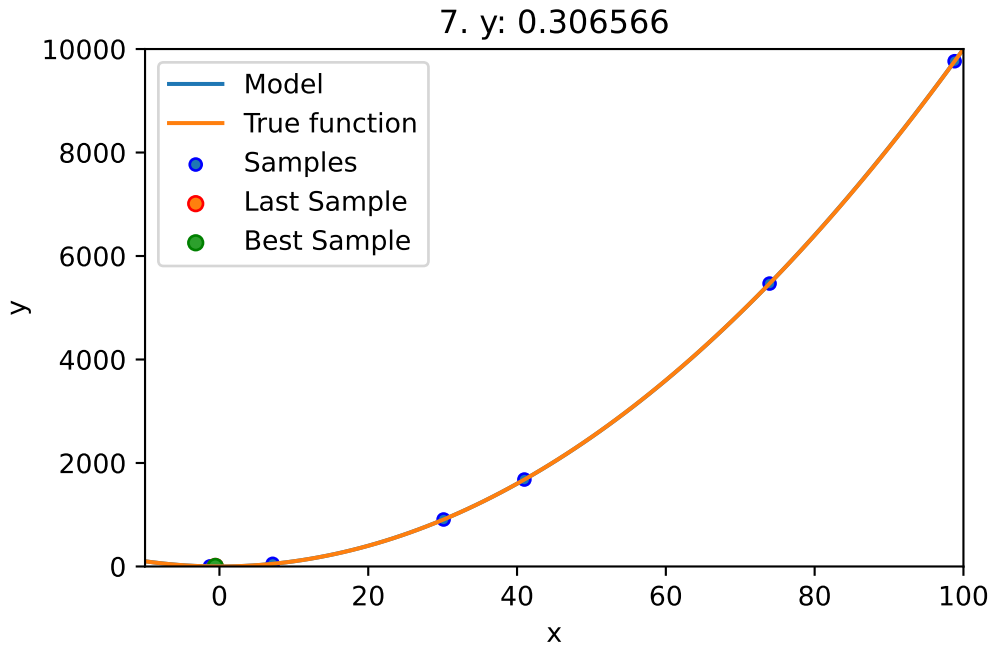
external parameter	type	description	default	mandatory
`max_iter`	int	max number of iterations. Note: these are the cheap evaluations on the surrogate.	`1000`	no

21.6 Run

```
spot_1.run()
```








```
<spotPython.spot.spot.Spot at 0x17ed8a9e0>
```

21.7 Print the Results

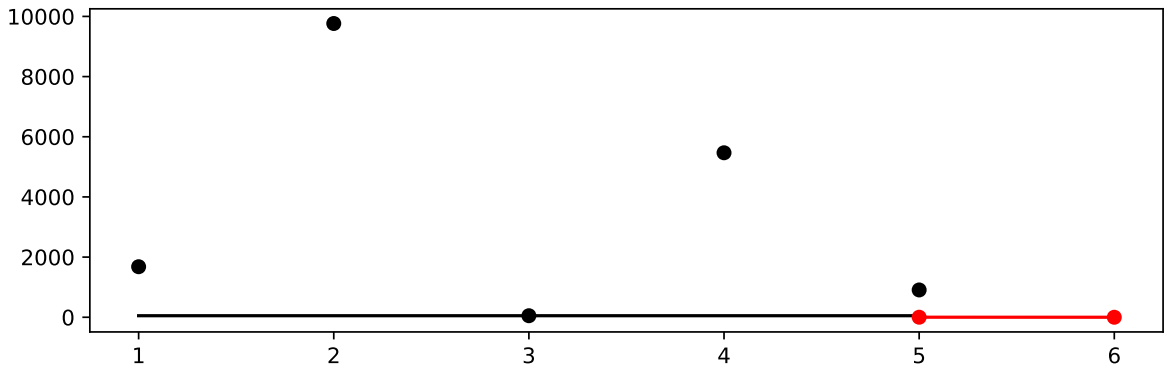
```
spot_1.print_results()
```

```
min y: 0.30656551286610595
x0: -0.5536835855126157

[['x0', -0.5536835855126157]]
```

21.8 Show the Progress

```
spot_1.plot_progress()
```

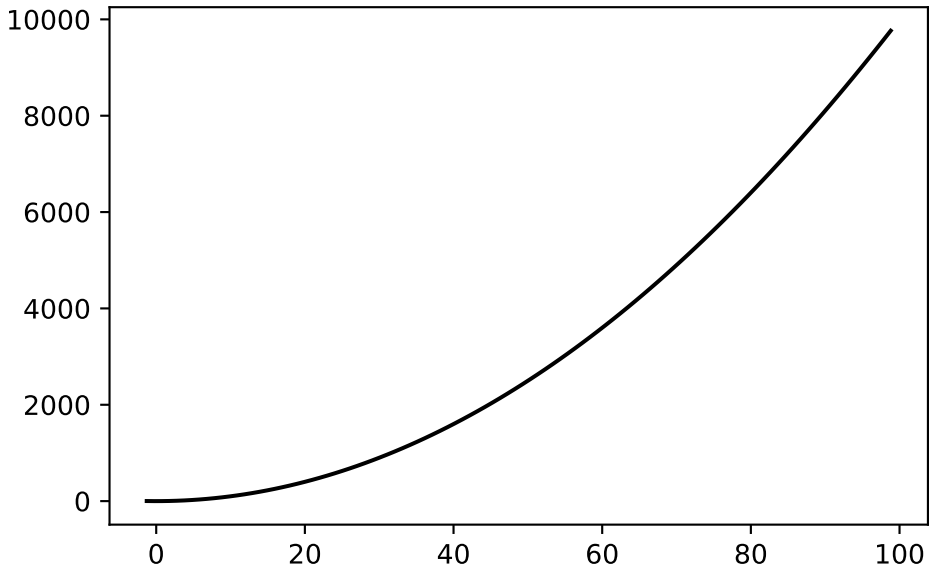


21.9 Visualize the Surrogate

- The plot method of the `kriging` surrogate is used.
- Note: the plot uses the interval defined by the ranges of the natural variables.

```
spot_1.surrogate.plot()
```

```
<Figure size 2700x1800 with 0 Axes>
```



21.10 Init: Build Initial Design

```
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
from spotPython.fun.objectivefunctions import analytical
gen = spacefilling(2)
rng = np.random.RandomState(1)
lower = np.array([-5,-0])
upper = np.array([10,15])
fun = analytical().fun_branin
fun_control = {"sigma": 0,
               "seed": 123}

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
```

```
[[ 8.97647221 13.41926847]
 [ 0.66946019  1.22344228]
 [ 5.23614115 13.78185824]
 [ 5.6149825  11.5851384 ]
```

```
 [-1.72963184  1.66516096]
 [-4.26945568  7.1325531 ]
 [ 1.26363761 10.17935555]
 [ 2.88779942  8.05508969]
 [-3.39111089  4.15213772]
 [ 7.30131231  5.22275244]]
[128.95676449  31.73474356 172.89678121 126.71295908  64.34349975
  70.16178611  48.71407916  31.77322887  76.91788181  30.69410529]
```

21.11 Replicability

Seed

```
gen = spacefilling(2, seed=123)
X0 = gen.scipy_lhd(3)
gen = spacefilling(2, seed=345)
X1 = gen.scipy_lhd(3)
X2 = gen.scipy_lhd(3)
gen = spacefilling(2, seed=123)
X3 = gen.scipy_lhd(3)
X0, X1, X2, X3
```

```
(array([[0.77254938, 0.31539299],
        [0.59321338, 0.93854273],
        [0.27469803, 0.3959685 ]]),
 array([[0.78373509, 0.86811887],
        [0.06692621, 0.6058029 ],
        [0.41374778, 0.00525456]]),
 array([[0.121357  , 0.69043832],
        [0.41906219, 0.32838498],
        [0.86742658, 0.52910374]]),
 array([[0.77254938, 0.31539299],
        [0.59321338, 0.93854273],
        [0.27469803, 0.3959685 ]]))
```

21.12 Surrogates

21.12.1 A Simple Predictor

The code below shows how to use a simple model for prediction. Assume that only two (very costly) measurements are available:

1. f(0) = 0.5
2. f(2) = 2.5

We are interested in the value at $x_0 = 1$, i.e., $f(x_0 = 1)$, but cannot run an additional, third experiment.

```
from sklearn import linear_model
X = np.array([[0], [2]])
y = np.array([0.5, 2.5])
S_lm = linear_model.LinearRegression()
S_lm = S_lm.fit(X, y)
X0 = np.array([[1]])
y0 = S_lm.predict(X0)
print(y0)
```

```
[1.5]
```

Central Idea: Evaluation of the surrogate model `S_lm` is much cheaper (or / and much faster) than running the real-world experiment f.

21.13 Demo/Test: Objective Function Fails

SPOT expects `np.nan` values from failed objective function values. These are handled. Note: SPOT's counter considers only successful executions of the objective function.

```
import numpy as np
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
import numpy as np
from math import inf
# number of initial points:
ni = 20
# number of points
n = 30
```

```
fun = analytical().fun_random_error
lower = np.array([-1])
upper = np.array([1])
design_control={"init_size": ni}

spot_1 = spot.Spot(fun=fun,
            lower = lower,
            upper= upper,
            fun_evals = n,
            show_progress=False,
            design_control=design_control,)
spot_1.run()
# To check whether the run was successfully completed,
# we compare the number of evaluated points to the specified
# number of points.
assert spot_1.y.shape[0] == n
```

```
[ 0.53176481 -0.9053821  -0.02203599 -0.21843718  0.78240941 -0.58120945
 -0.3923345   0.67234256  0.31802454 -0.68898927 -0.75129705  0.97550354
  0.41757584  0.0786237   0.82585329  0.23700598 -0.49274073 -0.82319082
         nan  0.1481835 ]
[-1.]

[0.17335968]


[-0.58552368]

[-0.20126111]
[-0.60100809]

[-0.97897336]

[-0.2748985]
[0.8359486]

[0.99035591]
[0.01641232]

[0.5629346]
```

21.14 PyTorch: Detailed Description of the Data Splitting

21.14.1 Description of the "train_hold_out" Setting

The "train_hold_out" setting is used by default. It uses the loss function specfied in fun_control and the metric specified in fun_control.

1. First, the method HyperTorch().fun_torch is called.
2. fun_torc(), which is implemented in the file hypertorch.py, calls evaluate_hold_out() as follows:

```
df_eval, _ = evaluate_hold_out(
    model,
    train_dataset=fun_control["train"],
    shuffle=self.fun_control["shuffle"],
    loss_function=self.fun_control["loss_function"],
    metric=self.fun_control["metric_torch"],
    device=self.fun_control["device"],
    show_batch_interval=self.fun_control["show_batch_interval"],
    path=self.fun_control["path"],
    task=self.fun_control["task"],
    writer=self.fun_control["writer"],
    writerId=config_id,
)
```

Note: Only the data set fun_control["train"] is used for training and validation. It is used in evaluate_hold_out as follows:

```
trainloader, valloader = create_train_val_data_loaders(
                dataset=train_dataset, batch_size=batch_size_instance, shuffle=shuffle
            )
```

create_train_val_data_loaders() splits the train_dataset into trainloader and valloader using torch.utils.data.random_split() as follows:

```
def create_train_val_data_loaders(dataset, batch_size, shuffle, num_workers=0):
    test_abs = int(len(dataset) * 0.6)
    train_subset, val_subset = random_split(dataset, [test_abs, len(dataset) - test_abs])
    trainloader = torch.utils.data.DataLoader(
        train_subset, batch_size=int(batch_size), shuffle=shuffle, num_workers=num_workers
    )
    valloader = torch.utils.data.DataLoader(
```

```
        val_subset, batch_size=int(batch_size), shuffle=shuffle, num_workers=num_workers
    )
    return trainloader, valloader
```

The optimizer is set up as follows:

```
optimizer_instance = net.optimizer
lr_mult_instance = net.lr_mult
sgd_momentum_instance = net.sgd_momentum
optimizer = optimizer_handler(
    optimizer_name=optimizer_instance,
    params=net.parameters(),
    lr_mult=lr_mult_instance,
    sgd_momentum=sgd_momentum_instance,
)
```

3. `evaluate_hold_out()` sets the `net` attributes such as `epochs`, `batch_size`, `optimizer`, and `patience`. For each epoch, the methods `train_one_epoch()` and `validate_one_epoch()` are called, the former for training and the latter for validation and early stopping. The validation loss from the last epoch (not the best validation loss) is returned from `evaluate_hold_out`.
4. The method `train_one_epoch()` is implemented as follows:

```
def train_one_epoch(
    net,
    trainloader,
    batch_size,
    loss_function,
    optimizer,
    device,
    show_batch_interval=10_000,
    task=None,
):
    running_loss = 0.0
    epoch_steps = 0
    for batch_nr, data in enumerate(trainloader, 0):
        input, target = data
        input, target = input.to(device), target.to(device)
        optimizer.zero_grad()
        output = net(input)
        if task == "regression":
```

```
            target = target.unsqueeze(1)
            if target.shape == output.shape:
                loss = loss_function(output, target)
            else:
                raise ValueError(f"Shapes of target and output do not match:
                 {target.shape} vs {output.shape}")
        elif task == "classification":
            loss = loss_function(output, target)
        else:
            raise ValueError(f"Unknown task: {task}")
        loss.backward()
        torch.nn.utils.clip_grad_norm_(net.parameters(), max_norm=1.0)
        optimizer.step()
        running_loss += loss.item()
        epoch_steps += 1
        if batch_nr % show_batch_interval == (show_batch_interval - 1):
            print(
                "Batch: %5d. Batch Size: %d. Training Loss (running): %.3f"
                % (batch_nr + 1, int(batch_size), running_loss / epoch_steps)
            )
            running_loss = 0.0
    return loss.item()
```

5. The method `validate_one_epoch()` is implemented as follows:

```
def validate_one_epoch(net, valloader, loss_function, metric, device, task):
    val_loss = 0.0
    val_steps = 0
    total = 0
    correct = 0
    metric.reset()
    for i, data in enumerate(valloader, 0):
        # get batches
        with torch.no_grad():
            input, target = data
            input, target = input.to(device), target.to(device)
            output = net(input)
            # print(f"target: {target}")
            # print(f"output: {output}")
            if task == "regression":
                target = target.unsqueeze(1)
```

```
                if target.shape == output.shape:
                    loss = loss_function(output, target)
                else:
                    raise ValueError(f"Shapes of target and output
                        do not match: {target.shape} vs {output.shape}")
                metric_value = metric.update(output, target)
            elif task == "classification":
                loss = loss_function(output, target)
                metric_value = metric.update(output, target)
                _, predicted = torch.max(output.data, 1)
                total += target.size(0)
                correct += (predicted == target).sum().item()
            else:
                raise ValueError(f"Unknown task: {task}")
            val_loss += loss.cpu().numpy()
            val_steps += 1
    loss = val_loss / val_steps
    print(f"Loss on hold-out set: {loss}")
    if task == "classification":
        accuracy = correct / total
        print(f"Accuracy on hold-out set: {accuracy}")
    # metric on all batches using custom accumulation
    metric_value = metric.compute()
    metric_name = type(metric).__name__
    print(f"{metric_name} value on hold-out data: {metric_value}")
    return metric_value, loss
```

21.14.1.1 Description of the `"test_hold_out"` Setting

It uses the loss function specfied in `fun_control` and the metric specified in `fun_control`.

1. First, the method `HyperTorch().fun_torch` is called.
2. `fun_torc()` calls `spotPython.torch.traintest.evaluate_hold_out()` similar to the `"train_hold_out"` setting with one exception: It passes an additional `test` data set to `evaluate_hold_out()` as follows:

```
test_dataset=fun_control["test"]
```

`evaluate_hold_out()` calls `create_train_test_data_loaders` instead of `create_train_val_data_loaders`: The two data sets are used in `create_train_test_data_loaders` as follows:

```
def create_train_test_data_loaders(dataset, batch_size, shuffle, test_dataset,
        num_workers=0):
    trainloader = torch.utils.data.DataLoader(
        dataset, batch_size=int(batch_size), shuffle=shuffle,
        num_workers=num_workers
    )
    testloader = torch.utils.data.DataLoader(
        test_dataset, batch_size=int(batch_size), shuffle=shuffle,
        num_workers=num_workers
    )
    return trainloader, testloader
```

3. The following steps are identical to the `"train_hold_out"` setting. Only a different data loader is used for testing.

21.14.1.2 Detailed Description of the `"train_cv"` Setting

It uses the loss function specfied in `fun_control` and the metric specified in `fun_control`.

1. First, the method `HyperTorch().fun_torch` is called.
2. `fun_torc()` calls `spotPython.torch.traintest.evaluate_cv()` as follows (Note: Only the data set `fun_control["train"]` is used for CV.):

```
df_eval, _ = evaluate_cv(
    model,
    dataset=fun_control["train"],
    shuffle=self.fun_control["shuffle"],
    device=self.fun_control["device"],
    show_batch_interval=self.fun_control["show_batch_interval"],
    task=self.fun_control["task"],
    writer=self.fun_control["writer"],
    writerId=config_id,
)
```

3. In ‘evaluate_cv(), the following steps are performed: The optimizer is set up as follows:

```
optimizer_instance = net.optimizer
lr_instance = net.lr
sgd_momentum_instance = net.sgd_momentum
optimizer = optimizer_handler(optimizer_name=optimizer_instance,
     params=net.parameters(), lr_mult=lr_mult_instance)
```

`evaluate_cv()` sets the `net` attributes such as `epochs`, `batch_size`, `optimizer`, and `patience`. CV is implemented as follows:

```
def evaluate_cv(
    net,
    dataset,
    shuffle=False,
    loss_function=None,
    num_workers=0,
    device=None,
    show_batch_interval=10_000,
    metric=None,
    path=None,
    task=None,
    writer=None,
    writerId=None,
):
    lr_mult_instance = net.lr_mult
    epochs_instance = net.epochs
    batch_size_instance = net.batch_size
    k_folds_instance = net.k_folds
    optimizer_instance = net.optimizer
    patience_instance = net.patience
    sgd_momentum_instance = net.sgd_momentum
    removed_attributes, net = get_removed_attributes_and_base_net(net)
    metric_values = {}
    loss_values = {}
    try:
        device = getDevice(device=device)
        if torch.cuda.is_available():
            device = "cuda:0"
            if torch.cuda.device_count() > 1:
                print("We will use", torch.cuda.device_count(), "GPUs!")
                net = nn.DataParallel(net)
        net.to(device)
        optimizer = optimizer_handler(
            optimizer_name=optimizer_instance,
            params=net.parameters(),
            lr_mult=lr_mult_instance,
            sgd_momentum=sgd_momentum_instance,
        )
        kfold = KFold(n_splits=k_folds_instance, shuffle=shuffle)
```

```
        for fold, (train_ids, val_ids) in enumerate(kfold.split(dataset)):
            print(f"Fold: {fold + 1}")
            train_subsampler = torch.utils.data.SubsetRandomSampler(train_ids)
            val_subsampler = torch.utils.data.SubsetRandomSampler(val_ids)
            trainloader = torch.utils.data.DataLoader(
                dataset, batch_size=batch_size_instance,
                sampler=train_subsampler, num_workers=num_workers
            )
            valloader = torch.utils.data.DataLoader(
                dataset, batch_size=batch_size_instance,
                sampler=val_subsampler, num_workers=num_workers
            )
            # each fold starts with new weights:
            reset_weights(net)
            # Early stopping parameters
            best_val_loss = float("inf")
            counter = 0
            for epoch in range(epochs_instance):
                print(f"Epoch: {epoch + 1}")
                # training loss from one epoch:
                training_loss = train_one_epoch(
                    net=net,
                    trainloader=trainloader,
                    batch_size=batch_size_instance,
                    loss_function=loss_function,
                    optimizer=optimizer,
                    device=device,
                    show_batch_interval=show_batch_interval,
                    task=task,
                )
                # Early stopping check. Calculate validation loss from one epoch:
                metric_values[fold], loss_values[fold] = validate_one_epoch(
                    net, valloader=valloader, loss_function=loss_function,
                    metric=metric, device=device, task=task
                )
                # Log the running loss averaged per batch
                metric_name = "Metric"
                if metric is None:
                    metric_name = type(metric).__name__
                    print(f"{metric_name} value on hold-out data:
                        {metric_values[fold]}")
```

```
                if writer is not None:
                    writer.add_scalars(
                        "evaluate_cv fold:" + str(fold + 1) +
                        ". Train & Val Loss and Val Metric" + writerId,
                        {"Train loss": training_loss, "Val loss":
                        loss_values[fold], metric_name: metric_values[fold]},
                        epoch + 1,
                    )
                    writer.flush()
                if loss_values[fold] < best_val_loss:
                    best_val_loss = loss_values[fold]
                    counter = 0
                    # save model:
                    if path is not None:
                        torch.save(net.state_dict(), path)
                else:
                    counter += 1
                    if counter >= patience_instance:
                        print(f"Early stopping at epoch {epoch}")
                        break
        df_eval = sum(loss_values.values()) / len(loss_values.values())
        df_metrics = sum(metric_values.values()) / len(metric_values.values())
        df_preds = np.nan
    except Exception as err:
        print(f"Error in Net_Core. Call to evaluate_cv() failed. {err=},
            {type(err)=}")
        df_eval = np.nan
        df_preds = np.nan
    add_attributes(net, removed_attributes)
    if writer is not None:
        metric_name = "Metric"
        if metric is None:
            metric_name = type(metric).__name__
        writer.add_scalars(
            "CV: Val Loss and Val Metric" + writerId,
            {"CV-loss": df_eval, metric_name: df_metrics},
            epoch + 1,
        )
        writer.flush()
    return df_eval, df_preds, df_metrics
```

4. The method `train_fold()` is implemented as shown above.

5. The method `validate_one_epoch()` is implemented as shown above. In contrast to the hold-out setting, it is called for each of the k folds. The results are stored in a dictionaries `metric_values` and `loss_values`. The results are averaged over the k folds and returned as `df_eval`.

21.14.1.3 Detailed Description of the `"test_cv"` Setting

It uses the loss function specfied in `fun_control` and the metric specified in `fun_control`.

1. First, the method `HyperTorch().fun_torch` is called.
2. `fun_torc()` calls `spotPython.torch.traintest.evaluate_cv()` as follows:

```
df_eval, _ = evaluate_cv(
    model,
    dataset=fun_control["test"],
    shuffle=self.fun_control["shuffle"],
    device=self.fun_control["device"],
    show_batch_interval=self.fun_control["show_batch_interval"],
    task=self.fun_control["task"],
    writer=self.fun_control["writer"],
    writerId=config_id,
)
```

Note: The data set `fun_control["test"]` is used for CV. The rest is the same as for the `"train_cv"` setting.

21.14.1.4 Detailed Description of the Final Model Training and Evaluation

There are two methods that can be used for the final evaluation of a Pytorch model:

1. `"train_tuned` and
2. `"test_tuned"`.

`train_tuned()` is just a wrapper to `evaluate_hold_out` using the `train` data set. It is implemented as follows:

```
def train_tuned(
    net,
    train_dataset,
    shuffle,
    loss_function,
    metric,
```

```
    device=None,
    show_batch_interval=10_000,
    path=None,
    task=None,
    writer=None,
):
    evaluate_hold_out(
        net=net,
        train_dataset=train_dataset,
        shuffle=shuffle,
        test_dataset=None,
        loss_function=loss_function,
        metric=metric,
        device=device,
        show_batch_interval=show_batch_interval,
        path=path,
        task=task,
        writer=writer,
    )
```

The `test_tuned()` procedure is implemented as follows:

```
def test_tuned(net, shuffle, test_dataset=None, loss_function=None,
    metric=None, device=None, path=None, task=None):
    batch_size_instance = net.batch_size
    removed_attributes, net = get_removed_attributes_and_base_net(net)
    if path is not None:
        net.load_state_dict(torch.load(path))
        net.eval()
    try:
        device = getDevice(device=device)
        if torch.cuda.is_available():
            device = "cuda:0"
            if torch.cuda.device_count() > 1:
                print("We will use", torch.cuda.device_count(), "GPUs!")
                net = nn.DataParallel(net)
        net.to(device)
        valloader = torch.utils.data.DataLoader(
            test_dataset, batch_size=int(batch_size_instance),
            shuffle=shuffle,
            num_workers=0
        )
```

```
        metric_value, loss = validate_one_epoch(
            net, valloader=valloader, loss_function=loss_function,
            metric=metric, device=device, task=task
        )
        df_eval = loss
        df_metric = metric_value
        df_preds = np.nan
    except Exception as err:
        print(f"Error in Net_Core. Call to test_tuned() failed. {err=},
            {type(err)=}")
        df_eval = np.nan
        df_metric = np.nan
        df_preds = np.nan
    add_attributes(net, removed_attributes)
    print(f"Final evaluation: Validation loss: {df_eval}")
    print(f"Final evaluation: Validation metric: {df_metric}")
    print("------------------------------------------------")
    return df_eval, df_preds, df_metric
```

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