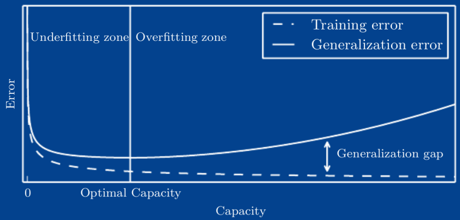
AARHUS
UNIVERSITY
SCHOOL OF ENGINEERING

LESSON 08: Model-capacity, Under/over-fitting, Generalization

CARSTEN EIE FRIGAARD

SPRING 2022



"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P , if its performance at tasks in T , as measured by P , improves with experience E." — Mitchell (1997).

L08: Model-capacity, Under/over-fitting, Generalization

Agenda

- Resumé af GD og NN's.
- Model Capacity,
- Under/over-fitting,
  Exercise: `L08/capacity_under_overfitting.ipynb`
  [OPTIONAL]
- Generalization Error,
  Exercise: `L08/generalization_error.ipynb`

RESUMÉ: GD

The numerically Gradient decent [GD] method is based on the gradient vector

$$\nabla_{\mathbf{w}} J(\mathbf{w})$$

for the gradient oprator

$$\nabla_{\mathbf{w}} = \left[\frac{\partial}{\partial w_1}, \frac{\partial}{\partial w_2}, \ldots, \frac{\partial}{\partial w_m}\right]^\top$$

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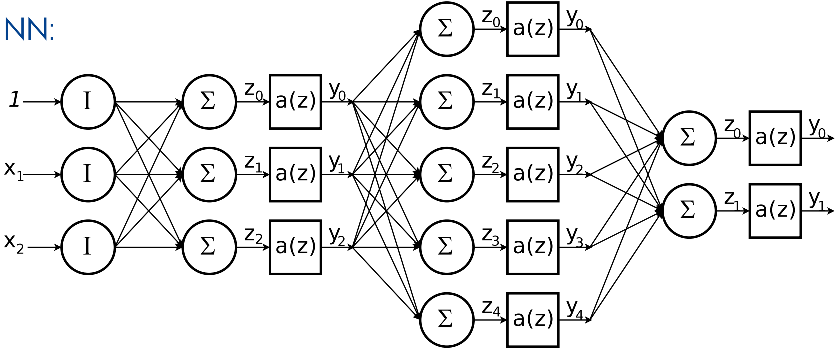
The algoritmn for updating via steps reads

$$\mathbf{w}^{(\text{next step})} = \mathbf{w} - \eta \nabla_{\mathbf{w}} J(\mathbf{w})$$

with η being the step size.

RESUMÉ: Training Deep Neural Networks

NN:



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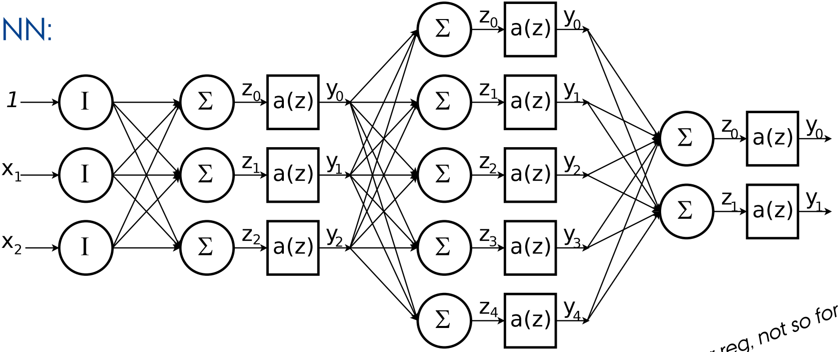
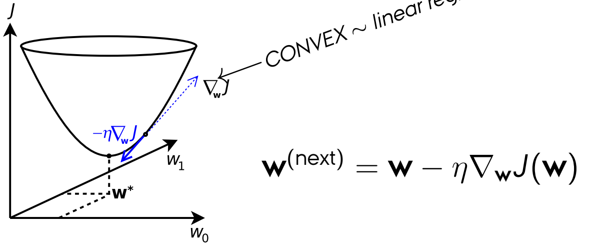


GD (via BPROP):

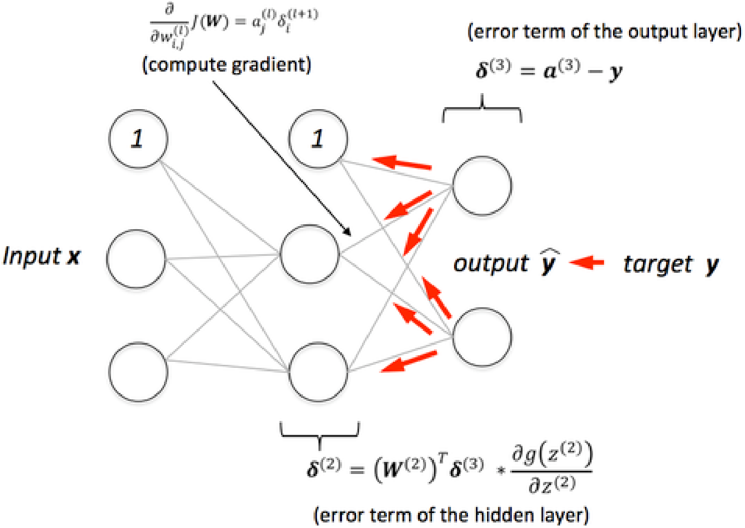


$$\mathbf{w}^{(\text{next})} = \mathbf{w} - \eta \nabla_{\mathbf{w}} J(\mathbf{w})$$

NOTE: NN: Neural net, GD: Gradient Descent, BPROP: Back Propagation

Backpropagation (BProp)

Training MLPs



NOTE: [`https://sebastianraschka.com/images/faq/visual-backpropagation/backpropagation.png`

RESUMÉ: Training Deep Neural Networks

Equation 4-6. Gradient vector of the cost function

$$\nabla_{\boldsymbol{\theta}} \text{MSE}(\boldsymbol{\theta}) = \begin{pmatrix} \frac{\partial}{\partial \theta_0} \text{MSE}(\boldsymbol{\theta}) \\ \frac{\partial}{\partial \theta_1} \text{MSE}(\boldsymbol{\theta}) \\ \vdots \\ \frac{\partial}{\partial \theta_n} \text{MSE}(\boldsymbol{\theta}) \end{pmatrix} = \frac{2}{m} \mathbf{X}^T (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$$

Notice that this formula involves calculations over the full training set **X**, at each Gradient Descent step! This is why the algorithm is called *Batch Gradient Descent*: it uses the whole batch of training data at every step (actually, *Full Gradient Descent* would probably be a better name). As a result it is terribly slow on very large training sets (but we will see much faster Gradient Descent algorithms shortly). However, Gradient Descent scales well with the number of features; training a Linear Regression model when there are hundreds of thousands of features is much faster using Gradient Descent than using the Normal Equation or SVD decomposition.

Once you have the gradient vector, which points uphill, just go in the opposite direction to go downhill. This means subtracting $\nabla_{\boldsymbol{\theta}}\text{MSE}(\boldsymbol{\theta})$ from $\boldsymbol{\theta}$. This is where the learning rate η comes into play:[6] multiply the gradient vector by η to determine the size of the downhill step (Equation 4-7).

Equation 4-7. Gradient Descent step

$$\boldsymbol{\theta}^{(\text{next step})} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \text{MSE}(\boldsymbol{\theta})$$

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RESUMÉ: Training Deep Neural Networks

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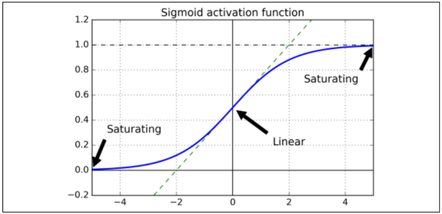

Figure 11-1. Logistic activation function saturation

Once you have the gradient vector, which points uphill, just go in the opposite direction to go downhill. This means subtracting $\nabla_{\boldsymbol{\theta}}\mathrm{MSE}(\boldsymbol{\theta})$ from $\boldsymbol{\theta}$. This is where the learning rate η comes into play:[6] multiply the gradient vector by η to determine the size of the downhill step (Equation 4-7).

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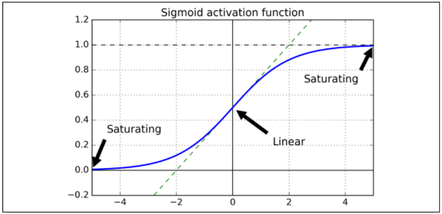

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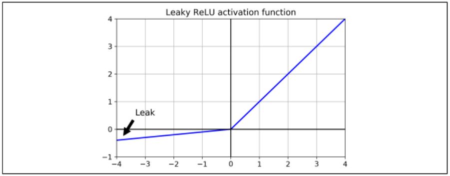

Figure 11-2. Leaky ReLU

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MODEL CAPACITY

Model capacity

Exercise: `capacity_under_overfitting.ipynb`

Dummy and Paradox classifier:

capacity fixed ~ 0, cannot generalize at all!

Model capacity

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Linear regression for a polynomial model:
capacity $\sim$ degree of the polynomial, x^n

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Homo sabiens ("modern humans"):
capacity $\propto$ the IQ 'score' function?

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$\Rightarrow$ **Capacity** can be hard to express as a quantity for some models, but you need to choose..

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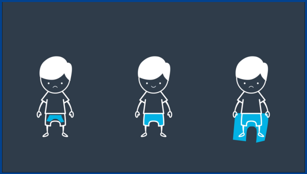
$\Rightarrow$ **Capacity** can be hard to express as a quantity for some models, but you need to choose..

$\Longrightarrow$ how to choose the **optimal** *capacity*?

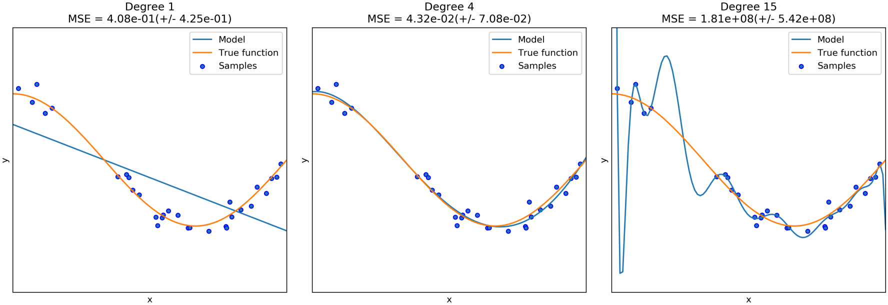
UNDER- AND OVERFITTING



Under- and overfitting

Exercise: `capacity_under_overfitting.ipynb`

Polynomial linear reg. fit for underlying model: `cos(x)`



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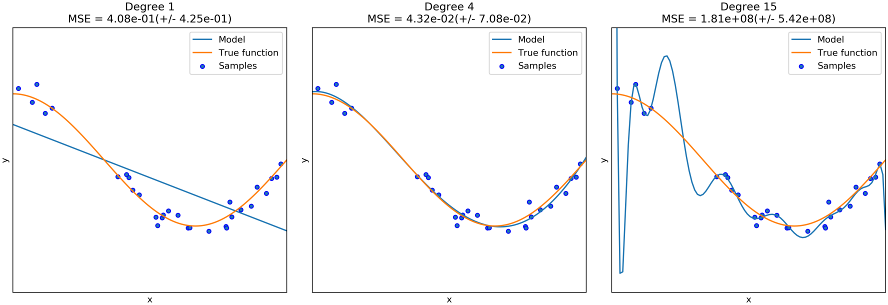
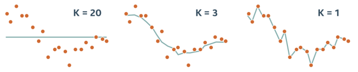


k-NN from L01:



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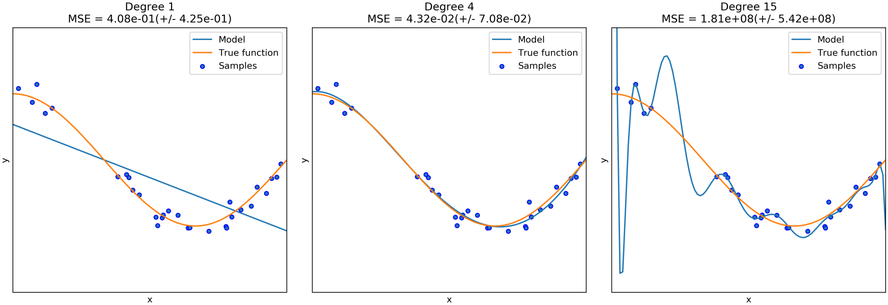

- underfitting:
  capacity of model too low,
- overfitting:
  capacity to high.

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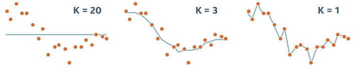

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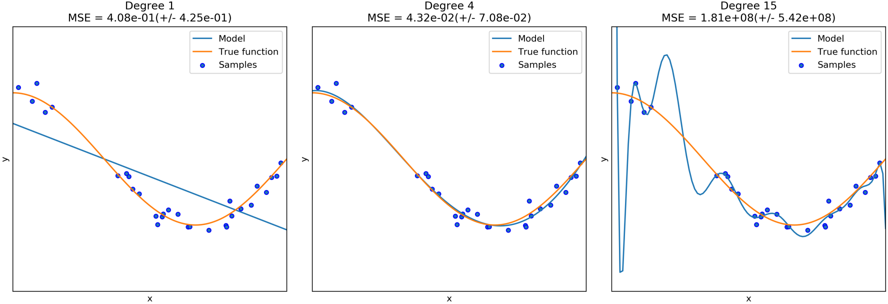

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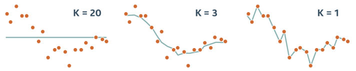
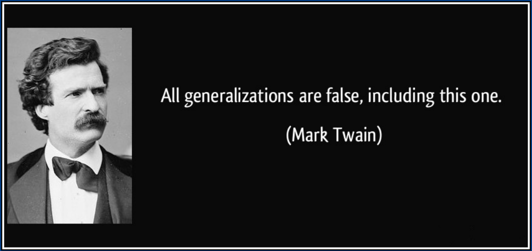


$\Longrightarrow$ how to choose the **optimal** capacity?

NOTE: HOML: *Constraining a model [..] reduce risk of overfitting [via] regularization => L10*

GENERALIZATION ERROR

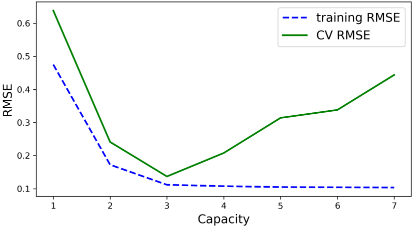


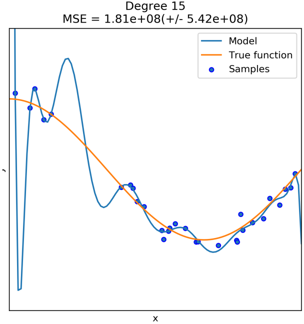
Generalization Error

Exercise: `generalization_error.ipynb`

RMSE-capacity plot for lin. reg. with polynomial features

(capacity $\sim$ degree of poly)





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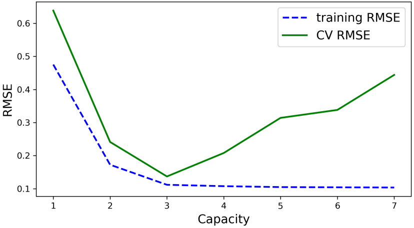
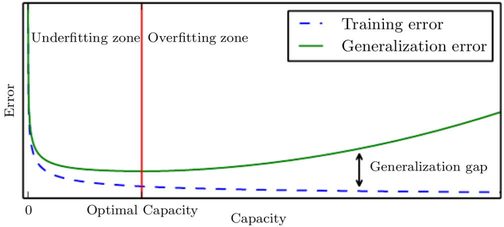


(Figure 5.3 from [DL])



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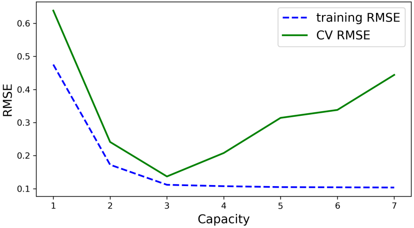

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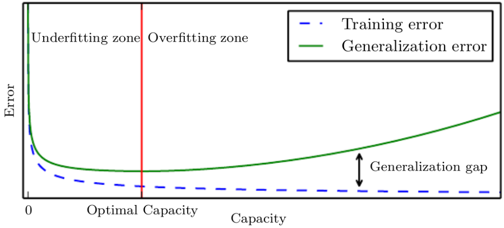

Inspecting the plots from the exercise (`.ipynb`) and [DL], extracting the concepts:

- training/generalization error,
- generalization gab,
- underfit/overfit zone,
- optimal capacity (best-model, early stop),
- (and the two axes: x/capacity, y/error.)

Generalization Error

Definition of ML:

> "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P , if its performance at tasks in T, as measured by P, improves with experience E."
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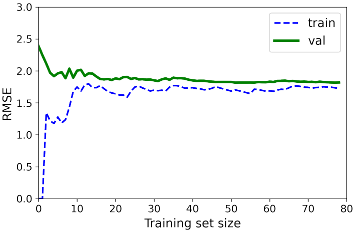
Generalization Error

Exercise: `generalization_error.ipynb`

NOTE: three methods/plots:

i) via **learning curves** as in [HOML],



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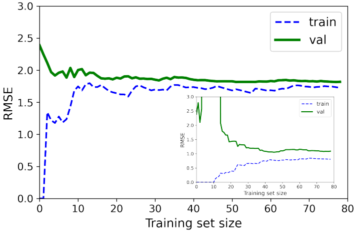

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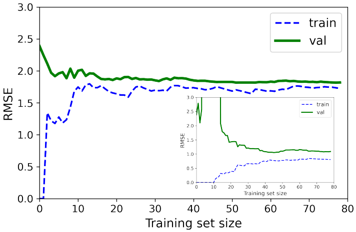

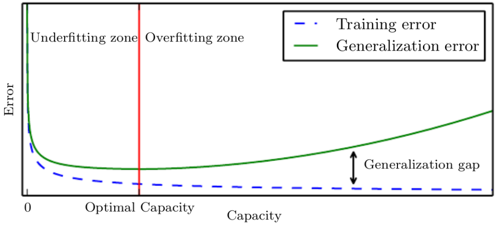

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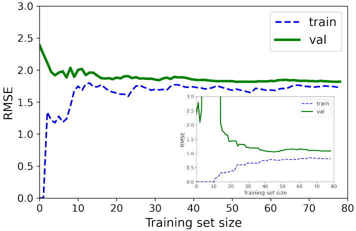

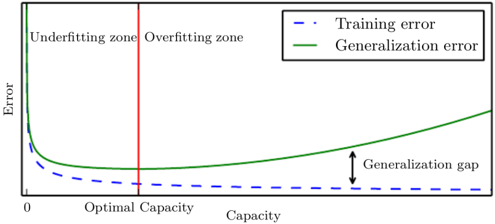

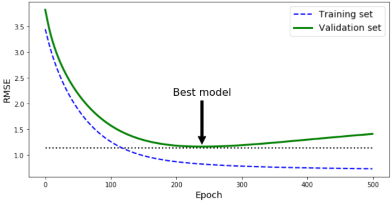

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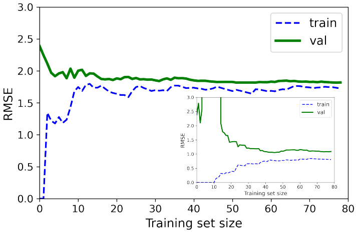

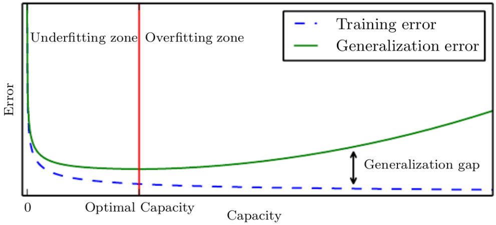

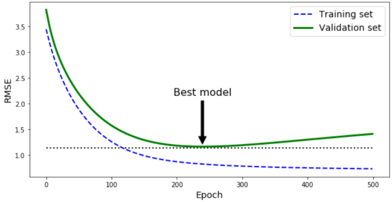

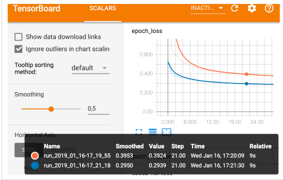

Figure 10-16. Visualizing Learning Curves with TensorBoard