Regression

6. Gradient descent

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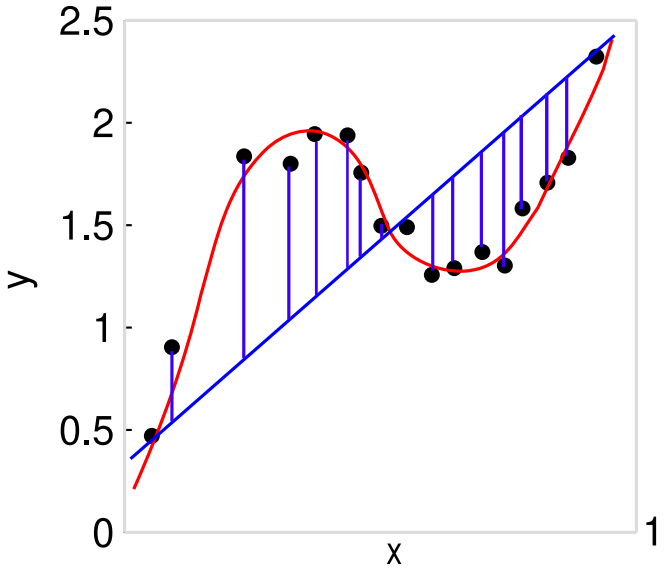
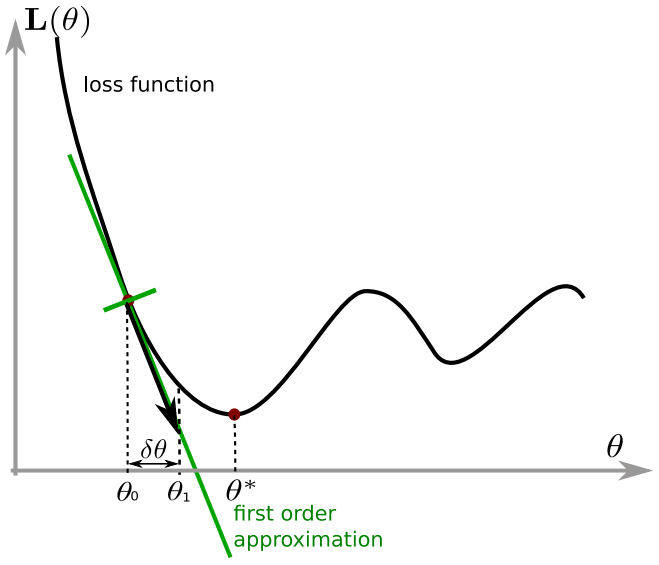
Outline

- In this class, we will see:
  - How regression can be cast as a gradient descent problem
  - What are the gradient descent properties independently from regression
  - What is the difference between batch and stochastic gradient descent
- More advanced methods will be explained in the next class

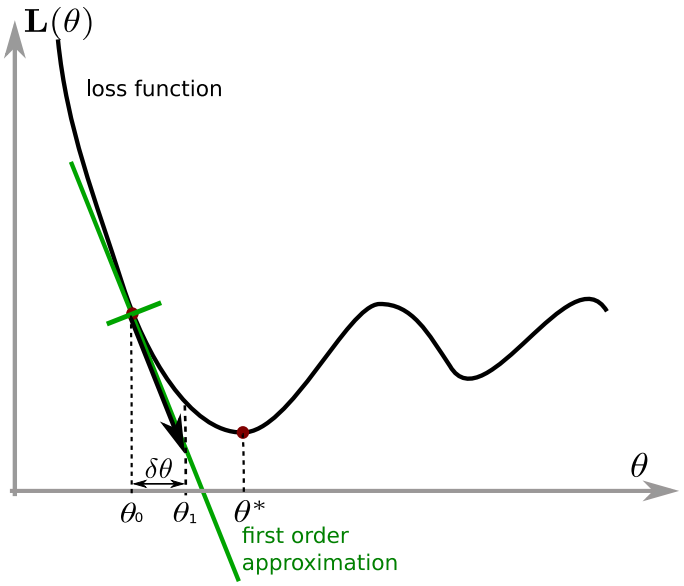
Regression through gradient descent





- We want to minimize a regression error (left)
- Thus find the minimum of a **loss function** $\mathbf{L}(\boldsymbol{\theta})$ (right)
- Instead of solving $\boldsymbol{\theta}^* = \min_{\boldsymbol{\theta}} \mathbf{L}(\boldsymbol{\theta})$ (immediate, but expensive)
- Rather perform local steps using an iterative approach
- The iteration equation is $\boldsymbol{\theta}_{i+1} \leftarrow \boldsymbol{\theta}_i + \delta\boldsymbol{\theta}_i$
- This is the essence of gradient descent

Gradient descent iteration

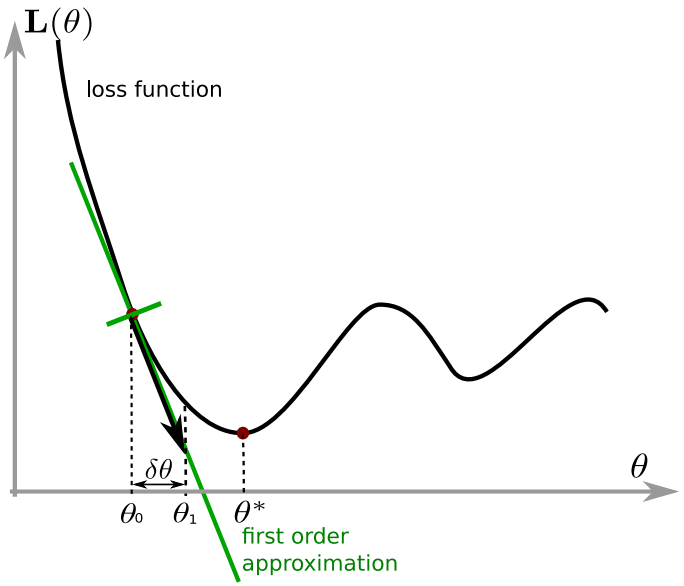


- Now we want to minimize $\mathbf{L}(\boldsymbol{\theta}_i + \delta\boldsymbol{\theta}_i)$ over $\delta\boldsymbol{\theta}_i$.
- How to choose $\delta\boldsymbol{\theta}_i$?

First order approximation of the loss

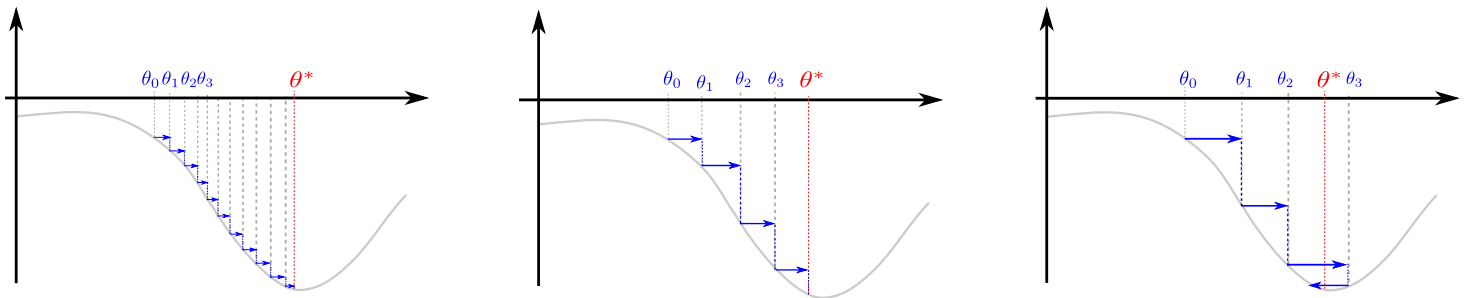
- The optimum on $\delta\boldsymbol{\theta}$ is reached when $\frac{\partial \mathbf{L}(\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{\partial \delta\boldsymbol{\theta}} = 0$
- $\mathbf{L}(\boldsymbol{\theta}+\delta\boldsymbol{\theta})$ can be approximated at the first order as $\mathbf{L}(\boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}}\mathbf{L}(\boldsymbol{\theta})^T\delta\boldsymbol{\theta} + \nu\delta\boldsymbol{\theta}^T\delta\boldsymbol{\theta} +$ higher order terms
- $\frac{\partial \mathbf{L}(\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{\partial \delta\boldsymbol{\theta}} \sim \nabla_{\boldsymbol{\theta}}\mathbf{L}(\boldsymbol{\theta})^T\delta\boldsymbol{\theta} + 2\nu\delta\boldsymbol{\theta}$
- Thus $\delta\boldsymbol{\theta}^* = -\frac{1}{2\nu}\nabla_{\boldsymbol{\theta}}\mathbf{L}(\boldsymbol{\theta})$
- We rewrite it $\delta\boldsymbol{\theta}^* = -\alpha\nabla_{\boldsymbol{\theta}}\mathbf{L}(\boldsymbol{\theta})$
- And the iteration rule is $\boldsymbol{\theta}_{i+1} \leftarrow \boldsymbol{\theta}_i - \alpha_i\nabla_{\boldsymbol{\theta}}\mathbf{L}(\boldsymbol{\theta})$
- Thus the steepest descent direction is given by the first order derivative

Gradient descent iteration



- The first order local derivative $\nabla_{\boldsymbol{\theta}}\mathbf{L}(\boldsymbol{\theta})|_{\boldsymbol{\theta}=\boldsymbol{\theta}_i}$ gives the right direction (move left or right)
- But minimizing the first order derivative is not lower bounded
- We need a step size α to determine how far to go

Tuning the step size

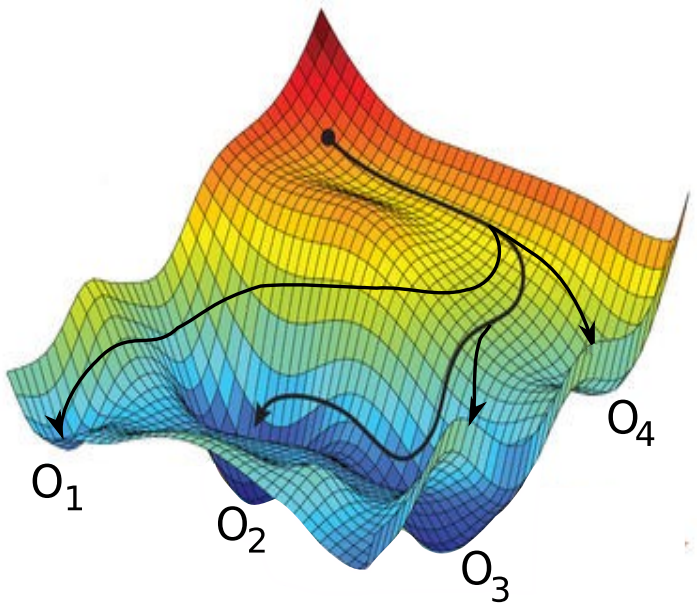


(a) (b) (c)

- (a) α_i are too small, (b) α_i are adequate, (c) α_i are too large
- If too small, too many steps. If too large, may miss a local optimum
- Line search: iterate to find the best step size (used e.g. in TRPO)

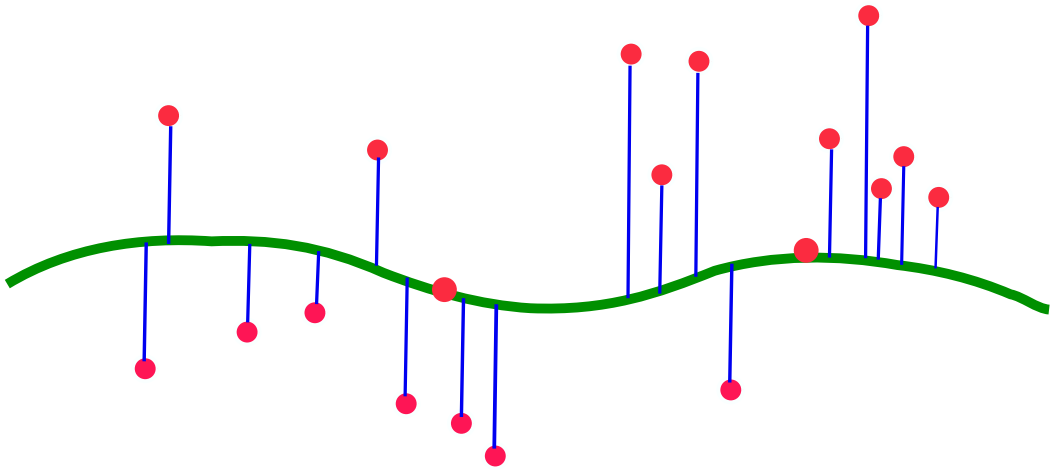
Schulman, J., Levine, S., Moritz, P., Jordan, M. I., & Abbeel, P. (2015) Trust region policy optimization. *CoRR, abs/1502.05477*

Local Optima



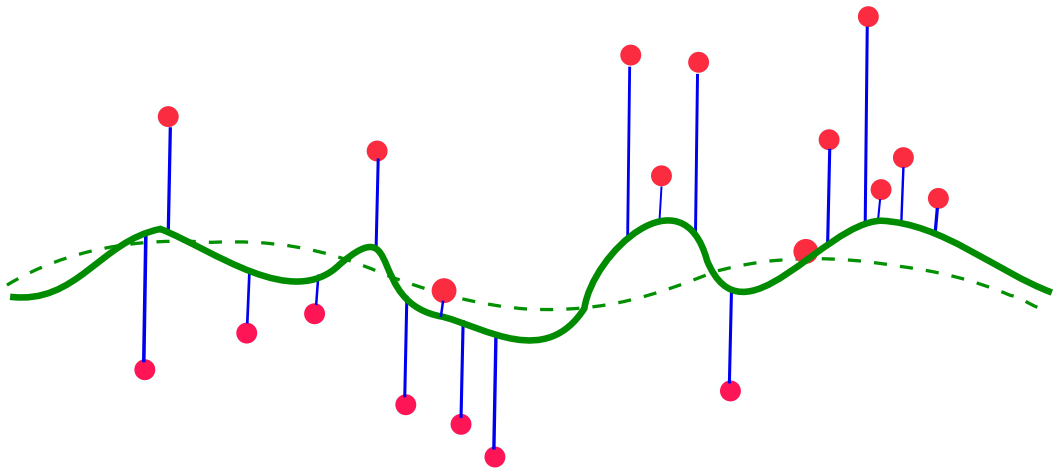
- Gradient descent is a local improvement approach where, at each step, we follow the steepest descent direction
- But we don't know where is the optimum we are targetting
- Unless the cost function is convex in the parameter space, gradient descent can end-up in different local optima depending on the starting point or noise
- Anything that basically goes down will end up somewhere low!

Batch regression through gradient descent



- The loss is the squared sum of all errors $\mathbf{L}(\boldsymbol{\theta}) = \|\mathbf{y} - \hat{f}(\mathbf{X})\|^2$
- The weights of the regressor $\hat{f}$ are updated so as to decrease all errors on average
- The maths make it so that the regressor is corrected more where it makes larger errors

Batch regression through gradient descent



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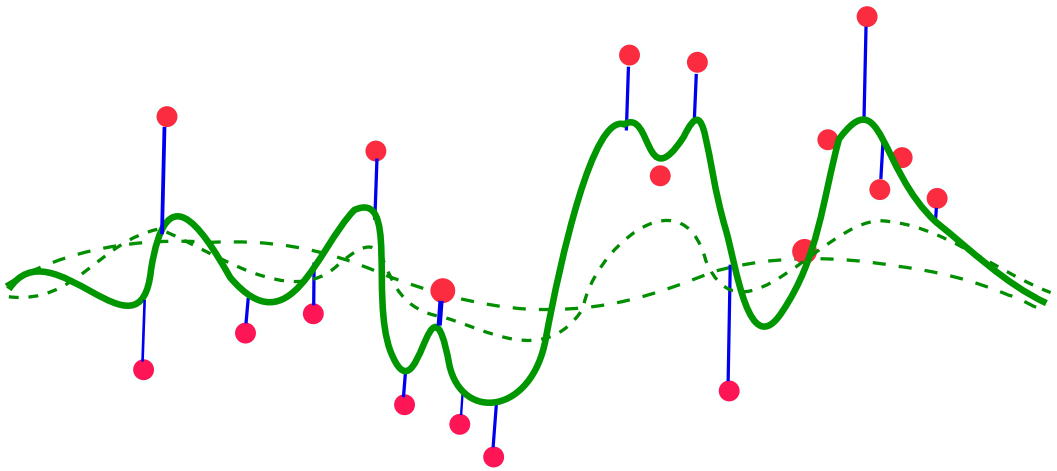

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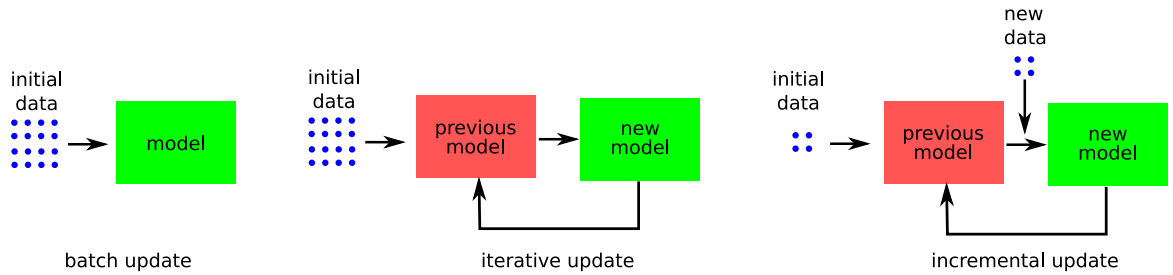
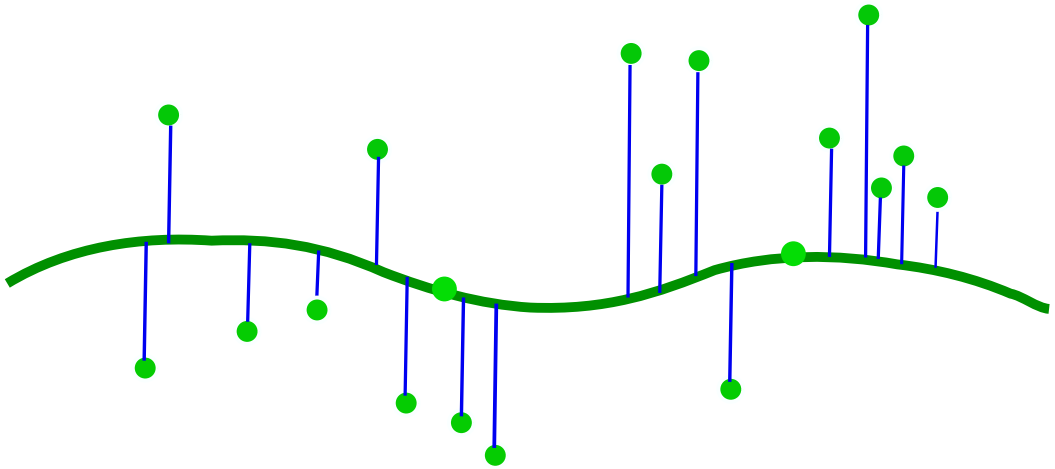
Reminder: Batch, Iterative, Incremental



- In regression, the cost function or loss is the regression error (e.g. $\mathbf{L}(\boldsymbol{\theta}) = \|\mathbf{y} - \hat{f}(\mathbf{X})\|^2$)
- The model function $\hat{f}(\mathbf{x})$ is known, so its derivative $\nabla_{\boldsymbol{\theta}} \hat{f}(\mathbf{x})$ can be computed analytically
- The values $\mathbf{y}$ and $\mathbf{X}$ are known too
- Hence batch gradient descent is only iterative: no need for additional data
- Stochastic gradient descent is a specific case of incremental ($\mathbf{y}$ and $\mathbf{X}$ change for each mini-batch)
- The new datapoints are taken randomly from the batch

Stochastic gradient descent (SGD)



- Batch gradient descent is expensive when the batch is large
- We can decrease the cost by using several mini-batches (extra gain with parallel computations)
- In SGD, each mini-batch gives a different (inaccurate) estimate of the local gradient
- Combining several inaccurate estimates can help being accurate
- Actually, being inaccurate is no big deal (see Class 7)
- Note that SGD converges more slowly. Use it only for large batches.

Bottou, L. (2012) Stochastic gradient descent tricks. *Neural networks: Tricks of the trade*, pp. 421–436. Springer

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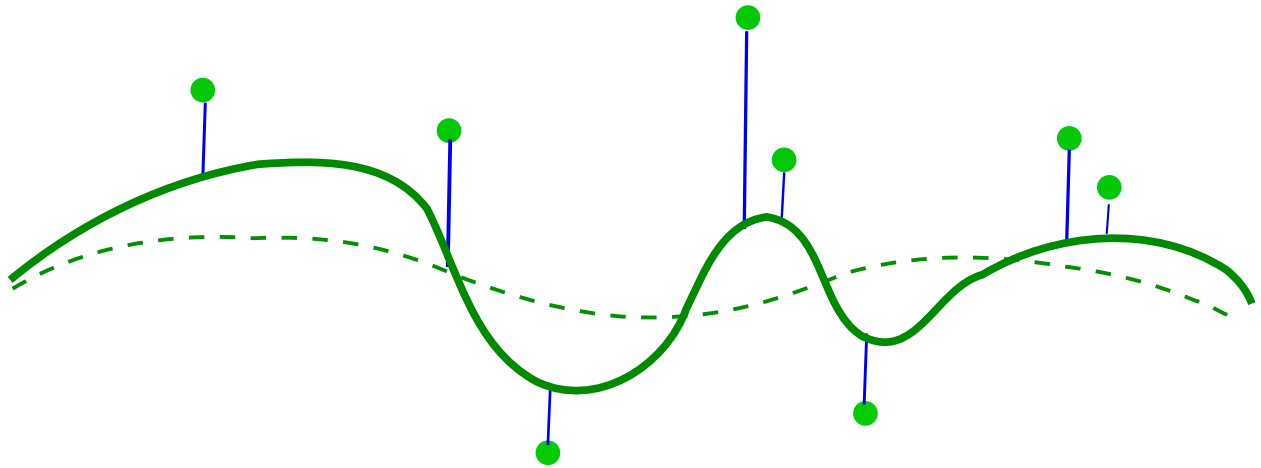

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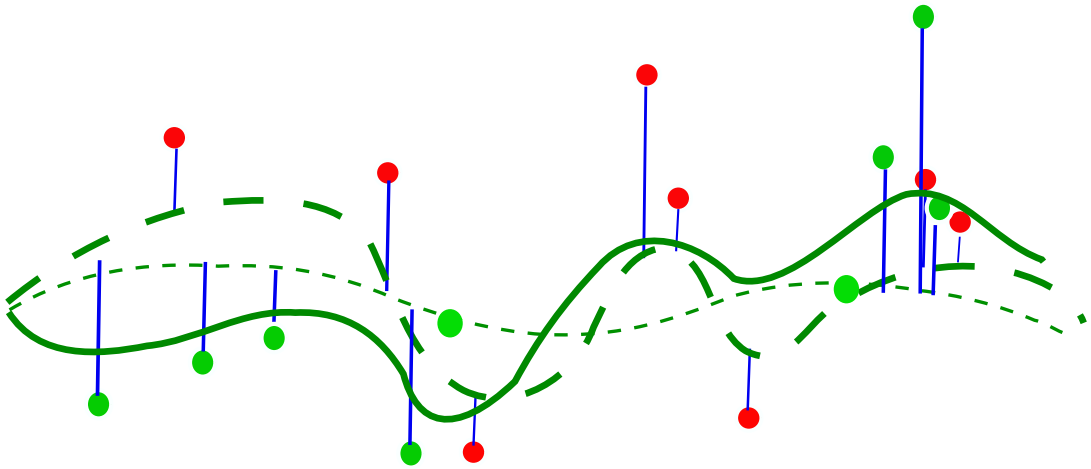

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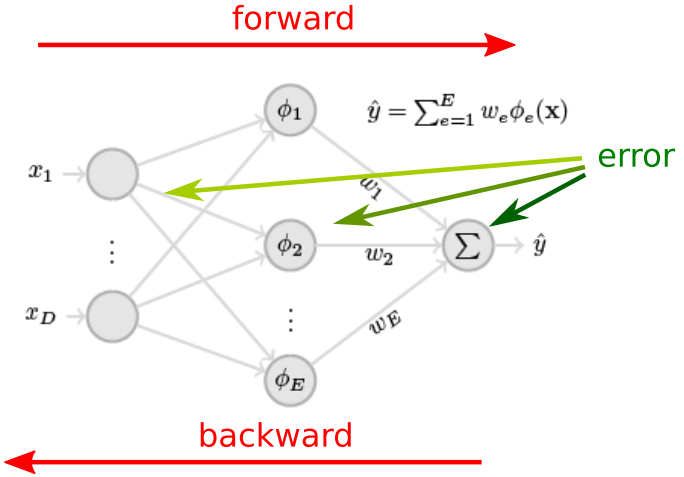
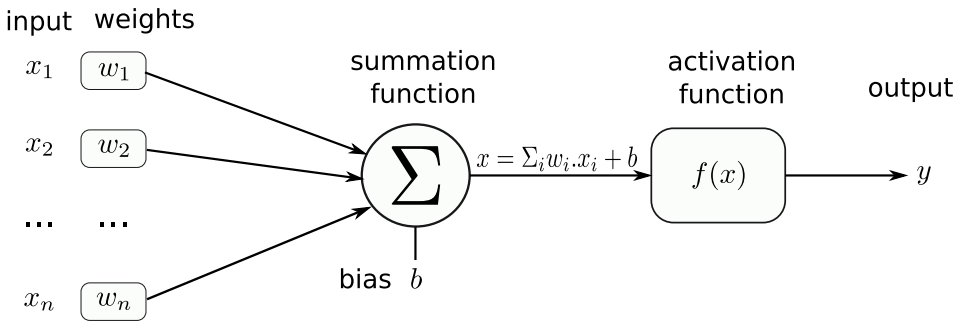
Gradient descent over multilayer neural networks





- The parameters $\boldsymbol{\theta}$ are the weights w_{ij} and biases b_i
- In $\nabla_{\boldsymbol{\theta}}(\mathbf{L}(\boldsymbol{\theta}))$, the errors at a layer depends on the errors at the next layers
- Gradient computation cannot be performed in a single step
- Compute the gradient with the gradient backpropagation algorithm (backprop)
- It is technical an a little tedious to code for each specific network structure
- TensorFlow, pytorch and their ancestors (theano, caffe...) are built to provide gradient backpropagation for any tensor structure

Nielsen, M. A. *Neural networks and deep learning*, volume 25. Determination press San Francisco, CA, 2015

http://neuralnetworksanddeeplearning.com/chap2.html

Creating an neural network in pytorch

```
class NeuralNetwork(nn.Module):

  def __init__(self, l1, l2, l3, l4, out, learning_rate):
    super(NeuralNetwork, self).__init__()
    self.relu = nn.ReLU()
    self.sigmoid = nn.Sigmoid()
    self.fc1 = nn.Linear(l1, l2)
    self.fc2 = nn.Linear(l2, l3)
    self.fc3 = nn.Linear(l3, l4)
    self.fc4 = nn.Linear(l4, out)
    self.optimizer = th.optim.Adam(self.parameters(), lr=learning_rate)

  def f(self, x):
      input = th.from_numpy(x).float()
      hidden1 = self.sigmoid(self.fc1(input))
      hidden2 = self.sigmoid(self.fc2(hidden1))
      hidden3 = self.sigmoid(self.fc3(hidden2))
      output = rescale(self.sigmoid(self.fc4(hidden3)))
      return output
```

- Adam does better than SGD
- f() is often called forward()
- Other functions not shown

Gradient descent in pytorch

- Computing the loss over a batch

```
for i in range(max_iter):
  output = model.f(xt)
  loss = func.mse_loss(output, yt)
  model.update(loss)
```

- Applying gradient descent

```
def update(self, loss) -> None:
    """
    Apply a loss to a network using gradient backpropagation
    :param loss: the applied loss
    :return: nothing
    """
    self.optimizer.zero_grad()
    loss.sum().backward()
    self.optimizer.step()
```

- The backprop in one line!

Any question?

Send mail to: Olivier.Sigaud@upmc.fr

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In Bach, F. R. and Blei, D. M. (eds.), *Proceedings of the 32nd International Conference on Machine Learning, ICML 2015, Lille, France, 6-11 July 2015*, volume 37 of *JMLR Workshop and Conference Proceedings*, pp. 1889–1897. JMLR.org, 2015.
URL `http://proceedings.mlr.press/v37/schulman15.html`.