Hyperparameter-tuning Cookbook

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

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Table of contents

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:

```
@ARTICLE{bart23earxiv,
       author = {{Bartz-Beielstein}, Thomas},
        title = "{PyTorch Hyperparameter Tuning -- A Tutorial for spotPython}",
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         year = 2023,
        month = may,
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          doi = {10.48550/arXiv.2305.11930},
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      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 18 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 18.1 describes the setup of the tuners. Section 18.3 describes the data loading. Section 18.4 describes the model to be tuned. The search space is introduced in Section 18.5. Optimizers are presented in Section 18.6. How to split the data in train, validation, and test sets is described in Section 18.7. The selection of the loss function and metrics is described in Section 18.8. @#sec-prepare-spot-call describes the preparation of the `spotPython` call. The objective function is described in Section 18.10. How to use results from previous runs and default hyperparameter configurations is described in Section 18.11. Starting the tuner is shown in Section 18.12. TensorBoard can be used to visualize the results as shown in Section 18.13. Results are discussed and explained in Section 18.14 Finally, Section 18.15 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 18.3.
2. Specification of the preprocessing model, see Section 18.4.1. 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 18.4.2. 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 18.5.3.1. 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 18.8.
6. Calling SPOT with the corresponding parameters, see Section 18.12. The results are stored in a dictionary and are available for further analysis.
7. Presentation, visualization and interpretation of the results, see Section 18.14.

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

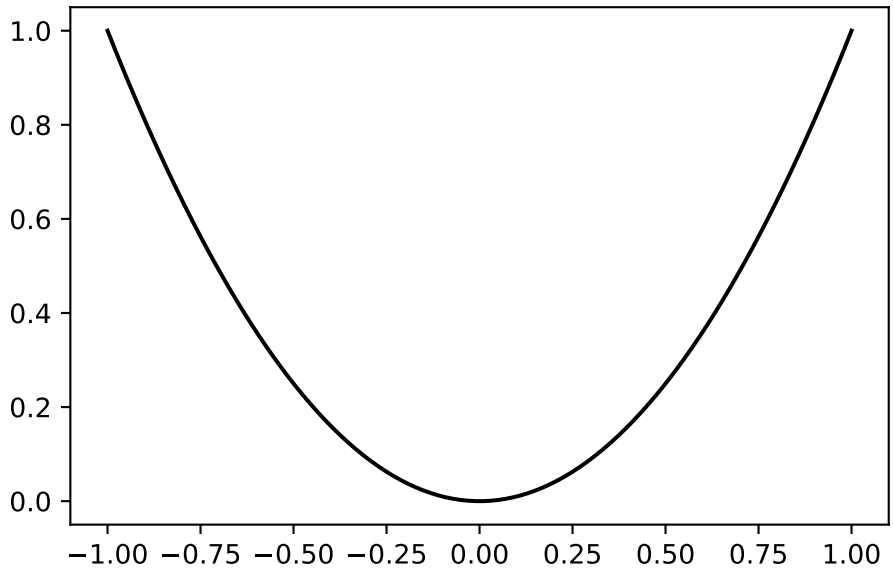
The `spotPython` package provides several classes of objective functions. We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

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

```
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]))
```

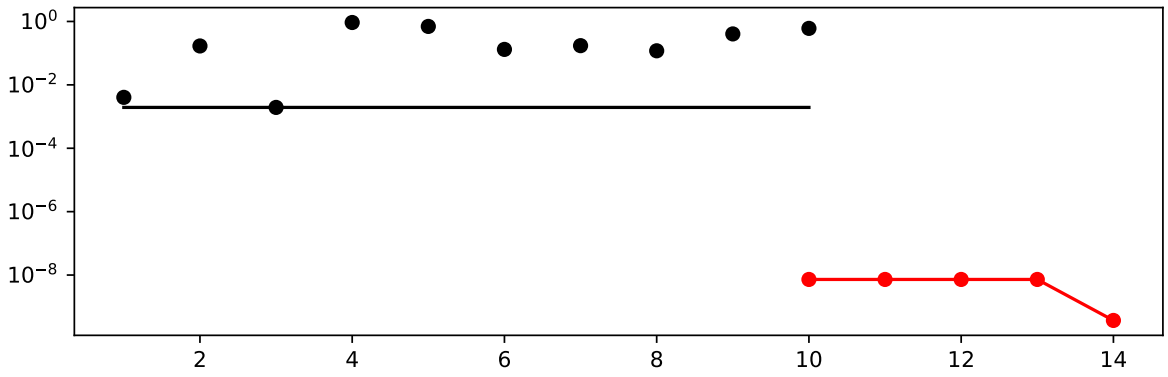
```
spot_0.run()
```

```
<spotPython.spot.spot.Spot at 0x10755cc70>
```

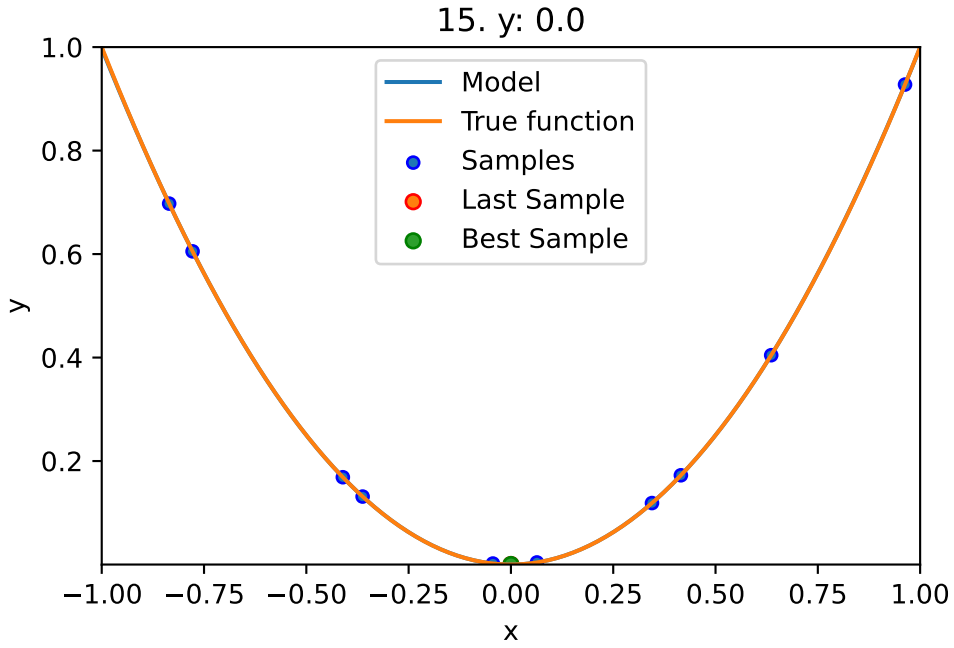
```
spot_0.print_results()
```

```
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`

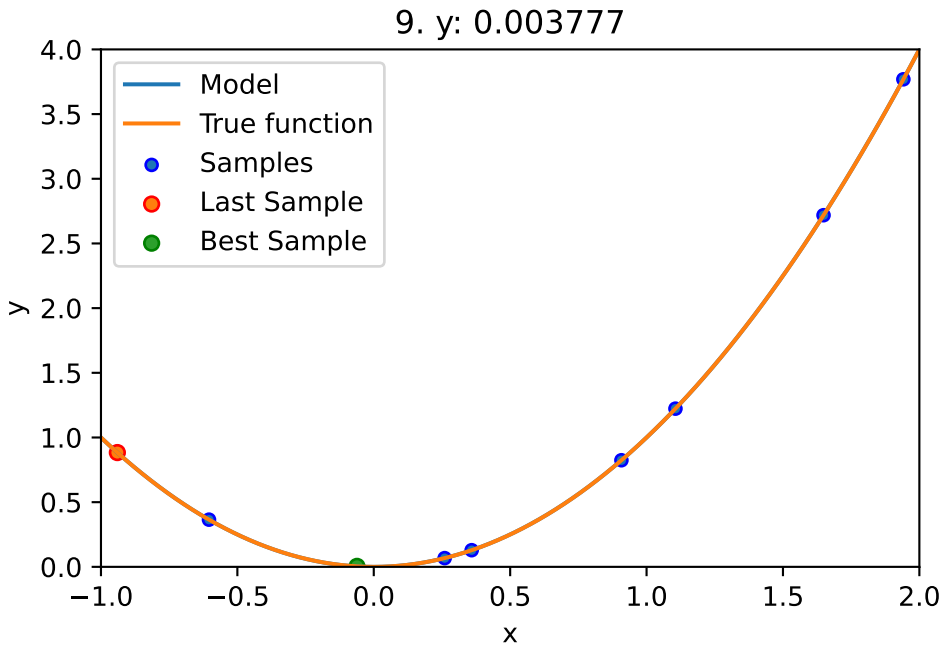
We will modify three parameters:

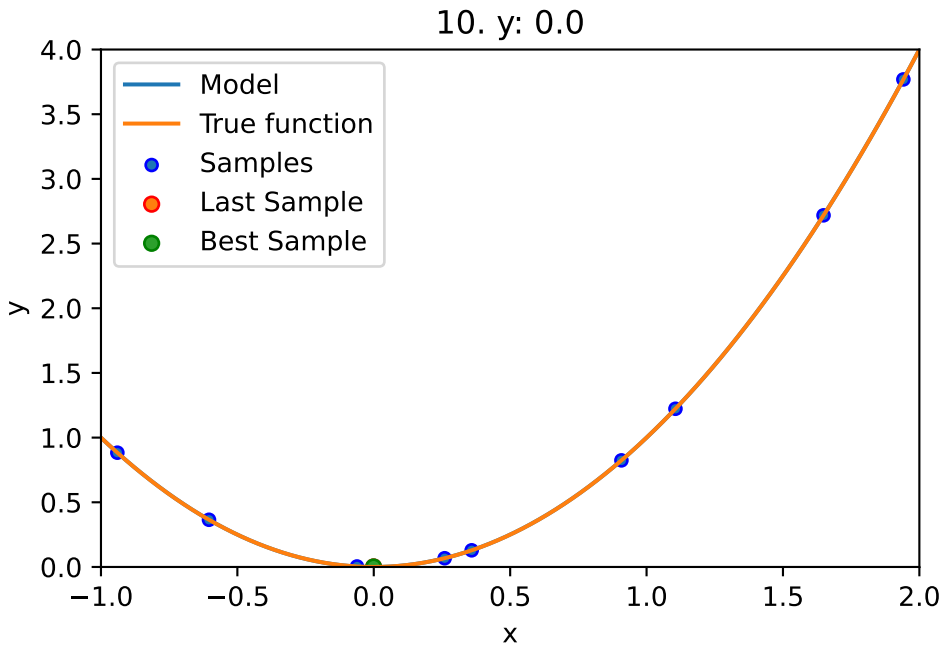
1. The number of function evaluations (`fun_evals`)
2. The size of the initial design (`init_size`)

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 0x13999d660>
```

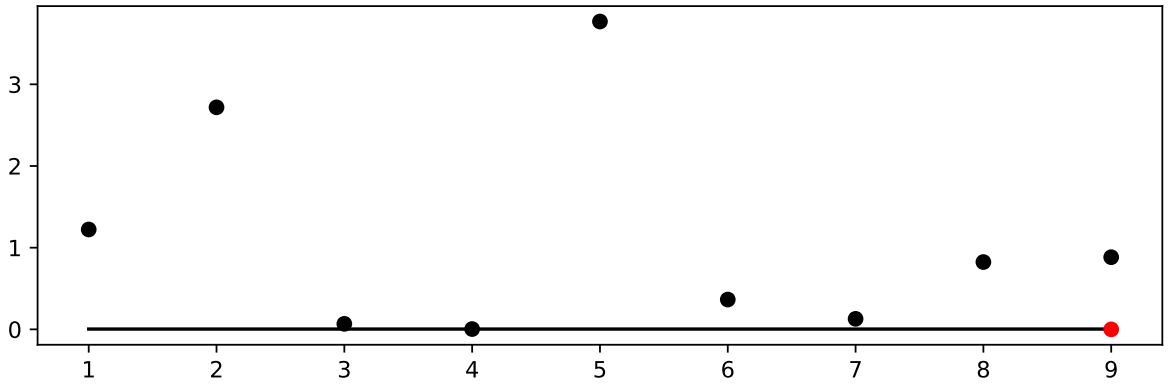
1.5 Print the Results

```
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()
```

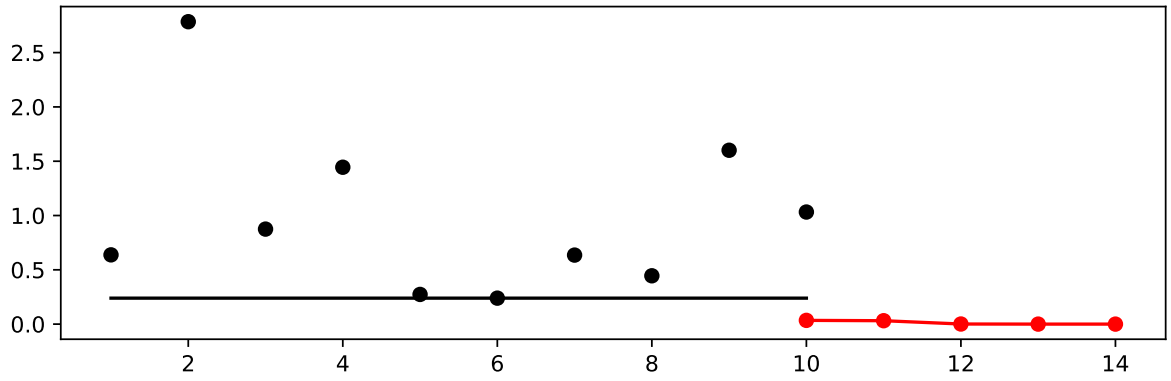
```
spotPython tuning: 0.03443344056467332 [#######---] 73.33%

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 0x10505c070>
```

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]]
```

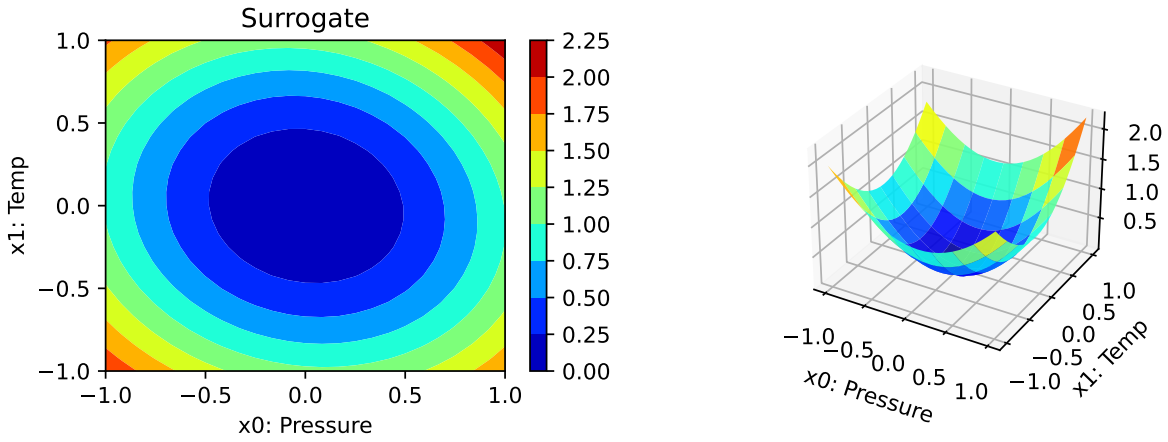
```
spot_3.plot_progress()
```



2.1.3 A Contour Plot

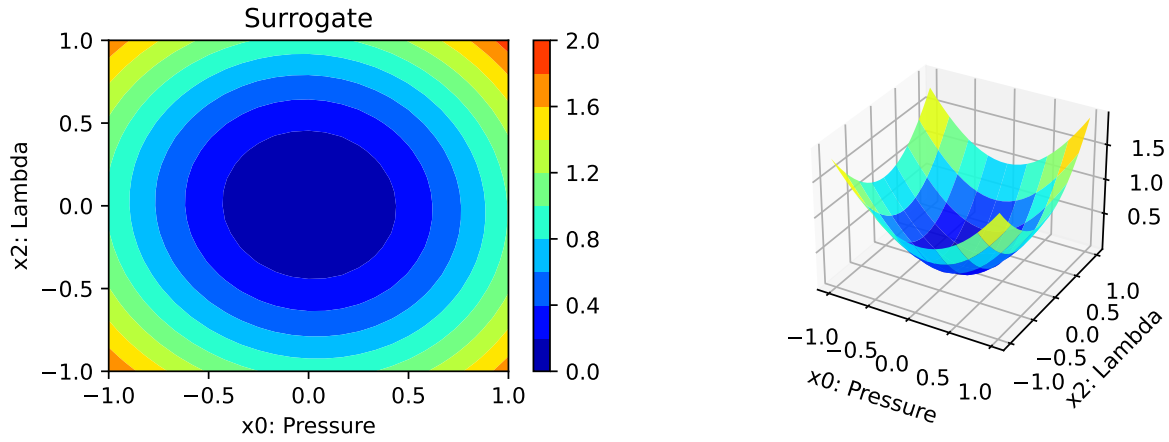
- We can select two dimensions, say $i = 0$ and $j = 1$, and generate a contour plot as follows.
  - Note: We have specified identical `min_z` and `max_z` values to generate comparable plots!

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



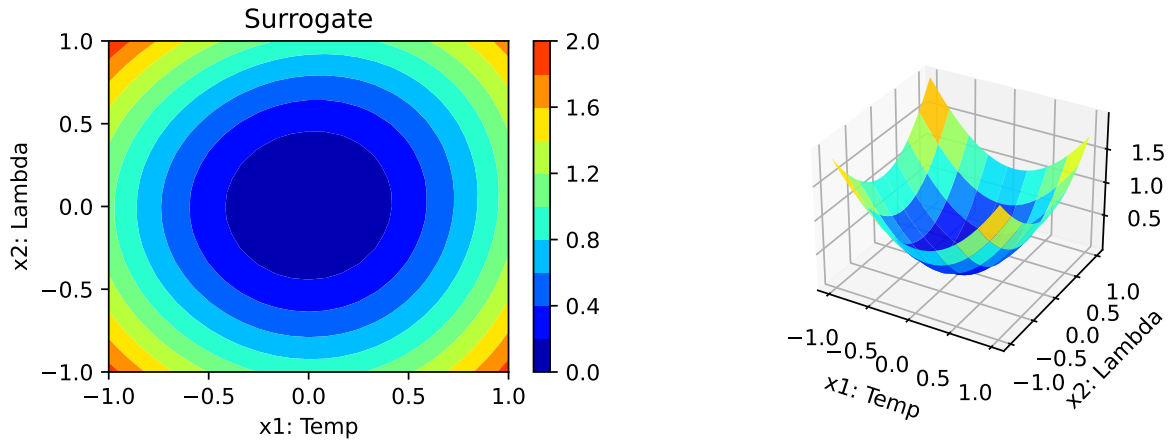
- In a similar manner, we can plot dimension $i = 0$ and $j = 2$:

```
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()
```

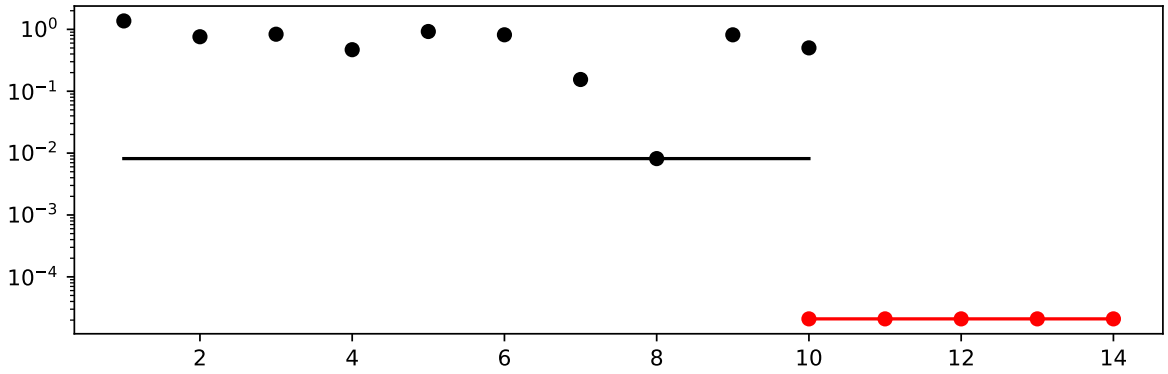
```
<spotPython.spot.spot.Spot at 0x29775bb50>
```

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 0x2b353f6d0>
```

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])
```

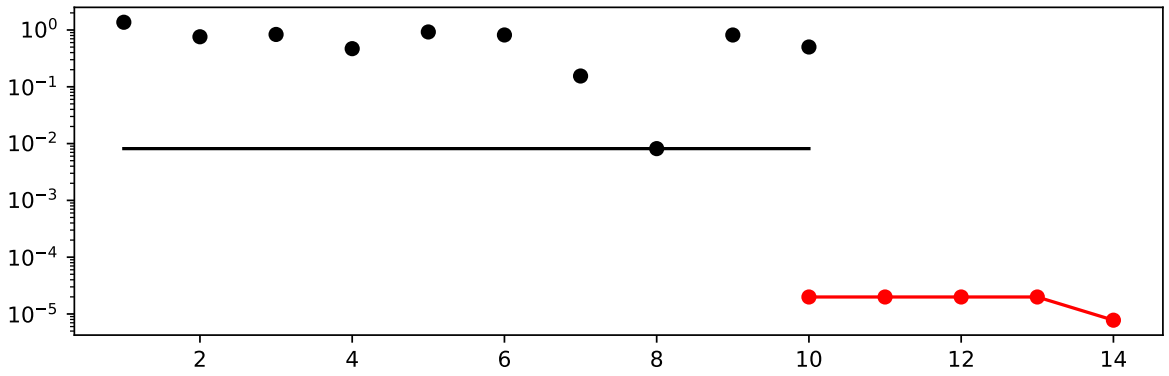
- Since the surrogate from the isotropic setting was stored as `spot_2`, we can also take a look at the `theta` value from this model:

```
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)
```

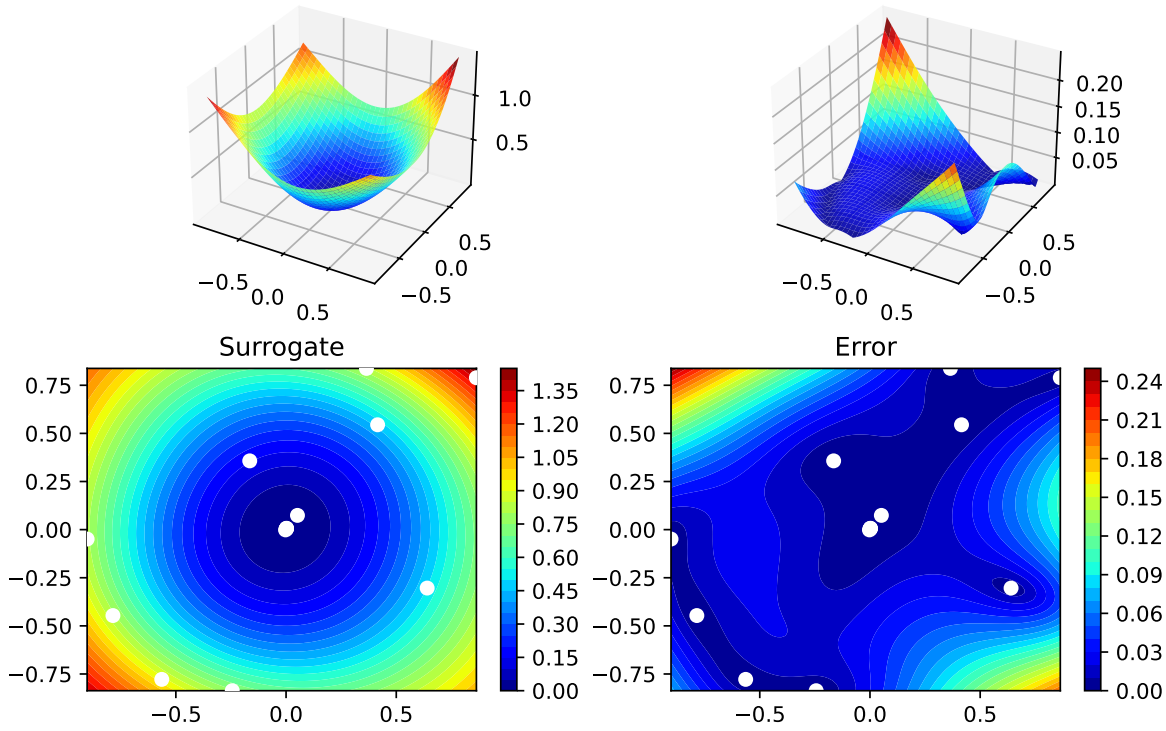


```
spot_2_anisotropic.print_results()
```

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

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

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



4 Exercises

4.1 `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,
```

4.2 `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`.

4.3 `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`.

4.4 `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`.

5 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
```

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

5.1.1 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
```

5.1.2 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 0x103e5dae0>
```

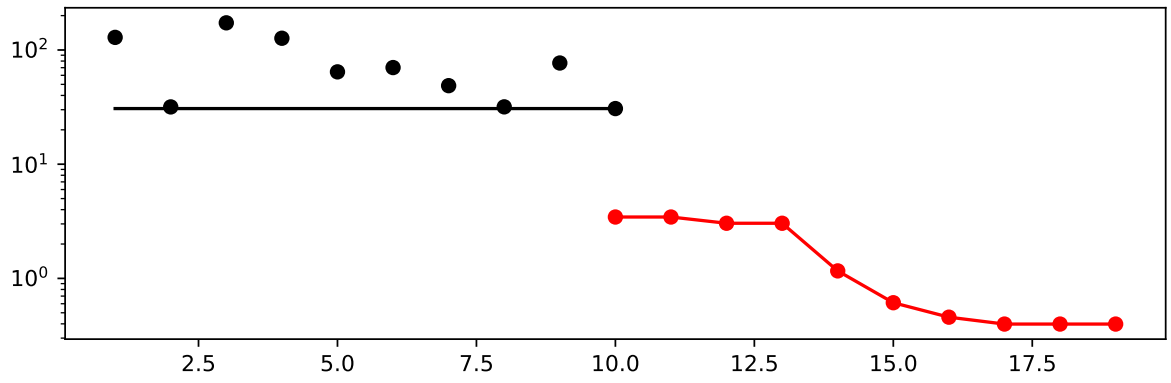
5.1.3 Print the Results

```
spot_2.print_results()
```

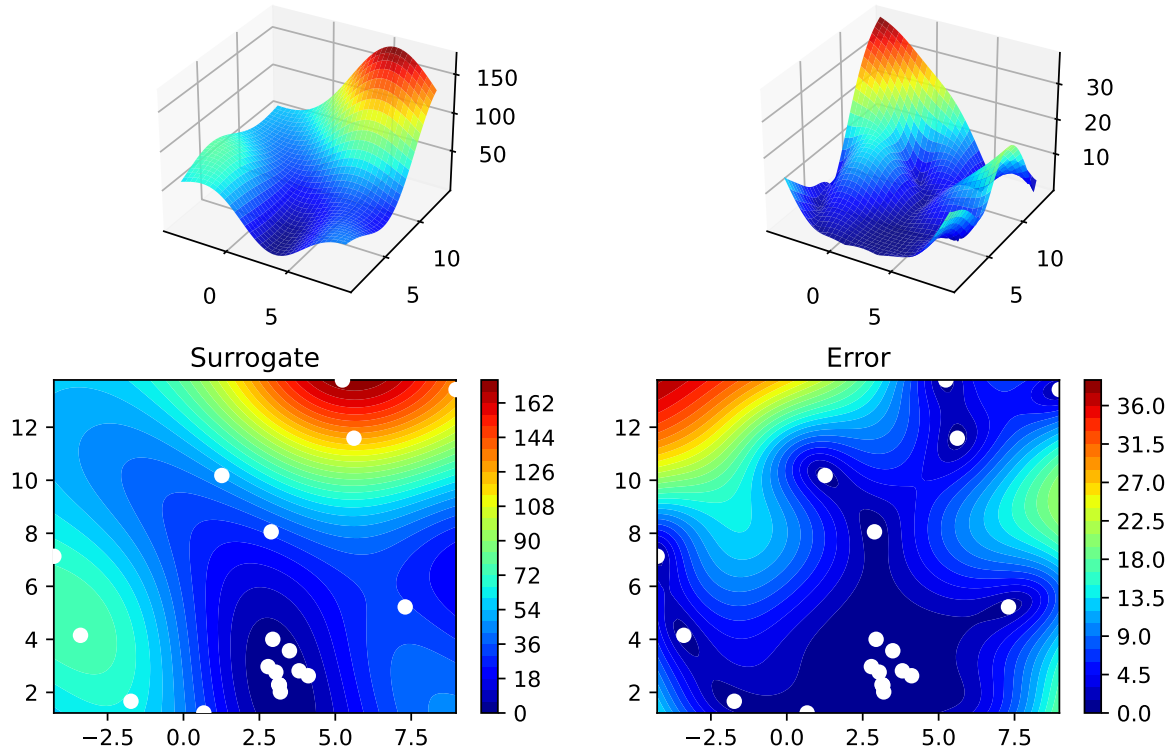
```
min y: 0.3982295132785083
x0: 3.135528626303215
x1: 2.2926027772585886

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

5.1.4 Show the Progress and the Surrogate

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




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



5.2 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)
```

5.2.1 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)
```

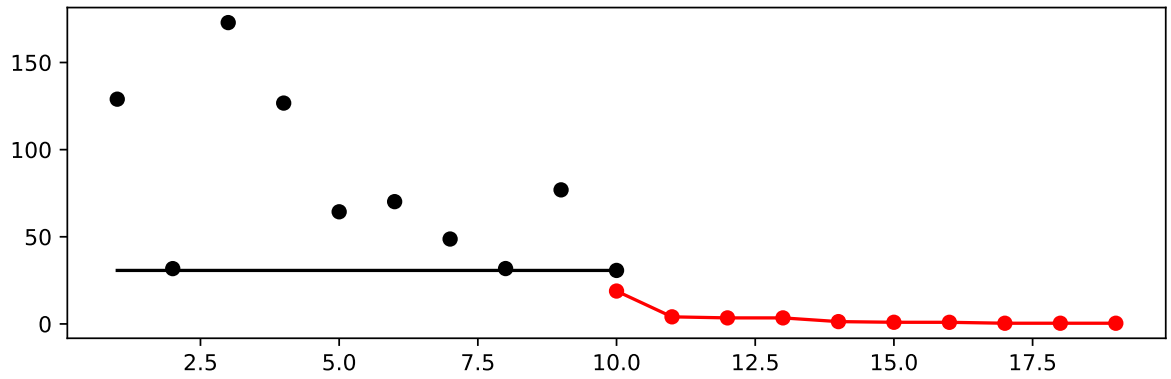
```
True
```

- 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 0x2a50626b0>
```

```
spot_2_GP.plot_progress()
```




```
spot_2_GP.print_results()
```

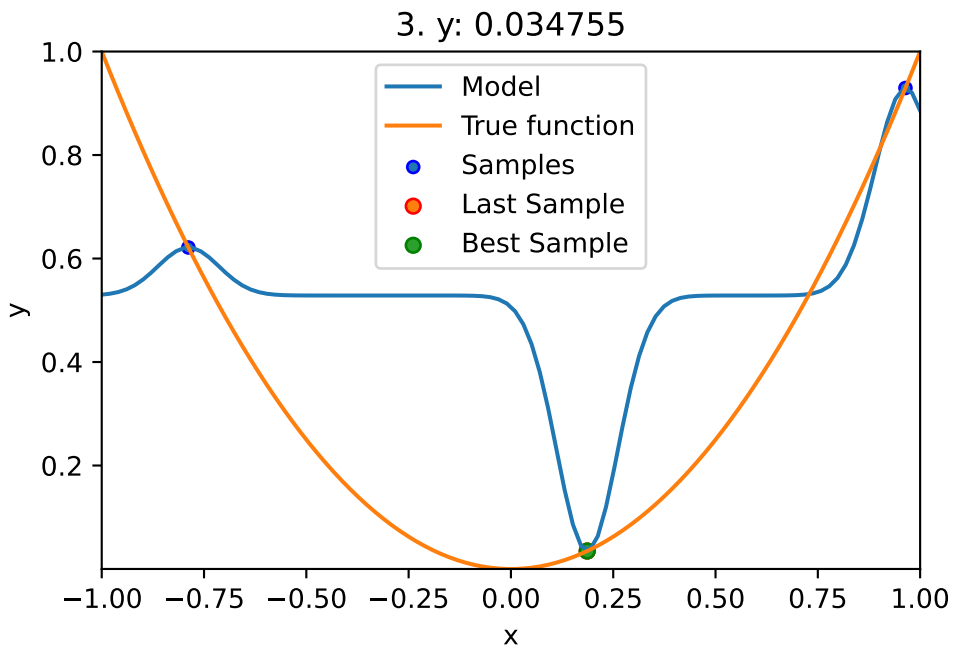
```
min y: 0.39818703958416535
x0: 3.1490973266645073
x1: 2.2745664396908745

[['x0', 3.1490973266645073], ['x1', 2.2745664396908745]]
```

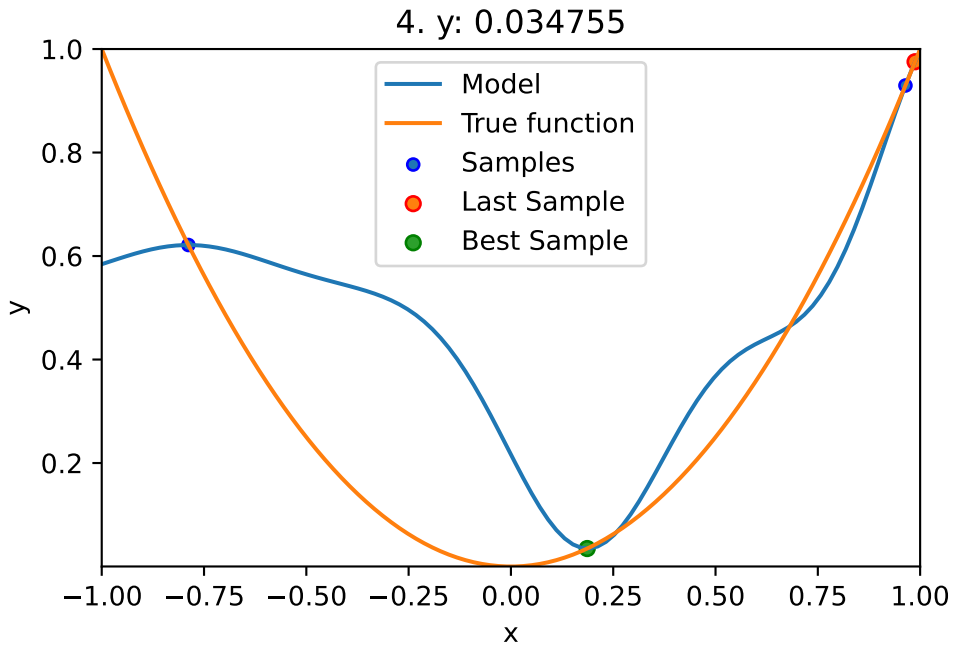
6 Example: One-dimensional Sphere Function With spotPython's Kriging

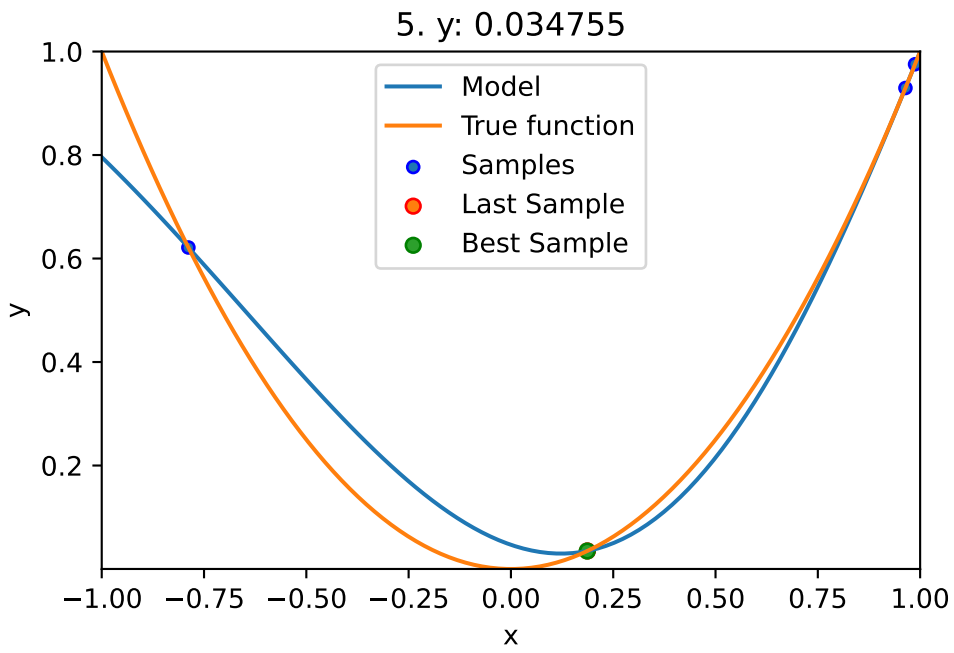
- In this example, we will use an one-dimensional function, which allows us to visualize the optimization process.
  - `show_models= True` is added to the argument list.

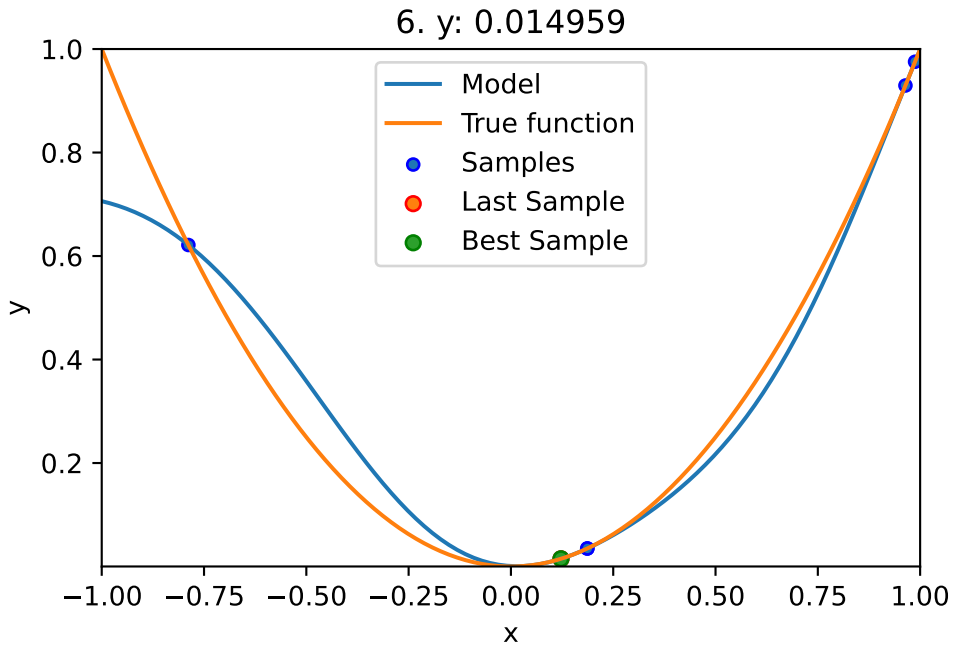
```
from spotPython.fun.objectivefunctions import analytical
lower = np.array([-1])
upper = np.array([1])
fun = analytical(seed=123).fun_sphere
```

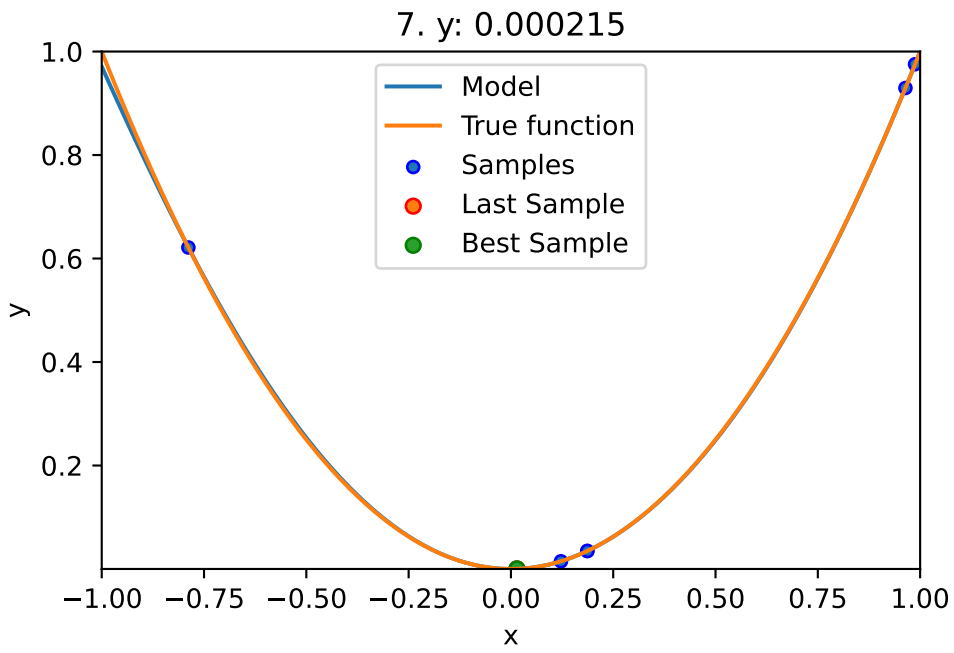
```
spot_1 = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = 10,
                   max_time = inf,
                   seed=123,
                   show_models= True,
                   tolerance_x = np.sqrt(np.spacing(1)),
      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

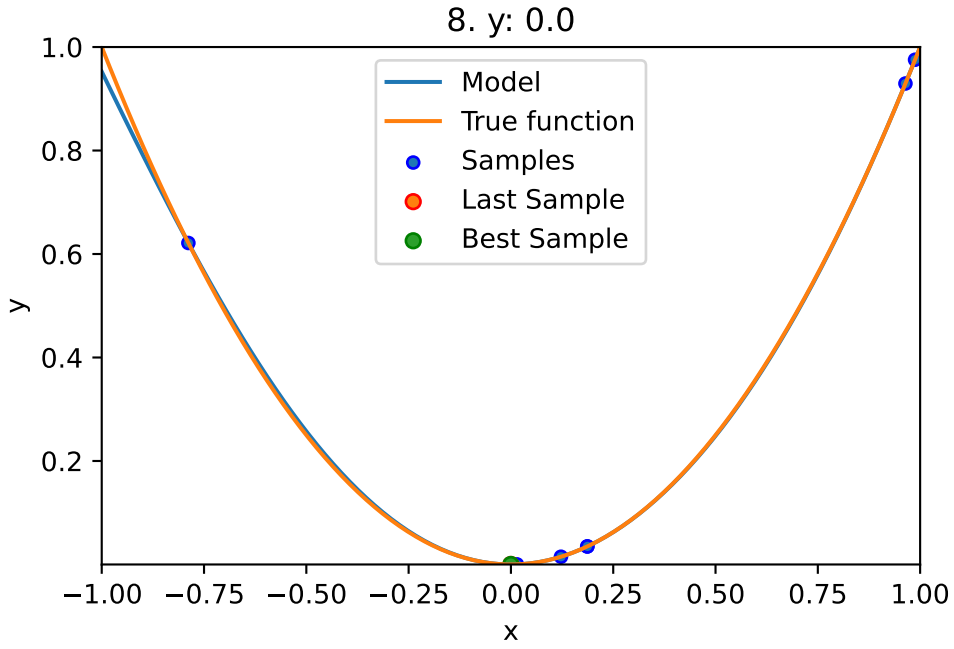

3. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

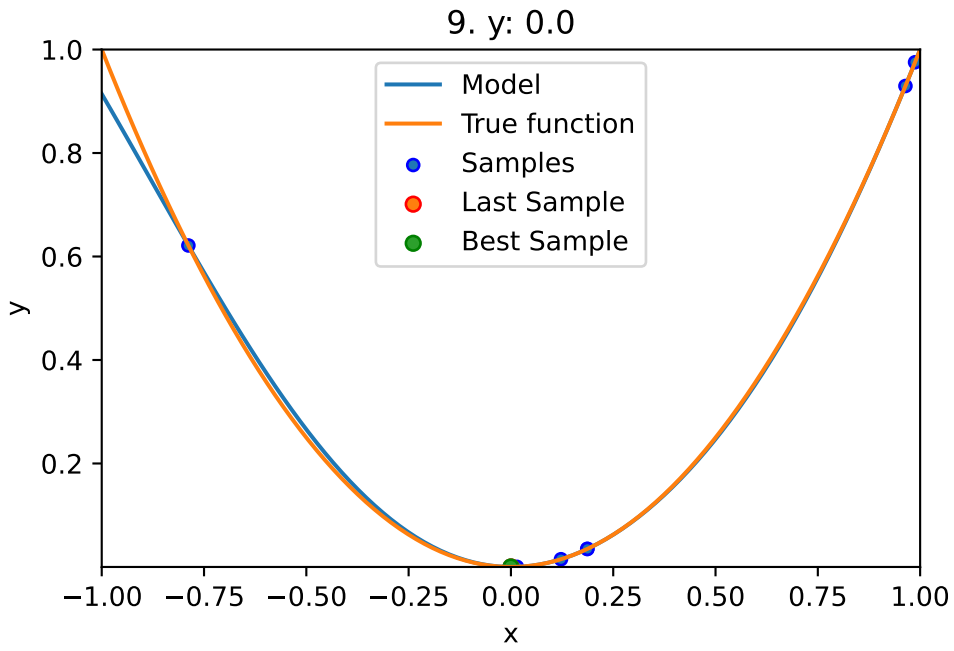

4. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

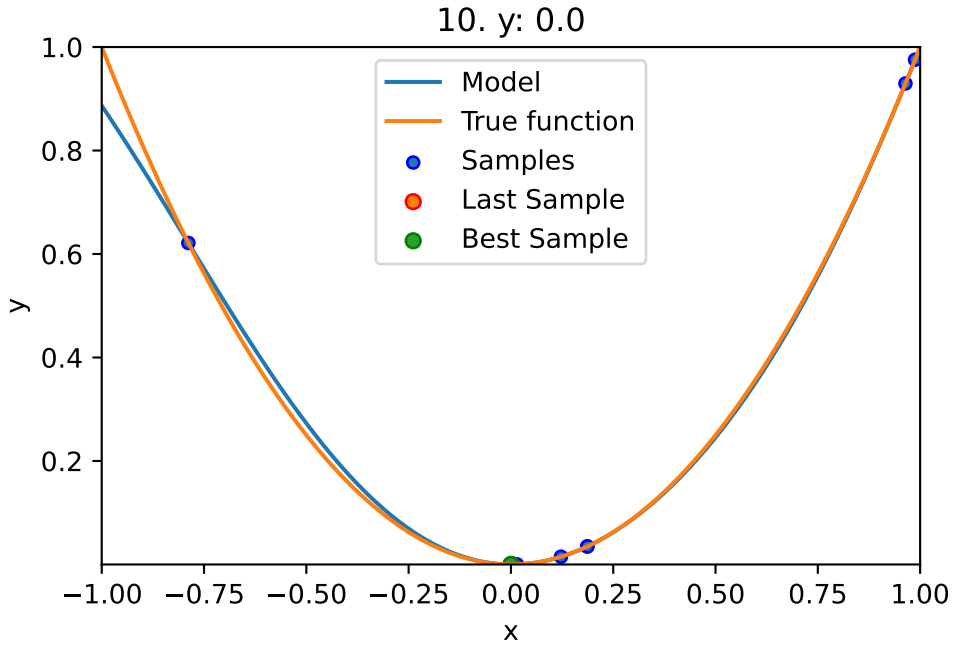

5. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


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





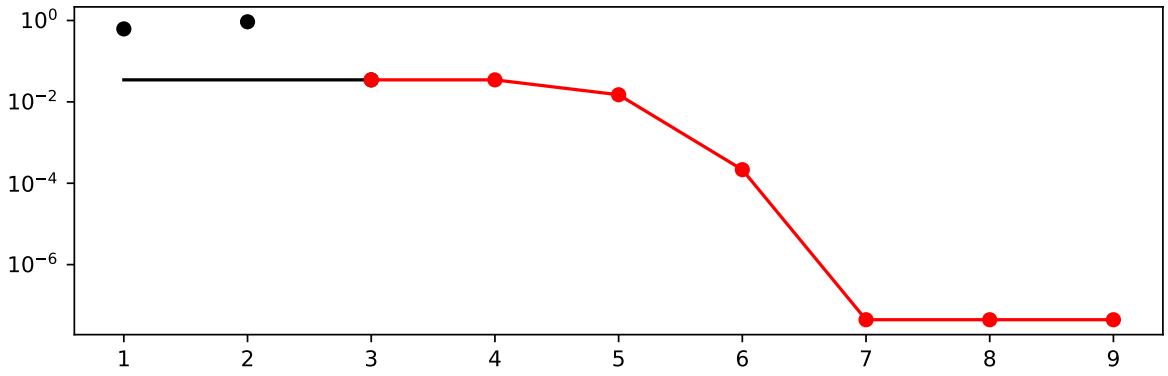

```
<spotPython.spot.spot.Spot at 0x2a50627a0>
```

6.0.1 Results

```
spot_1.print_results()
```

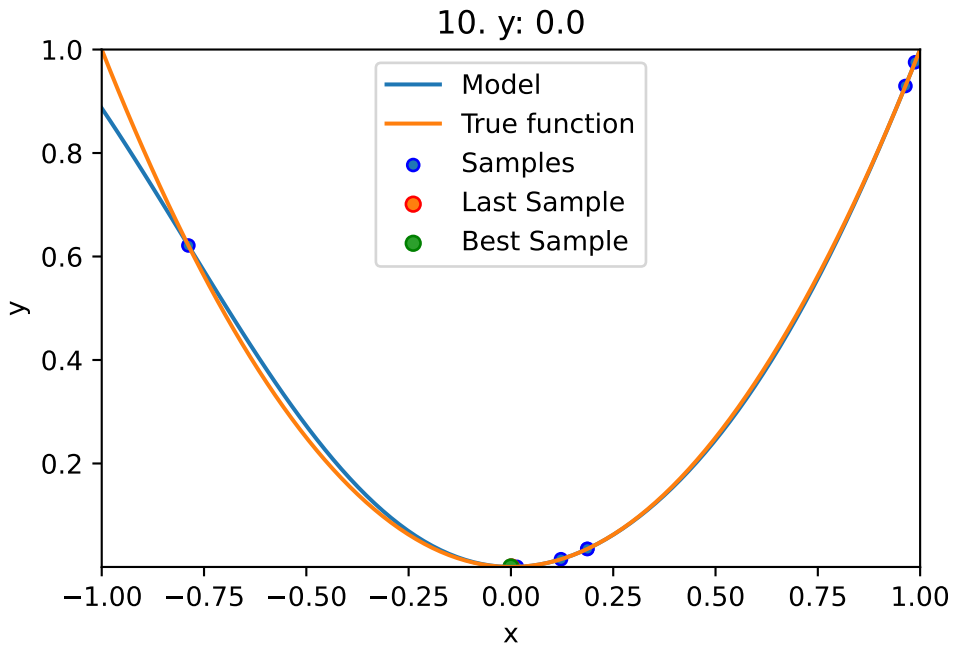
```
min y: 4.41925228274096e-08
x0: -0.00021022017702259125

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

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



- The method `plot_model` plots the final surrogate:

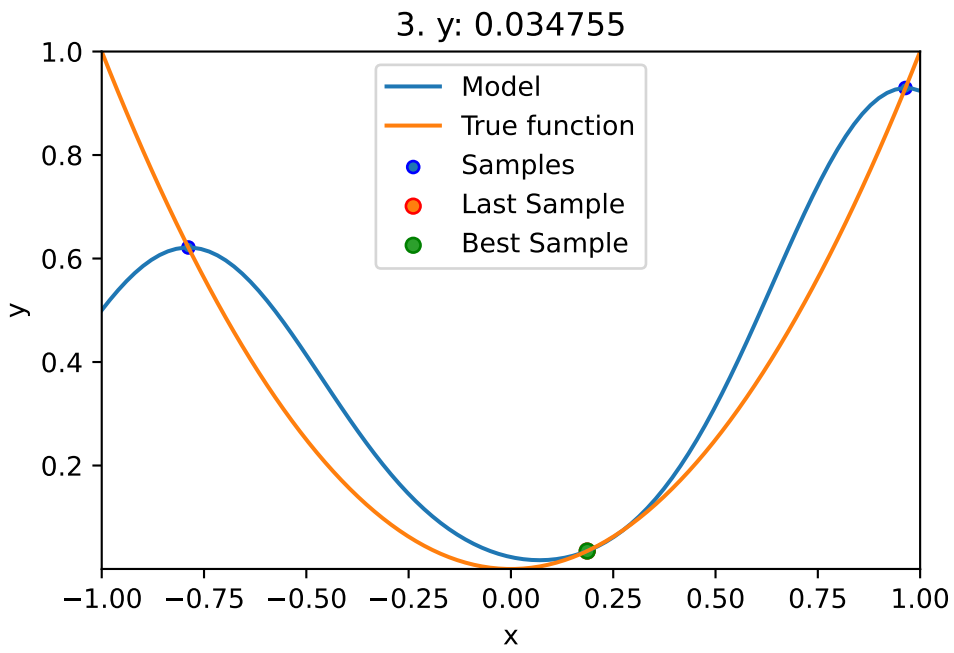
```
spot_1.plot_model()
```

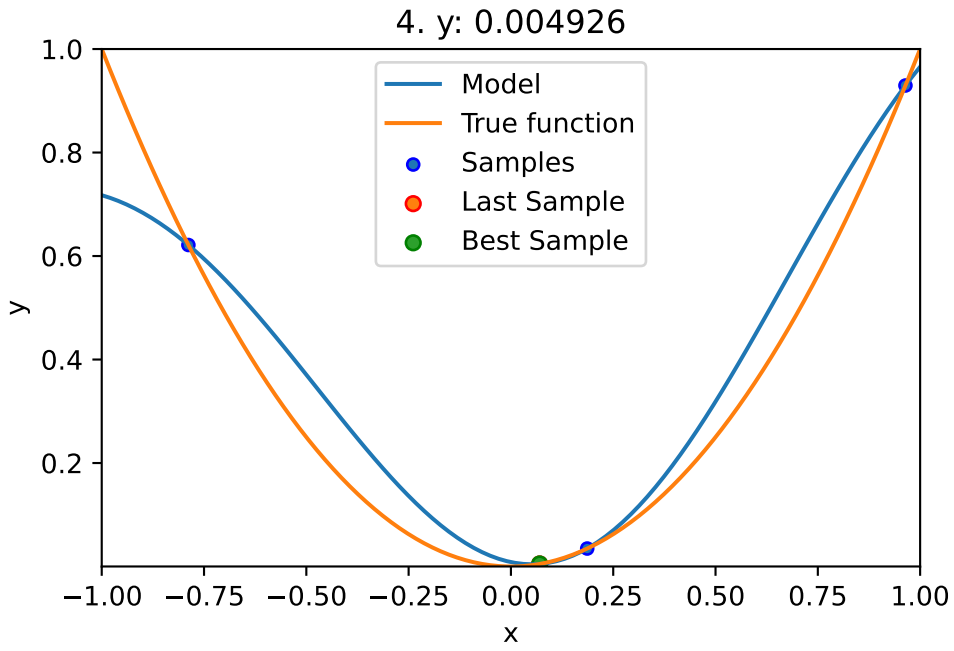


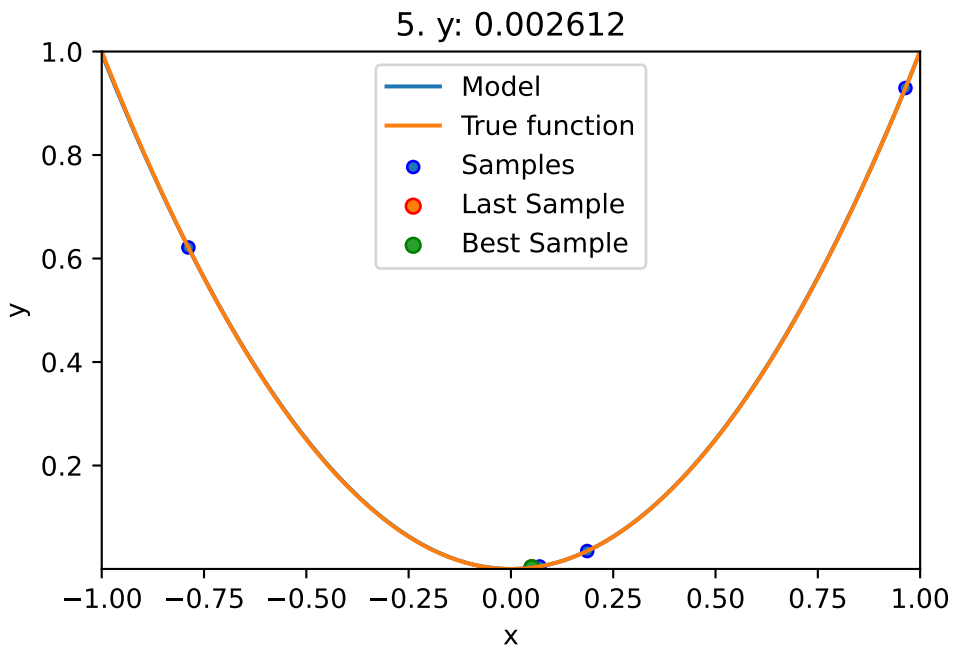
6.1 Example: `Sklearn` Model GaussianProcess

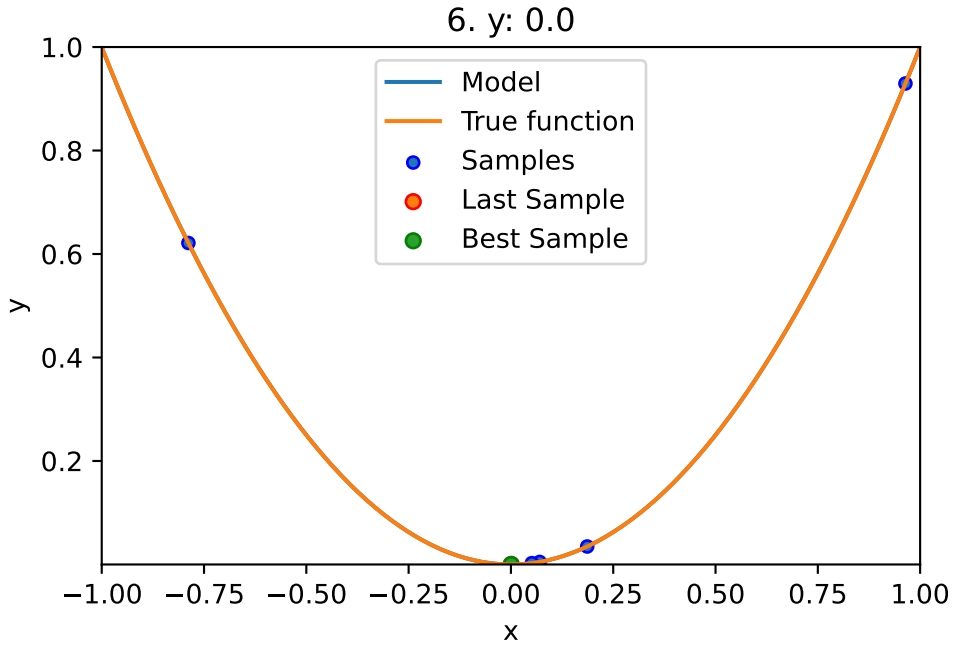
- This example visualizes the search process on the `GaussianProcessRegression` surrogate from `sklearn`.
- Therefore `surrogate = S_GP` is added to the argument list.

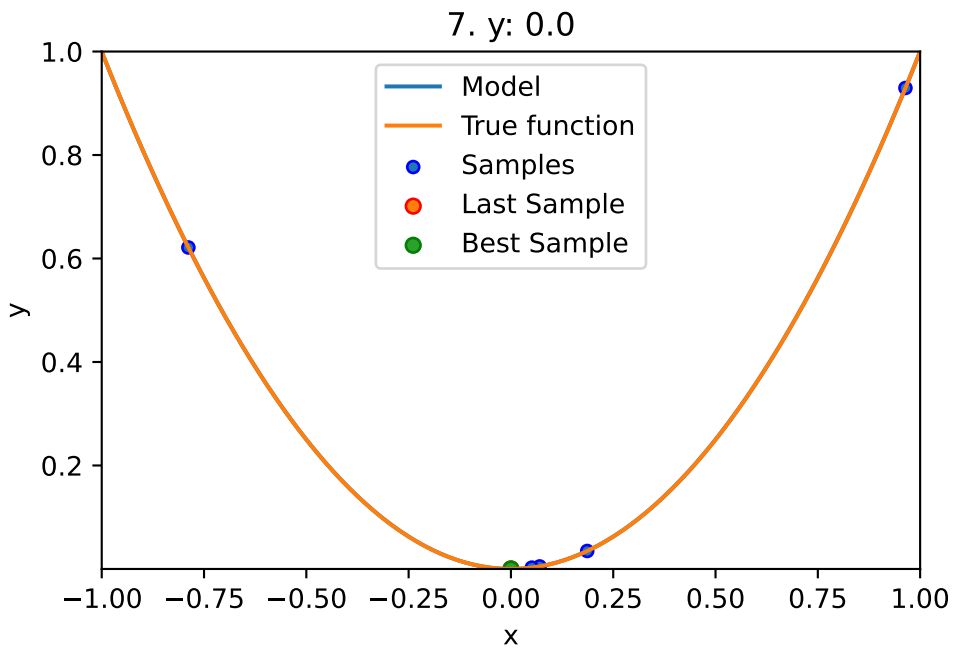
```
fun = analytical(seed=123).fun_sphere
spot_1_GP = spot.Spot(fun=fun,
                      lower = lower,
                      upper = upper,
                      fun_evals = 10,
                      max_time = inf,
                      seed=123,
                      show_models= True,
    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

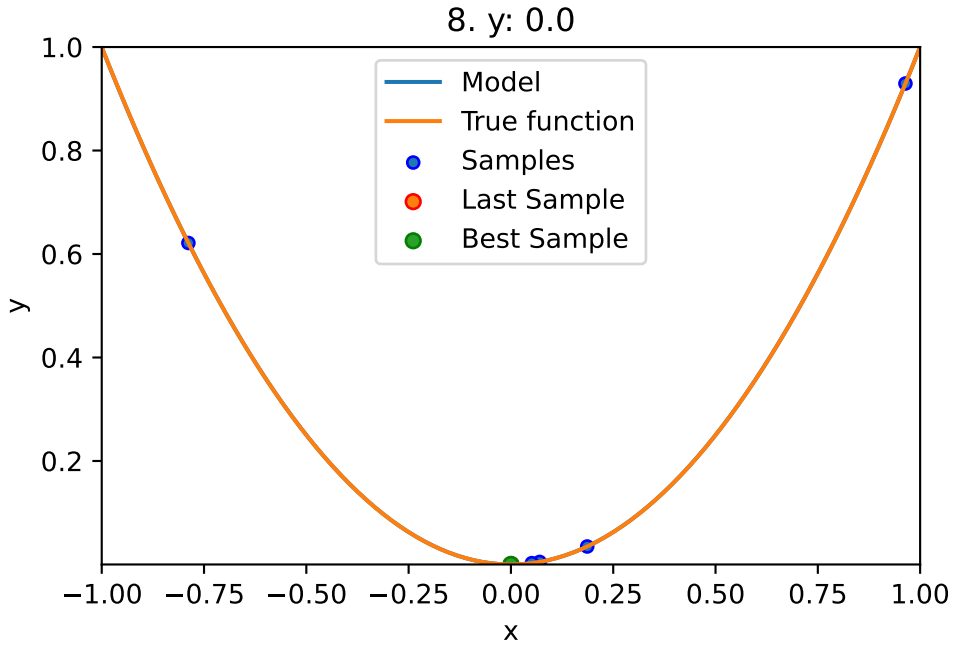

3. y: 0.034755
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

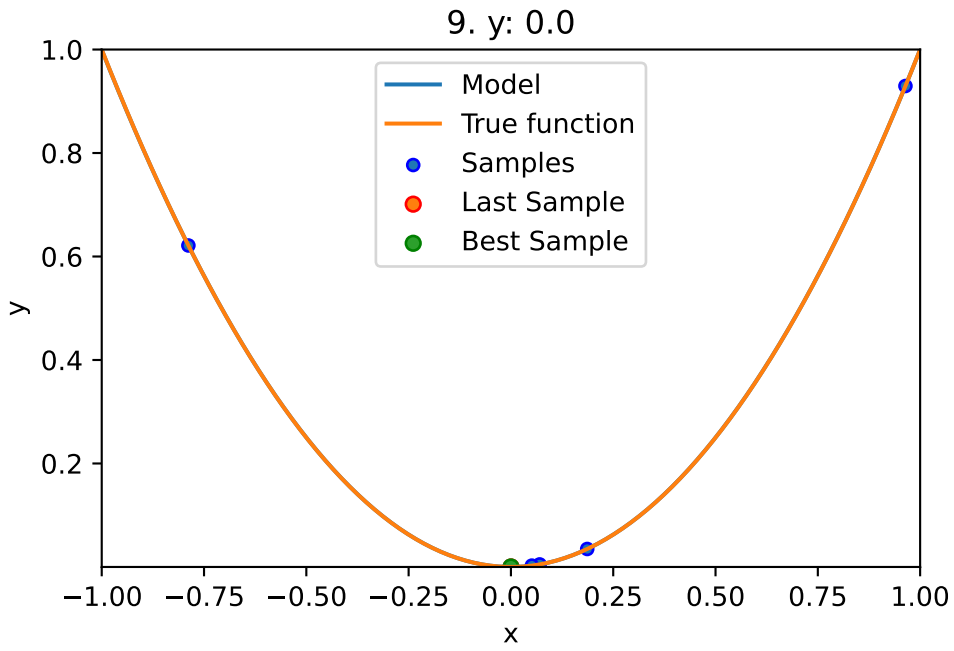

4. y: 0.004926
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x

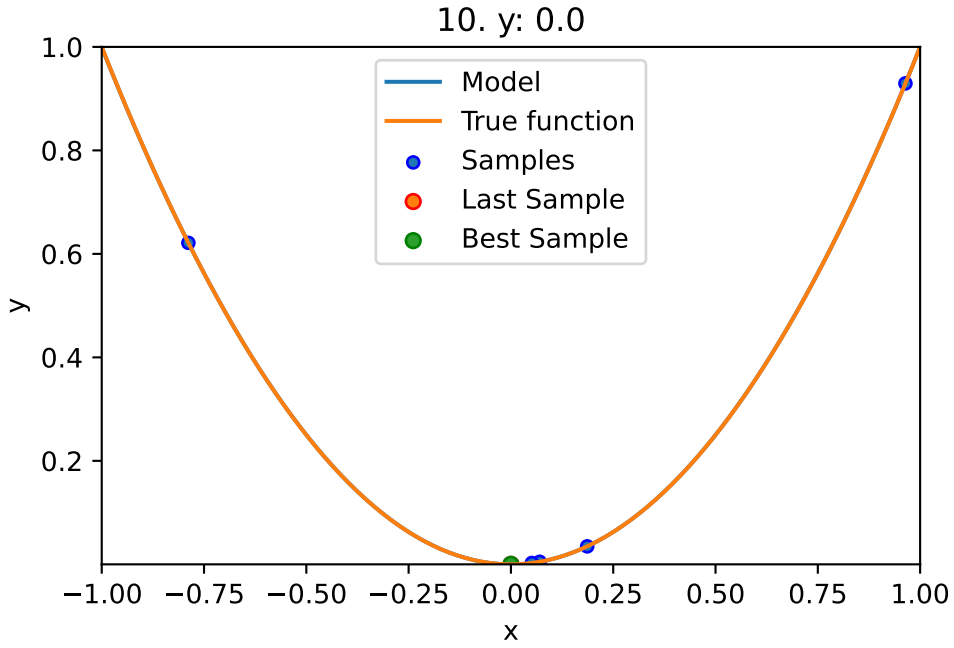

5. y: 0.002612
Model
True function
Samples
Last Sample
Best Sample
1.0
0.8
0.6
0.4
0.2
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


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



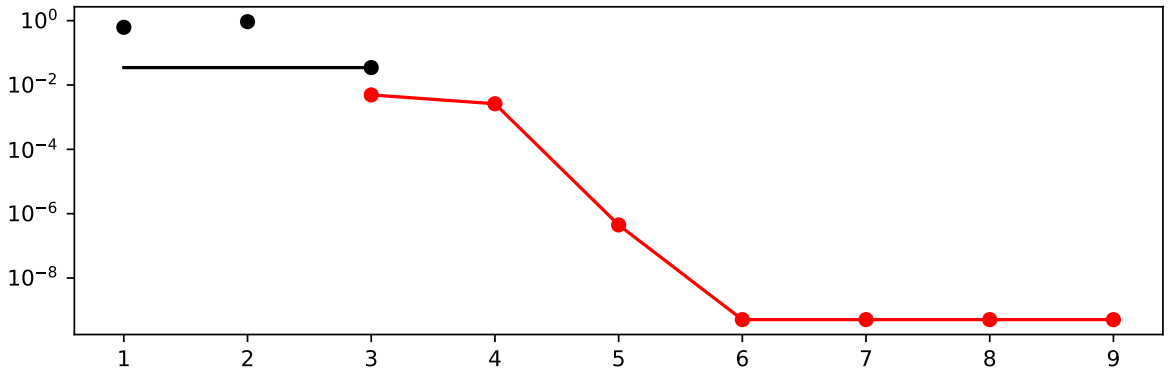



```
<spotPython.spot.spot.Spot at 0x2a747bfa0>
```

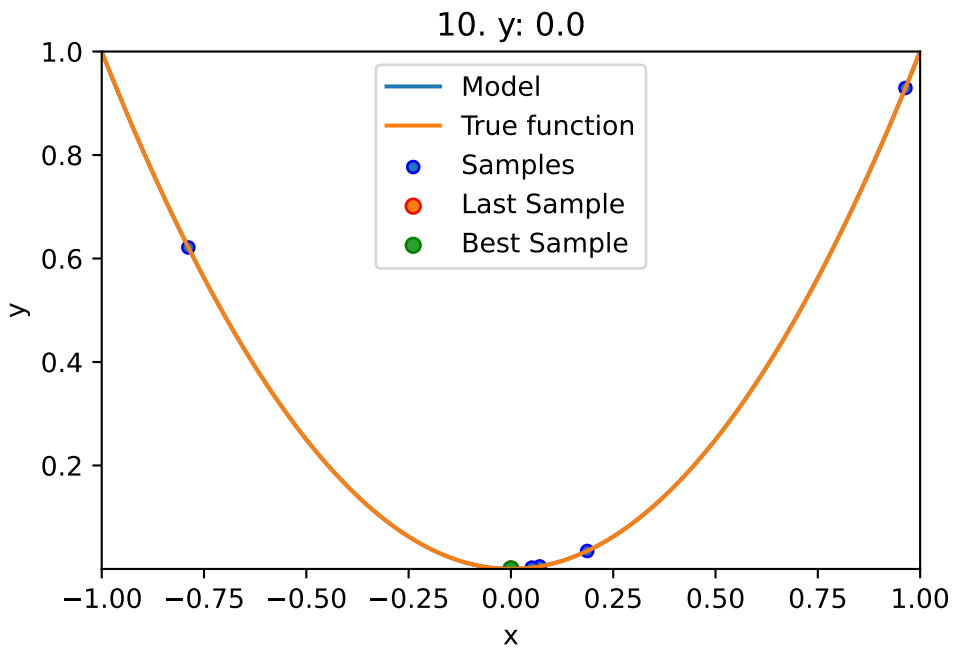
```
spot_1_GP.print_results()
```

```
min y: 5.09793870674032e-10
x0: 2.257861534005201e-05

[['x0', 2.257861534005201e-05]]
```

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




```
spot_1_GP.plot_model()
```


10. 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 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.

7.0.1 `DecisionTreeRegressor`

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

7.0.2 `RandomForestRegressor`

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

7.0.3 `linear_model.LinearRegression`

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

7.0.4 `linear_model.Ridge`

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

7.1 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`

8 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
```

8.1 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
```

8.2 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 0x107b5ca30>
```

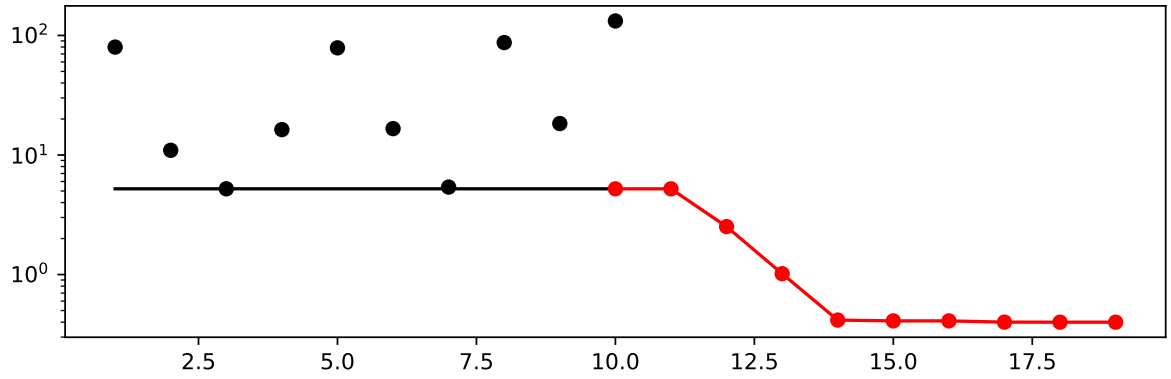
8.3 Print the Results

```
spot_de.print_results()
```

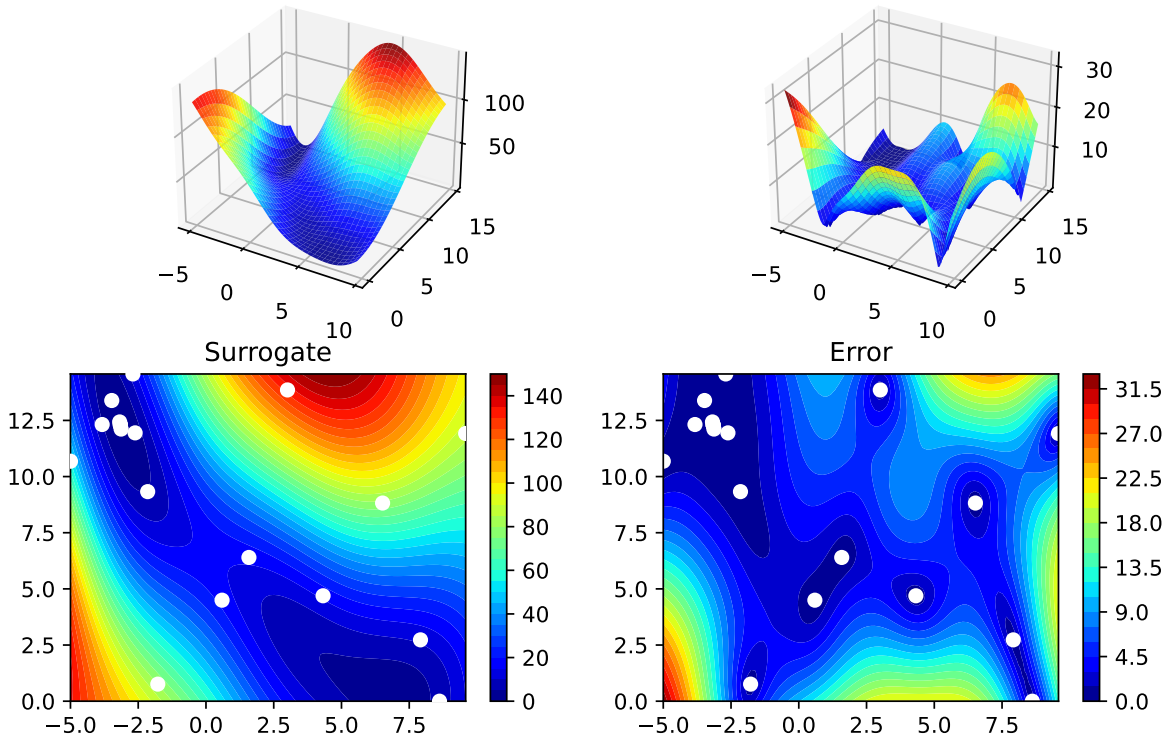
```
min y: 0.39951958110619046
x0: -3.1570201165683587
x1: 12.289980569430284

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

8.4 Show the Progress

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



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



9 Exercises

9.1 `dual_annealing`

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

9.2 `direct`

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

9.3 `shgo`

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

9.4 `basinhopping`

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

9.5 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?

10 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
```

10.1 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.

10.1.1 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]
```

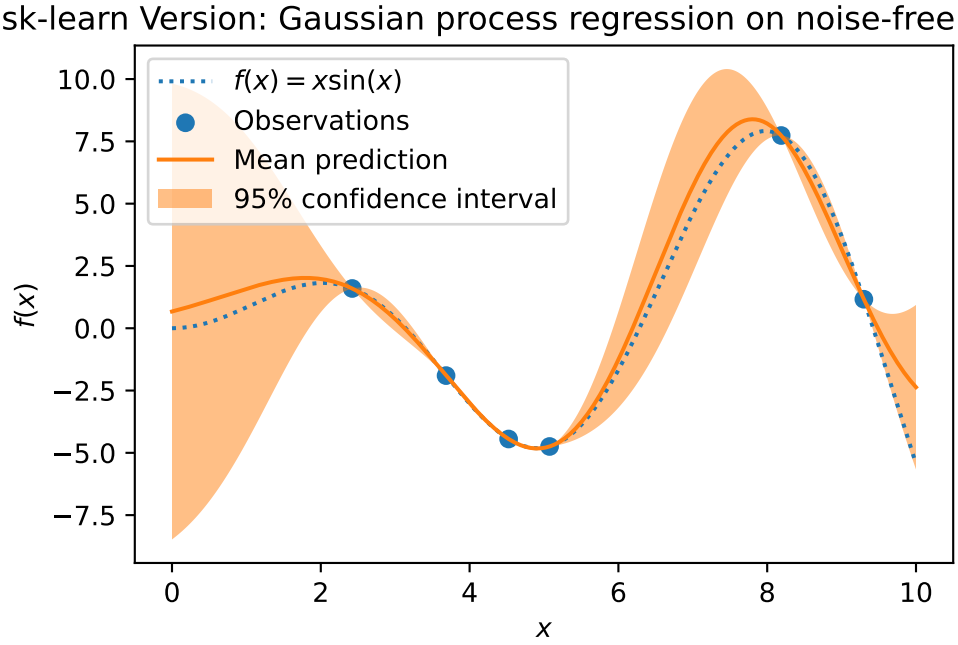
10.1.2 Building the Surrogate With `Sklearn`

- 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)
```

10.1.3 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")
```



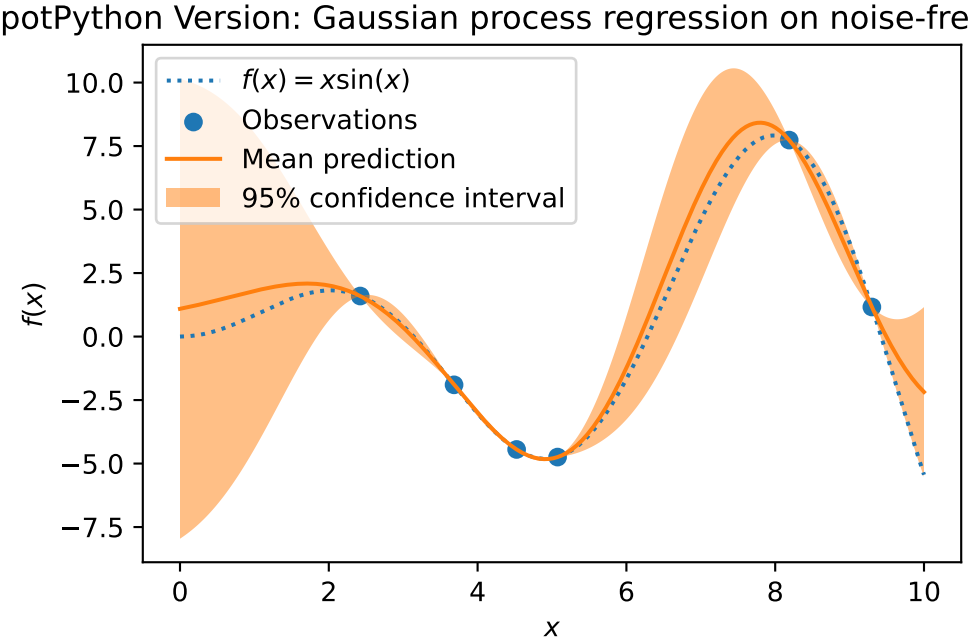
10.1.4 The `spotPython` Version

- 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")
```

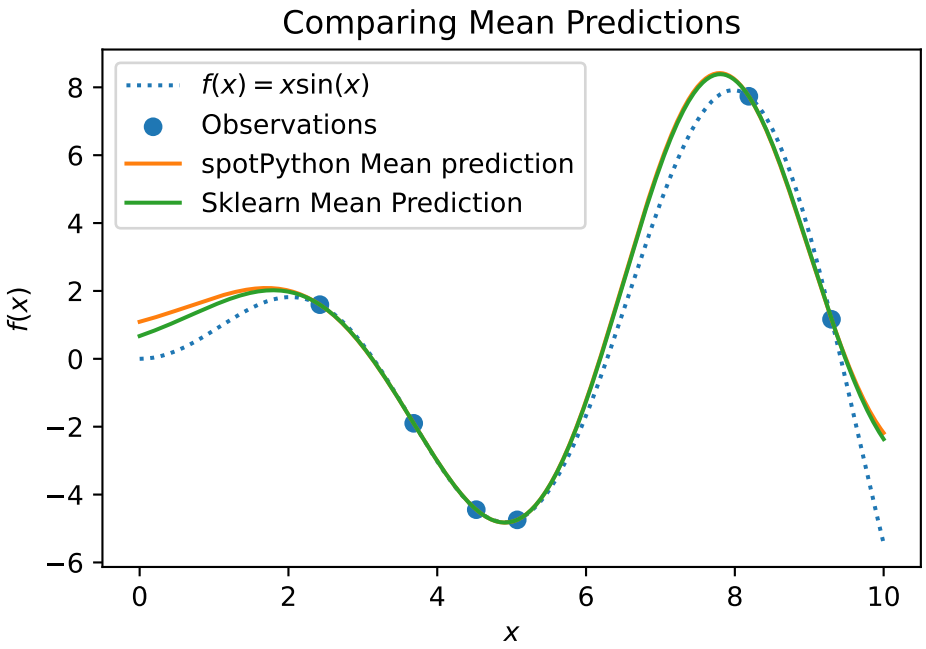
```
plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, S_mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
    S_mean_prediction - 1.96 * S_std_prediction,
    S_mean_prediction + 1.96 * S_std_prediction,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



10.1.5 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")
```


Comparing Mean Predictions
$f(x) = x\sin(x)$
Observations
spotPython Mean prediction
Sklearn Mean Prediction
$f(x)$
x
8
6
4
2
0
−2
−4
−6
0
2
4
6
8
10

11 Exercises

11.1 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.

11.2 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}
```

11.3 `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}
```

11.4 `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}
```

11.5 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?

12 Expected Improvement

12.1 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
```

12.1.1 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()
```

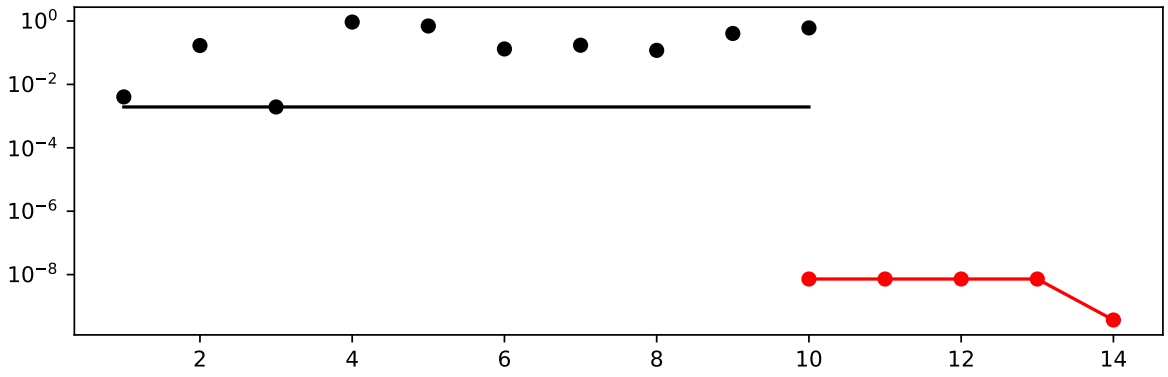
```
<spotPython.spot.spot.Spot at 0x17f91b760>
```

12.1.2 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)
```

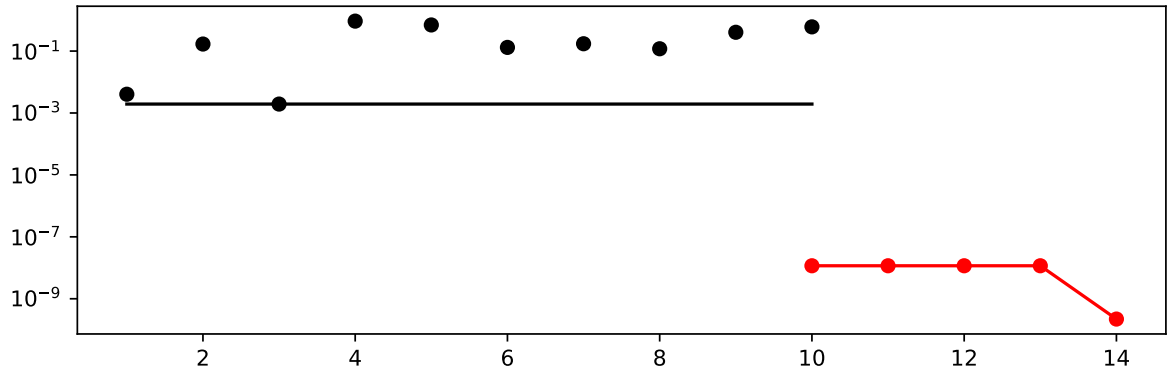


12.2 Same, but with EI as infill_criterion

```
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 0x2b4ec9c30>
```

```
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]]
```

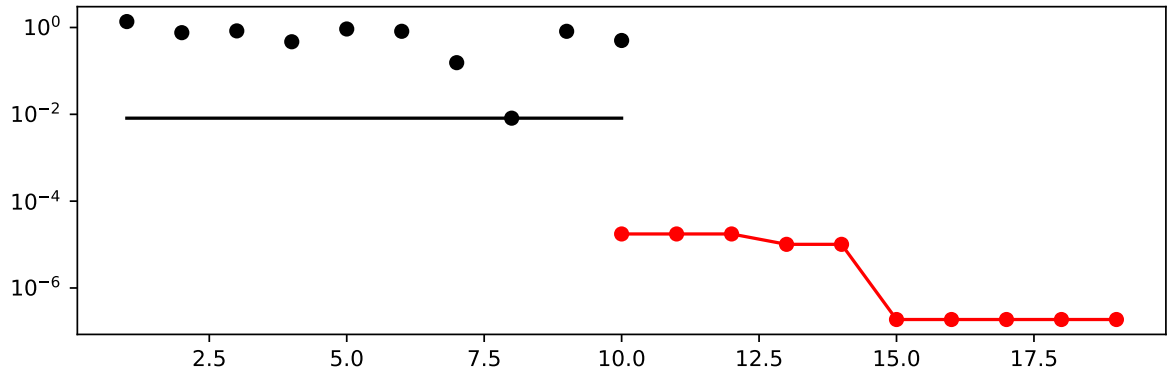
12.3 Non-isotropic Kriging

```
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 0x2b5108e50>
```

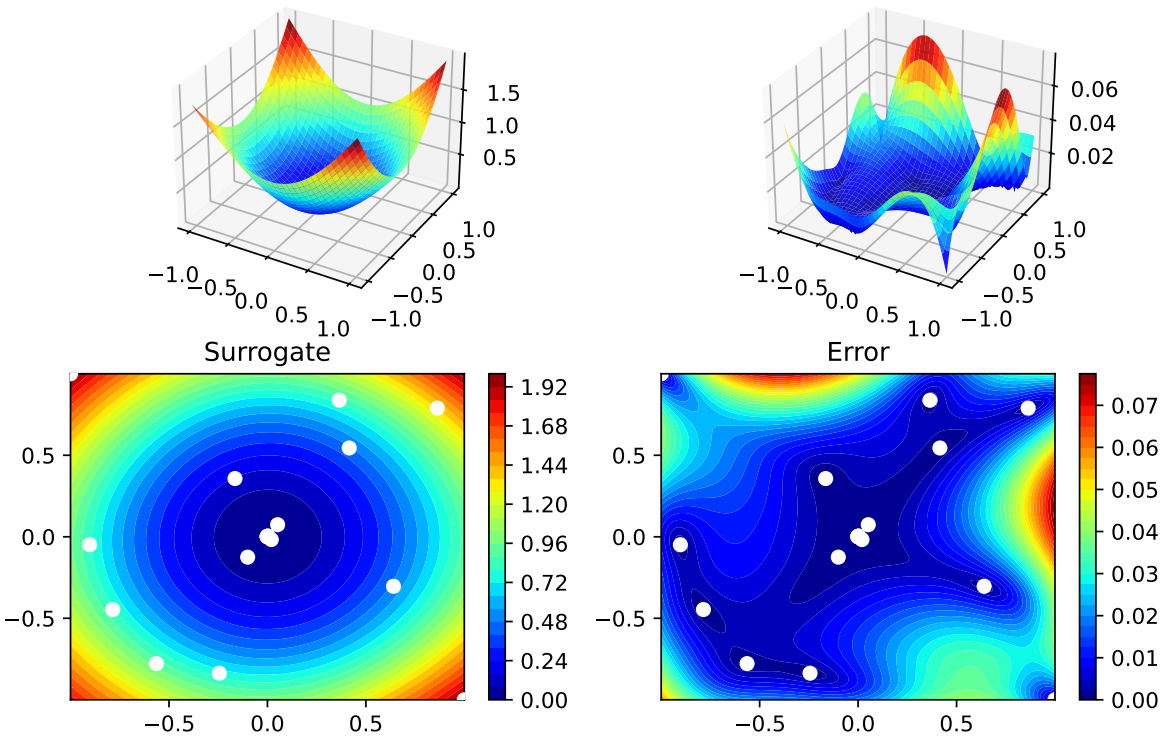
```
spot_2_ei_noniso.plot_progress(log_y=True)
```




```
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()
```



12.4 Using `sklearn` Surrogates

12.4.1 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:

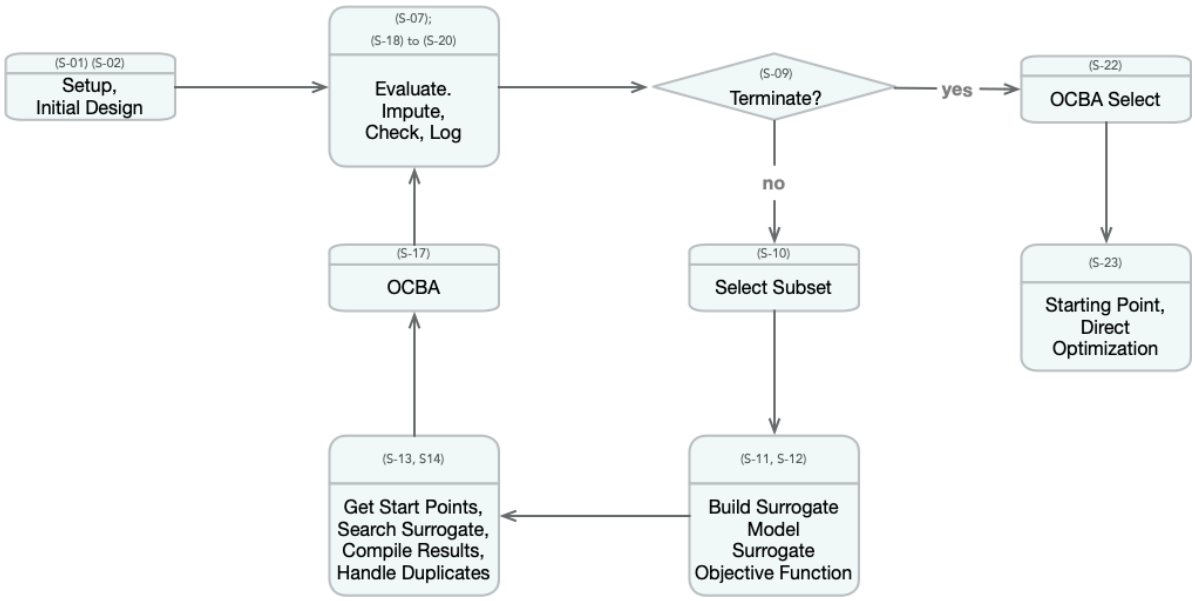


Figure 12.1: Visual representation of the model based search with SPOT. Taken from: Bartz-Beielstein, T., and Zaefferer, M. Hyperparameter tuning approaches. In Hyperparameter Tuning for Machine and Deep Learning with R - A Practical Guide, E. Bartz, T. Bartz-Beielstein, M. Zaefferer, and O. Mersmann, Eds. Springer, 2022, ch. 4, pp. 67–114.

12.4.2 spot: The Initial Model

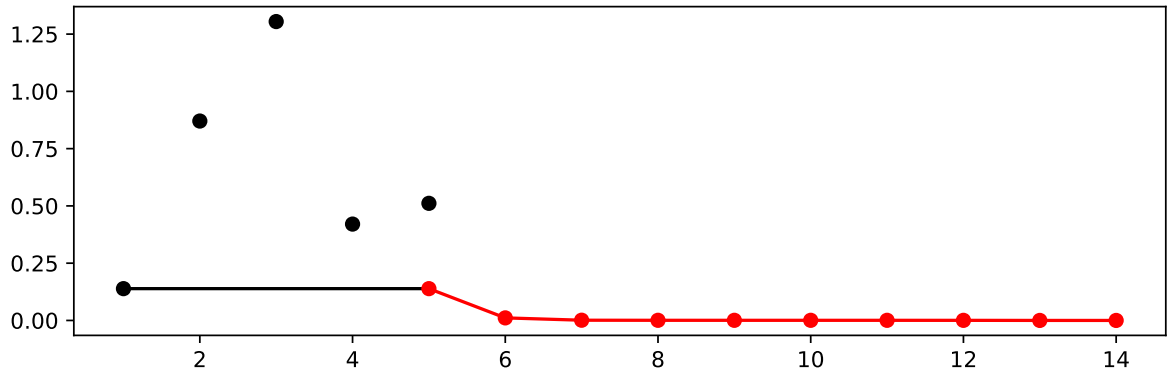
12.4.2.1 Example: Modifying the initial design size

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 0x2b9125c30>
```

```
spot_ei.plot_progress()
```




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

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

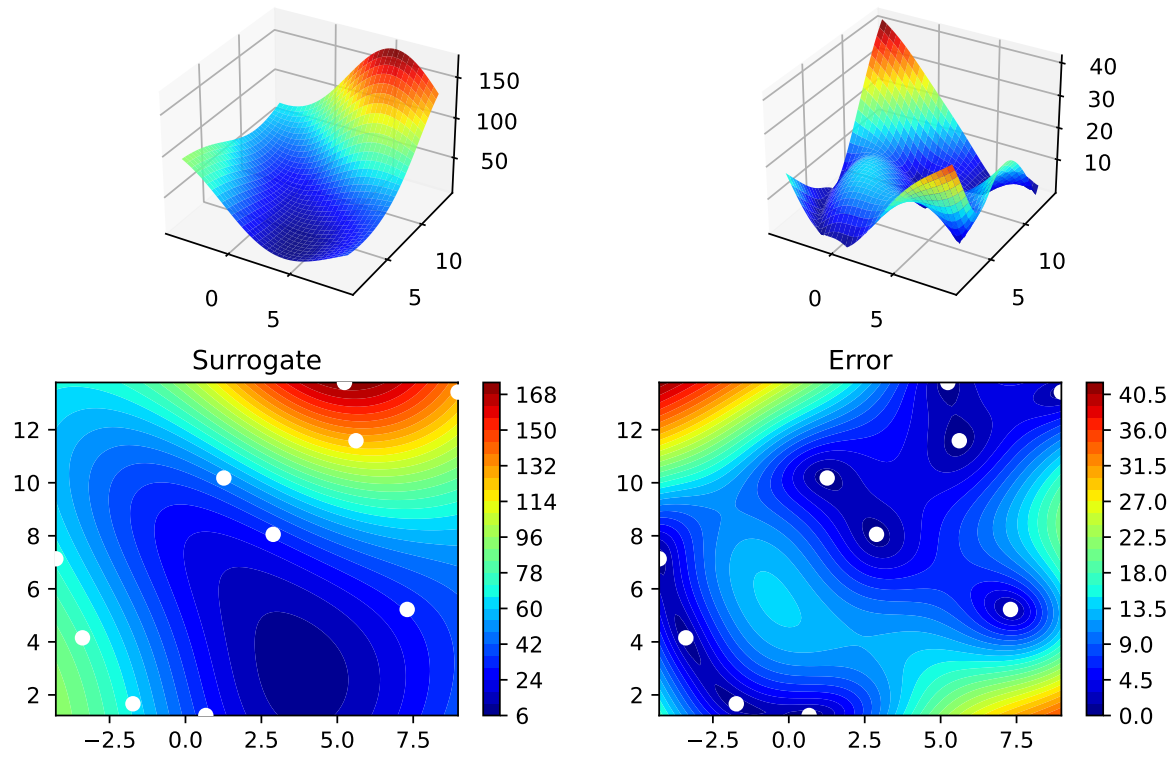
12.4.3 Init: Build Initial Design

```
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 ]]))
```

12.4.4 Evaluate

12.4.5 Build Surrogate

12.4.6 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)
```

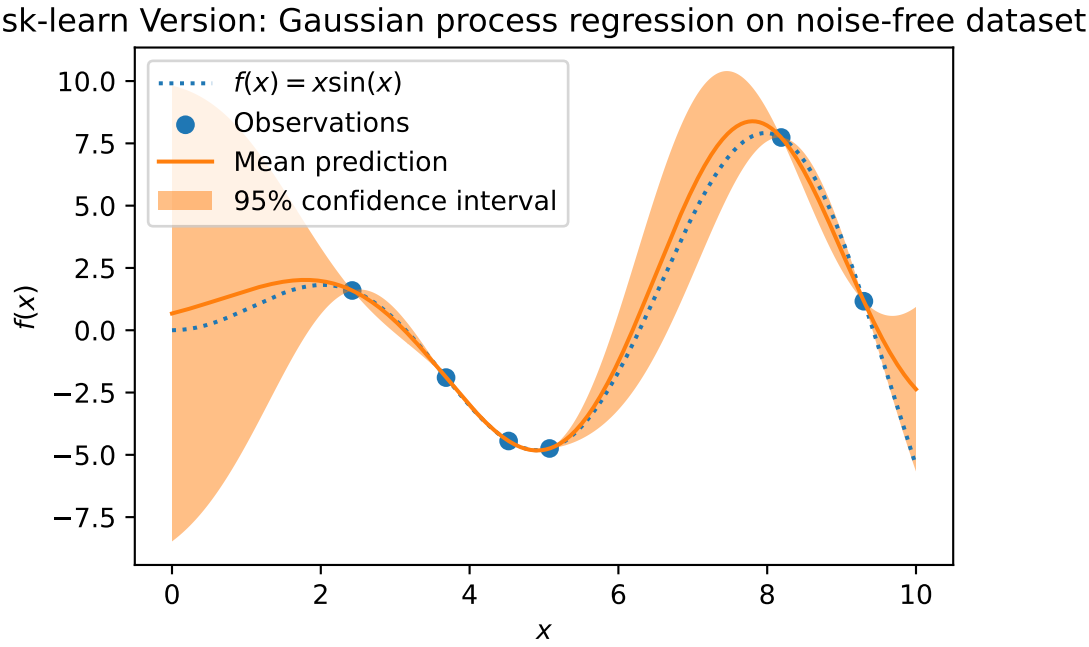
```
[1.5]
```

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

12.5 Gaussian Processes regression: basic introductory example

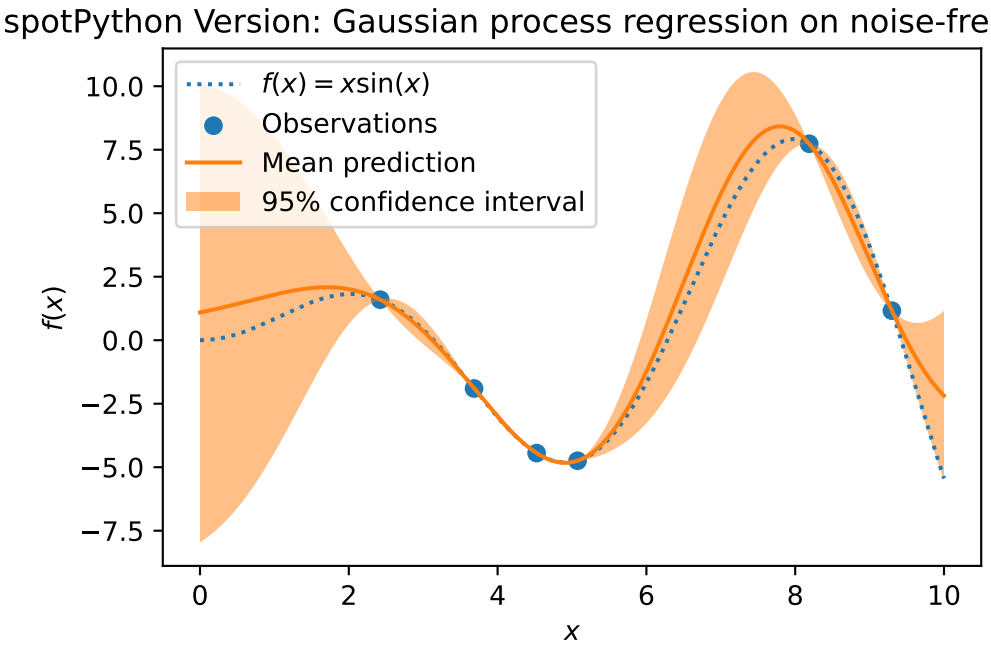
This example was taken from scikit-learn. After fitting our model, we see that the hyperparameters of the kernel have been optimized. Now, we will use our kernel to compute the mean prediction of the full dataset and plot the 95% confidence interval.

```
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")
```



12.6 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)
```

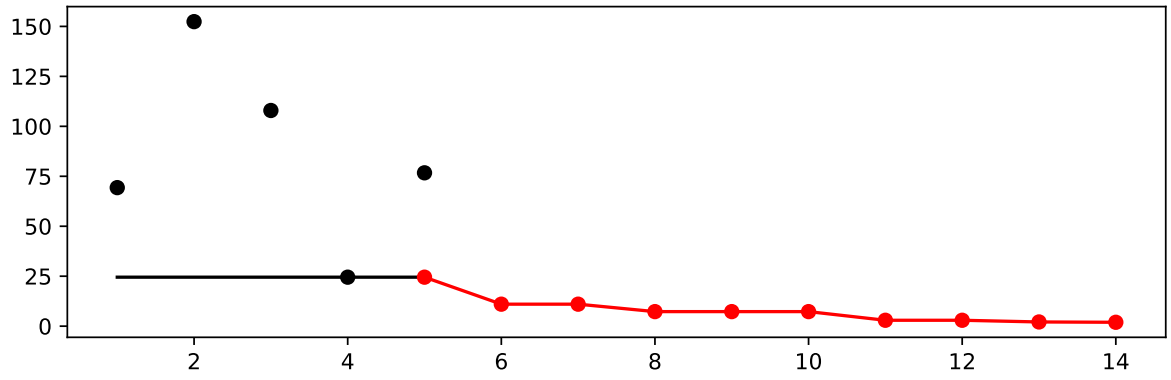
```
spot_GP.run()
```

```
<spotPython.spot.spot.Spot at 0x2b517bd60>
```

```
spot_GP.y
```

```
array([ 69.32459936, 152.38491454, 107.92560483,  24.51465459,
        76.73500031,  86.30426229,  11.00310775,  16.11745799,
         7.2811522 ,  21.82317675,  10.96088904,   2.95191763,
         3.02909859,   2.10497646,   1.94315945])
```

```
spot_GP.plot_progress()
```




```
spot_GP.print_results()
```

```
min y: 1.9431594518946582
x0: 10.0
x1: 2.9986219761932014

[['x0', 10.0], ['x1', 2.9986219761932014]]
```

12.7 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
```

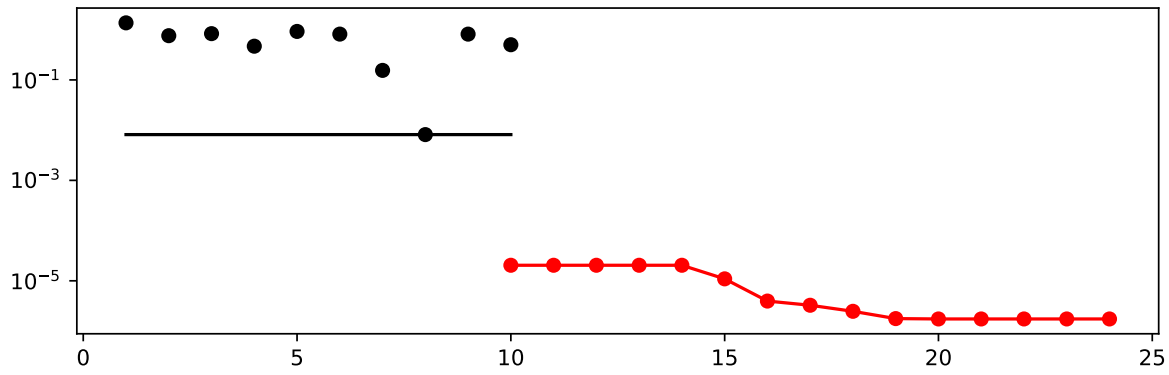
```
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
S_GP = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
```

```
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,
```

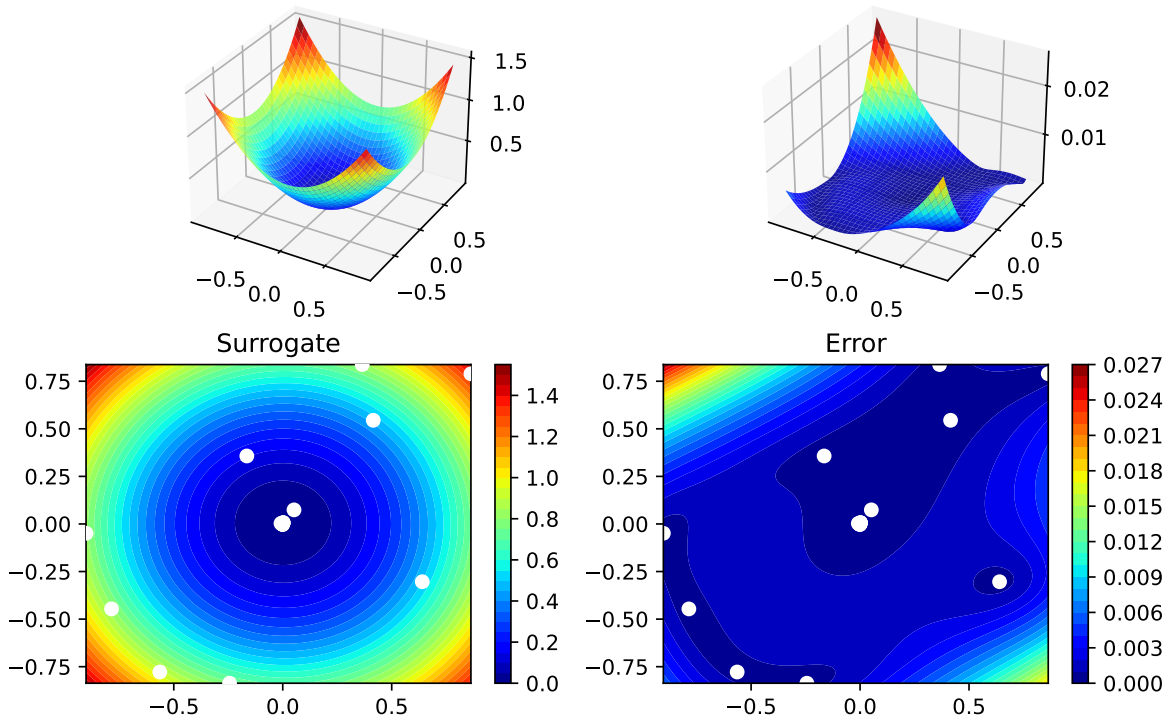
```
                    design_control=design_control,
                    surrogate_control=surrogate_control)

spot_S_K.run()
```

```
<spotPython.spot.spot.Spot at 0x2b65d9660>
```

```
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]]
```

12.7.1 Optimize on Surrogate

12.7.2 Evaluate on Real Objective

12.7.3 Impute / Infill new Points

12.8 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]]
```

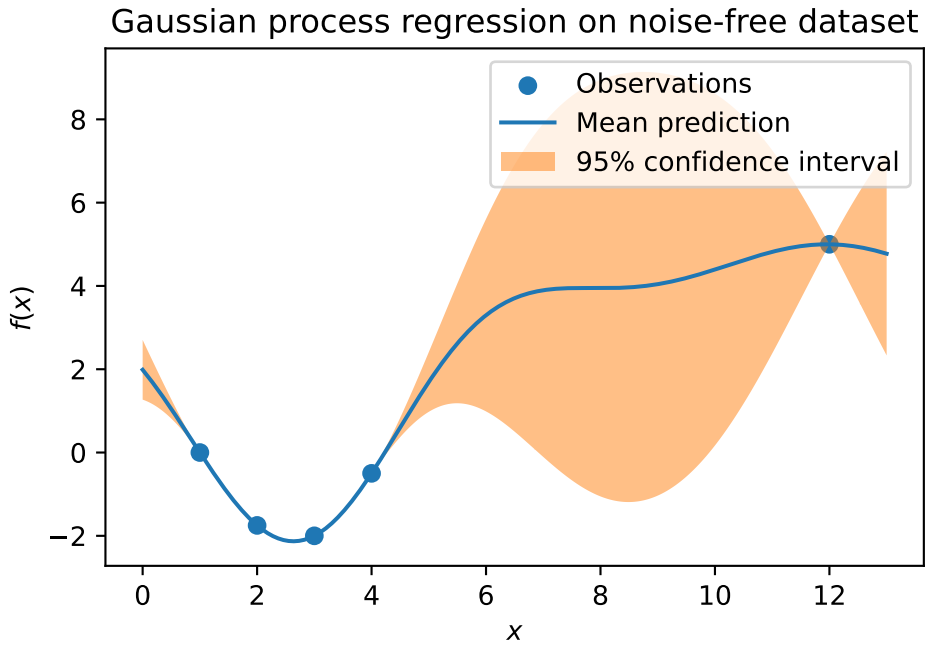
```
 [-0.16484832  0.35724741]
 [ 0.05170659  0.07401196]
 [-0.78548145 -0.44638164]
 [ 0.64017497 -0.30363301]]
[1.36857656 0.75992983 0.83463487 0.46918172 0.92329124 0.8170764
 0.15480068 0.00815134 0.81623768 0.502017  ]
[[0.00160553 0.00428429]
 [0.00160553 0.00428429]]
```

12.9 EI: The Famous Schonlau Example

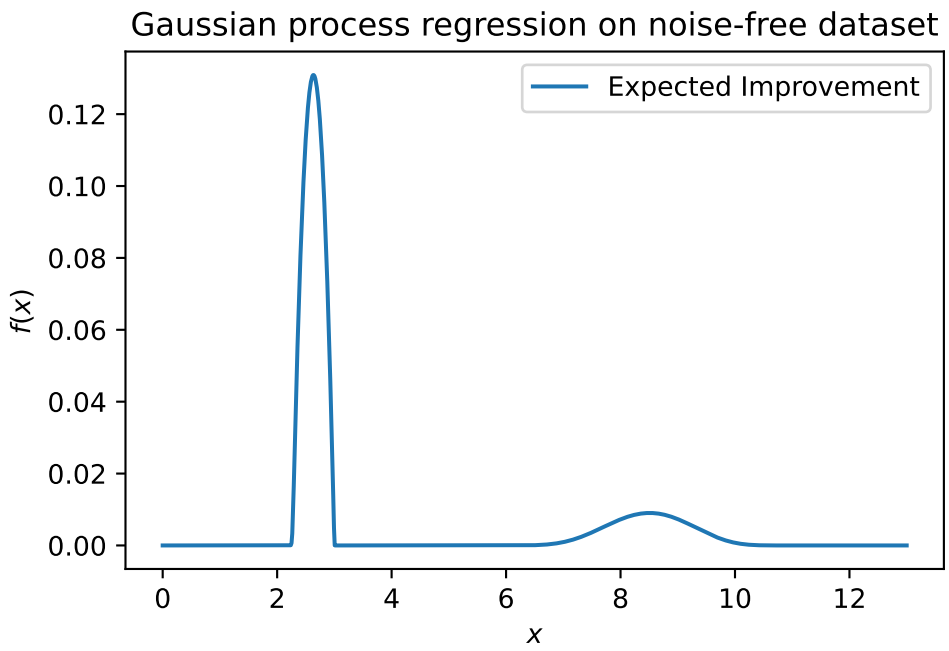
```
X_train0 = np.array([1, 2, 3, 4, 12]).reshape(-1,1)
X_train = np.linspace(start=0, stop=10, num=5).reshape(-1, 1)
```

```
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")
```



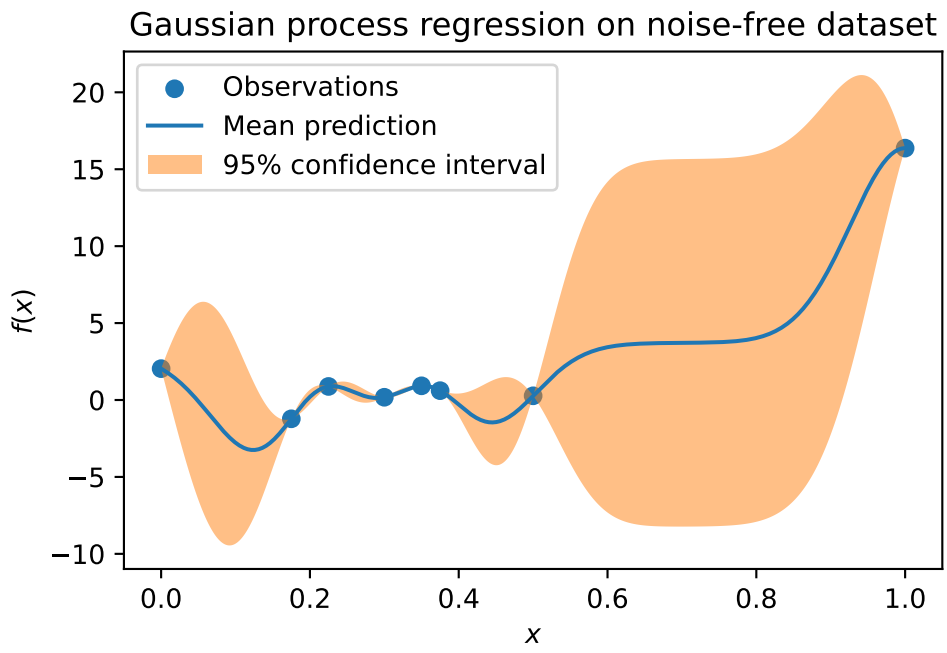

```
S.log
```

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

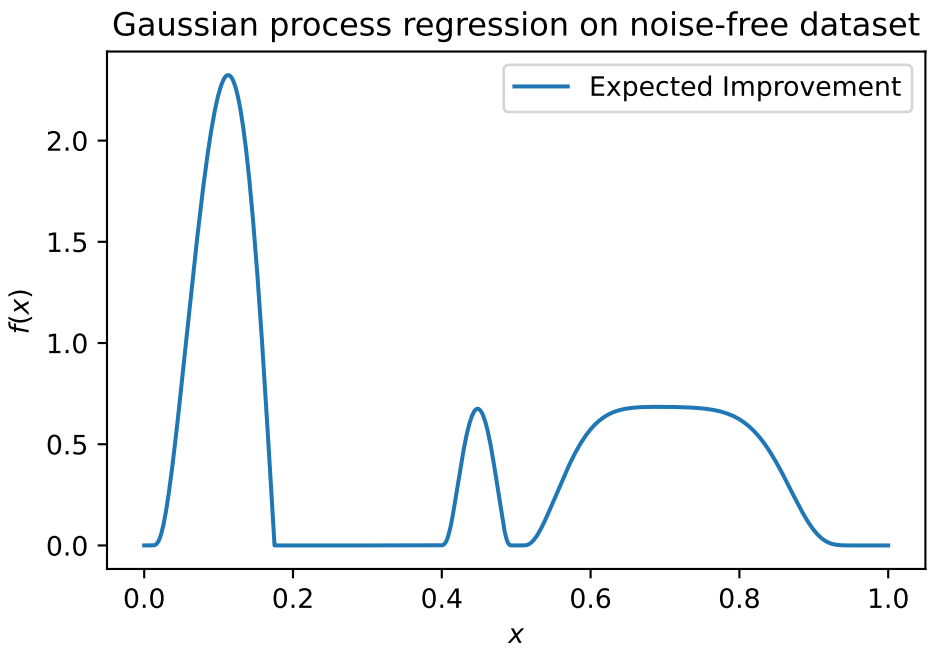
12.10 EI: The Forrester Example

```
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")
```

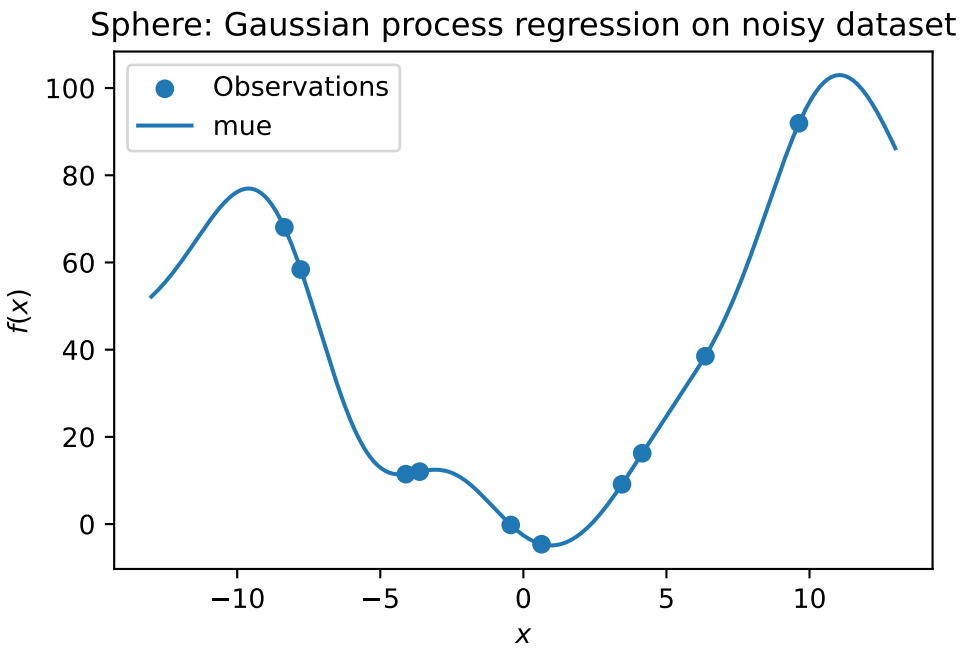


12.11 Noise

```
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]
```

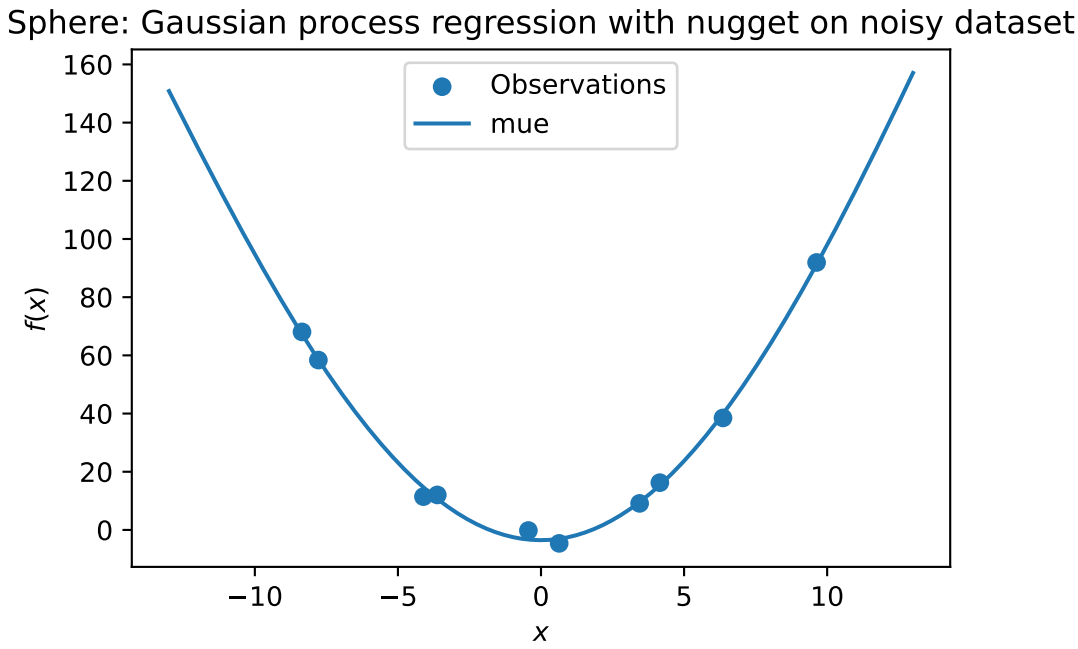



```
S.log
```

```
{'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])}
```

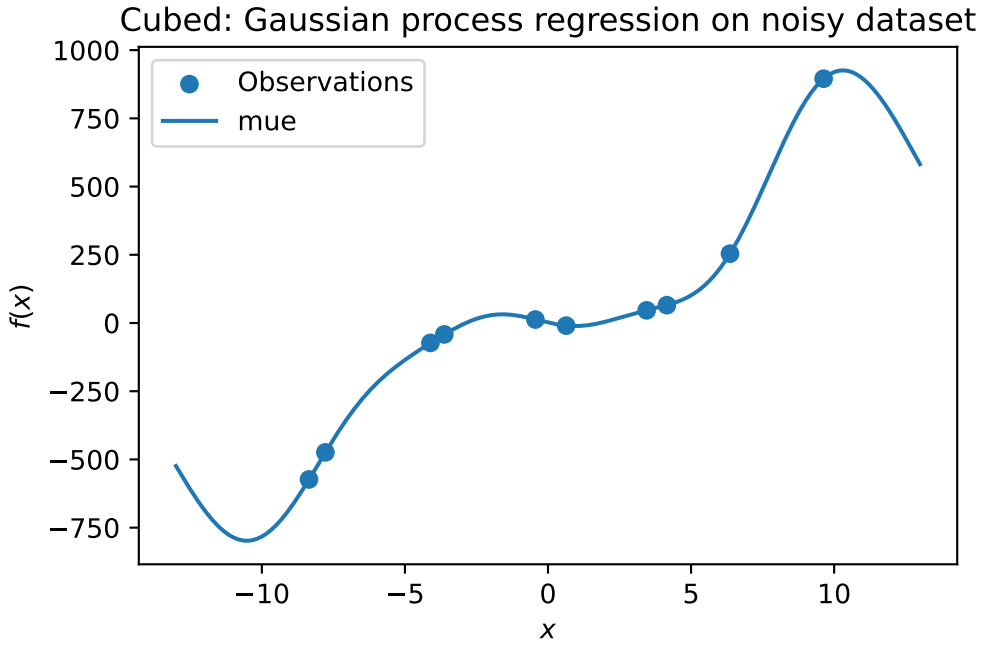
12.12 Cubic Function

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

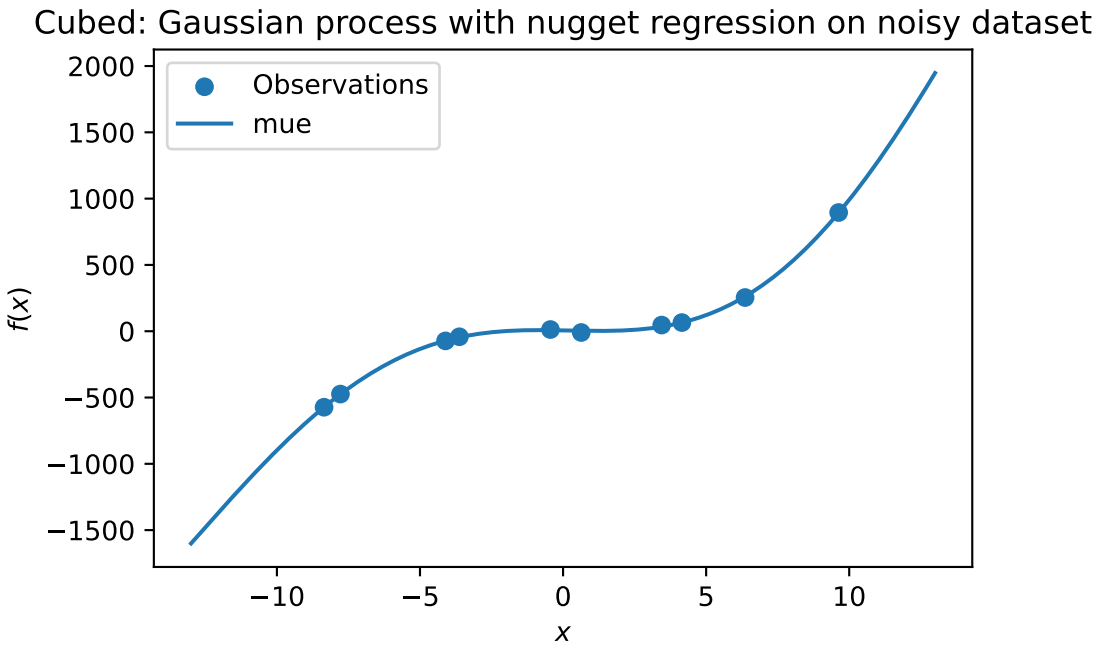
```
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

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]
```



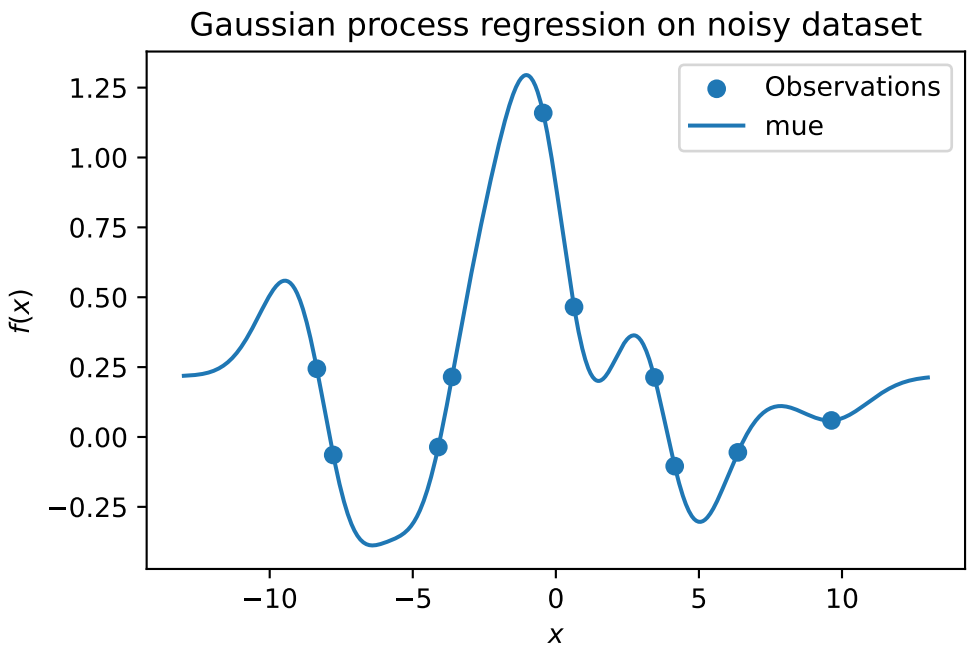

```
S = Kriging(name='kriging',  seed=123, log_level=0, n_theta=1, noise=True)
S.fit(X_train, y_train)

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")
```



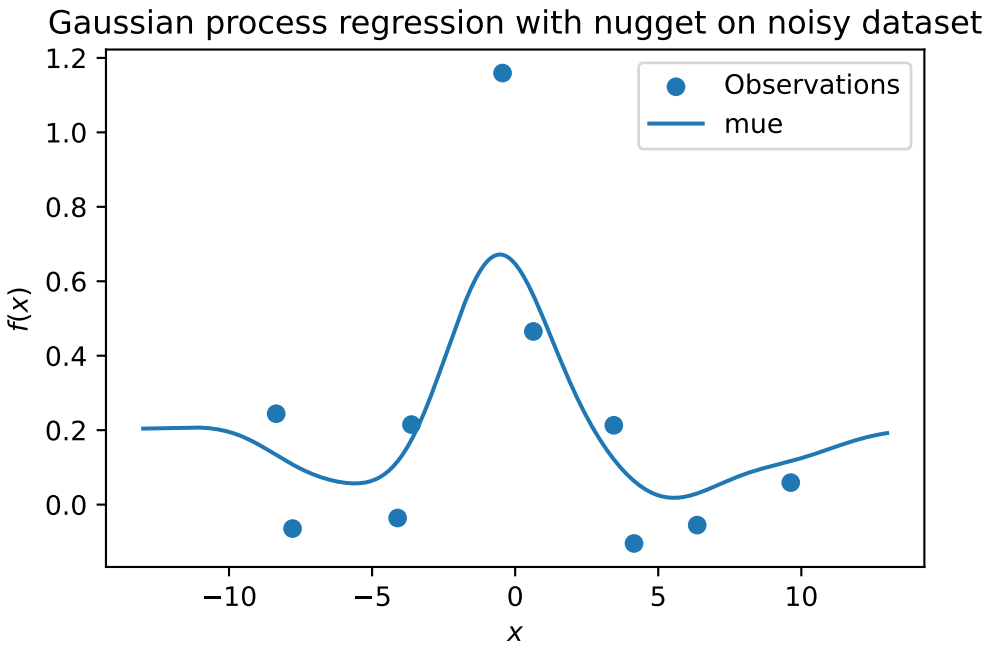

```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

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")
```



12.13 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
```

```
-13.631795005659114
```

```
# vars(S)
```

```
# vars(Sf)
```

13 Hyperparameter Tuning and Noise

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

13.1 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
```

13.1.1 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:

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

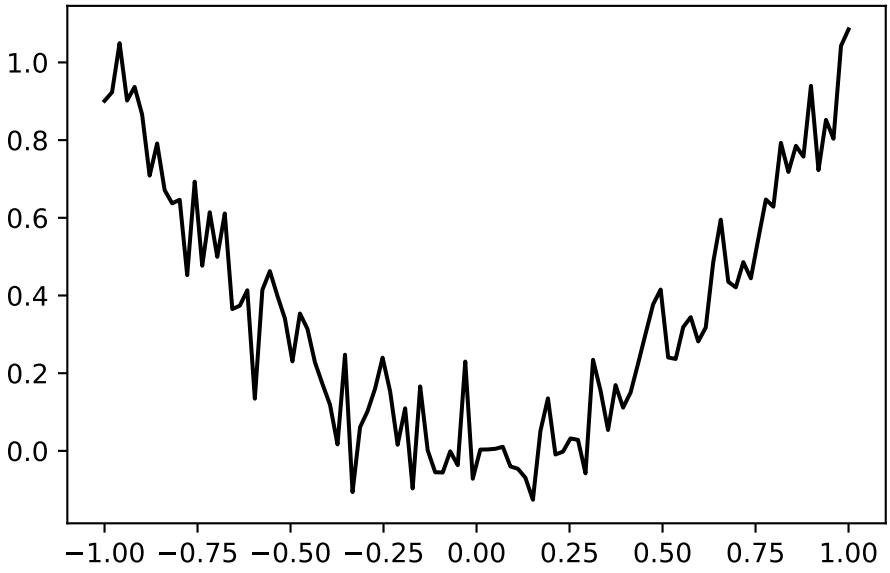
- Since `sigma` is set to `0.1`, noise is added to the function:

```
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()
```

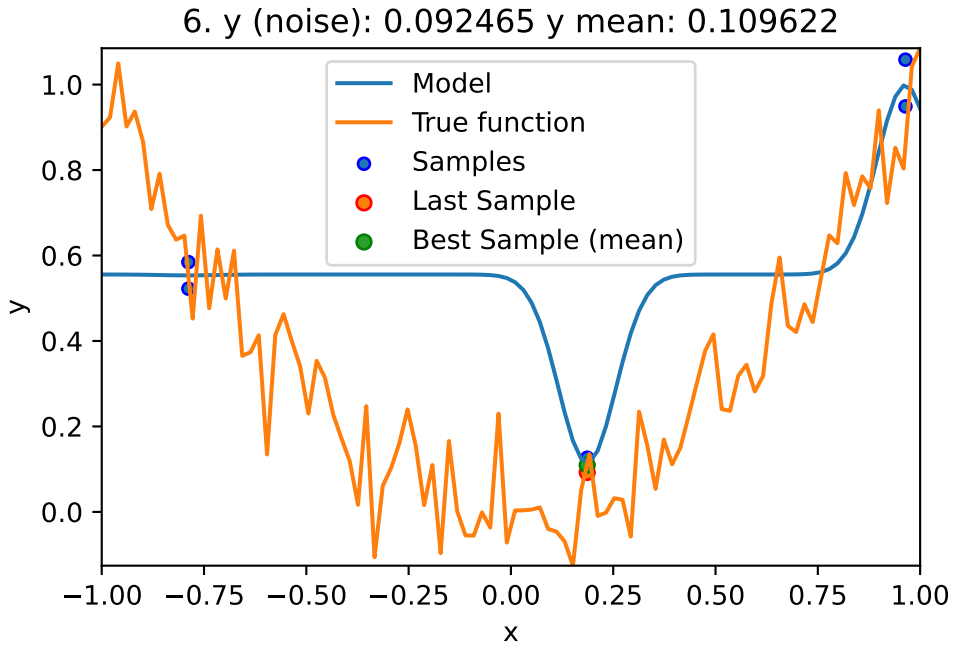


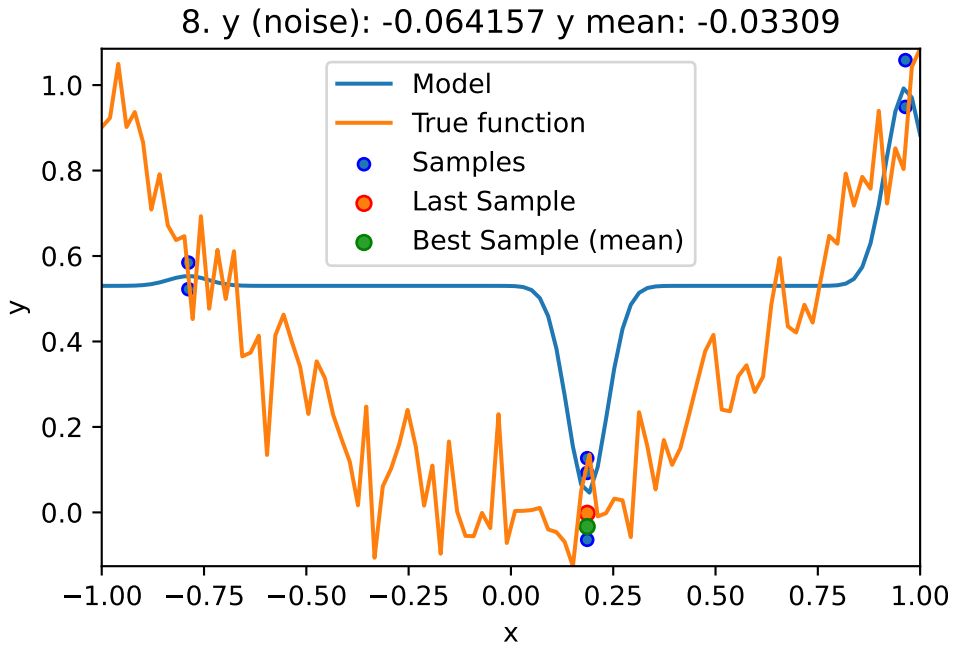
`Spot` is adopted as follows to cope with noisy functions:

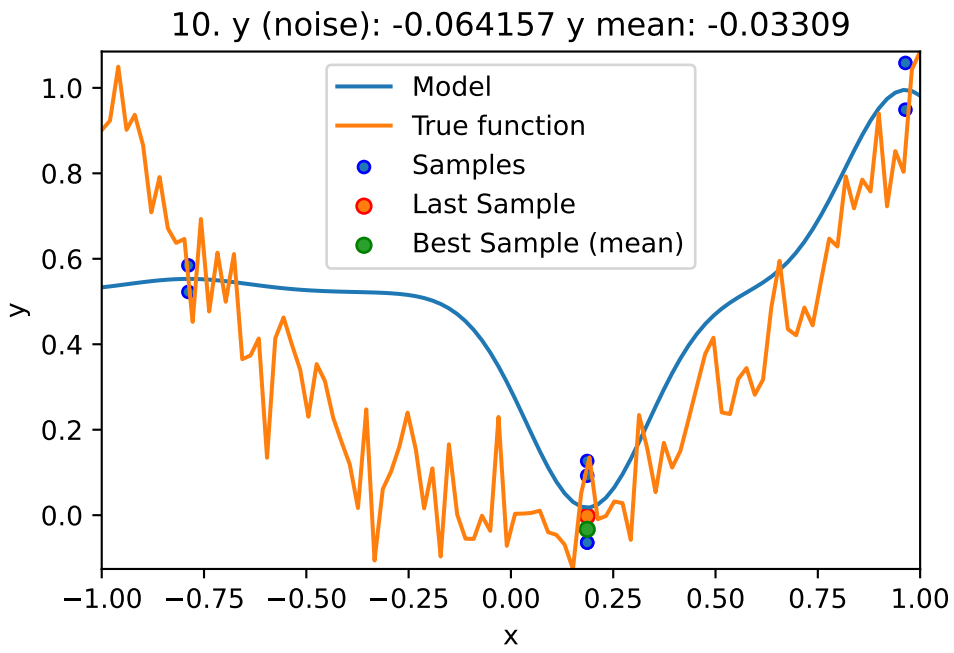
1. `fun_repeats` is set to a value larger than 1 (here: 2)
2. `noise` is set to `true`. Therefore, a nugget (`Lambda`) term is added to the correlation matrix
3. `init size` (of the `design_control` dictionary) is set to a value larger than 1 (here: 2)

```
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()
```







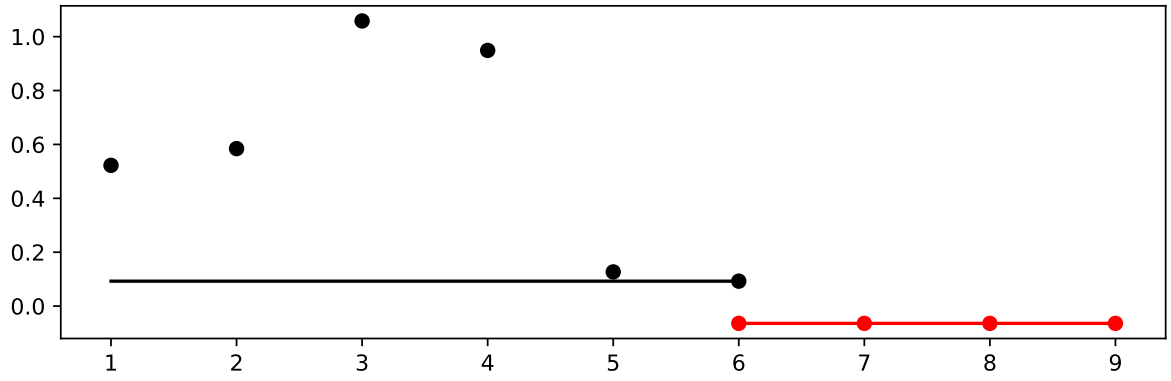

```
<spotPython.spot.spot.Spot at 0x29a4ff6d0>
```

13.2 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)
```



13.3 Noise and Surrogates: The Nugget Effect

13.3.1 The Noisy Sphere

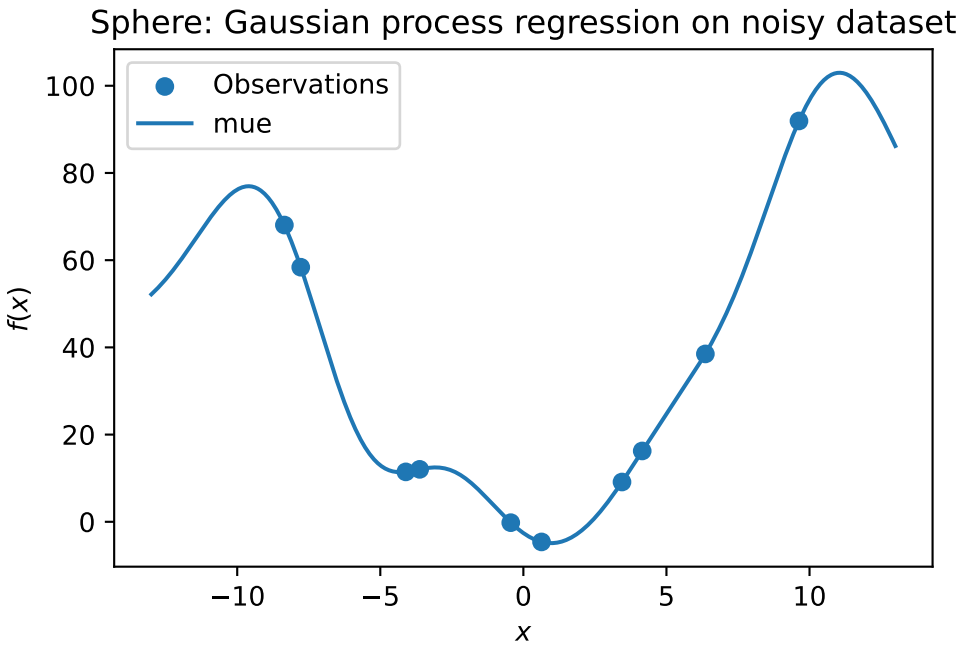
13.3.1.1 The Data

- 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
```

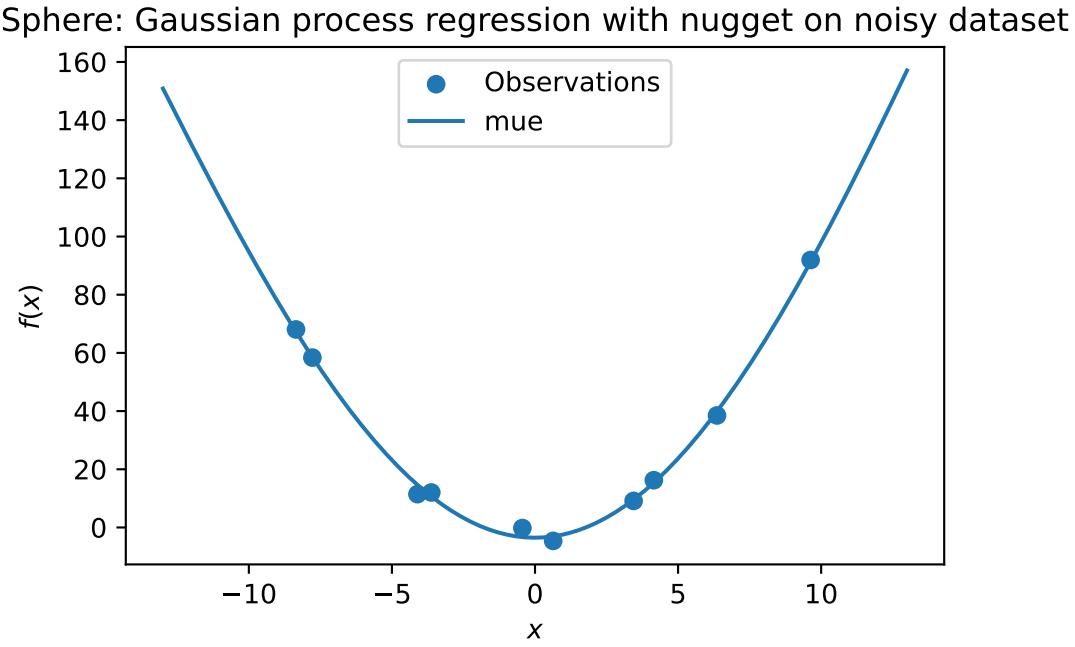
- A surrogate without nugget is fitted to these data:

```
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.

13.4 Exercises

13.4.1 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])
```

13.4.2 `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}
```

13.4.3 `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}
```

13.4.4 `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}
```

14 Handling Noise: Optimal Computational Budget Allocation in Spot

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

14.1 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
```

14.1.1 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:

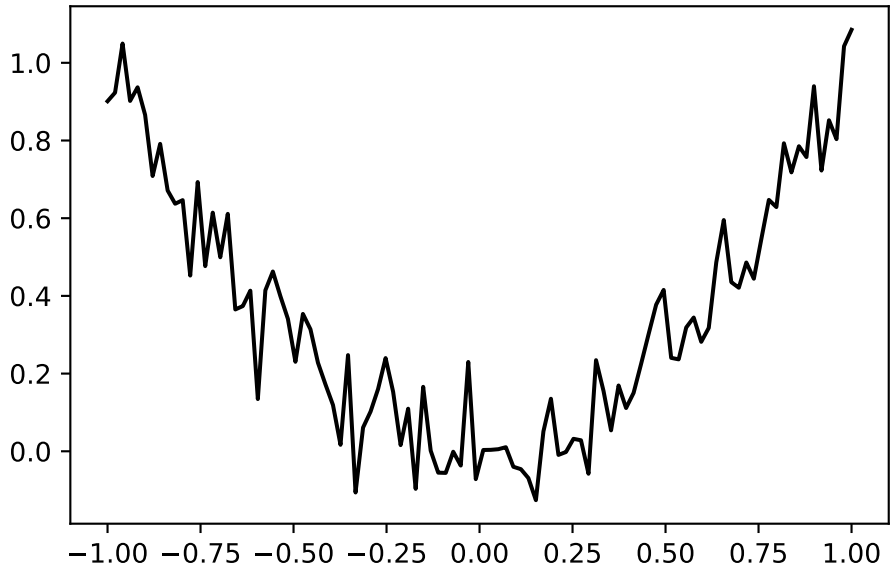
$$f(x) = x^2 + \epsilon$$

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()
```



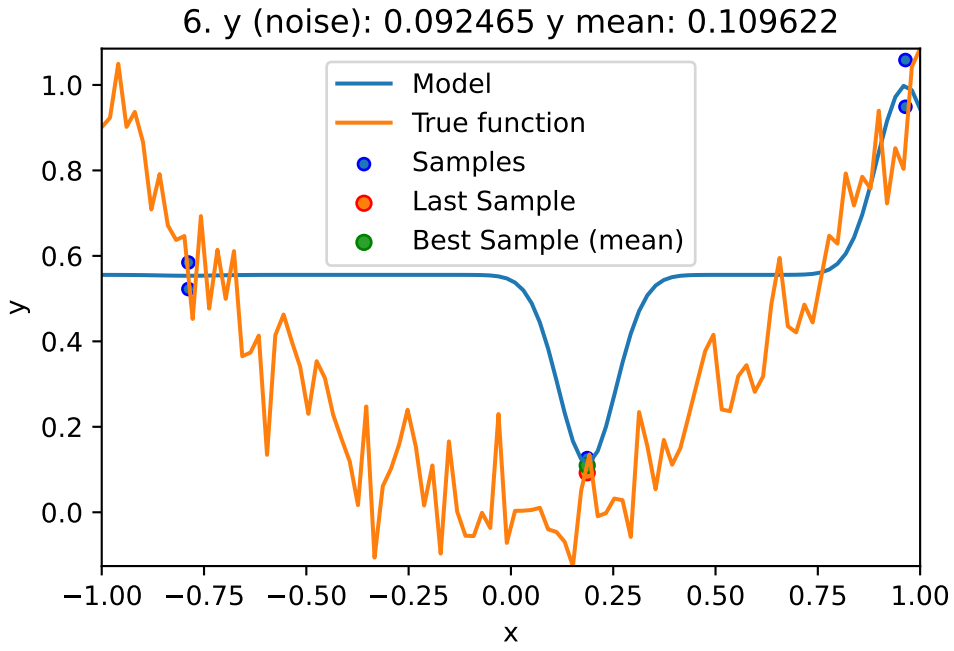
`Spot` is adopted as follows to cope with noisy functions:

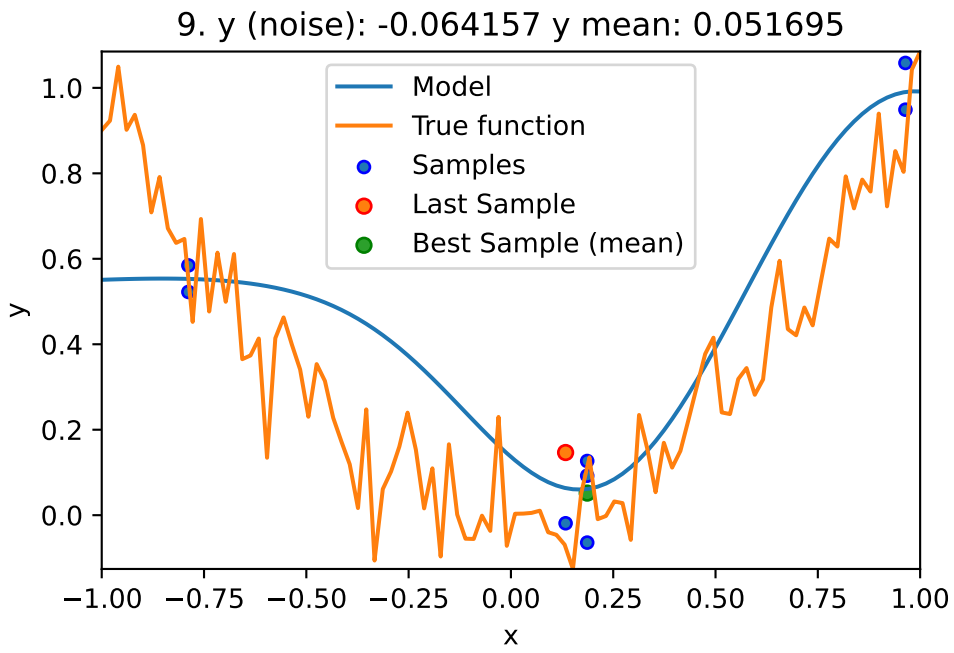
1. `fun_repeats` is set to a value larger than 1 (here: 2)
2. `noise` is set to `true`. Therefore, a nugget (`Lambda`) term is added to the correlation matrix
3. `init size` (of the `design_control` dictionary) is set to a value larger than 1 (here: 2)

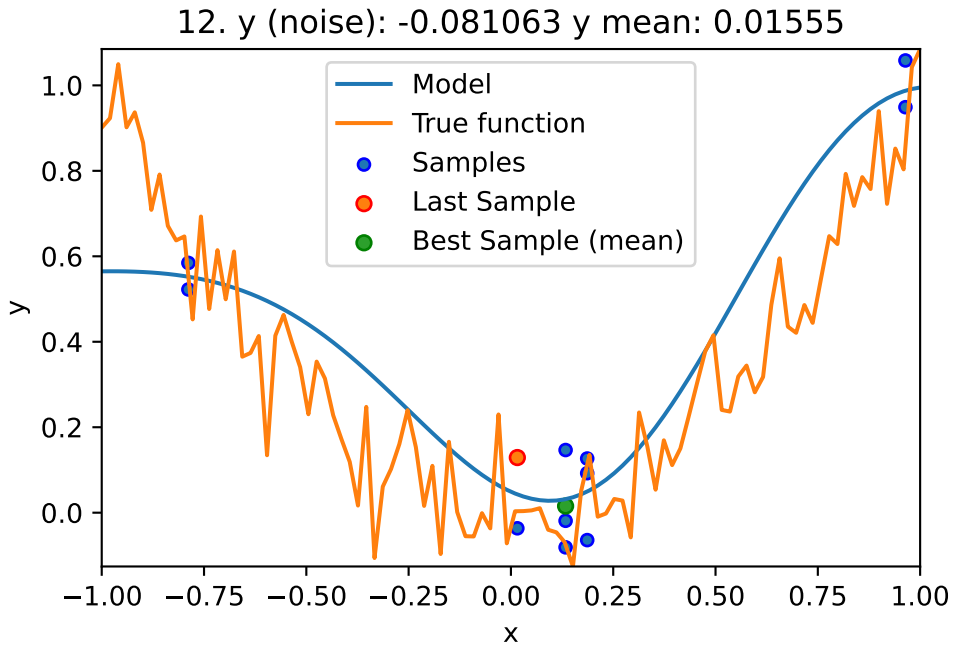
```
spot_1_noisy = spot.Spot(fun=fun,
                    lower = np.array([-1]),
                    upper = np.array([1]),
                    fun_evals = 50,
                    fun_repeats = 2,
                    infill_criterion="ei",
                    noise = True,
                    tolerance_x=0.0,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

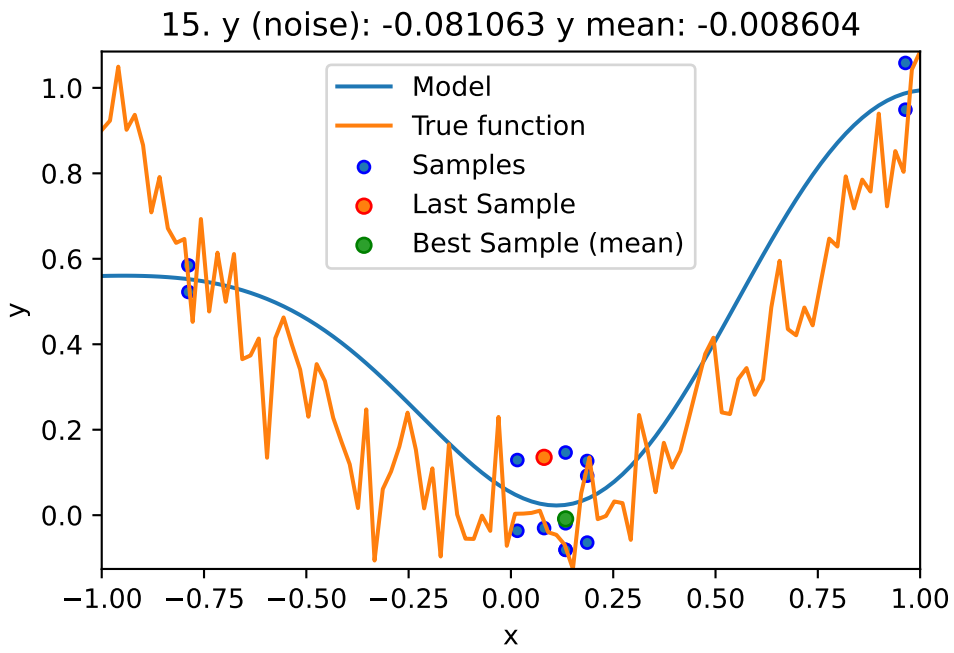
```
                    show_models=True,
                    fun_control = fun_control,
                    design_control={"init_size": 3,
                                    "repeats": 2},
                    surrogate_control={"noise": True})
```

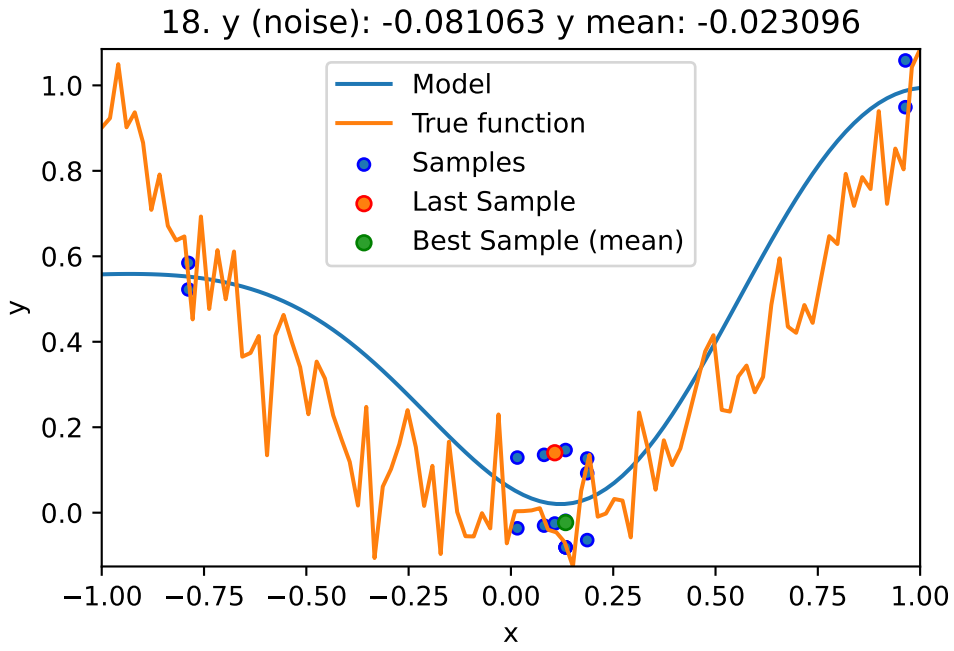
```
spot_1_noisy.run()
```

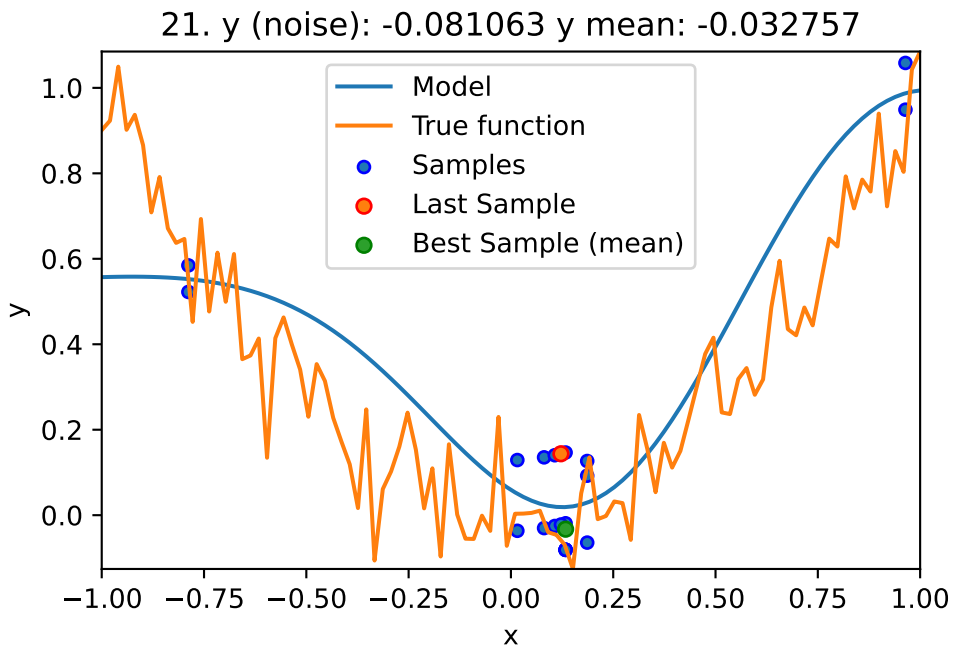


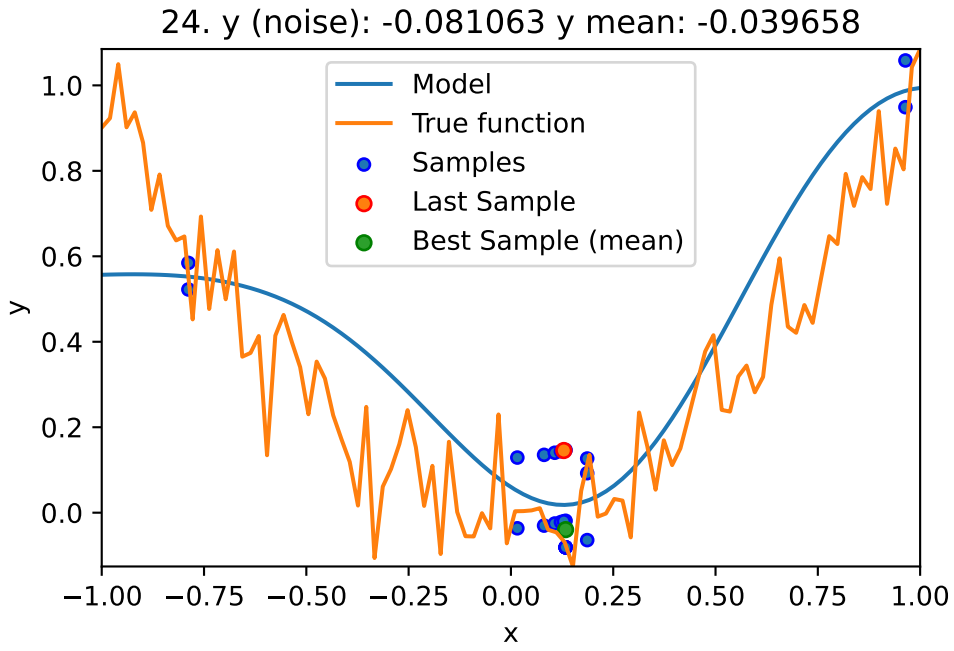

9. y (noise): -0.064157 y mean: 0.051695
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

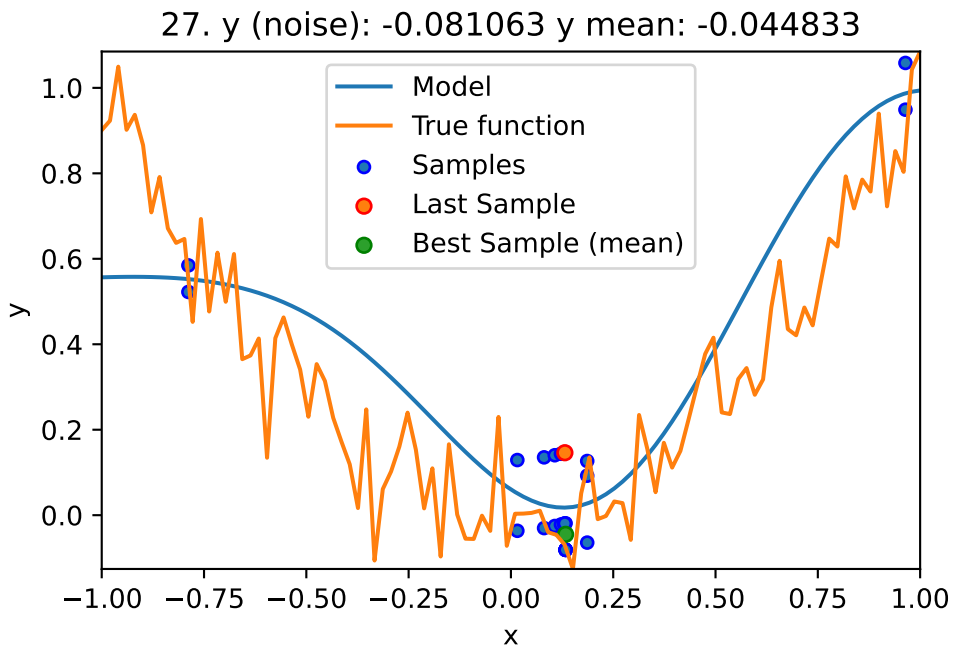

12. y (noise): -0.081063 y mean: 0.01555
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

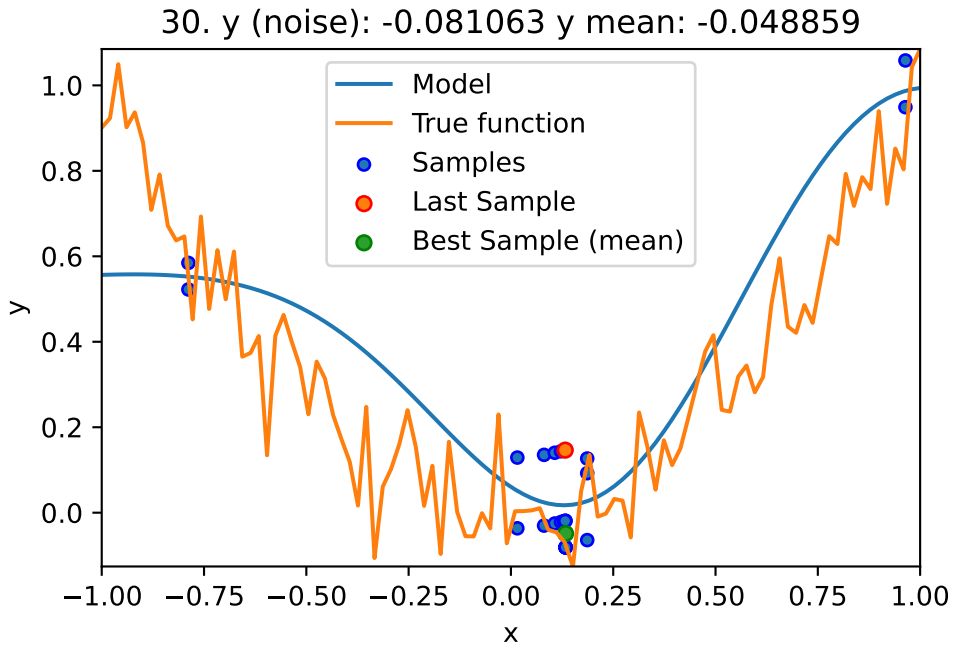

15. y (noise): -0.081063 y mean: -0.008604
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

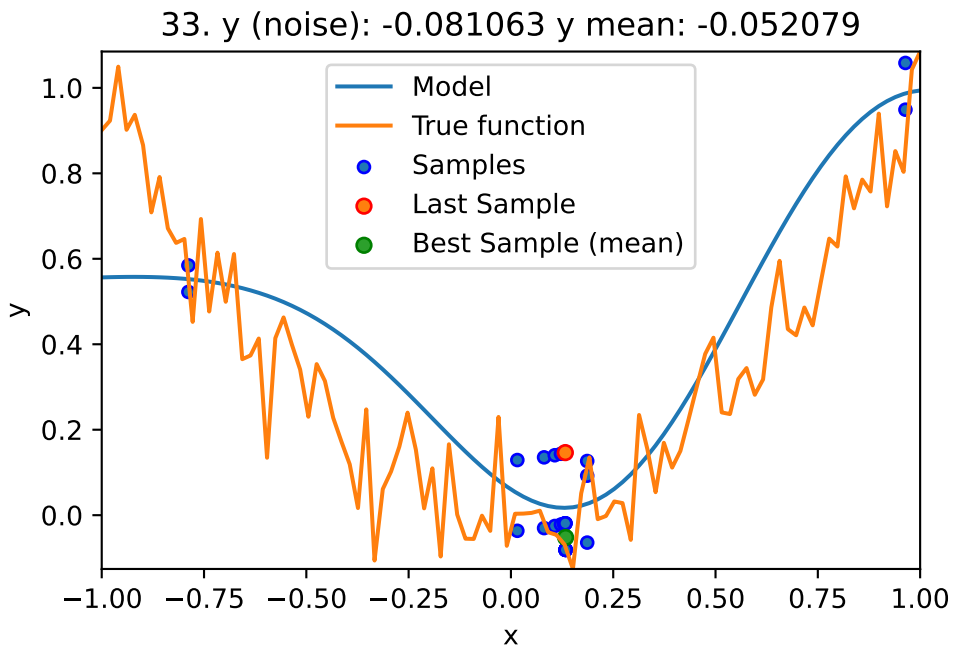

18. y (noise): -0.081063 y mean: -0.023096
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

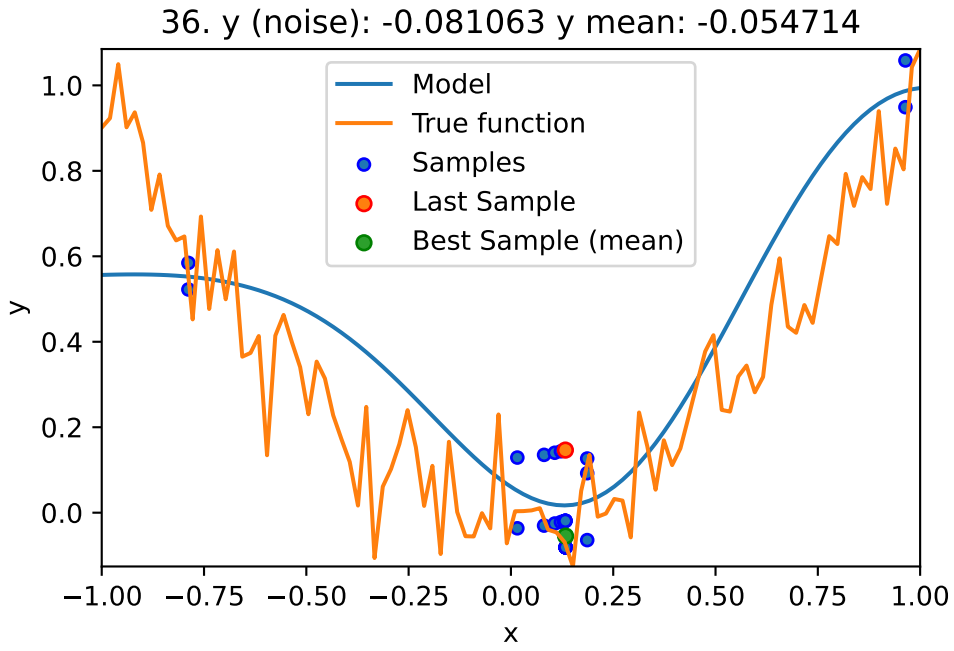

21. y (noise): -0.081063 y mean: -0.032757
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

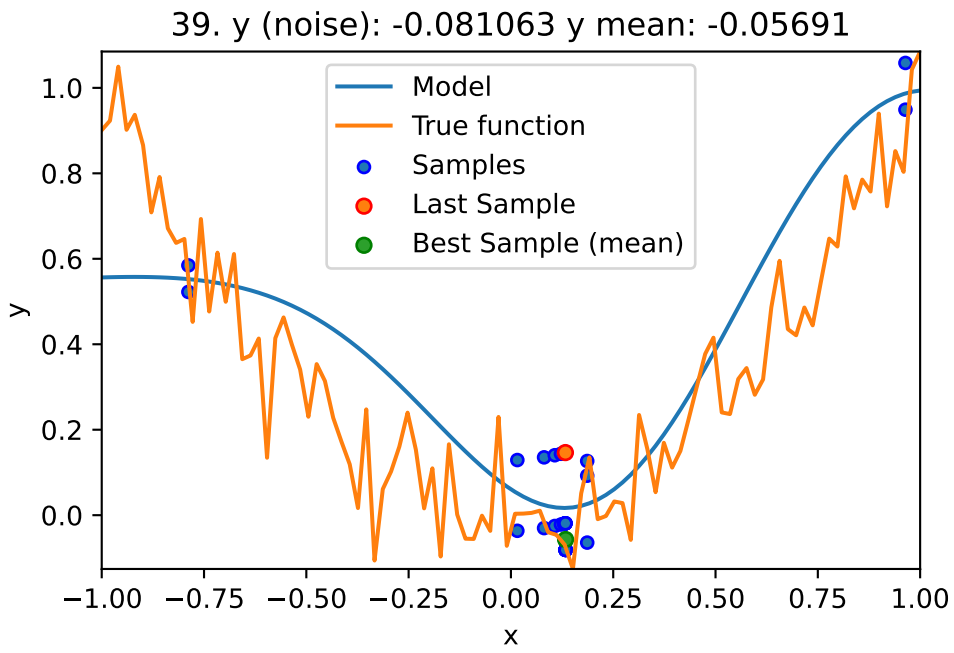

24. y (noise): -0.081063 y mean: -0.039658
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

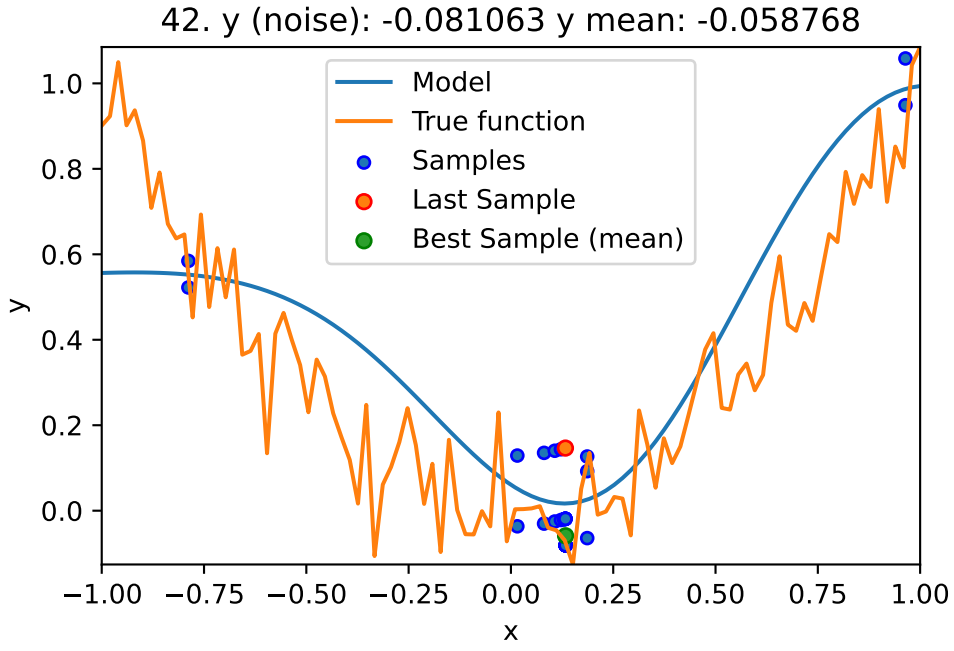

27. y (noise): -0.081063 y mean: -0.044833
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

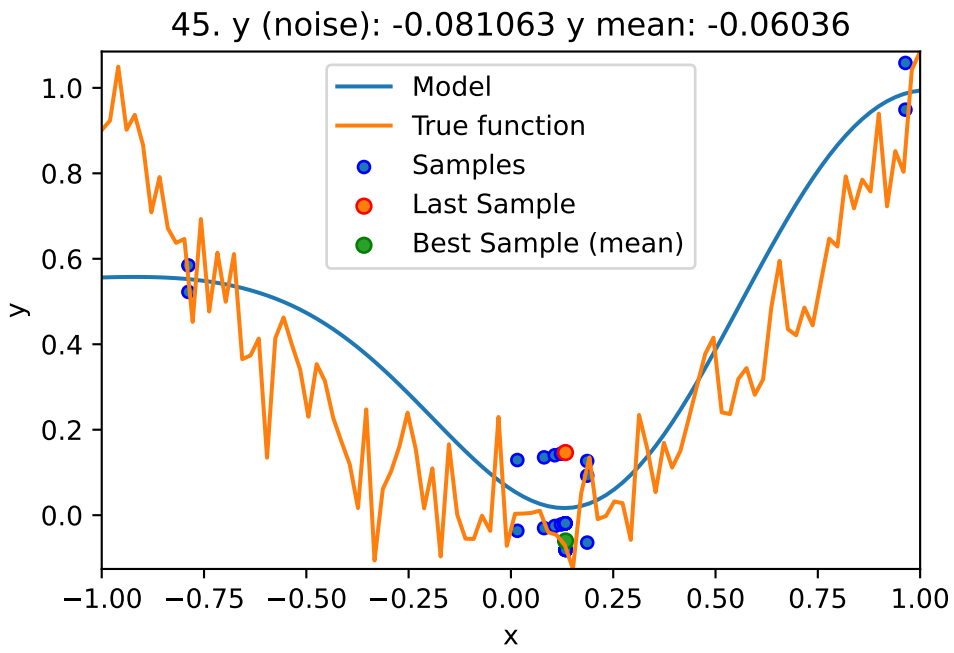

30. y (noise): -0.081063 y mean: -0.048859
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

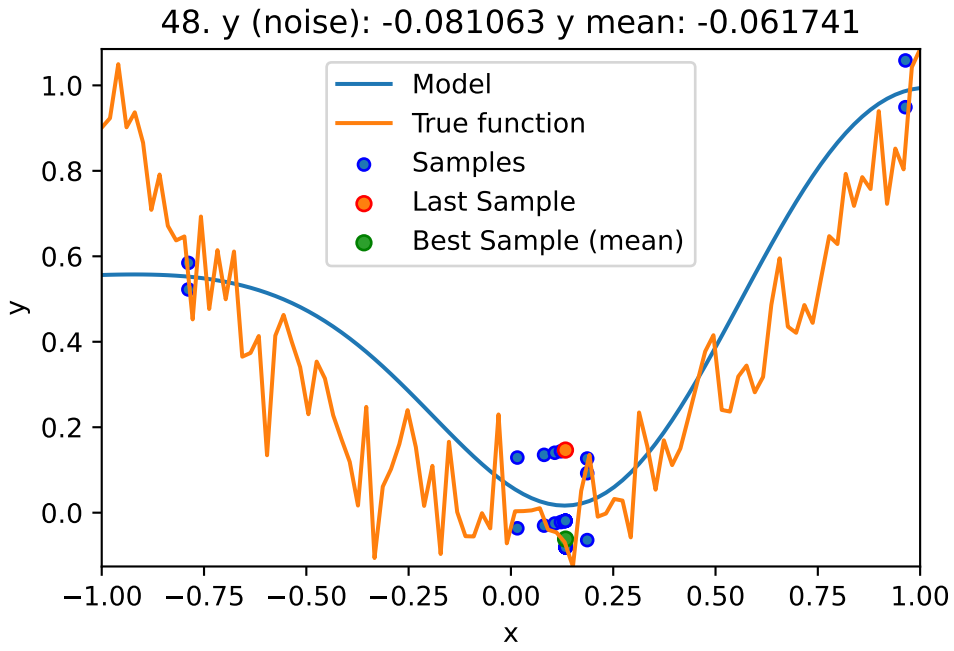

33. y (noise): -0.081063 y mean: -0.052079
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

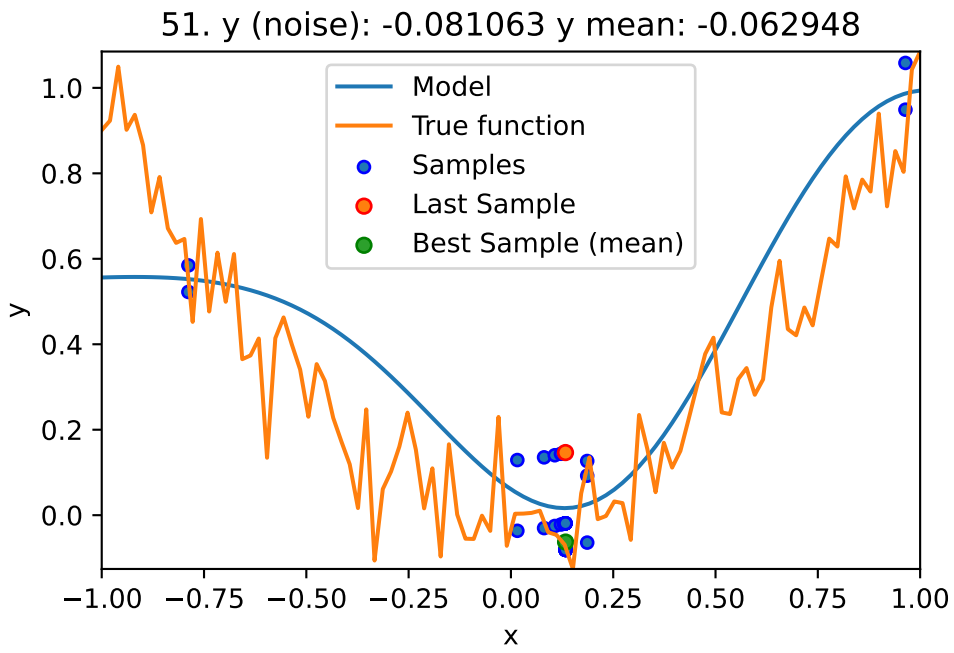

36. y (noise): -0.081063 y mean: -0.054714
Model
True function
Samples
Last Sample
Best Sample (mean)
y
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00


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


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


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



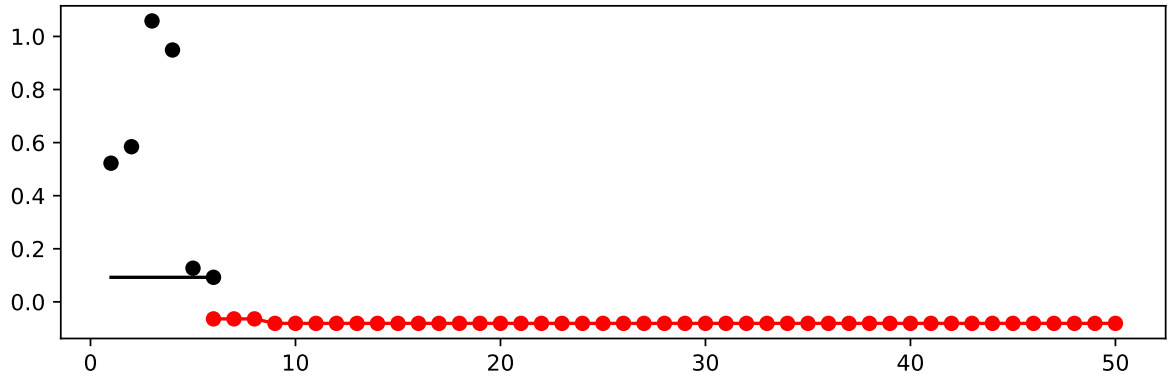

```
<spotPython.spot.spot.Spot at 0x15d187610>
```

14.2 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)
```



14.3 Noise and Surrogates: The Nugget Effect

14.3.1 The Noisy Sphere

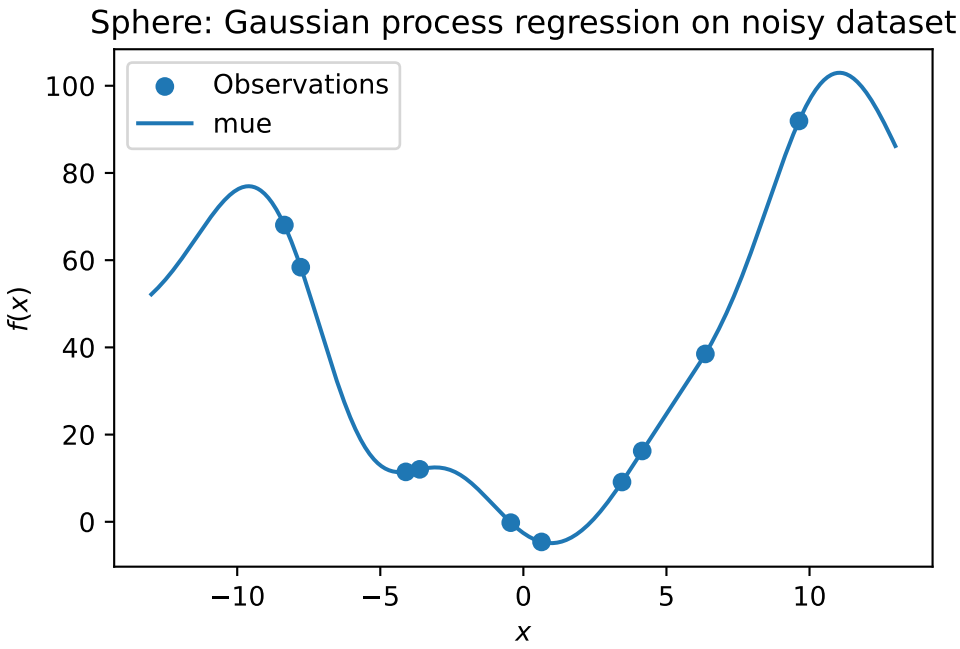
14.3.1.1 The Data

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
```

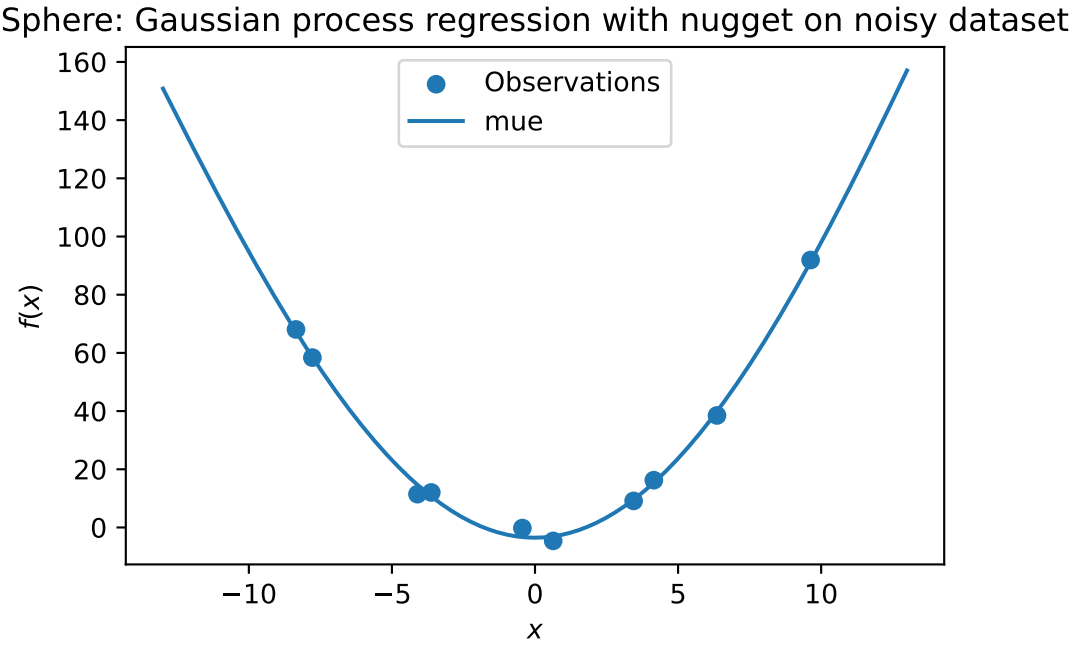
A surrogate without nugget is fitted to these data:

```
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.

14.4 Exercises

14.4.1 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])
```

14.4.2 `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}
```

14.4.3 `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}
```

14.4.4 `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
```

15 Hyperparameter Tuning: sklearn

```
MAX_TIME = 5 # Time in minutes. Counter starts, after the initial design is evaluated. So,
INIT_SIZE = 20 # Initial number of designs to evaluate, before the surrogate is build.
```

```
import pickle
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(':', '-')
experiment_name
```

This notebook exemplifies hyperparameter tuning with SPOT (spotPython). 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.

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

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

```
from tabulate import tabulate
import warnings
import numpy as np
from math import inf
import pandas as pd

from scipy.optimize import differential_evolution
```

```
import matplotlib.pyplot as plt

from sklearn.preprocessing import OneHotEncoder , MinMaxScaler, StandardScaler
from sklearn.preprocessing import OrdinalEncoder
from sklearn.linear_model import RidgeCV
from sklearn.pipeline import make_pipeline , Pipeline
from sklearn.compose import ColumnTransformer
from sklearn.ensemble import HistGradientBoostingRegressor
from sklearn.model_selection import cross_validate
from sklearn.datasets import fetch_openml
from sklearn.metrics import mean_absolute_error, accuracy_score, roc_curve, roc_auc_score,
from sklearn.tree import DecisionTreeRegressor
from sklearn.datasets import make_regression
from sklearn.preprocessing import OneHotEncoder
from sklearn.preprocessing import MinMaxScaler
from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split
from sklearn.datasets import make_moons, make_circles, make_classification
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

warnings.filterwarnings("ignore")

from spotPython.spot import spot
from spotPython.hyperparameters.values import (
    add_core_model_to_fun_control,
    assign_values,
    convert_keys,
    get_bound_values,
    get_default_hyperparameters_for_core_model,
    get_default_values,
    get_dict_with_levels_and_types,
    get_values_from_dict,
    get_var_name,
    get_var_type,
```

```
    iterate_dict_values,
    modify_hyper_parameter_levels,
    modify_hyper_parameter_bounds,
    replace_levels_with_positions,
    return_conf_list_from_var_dict,
    get_one_core_model_from_X,
    transform_hyper_parameter_values,
    get_dict_with_levels_and_types,
    convert_keys,
    iterate_dict_values,
    get_one_sklearn_model_from_X
)

from spotPython.utils.convert import class_for_name
from spotPython.utils.eda import (
    get_stars,
    gen_design_table)
from spotPython.utils.transform import transform_hyper_parameter_values
from spotPython.utils.convert import get_Xy_from_df
from spotPython.plot.validation import plot_cv_predictions, plot_roc, plot_confusion_matri
from spotPython.utils.init import fun_control_init

from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
from spotPython.utils.metrics import mapk, apk
```

15.1 Step 1: Initialization of the Empty `fun_control` Dictionary

```
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/10_spot_hpt_sklearn_classification")
```

15.2 Step 2: Load Data (Classification)

Randomly generate classification data.

```
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()
```

```
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

# just plot the dataset first
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})
```

15.3 Step 3: 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(),
#     )
```

15.4 Step 4: Select `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:

```
# 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:

```
    "SVC":
    {
        "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": 1e-3,
            "transform": "None",
            "lower": 1e-4,
            "upper": 1e-2},
        "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}
    }
```

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

15.5.1 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:

```
fun_control = modify_hyper_parameter_levels(fun_control, "kernel", ["linear", "poly", "rbf
fun_control["core_model_hyper_dict"]["kernel"]
```

15.5.2 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])
# 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"]
```

15.6 Step 6: 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.
```

```
fun = HyperSklearn(seed=123, log_level=50).fun_sklearn
# metric_sklearn = roc_auc_score
# weights = -1.0
metric_sklearn = log_loss
weights = 1.0
# k = None
# custom_metric = mapk
```

```
fun_control.update({
                "horizon": None,
                "oml_grace_period": None,
                "weights": weights,
                "step": None,
                "log_level": 50,
                "weight_coeff": None,
                "metric_river": None,
                "metric_sklearn": metric_sklearn,
                # "metric_params": {"k": k},
                })
```

15.6.1 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,
                })
```

15.7 Step 7: Calling the SPOT Function

15.7.1 Prepare the SPOT Parameters

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
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")
```

```
print(gen_design_table(fun_control))
```

15.7.2 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=SklearnHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
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_optimizer": differential_evolution,
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

15.7.3 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)
```

- Show the Progress of the hyperparameter tuning:

```
spot_tuner.plot_progress(log_y=False, filename="../Figures.d/" + experiment_name+"_progres
```

Print the results.

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

15.8 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="../Figures.d/" + experiment_name+"_i
```

15.9 Get Default Hyperparameters

```
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

15.10 Get SPOT Results

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

```
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

15.11 Plot: Compare Predictions

```
plot_roc([model_default, model_spot], fun_control, model_names=["Default", "Spot"])
```

```
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)
```

15.12 Detailed Hyperparameter Plots

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

15.13 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

15.14 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 Hyperparameter Tuning: PyTorch With fashionMNIST Data Using Hold-out Data Sets

```
MAX_TIME = 60
INIT_SIZE = 10
DEVICE = "cpu" # "cuda:0"
```

```
import pickle
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(':', '-')
experiment_name
```

This notebook exemplifies hyperparameter tuning with SPOT (spotPython). 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.

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

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

```
from tabulate import tabulate
import copy
import warnings
import numbers
```

```
import json
import calendar
import math
import datetime as dt
import numpy as np
from math import inf
import pandas as pd

from scipy.optimize import differential_evolution

import matplotlib.pyplot as plt

import torch
from torch import nn
from torch.utils.data import DataLoader
from torchvision import datasets
from torchvision.transforms import ToTensor
from functools import partial
import torch.nn.functional as F
import torch.optim as optim
from torch.utils.data import random_split
import torchvision
import torchvision.transforms as transforms

from spotPython.spot import spot
from spotPython.hyperparameters.values import (
    add_core_model_to_fun_control,
    assign_values,
    convert_keys,
    get_bound_values,
    get_default_hyperparameters_for_core_model,
    get_default_values,
    get_dict_with_levels_and_types,
    get_values_from_dict,
    get_var_name,
    get_var_type,
    iterate_dict_values,
    modify_hyper_parameter_levels,
    modify_hyper_parameter_bounds,
    replace_levels_with_positions,
    return_conf_list_from_var_dict,
```

```
    get_one_core_model_from_X,
    transform_hyper_parameter_values,
    get_dict_with_levels_and_types,
    convert_keys,
    iterate_dict_values,
)

from spotPython.torch.traintest import evaluate_cv, evaluate_hold_out
from spotPython.utils.convert import class_for_name
from spotPython.utils.eda import (
    get_stars,
    gen_design_table)
from spotPython.utils.transform import transform_hyper_parameter_values

from spotPython.utils.convert import get_Xy_from_df
from spotPython.utils.init import fun_control_init
from spotPython.plot.validation import plot_cv_predictions, plot_roc, plot_confusion_matri

from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.fun.hypertorch import HyperTorch

warnings.filterwarnings("ignore")

# Neural Net specific imports:
from spotPython.torch.netfashionMNIST import Net_fashionMNIST
```

```
print(torch.__version__)
# Check that MPS is available
if not torch.backends.mps.is_available():
    if not torch.backends.mps.is_built():
        print("MPS not available because the current PyTorch install was not "
              "built with MPS enabled.")
    else:
        print("MPS not available because the current MacOS version is not 12.3+ "
              "and/or you do not have an MPS-enabled device on this machine.")

else:
    mps_device = torch.device("mps")
    print("MPS device: ", mps_device)
```

16.1 Step 1: Initialization of the Empty `fun_control` Dictionary

```
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/10_spot_hpt_sklearn_classification")
```

16.2 Step 2: Load fashionMNIST Data

```
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
```

```
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})
```

16.3 Step 3: Specification of the Preprocessing Model

```
# categorical_columns = []
# one_hot_encoder = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
# prep_model = ColumnTransformer(
#         transformers=[
#             ("categorical", one_hot_encoder, categorical_columns),
#         ],
#         remainder=StandardScaler(),
#     )
prep_model = None
fun_control.update({"prep_model": prep_model})
```

16.4 Step 4: Select `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 `netcifar10.py`. The class is imported here.

Note: In addition to the class Net from the PyTorch tutorial, the class Net_CIFAR10 has additional attributes, namely:

- learning rate (`lr`),
- batchsize (`batch_size`),
- epochs (`epochs`), and
- k_folds (`k_folds`).

Further attributes can be easily added to the class, e.g., `optimizer` or `loss_function`.

```
core_model = Net_fashionMNIST
fun_control = add_core_model_to_fun_control(core_model=core_model,
                                fun_control=fun_control,
                                hyper_dict=TorchHyperDict,
                                filename=None)
```

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

16.5.1 Modify hyperparameter of type factor

```
# fun_control = modify_hyper_parameter_levels(fun_control, "leaf_model", ["LinearRegressio
# fun_control["core_model_hyper_dict"]
```

16.5.2 Modify hyperparameter of type numeric and integer (boolean)

```
# 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", bounds=[0, 0])
# fun_control["core_model_hyper_dict"]
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])
```

16.6 Step 6: Selection of the Objective (Loss) Function

```
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[1].

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:

[1] https://torchmetrics.readthedocs.io/en/latest/.

- 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)
```

> **i** Minimization and maximization:
>
> `spotPython` performs minimization by default. If accuracy should be maximized, then the objective function has to be multiplied by -1. Therefore, `weights` is set to -1 in this case.

```
fun = HyperTorch(seed=123, log_level=50).fun_torch
loss_function = CrossEntropyLoss()
weights = 1.0
metric_torch = torchmetrics.Accuracy(task="multiclass", num_classes=10)
shuffle = True
eval = "train_hold_out"
device = DEVICE
show_batch_interval = 100_000
path="torch_model.pt"

fun_control.update({
                "data_dir": None,
                "checkpoint_dir": None,
                "horizon": None,
                "oml_grace_period": None,
                "weights": weights,
                "step": None,
                "log_level": 50,
                "weight_coeff": None,
                "metric_torch": metric_torch,
                "metric_river": None,
                "metric_sklearn": None,
                "loss_function": loss_function,
                "shuffle": shuffle,
```

```
                "eval": eval,
                "device": device,
                "show_batch_interval": show_batch_interval,
                "path": path,
                })
```

```
fun_control
```

16.7 Step 7: Calling the SPOT Function

16.7.1 Prepare the SPOT Parameters

Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
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")
```

```
print(gen_design_table(fun_control))
```

16.7.2 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=TorchHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
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_optimizer": differential_evolution,
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

16.7.3 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)
```

- Show the Progress of the hyperparameter tuning:

```
spot_tuner.y
```

```
spot_tuner.plot_progress(log_y=False, filename="../Figures.d/" + experiment_name+"_progres
```

Print the results

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

16.8 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="../Figures.d/" + experiment_name+"_i
```

16.9 Get 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
```

16.10 Get 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
```

16.11 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,
    test_tuned,
    )
train_tuned(net=model_default, train_dataset=train, shuffle=True,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        device = 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 = DEVICE,
        task=fun_control["task"],)
```

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 = DEVICE,
        path=None,
        task=fun_control["task"],)
#| echo: true
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = DEVICE,
            task=fun_control["task"],)
```

16.12 Detailed Hyperparameter Plots

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

16.13 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

16.14 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 Hyperparameter Tuning: PyTorch wth cifar10 Data

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

```
import pickle
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(':', '-')
experiment_name
```

This notebook exemplifies hyperparameter tuning with SPOT (spotPython). 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.

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

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

```
from tabulate import tabulate
import copy
import warnings
import numbers
import json
import calendar
```

```
import math
import datetime as dt
import numpy as np
from math import inf
import pandas as pd

from scipy.optimize import differential_evolution

import matplotlib.pyplot as plt

from functools import partial

import torch
from torch import nn
from torch.utils.data import DataLoader
import torch.nn.functional as F
import torch.optim as optim
from torch.utils.data import random_split
from torchvision import datasets
import torchvision
import torchvision.transforms as transforms
from torchvision.transforms import ToTensor

from spotPython.spot import spot
from spotPython.hyperparameters.values import (
    add_core_model_to_fun_control,
    assign_values,
    convert_keys,
    get_bound_values,
    get_default_hyperparameters_for_core_model,
    get_default_values,
    get_dict_with_levels_and_types,
    get_values_from_dict,
    get_var_name,
    get_var_type,
    iterate_dict_values,
    modify_hyper_parameter_levels,
    modify_hyper_parameter_bounds,
    replace_levels_with_positions,
    return_conf_list_from_var_dict,
    get_one_core_model_from_X,
```

```
    transform_hyper_parameter_values,
    get_dict_with_levels_and_types,
    convert_keys,
    iterate_dict_values,
)

from spotPython.torch.traintest import evaluate_cv, evaluate_hold_out
from spotPython.utils.convert import class_for_name
from spotPython.utils.eda import (
    get_stars,
    gen_design_table)
from spotPython.utils.transform import transform_hyper_parameter_values
from spotPython.utils.convert import get_Xy_from_df
from spotPython.utils.init import fun_control_init
from spotPython.plot.validation import plot_cv_predictions, plot_roc, plot_confusion_matri

from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.fun.hypertorch import HyperTorch

warnings.filterwarnings("ignore")

from spotPython.torch.netcifar10 import Net_CIFAR10
```

```
print(torch.__version__)
# Check that MPS is available
if not torch.backends.mps.is_available():
    if not torch.backends.mps.is_built():
        print("MPS not available because the current PyTorch install was not "
              "built with MPS enabled.")
    else:
        print("MPS not available because the current MacOS version is not 12.3+ "
              "and/or you do not have an MPS-enabled device on this machine.")

else:
    mps_device = torch.device("mps")
    print("MPS device: ", mps_device)
```

17.1 0. Initialization of the Empty `fun_control` Dictionary

```
fun_control = fun_control_init(task="classification")
```

17.2 1. Load Data Cifar10 Data

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

```
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})
```

17.3 2. Specification of the Preprocessing Model

```
# categorical_columns = []
# one_hot_encoder = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
# prep_model = ColumnTransformer(
#         transformers=[
#             ("categorical", one_hot_encoder, categorical_columns),
#         ],
#         remainder=StandardScaler(),
#     )
prep_model = None
fun_control.update({"prep_model": prep_model})
```

17.4 3. Select `algorithm` and `core_model_hyper_dict`

Our implementation is based on the Section "Configurable neural network" in the PyTorch tutorial Hyperparameter Tuning with Ray Tune is used here. `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`. The class is imported here.

Note: In addition to the class Net from the PyTorch tutorial, the class Net_CIFAR10 has additional attributes, namely:

- learning rate (`lr`),
- batchsize (`batch_size`),
- epochs (`epochs`), and
- k_folds (`k_folds`).

Further attributes can be easily added to the class, e.g., `optimizer` or `loss_function`.

```
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)
```

17.4.1 The `hyper_dict` Hyperparameters for the Selected Algorithm

`spotPython` uses simple `JSON` files for the specification of the hyperparameters. The `JSON` file for the `core_model` is called `torch_hyper_dict.json`. The corresponding entries for the

`Net_CIFAR10` class are shown below.

```
{"Net_CIFAR10":
    {
        "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": {
            "type": "float",
            "default": 1e-03,
            "transform": "None",
            "lower": 1e-05,
            "upper": 1e-02},
        "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": 1,
                "upper": 4},
        "k_folds": {
            "type": "int",
            "default": 2,
            "transform": "None",
            "lower": 2,
            "upper": 3}
    }
}
```

Each entry in the JSON file represents one hyperparameter with the following structure: type, default, transform, lower, and upper.

17.4.2 Categorical Hyperparameters

In contrast to Ray Tune, spotPython can handle numerical, boolean, and categorical hyperparameters. Since Ray Tune does not tune categorical hyperparameters, they are not used here. However, they can be specified in the JSON file in a similar way as the numerical hyperparameters as shown below:

```
"factor_hyperparameter": {
    "levels": ["A", "B", "C"],
    "type": "factor",
    "default": "B",
    "transform": "None",
    "core_model_parameter_type": "str",
    "lower": 0,
    "upper": 2},
```

17.5 4. 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 clever 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.

17.5.1 Modify hyperparameter 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.

```
# 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", bounds=[0, 0])
```

```
# fun_control["core_model_hyper_dict"]
fun_control = modify_hyper_parameter_bounds(fun_control, "k_folds", bounds=[2, 2])
```

17.5.2 Modify hyperparameter of type factor

In a similar manner as for the numerical hyperparameters, the categorical hyperparameters can be modified. For example, the hyperparameter `leaf_model` is de-activated here by choosing only one value `"LinearRegression"`.

```
# fun_control = modify_hyper_parameter_levels(fun_control, "leaf_model", ["LinearRegressio
# fun_control["core_model_hyper_dict"]
```

17.6 5. Selection of the Objective (Loss) Function

```
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[1].

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

[1] https://torchmetrics.readthedocs.io/en/latest/.

- Automatic synchronization between multiple devices

Therefore, we set

```
import torchmetrics
metric_torch = torchmetrics.Accuracy(task="multiclass", num_classes=10)
```

Important:

- `spotPython` performs minimization by default.
- If accuracy should be maximized, then the objective function has to be multiplied by -1. Therefore, `weights` is set to -1 in this case.

```
loss_function = CrossEntropyLoss()
weights = 1.0
metric_torch = torchmetrics.Accuracy(task="multiclass", num_classes=10)
shuffle = True
eval = "train_hold_out"
device = DEVICE
show_batch_interval = 100_000
path="torch_model.pt"

fun_control.update({
                "data_dir": None,
                "checkpoint_dir": None,
                "horizon": None,
                "oml_grace_period": None,
                "weights": weights,
                "step": None,
                "log_level": 50,
                "weight_coeff": None,
                "metric_torch": metric_torch,
                "metric_river": None,
                "metric_sklearn": None,
                "loss_function": loss_function,
                "shuffle": shuffle,
                "eval": eval,
                "device": device,
                "show_batch_interval": show_batch_interval,
                "path": path,
                })
```

17.7 6. Calling the SPOT Function

17.7.1 Prepare the SPOT Parameters

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
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")
```

```
print(gen_design_table(fun_control))
```

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
```

17.7.2 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=TorchHyperDict().load()
X_start = get_default_hyperparameters_as_array(fun_control, hyper_dict)
X_start
```

```
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_optimizer": differential_evolution,
                                       "model_fun_evals": 10_000,
                                       "log_level": 50
                                       })
spot_tuner.run(X_start=X_start)
```

17.7.3 4 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)
```

- Show the Progress of the hyperparameter tuning:

```
spot_tuner.y
```

```
spot_tuner.plot_progress(log_y=False, filename="../Figures.d/" + experiment_name+"_progres
```

- Print the Results

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

17.8 Show variable importance

```
spot_tuner.plot_importance(threshold=0.025, filename="../Figures.d/" + experiment_name+"_i
```

17.9 Get Default Hyperparameters

```
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
model_default = fun_control["core_model"](**values_default)
model_default
```

17.10 Get 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
```

17.11 Evaluation of the Tuned 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.

```
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 = 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 = DEVICE,
        task=fun_control["task"],)
```

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 = DEVICE,
        path=None,
        task=fun_control["task"],)
#| echo: true
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = DEVICE,
```

```
            task=fun_control["task"],)
```

17.12 Detailed Hyperparameter Plots

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

17.13 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

17.14 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 Hyperparameter Tuning for PyTorch With spotPython

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
- spotPython: 0.2.15

spotPython can be installed via pip[1].

```
!pip install spotPython
```

Results that refer to the Ray Tune package are taken from https://PyTorch.org/tutorials/beginner/hyperparameter_tuning_tutorial.html[2].

18.1 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.

```
MAX_TIME = 60
INIT_SIZE = 20
DEVICE = "cpu" # "cuda:0"
```

[1] Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

[2] We were not able to install Ray Tune on our system. Therefore, we used the results from the PyTorch tutorial.

18.2 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.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="classification",
    tensorboard_path="runs/14_spot_ray_hpt_torch_cifar10")
```

18.3 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})
```

18.4 The Model (Algorithm) to be Tuned

18.4.1 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})
```

18.4.2 Select `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 18.4.2.1 first, before the extended implementation with `spotPython` is shown in Section 18.4.2.2.

18.4.2.1 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)
```

18.4.2.2 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
```

18.4.3 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
```

18.4.4 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)
```

18.5 The Search Space: Hyperparameters

In Section 18.5.1, 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 Section 18.5.2.

18.5.1 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.

18.5.2 Configuring the Search Space With spotPython

18.5.2.1 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 `Net_CIFAR10` class are shown below.

```
{"Net_CIFAR10":
    {
        "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},
        "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": 1,
            "upper": 4},
        "k_folds": {
            "type": "int",
            "default": 2,
            "transform": "None",
            "lower": 2,
            "upper": 3},
        "patience": {
            "type": "int",
```

```
            "default": 5,
            "transform": "None",
            "lower": 2,
            "upper": 10},
        "optimizer": {
            "levels": ["Adadelta",
                       "Adagrad",
                       "Adam",
                       "AdamW",
                       "SparseAdam",
                       "Adamax",
                       "ASGD",
                       "LBFGS",
                       "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}
    }
}
```

18.5.3 Modifying the Hyperparameters

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.

18.5.3.1 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.

18.5.3.2 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])
```

18.5.3.3 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 18.6, 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"])
```

18.6 Optimizers

Table 19.1 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 18.1: 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	-	-	-	-	-
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])
```

18.7 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.

18.7.1 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.

`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).

18.7.2 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.

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.

18.7.3 Overview of the Evaluation Settings

18.7.3.1 Settings for the Hyperparameter Tuning

An overview of the training evaluations is shown in Table 19.2. `"train_cv"` and `"test_cv"` use `sklearn.model_selection.KFold()` internally. More details on the data splitting are provided in Section 20.14 (in the Appendix).

Table 18.2: 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.

18.7.3.2 Settings for the Final Evaluation of the Tuned Architecture

18.7.3.2.1 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.

18.7.3.2.2 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 20.14.1.4 describes the final evaluation of the tuned architecture.

18.8 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)
```

```
loss_function = CrossEntropyLoss()
weights = 1.0
metric_torch = torchmetrics.Accuracy(task="multiclass", num_classes=10)
shuffle = True
eval = "train_hold_out"
device = DEVICE
show_batch_interval = 100_000
path="torch_model.pt"

fun_control.update({
                "data_dir": None,
                "checkpoint_dir": None,
                "horizon": None,
                "oml_grace_period": None,
                "weights": weights,
                "step": None,
                "log_level": 50,
                "weight_coeff": None,
                "metric_torch": metric_torch,
                "metric_river": None,
                "metric_sklearn": None,
                "loss_function": loss_function,
                "shuffle": shuffle,
                "eval": eval,
                "device": device,
                "show_batch_interval": show_batch_interval,
                "path": path,
                })
```

18.9 Preparing the SPOT Call

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

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))
```

This allows to check if all information is available and if the information is correct. Table 19.3 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 $2^4 = 16$.

Table 18.3: Experimental design for the hyperparameter tuning.

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

18.10 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
```

18.11 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)
```

18.12 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`.

```
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)
```

During the run, the following output is shown:

```
config: {'l1': 128, 'l2': 8, 'lr_mult': 1.0, 'batch_size': 32,
    'epochs': 16, 'k_folds': 0, 'patience': 3,
    'optimizer': 'AdamW', 'sgd_momentum': 0.9}
Epoch: 1
Loss on hold-out set: 1.5143253986358642
Accuracy on hold-out set: 0.4447
MulticlassAccuracy value on hold-out data: 0.4447000026702881
Epoch: 2
...
Epoch: 15
Loss on hold-out set: 1.2061678514480592
Accuracy on hold-out set: 0.59505
MulticlassAccuracy value on hold-out data: 0.5950499773025513
Early stopping at epoch 14
Returned to Spot: Validation loss: 1.2061678514480592
-----------------------------------------------
```

18.13 Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard.

18.13.1 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.

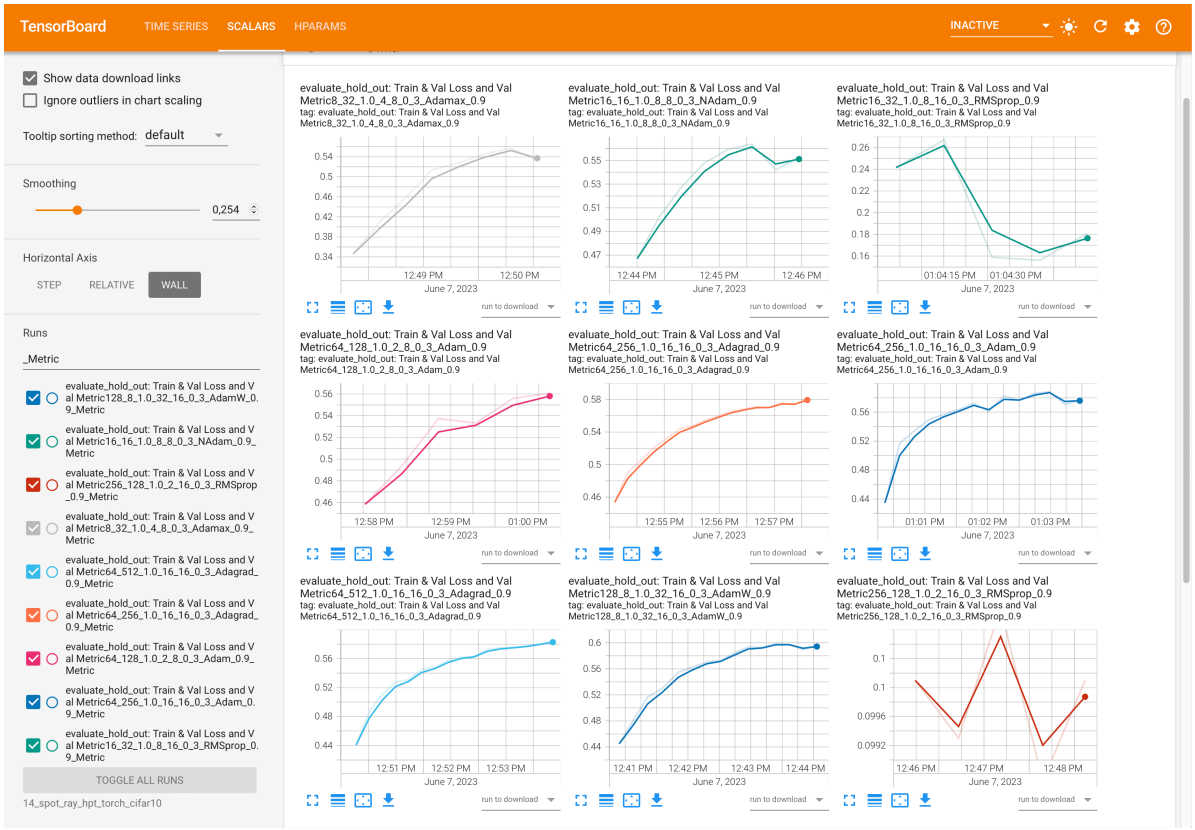


Figure 18.1: Tensorboard

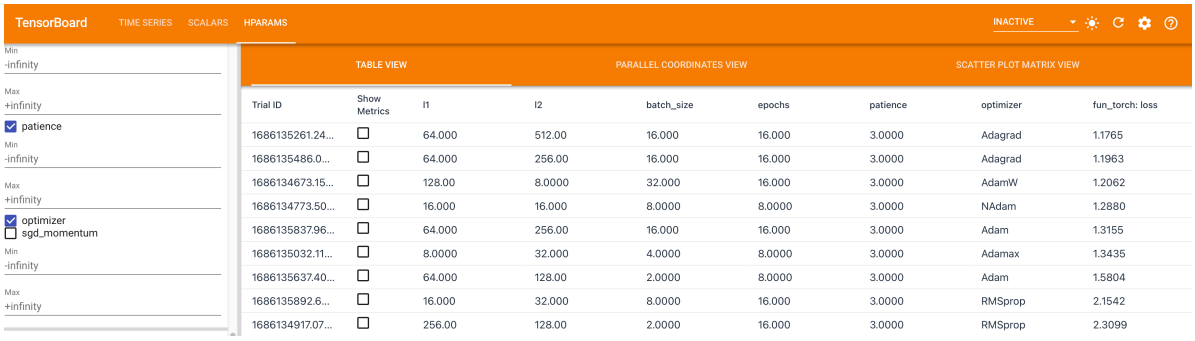


Figure 18.2: Tensorboard

18.13.2 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)
```

18.14 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 Figure 19.4.

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

Figure 19.4 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. Figure 19.4 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 Figure 19.4. 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 Table 19.4. The table shows the hyperparameters, their types, default values, lower and upper bounds, and the transformation function. The column "tuned"

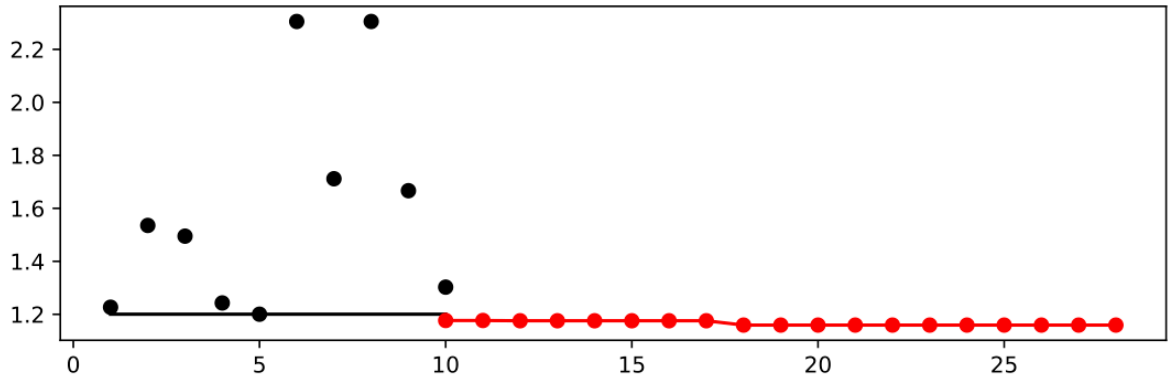


Figure 18.3: Progress plot. `Black` dots denote results from the initial design. `Red` dots illustrate the improvement found by the surrogate model based optimization (surrogate model based optimization).

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.

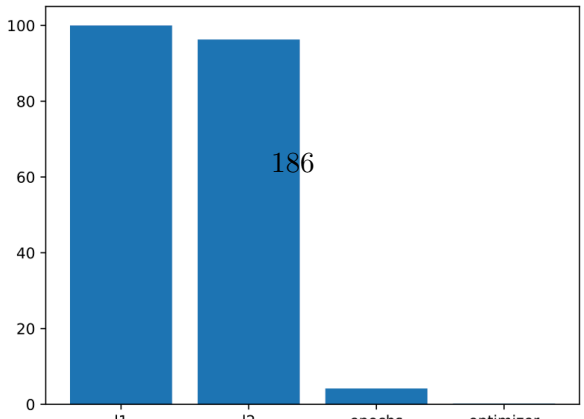
```
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

Table 18.4: Results of the hyperparameter tuning.

name	type	default	lower	upper	tuned	transform	importance	stars
l1	int	5	2.0	9.0	7.0	pow_2_int	100.00	***
l2	int	5	2.0	9.0	3.0	pow_2_int	96.29	***
lr_mult	float	1.0	0.1	10.0	0.1	None	0.00	
batchsize	int	4	1.0	5.0	4.0	pow_2_int	0.00	
epochs	int	3	3.0	4.0	4.0	pow_2_int	4.18	*
k_folds	int	2	0.0	0.0	0.0	None	0.00	
patience	int	5	3.0	3.0	3.0	None	0.00	
optimizer	factor	SGD	0.0	9.0	3.0	None	0.16	.

To visualize the most important hyperparameters, `spotPython` provides the function `plot_importance`. The following code generates the importance plot from Figure 19.5.

```
spot_tuner.plot_importance(threshold=0.025,
    filename="./figures/" + experiment_name+"_importance.png")
```



18.14.1 Get 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
```

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:

```
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=64, bias=True)
  (fc2): Linear(in_features=64, out_features=32, bias=True)
  (fc3): Linear(in_features=32, out_features=10, bias=True)
)
```

18.14.2 Get Default Hyperparameters

In a similar manner as in Section 18.14.1, 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)
```

The corresponding default model has the following architecture:

```
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)
)
```

18.14.3 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 = 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 = DEVICE,
        task=fun_control["task"],)
```

18.14.4 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.

```
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
```

```
        shuffle=True,
        device = 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 = DEVICE,
            task=fun_control["task"],)
```

These runs will generate output similar to the following:

```
Loss on hold-out set: 1.2267619131326675
Accuracy on hold-out set: 0.58955
Early stopping at epoch 13
```

18.14.5 Comparison with Default Hyperparameters and Ray Tune

Table 19.5 shows the loss and accuracy of the default model, the model with the hyperparameters from SPOT, and the model with the hyperparameters from `ray[tune]`. The table shows a comparison of the loss and accuracy of the default model, the model with the hyperparameters from SPOT, and the model with the hyperparameters from `ray[tune]`. `ray[tune]` only shows the validation loss, because training loss is not reported by `ray[tune]`

Table 18.5: Comparison.

Model	Validation Loss	Validation Accuracy	Loss	Accuracy
Default	2.1221	0.2452	2.1182	0.2425
`spotPython`	1.2268	0.5896	1.2426	0.5957
`ray[tune]`	1.1815	0.5836	-	0.5806

18.14.6 Detailed Hyperparameter Plots

The contour plots in this section visualize the interactions of the three most important hyperparameters, `l1`, `l2`, and `epochs`, and `optimizer` of the surrogate model used to optimize the 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. For this, again refer to the notebook (Bartz-Beielstein 2023).

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

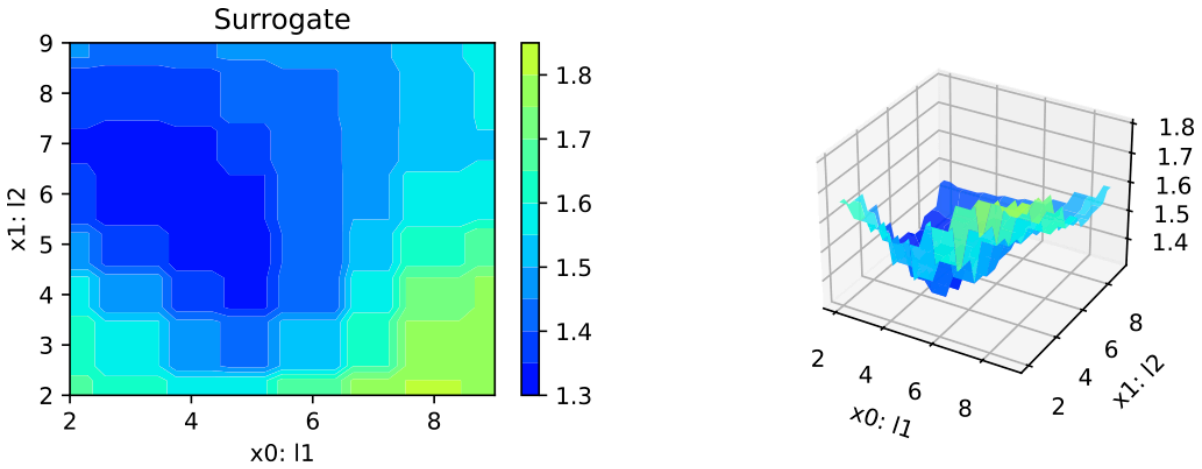


Figure 18.5: Contour plot of the loss as a function of `l1` and `l2`, i.e., the number of neurons in the layers.

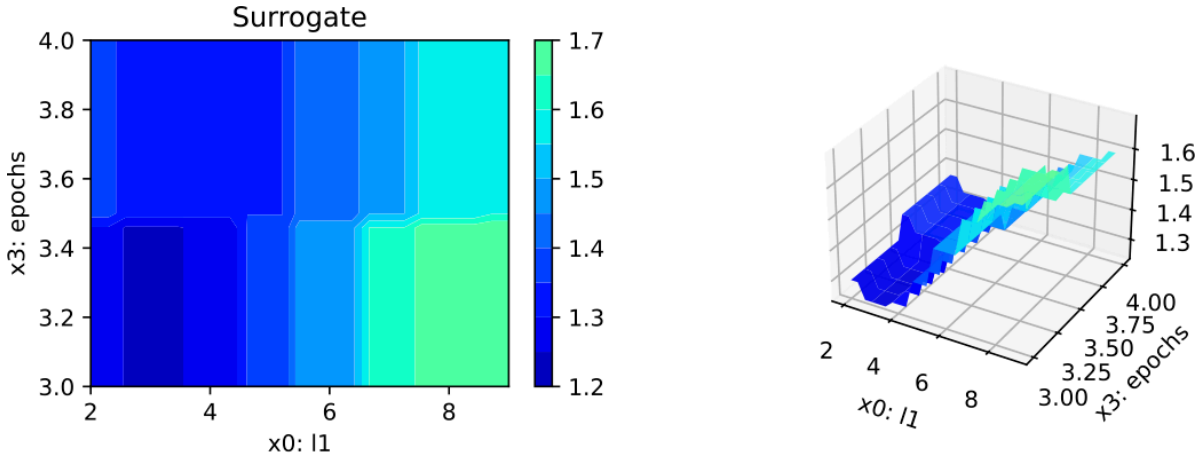


Figure 18.6: Contour plot of the loss as a function of the number of epochs and the neurons in layer `l1`.

The figures (Figure 18.5 to Figure 18.10) 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, Figure 19.7 shows the parallel plot of the hyperparameters.

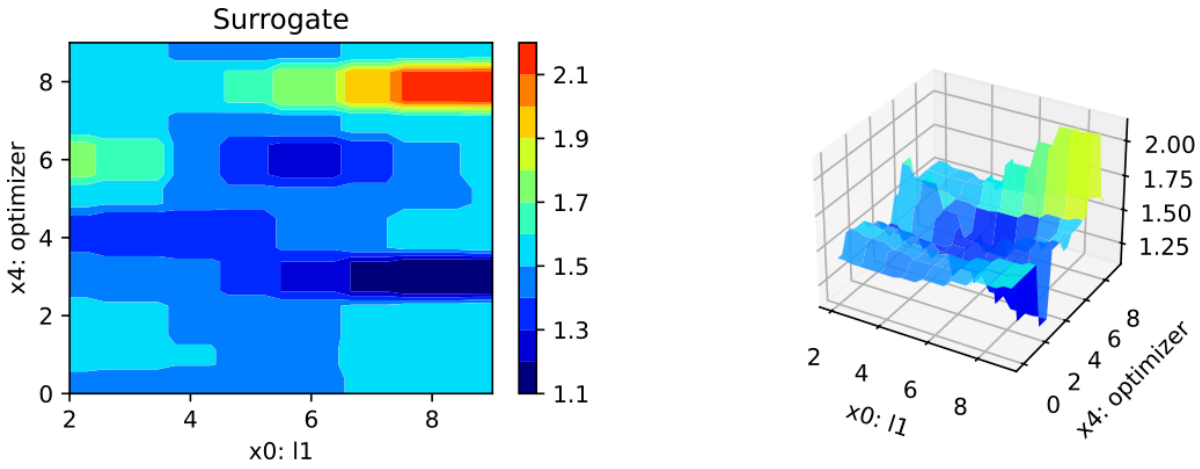


Figure 18.7: Contour plot of the loss as a function of the optimizer and the neurons in layer `l1`.

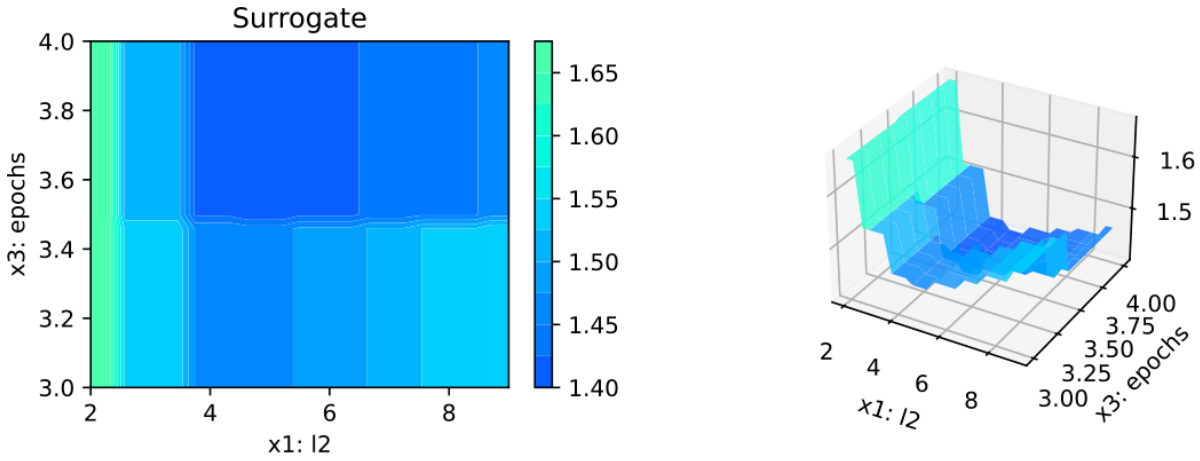


Figure 18.8: Contour plot of the loss as a function of the number of epochs and the neurons in layer `l2`.

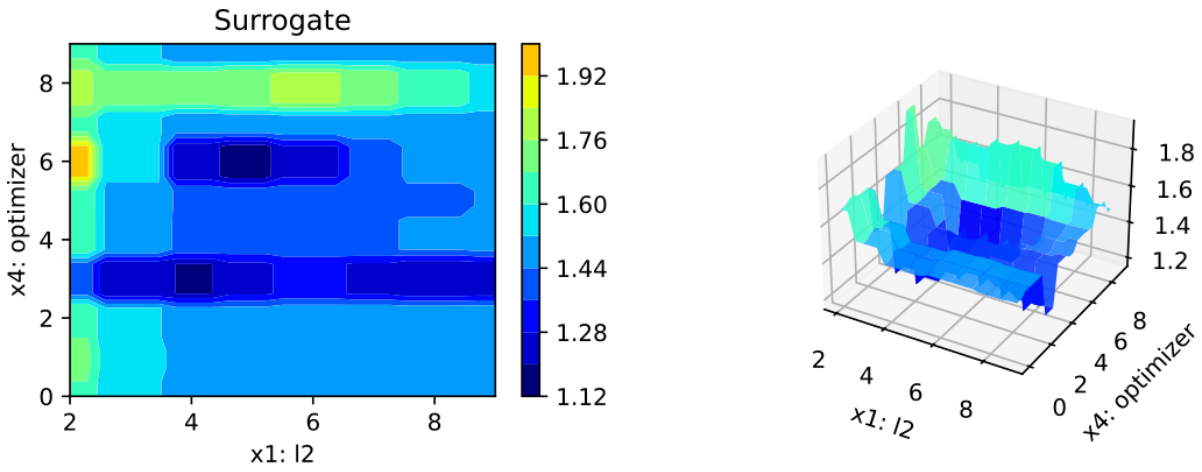


Figure 18.9: Contour plot of the loss as a function of the optimizer and the neurons in layer 12.

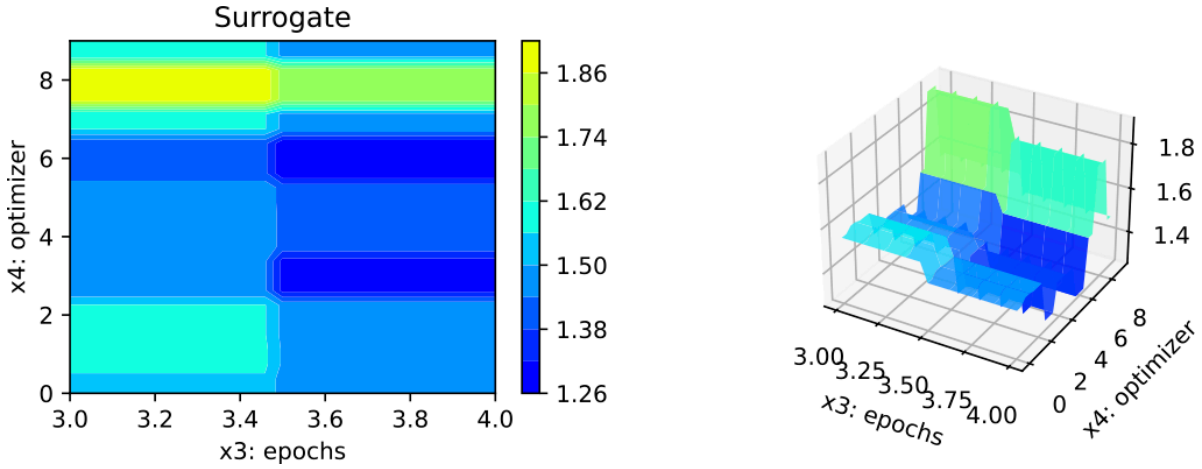


Figure 18.10: Contour plot of the loss as a function of the optimizer and the number of epochs.

```
spot_tuner.parallel_plot()
```

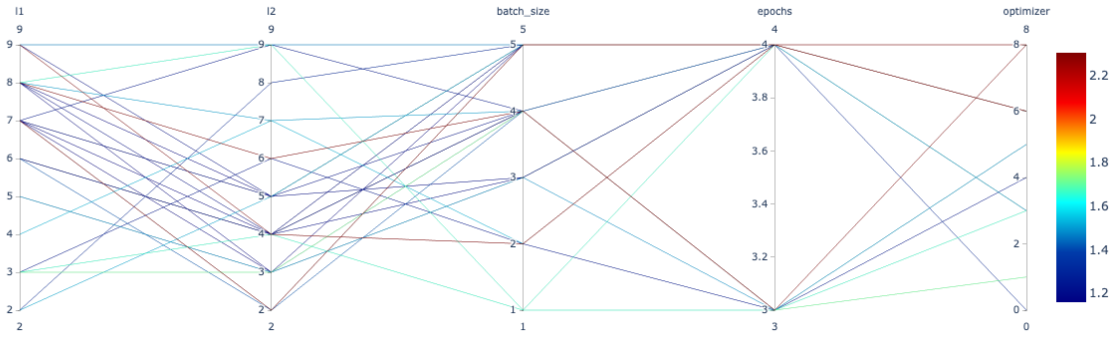


Figure 18.11: Parallel plot

18.15 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.

18.16 Appendix

18.16.1 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
```

19 Hyperparameter Tuning for PyTorch With spotPython: Regression

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
- spotPython: 0.2.15

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
```

19.1 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.

```
MAX_TIME = 10
INIT_SIZE = 20
DEVICE = "cpu" # "cuda:0"
```

19.2 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.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="regression",
 tensorboard_path="runs/24_spot_torch_regression")
```

19.3 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)
```

```
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
```

- 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 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(),
     )
```

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

19.5 Select `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`.

```
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`. 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
```

:::{.callout-note}

We see that the class `Net_lin_reg` 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_lin_reg` 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.netregression import Net_lin_reg
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
core_model = Net_lin_reg
fun_control = add_core_model_to_fun_control(core_model=core_model,
                               fun_control=fun_control,
                               hyper_dict=TorchHyperDict,
                               filename=None)
```

19.6 The Search Space

19.6.1 Configuring the Search Space With spotPython

19.6.1.1 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`.

`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 `Net_lin_reg` class are shown below.

```
    "Net_lin_reg":
    {
        "_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}
    },
```

19.7 Modifying the Hyperparameters

`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.

19.7.1 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.

19.7.2 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".

```
# modify the hyperparameter levels

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])
```

19.7.3 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 19.7.4, 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"])


fun_control.update({
                "_L_in": n_features,
                "_L_out": 1,})
```

19.7.4 Optimizers

Table 19.1 shows some of the optimizers available in `PyTorch`:

Table 19.1: Optimizers available in PyTorch (selection). "mom" denotes `momentum`, "weight" `weight_decay`, "damp" `dampening`, "nest" `nesterov`, "lr_sc" `learning rate for scaling delta`, "mom_dec" for `momentum_decay`, and "step_s" for `step_sizes`. The default values are shown in the table.

Optimizer	lr	mom	weight	damp	nest	rho	lr_sc	lr_dec	betas	lambd	alpha	mom_dec	decay	step_s
Adadelta	-	-	0.	-	-	0.9	1.0	-	-	-	-	-	-	-
Adagrad	1e-2	-	0.	-	-	-	-	0.	-	-	-	-	-	-
Adam	1e-3	-	0.	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
AdamW	1e-3	-	1e-2	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
SparseAdam	1e-3	-	-	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
Adamax	2e-3	-	0.	-	-	-	-	-	(0.9, 0.999)	-	-	-	-	-
ASGD	1e-2	0.9	0.	-	False	-	-	-	-	1e-4	0.75	-	-	-
LBFGS	1.	-	-	-	-	-	-	-	-	-	-	-	-	-
NAdam	2e-3	-	0.	-	-	-	-	-	(0.9,0.999)	-	0	-	-	-
RAdam	1e-3	-	0.	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
RMSprop	1e-2	0.	0.	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-

Optimizer	lr	mom	weight_d	damp	nest	rho	lr_sc	lr_decay	amsgrad	lambd	alpha	mom_decay	decay	step_s
Rprop	1e-2	-	-	-	-	-	-	-	-	-	(0.5,1.2)	(1e-6, 50)	-	-
SGD	required	0.	0.	False	-	-	-	-	-	-	-	-	-	-

`spotPython` implements an `optimization` handler that maps the optimizer names to the corresponding `PyTorch` optimizers.

> **i** 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 10 optimizers in the portfolio, it is not recommended tuning the hyperparameters that effect one single optimizer only.

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

19.8 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).

19.8.1 Hold-out Data Split and Cross-Validation

As a default, `spotPython` provides a standard hold-out data split and cross validation.

19.8.1.1 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. The following splits are performed in the hold-out setting: $\{\text{train}_0, \text{test}\} \rightarrow \{\text{train}_1, \text{validation}_1, \text{test}\}$, where $\text{train}_1 \cup \text{validation}_1 = \text{train}_0$.

> **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 hyperpa-

rameter 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).

19.8.1.2 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.

19.8.1.3 Overview of the Evaluation Settings

19.8.1.3.1 Settings for the Hyperparameter Tuning

Table 19.2 provides an overview of the training evaluations.

Table 19.2: 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.

- "train_cv" and "test_cv" use sklearn.model_selection.KFold() internally.

19.8.1.4 Settings for the Final Evaluation of the Tuned Architecture

19.8.1.4.1 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 traindata 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_one_epoch(). The validation data is used for early stopping using validate_one_epoch() on the validation data set.

19.8.1.4.2 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_one_epoch() function.

Note: During training, shuffle is set to True, whereas during testing, shuffle is set to False.

19.8.2 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.

19.8.2.1 Loss Function

The loss function is specified by the key `"loss_function"`. We will use MSE loss for the regression task.

```
from torch.nn import MSELoss
loss_torch = MSELoss()
fun_control.update({"loss_function": loss_torch})
```

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[1].

```
from torchmetrics import MeanAbsoluteError
metric_torch = MeanAbsoluteError()
fun_control.update({"metric_torch": metric_torch})
```

19.9 Calling the SPOT Function

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))
```

[1] https://torchmetrics.readthedocs.io/en/latest/.

This allows to check if all information is available and if the information is correct. Table 19.3 shows the experimental design for the hyperparameter tuning. 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 $2^4 = 16$.

Table 19.3: 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.

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	0.001	0.001	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	0.9	0.9	None

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
```

```
fun_control.update({
                "device": "cpu",
                })
```

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`.

```
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)
```

During the run, the following output is shown:

```
config: {'_L_in': 10, '_L_out': 1, 'l1': 64, 'dropout_prob': 0.4475780541539,
    'lr_mult': 0.001, 'batch_size': 16, 'epochs': 512, 'k_folds': 1,
    'patience': 32,'optimizer': 'Adagrad', 'sgd_momentum': 0.9}
Epoch: 1
...
Epoch: 7002
Loss on hold-out set: 1.6959798782529844e-05
MeanAbsoluteError value on hold-out data: 0.0018855303060263395
```

```
Epoch: 7003
Loss on hold-out set: 1.6984027051769603e-05
MeanAbsoluteError value on hold-out data: 0.001883985591121018
Early stopping at epoch 7002
Returned to Spot: Validation loss: 1.6984027051769603e-05
```

19.10 Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard.

19.10.1 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.

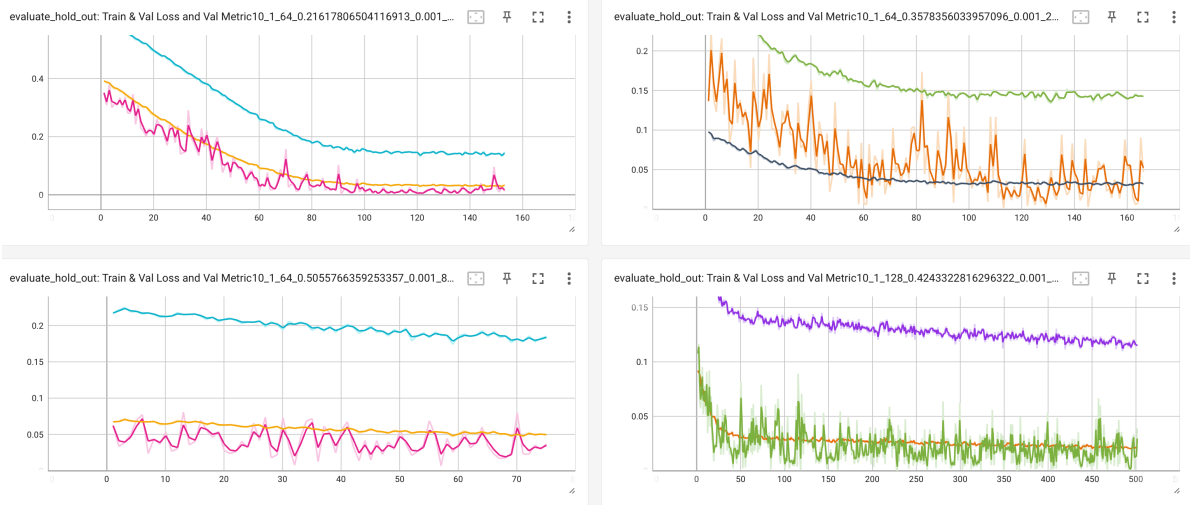


Figure 19.1: Tensorboard

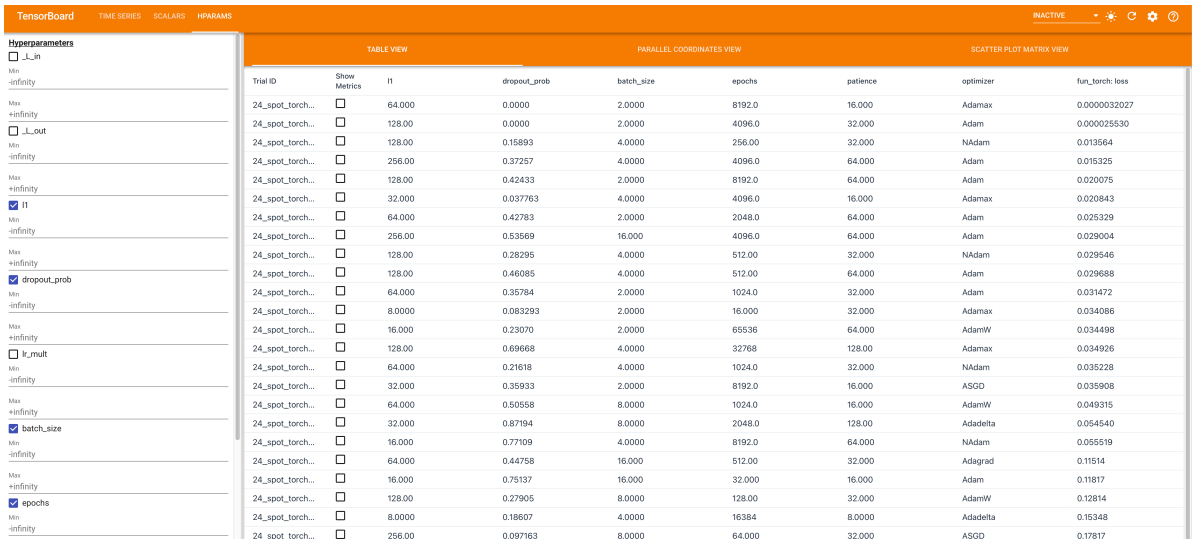


Figure 19.2: Tensorboard

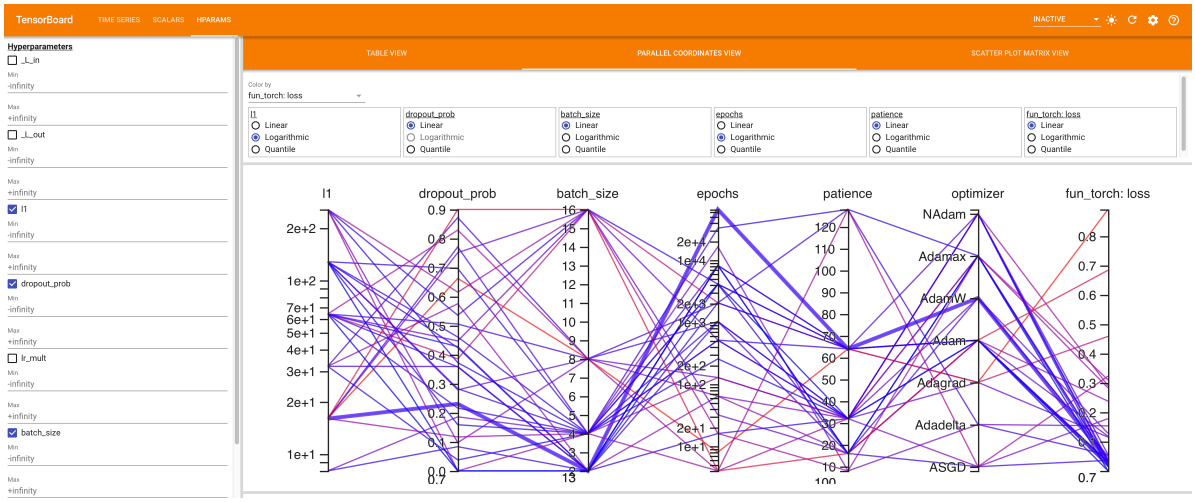


Figure 19.3: Tensorboard

19.11 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 Figure 19.4.

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

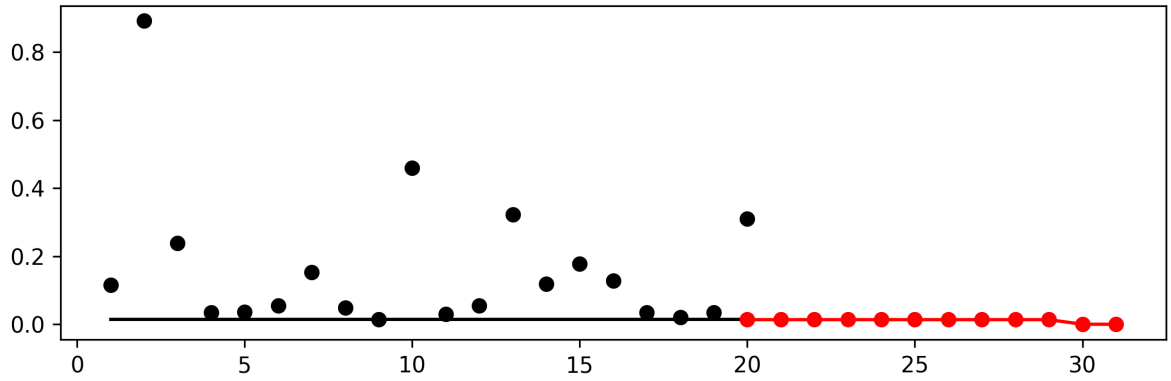


Figure 19.4: Progress plot. `Black` dots denote results from the initial design. `Red` dots illustrate the improvement found by the surrogate model based optimization (surrogate model based optimization).

Figure 19.4 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. Figure 19.4 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 Figure 19.4. 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 Table 19.4.

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

Table 19.4: Results of the hyperparameter tuning. 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.

name	type	default	lower	upper	tuned	transform	importance	stars
_L_in	int	10	10.0	10.0	10.0	None	0.00	
_L_out	int	1	1.0	1.0	1.0	None	0.00	
l1	int	3	3.0	8.0	6.0	power_2_int	1.42	*
drop_p	float	0.01	0.0	0.9	0.0	None	0.00	
lr_mult	float	1.0	0.001	0.001	0.001	None	0.00	
batch_s	int	4	1.0	4.0	1.0	power_2_int	0.01	
epochs	int	4	2.0	16.0	13.0	power_2_int	100.00	***
k_folds	int	1	1.0	1.0	1.0	None	0.00	
patience	int	2	3.0	7.0	4.0	power_2_int	0.00	
optim	factor	SGD	0.0	6.0	4.0	None	0.00	
sgd_mom	float	0.0	0.9	0.9	0.9	None	0.00	

To visualize the most important hyperparameters, `spotPython` provides the function `plot_importance`. The following code generates the importance plot from Figure 19.5.

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

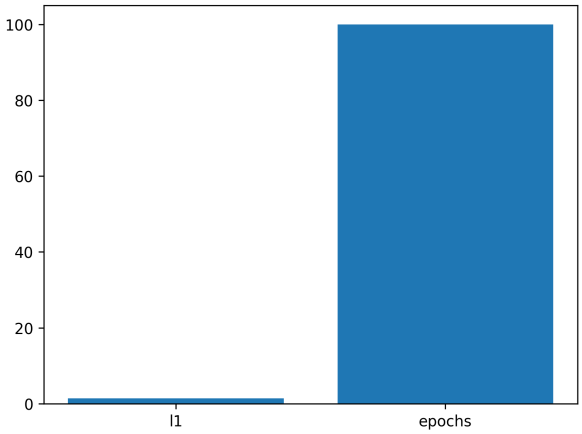


Figure 19.5: Variable importance

19.12 Get the Tuned Architecture

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
```

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:

```
Net_lin_reg(
  (fc1): Linear(in_features=10, out_features=64, bias=True)
  (fc2): Linear(in_features=64, out_features=32, bias=True)
  (fc3): Linear(in_features=32, out_features=1, bias=True)
  (relu): ReLU()
  (softmax): Softmax(dim=1)
  (dropout1): Dropout(p=0.0, inplace=False)
  (dropout2): Dropout(p=0.0, inplace=False)
)
```

19.13 Evaluation of the Tuned 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.

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.

```
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 = DEVICE,
        path=None,
        task=fun_control["task"],)
```

```
Epoch: 1
Loss on hold-out set: 0.17853929138431945
MeanAbsoluteError value on hold-out data: 0.3907899856567383
Epoch: 2
Loss on hold-out set: 0.17439044278115035
MeanAbsoluteError value on hold-out data: 0.38570401072502136
```

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 = DEVICE,
            task=fun_control["task"],)
```

```
Loss on hold-out set: 1.85966069472272e-05
MeanAbsoluteError value on hold-out data: 0.0021022311411798
Final evaluation: Validation loss: 1.85966069472272e-05
Final evaluation: Validation metric: 0.0021022311411798
---------------------------------------------
(1.85966069472272e-05, nan, tensor(0.0021))
```

19.14 Cross-validated Evaluations

```
from spotPython.torch.traintest import evaluate_cv
# modify k-kolds:
setattr(model_spot, "k_folds",  10)
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=DEVICE)
```

```
Fold: 1
Epoch: 1
Loss on hold-out set: 0.36993918985128404
MeanAbsoluteError value on hold-out data: 0.5827060341835022
Epoch: 2
Loss on hold-out set: 0.3583159705996513

(0.0027241395250238156, nan, tensor(0.0147))
```

Table 19.5 shows the loss and meric value (MAE) of the model with the tuned hyperparameters from SPOT.

Table 19.5: Comparison of the loss and metric values.

Model	Loss	Metric (MAE)
`Validation`	1.8597e-05	0.0021
`10-fold CV`	0.00272	0.0147

19.15 Detailed Hyperparameter Plots

The contour plot in this section visualize the interactions of the two most important hyperparameters, `l1`, and `epochs` of the surrogate model used to optimize the 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. For this, again refer to the notebook (Bartz-Beielstein 2023).

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

Figure 19.6 shows a contour plot 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, Figure 19.7 shows the parallel plot of the hyperparameters.

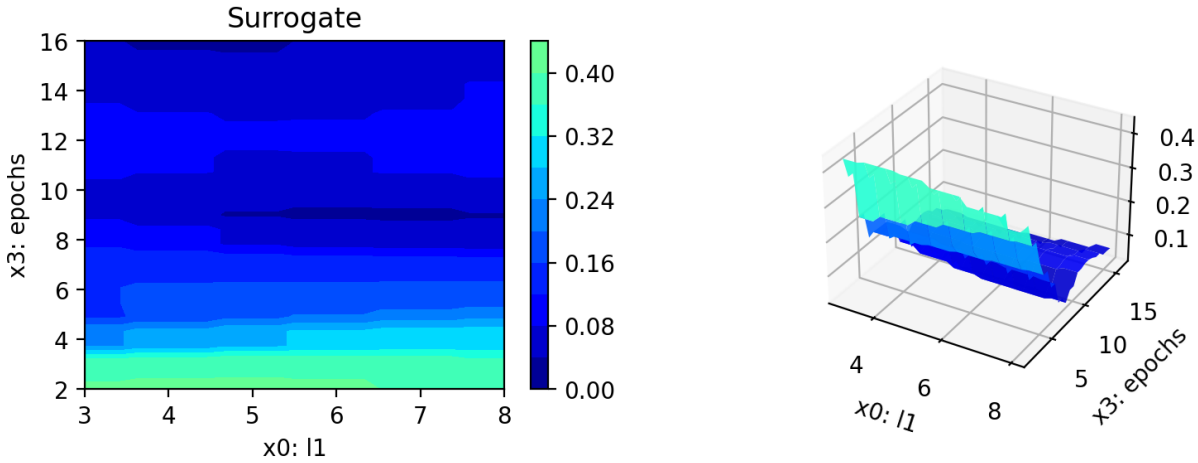


Figure 19.6: Contour plot of the loss as a function of `epochs` and `l1`, i.e., the number of neurons in the layers.

```
spot_tuner.parallel_plot()
```

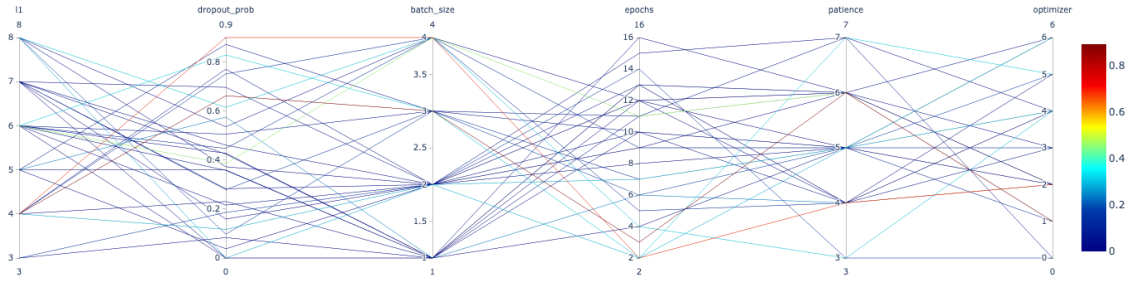


Figure 19.7: Parallel plot

19.16 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 Documentation of the Sequential Parameter Optimization

This document describes the `Spot` features.

20.1 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
```

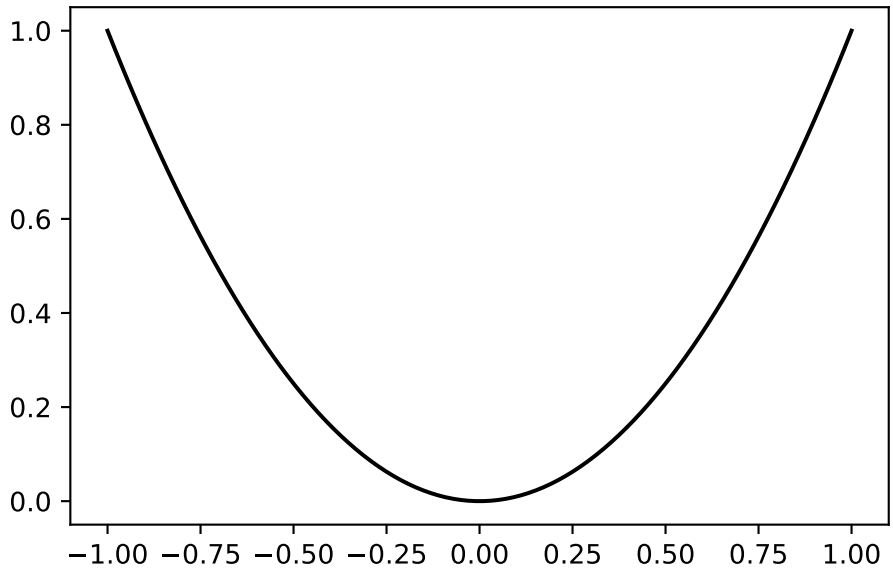
20.1.1 The Objective Function

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`.

20.1.2 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`

20.2 The `fun_control` Dictionary

external parameter	type	description	default	mandatory
`sigma`	float	noise: standard deviation	`0`	yes
`seed`	int	seed for rng	`124`	yes

20.3 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

20.4 The `surrogate_control` Dictionary

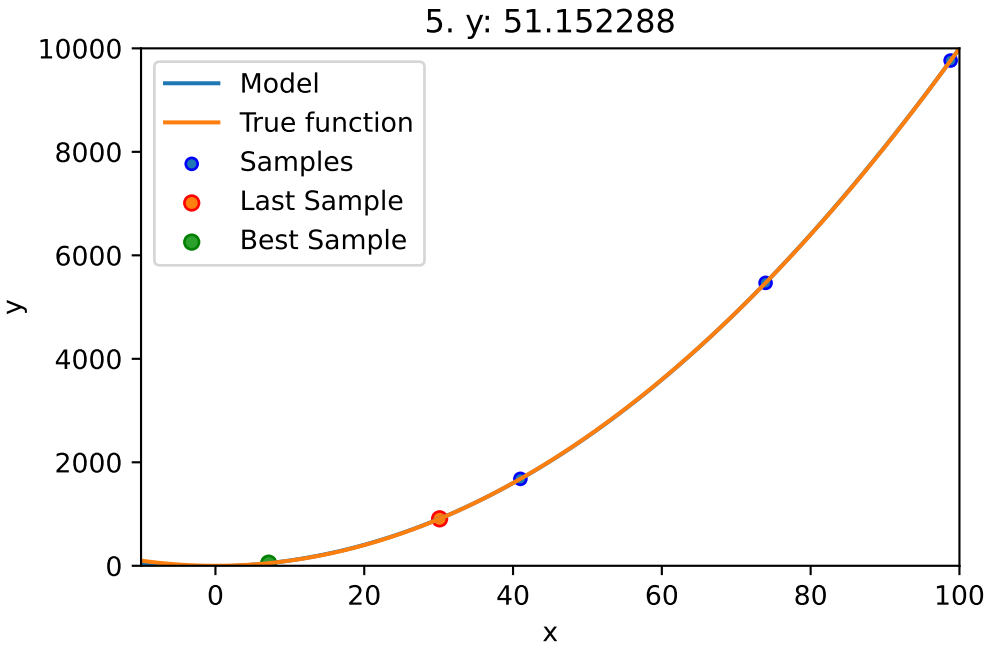
external parameter	type	description	default	mandatory
`noise_model_optimizer`	object	optimizer	`differential_evolution`	no
`model_fun_evals`				
`min_theta`			`-3.`	
`max_theta`			`3.`	
`n_theta`			`1`	
`n_p`			`1`	
`optim_p`			`False`	
`cod_type`			`"norm"`	
`var_type`				
`use_cod_y`	bool		`False`	

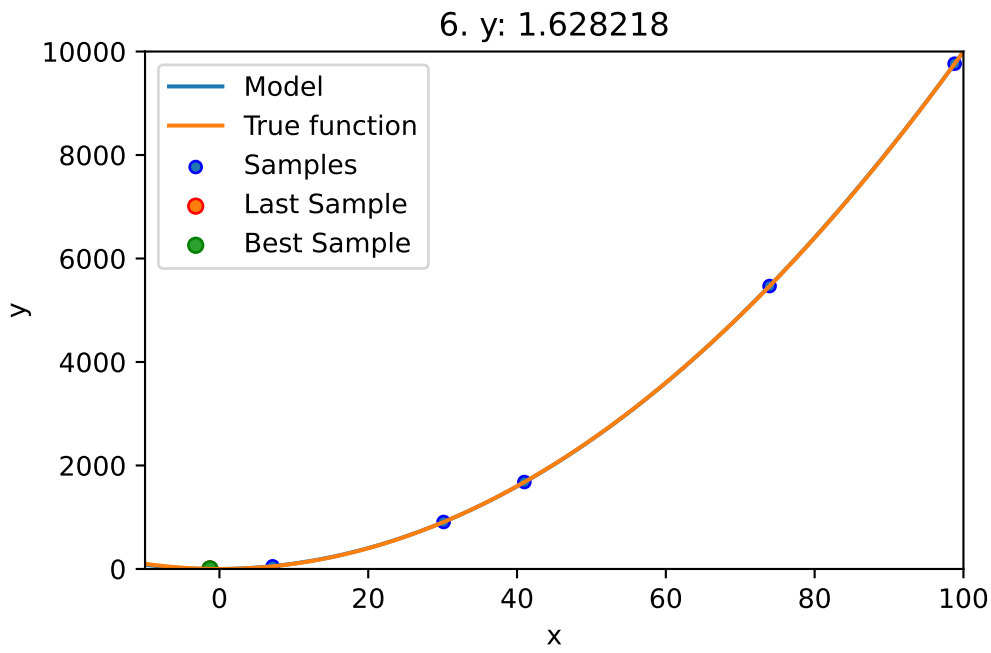
20.5 The `optimizer_control` Dictionary

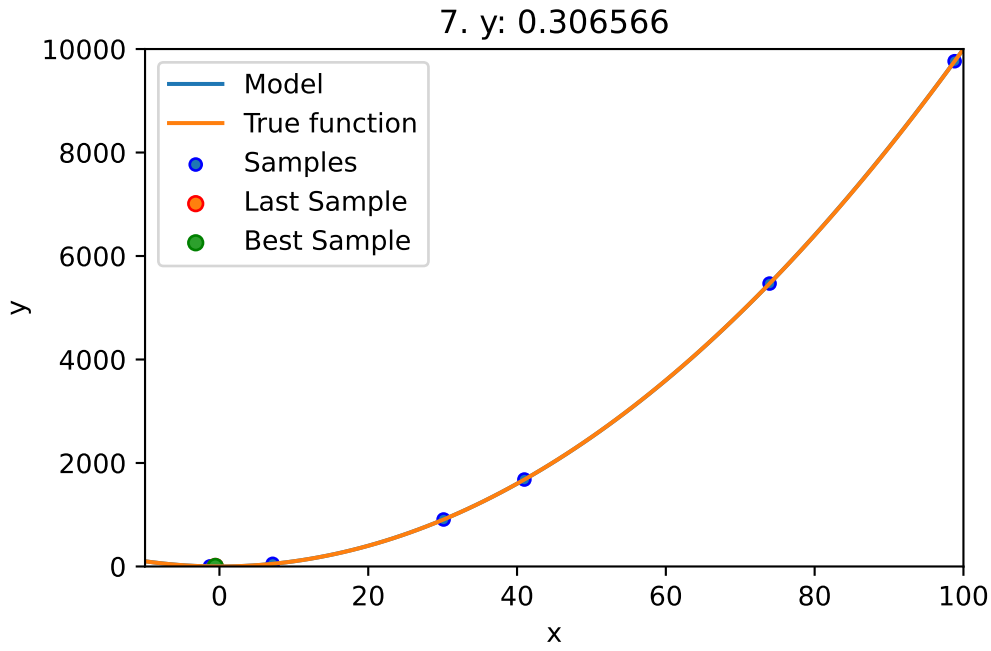
external parameter	type	description	default	mandatory
`max_iter`	int	max number of iterations. Note: these are the cheap evaluations on the surrogate.	`1000`	no

20.6 Run

```
spot_1.run()
```








```
<spotPython.spot.spot.Spot at 0x294486980>
```

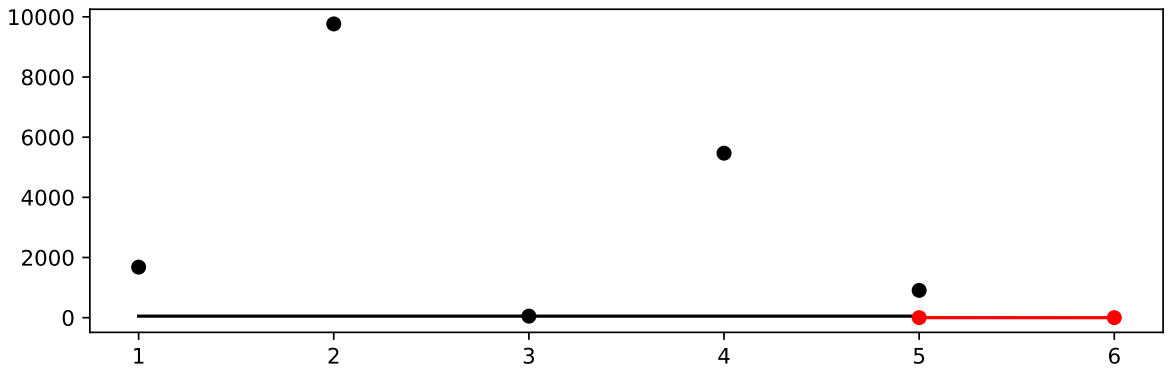
20.7 Print the Results

```
spot_1.print_results()
```

```
min y: 0.30656551286610595
x0: -0.5536835855126157

[['x0', -0.5536835855126157]]
```

20.8 Show the Progress

```
spot_1.plot_progress()
```

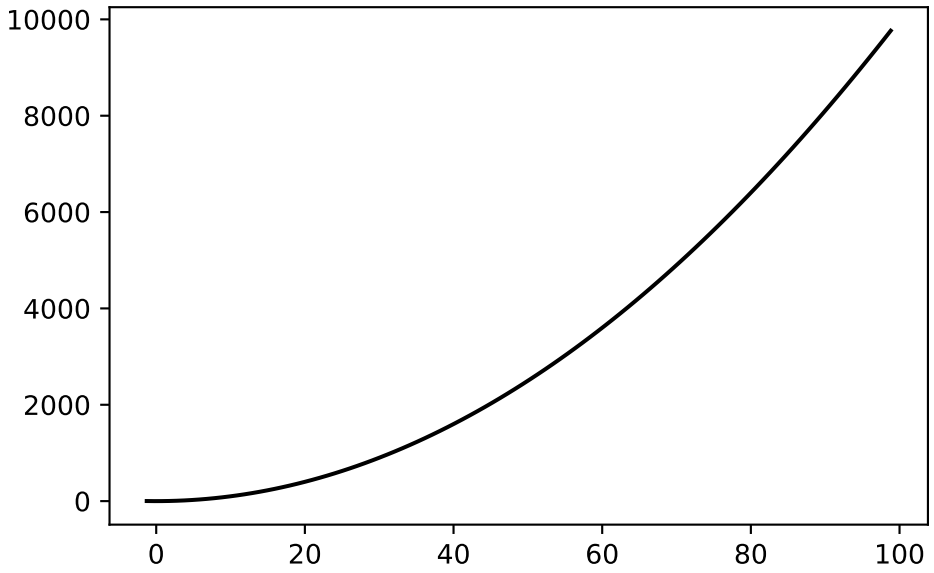


20.9 Visualize the Surrogate

- 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>
```



20.10 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]
```

20.11 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 ]]))
```

20.12 Surrogates

20.12.1 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.

20.13 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         nan
  0.41757584  0.0786237   0.82585329  0.23700598         nan -0.82319082
 -0.17991251  0.1481835 ]
[-1.]

[0.95541987]
[0.17335968]

[-0.58552368]
[-0.20126111]

[-0.60100809]
[-0.97897336]

[-0.2748985]
[nan]

[0.8359486]
[0.99035591]

[0.01641232]
[0.5629346]
```

20.14 PyTorch: Detailed Description of the Data Splitting

20.14.1 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
```

20.14.1.1 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.

20.14.1.2 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`.

20.14.1.3 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.

20.14.1.4 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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