AARHUS
UNIVERSITY
SCHOOL OF ENGINEERING

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

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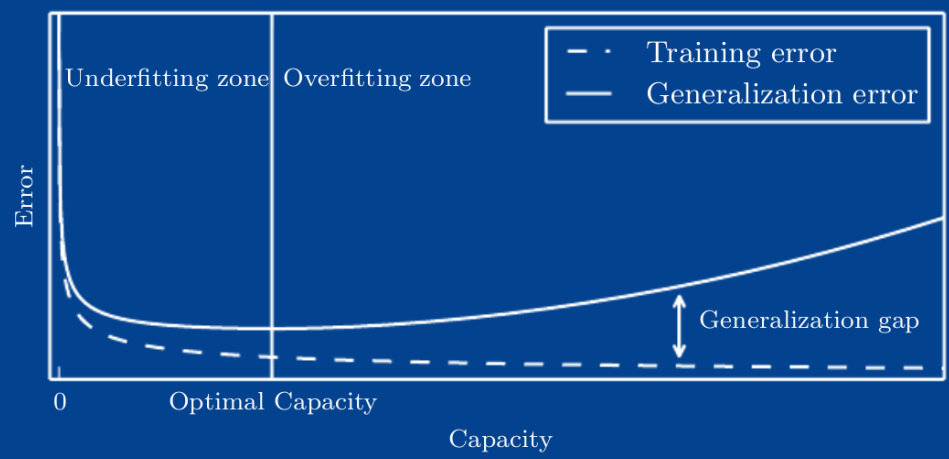


"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P , if its performance at tasks in T , as measured by P , improves with experience E." — Mitchell (1997).

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

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

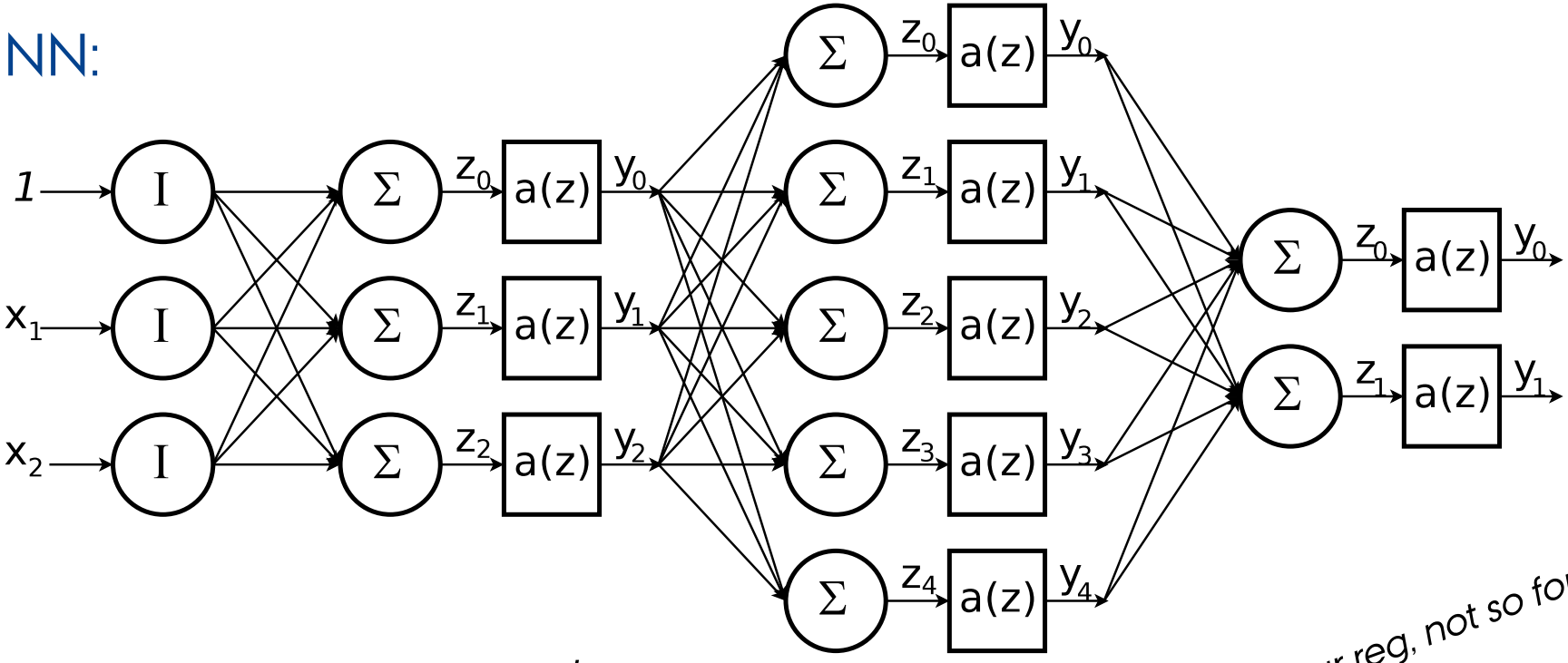
The algoritmn for updating via steps reads

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

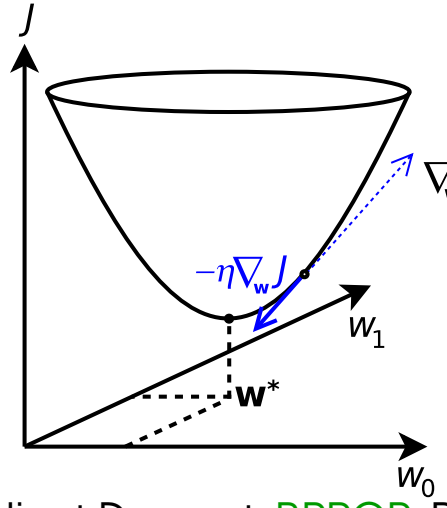
with η being the step size.

RESUMÉ: Training Deep Neural Networks

NN:



GD (via BPROP):



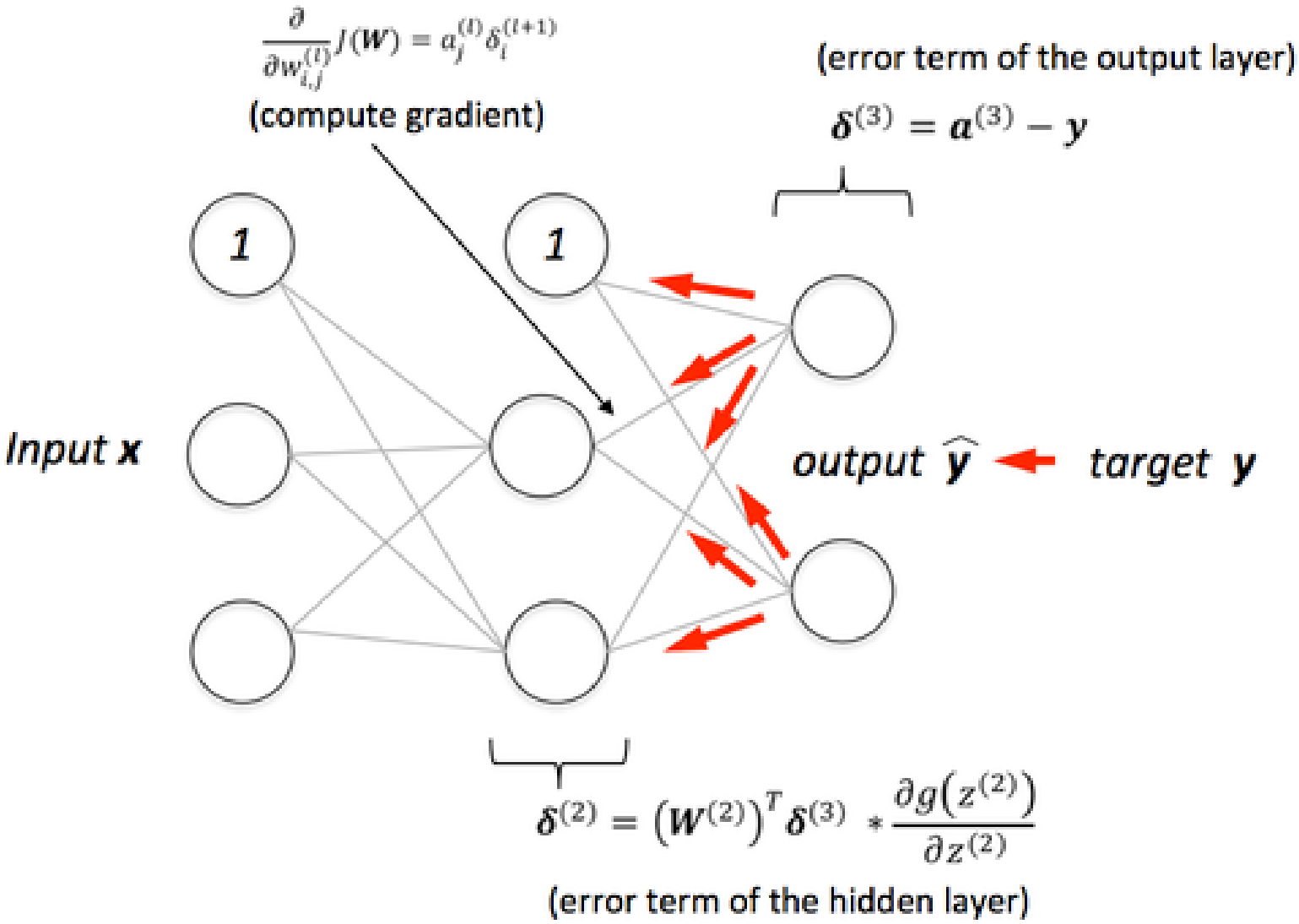
CONVEX ~ linear reg, not so for NNs

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

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

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

Notice that this formula involves calculation
set **X**, at each Gradient Descent step! This i
called *Batch Gradient Descent*: it uses the w
data at every step (actually, *Full Gradient D*
be a better name). As a result it is terribly sl
ing sets (but we will see much faster Gradient Descent algorithms
shortly). However, Gradient Descent scales we
features; training a Linear Regression model
dreds of thousands of features is much fa
Descent than using the Normal Equation or S

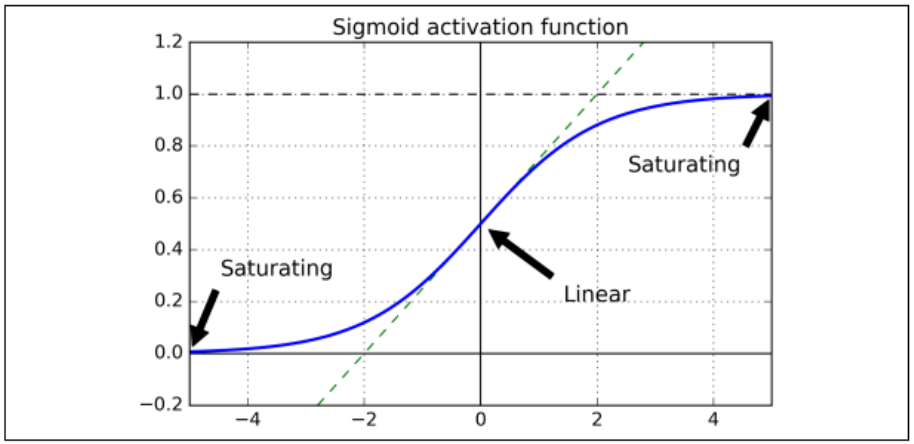


Figure 11-1. Logistic activation function saturation

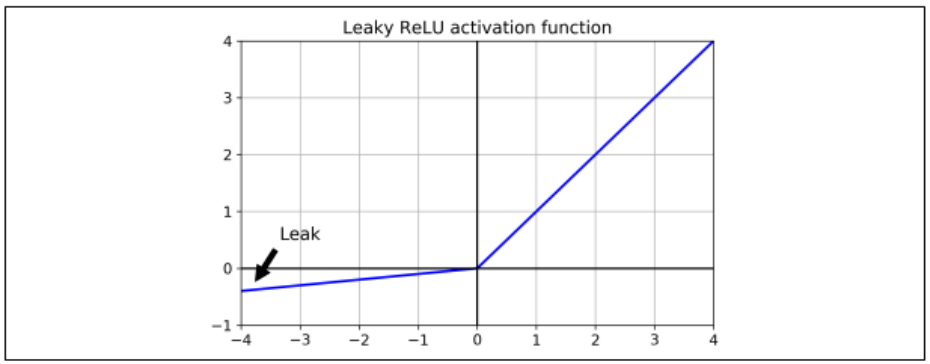


Figure 11-2. Leaky ReLU

Once you have the gradient vector, which points uphill, ju
tion to go downhill. This means subtracting $\nabla_{\boldsymbol{\theta}}\mathrm{MSE}(\boldsymbol{\theta})$
learning rate η comes into play:[6] multiply the gradient v
size of the downhill step (Equation 4-7).

Equation 4-7. Gradient Descent step

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

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

MODEL CAPACITY

Model capacity

Exercise: `capacity_under_overfitting.ipynb`

Dummy and Paradox classifier:
capacity fixed ~ 0, cannot generalize at all!

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

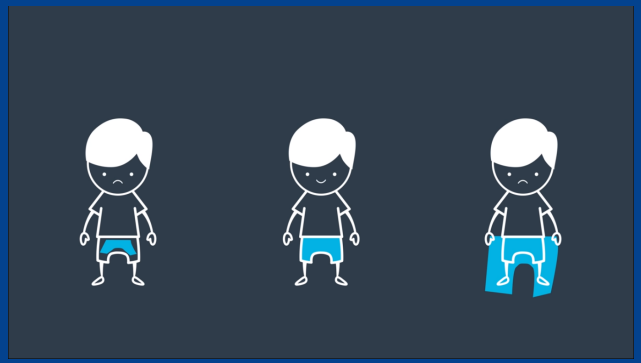
Neural Network model:
capacity $\propto$ number of neurons/layers

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

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

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

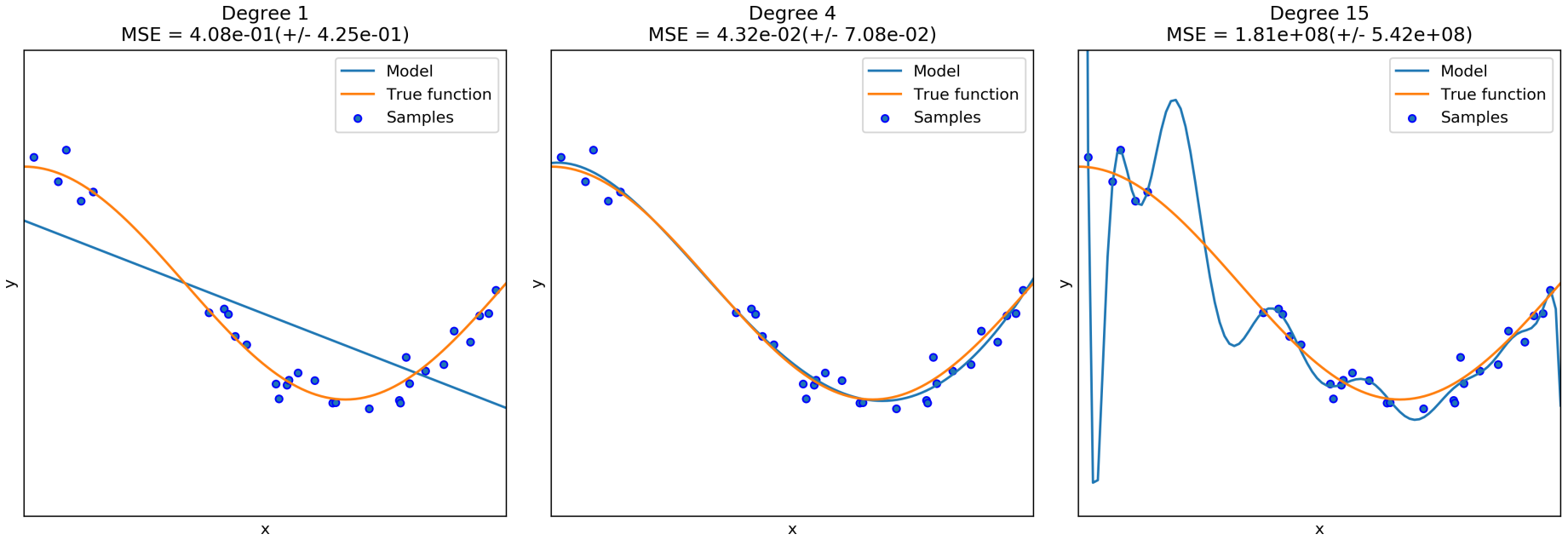
UNDER- AND OVERFITTING



Under- and overfitting

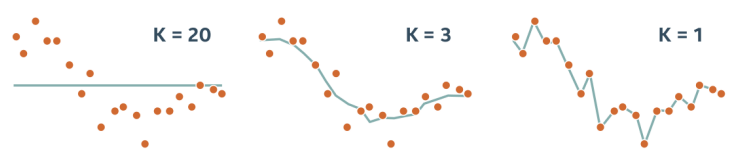
Exercise: `capacity_under_overfitting.ipynb`

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



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

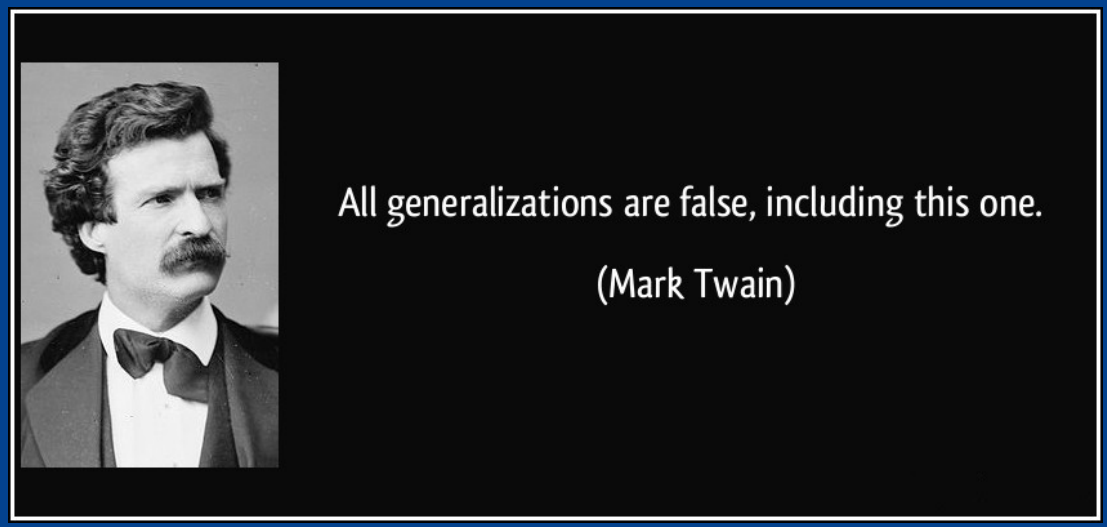
k-NN from L01:



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

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

GENERALIZATION ERROR

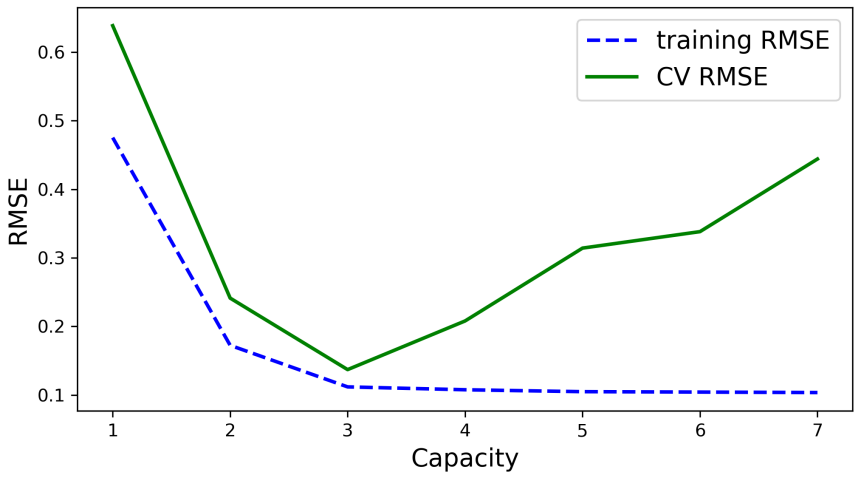


Generalization Error

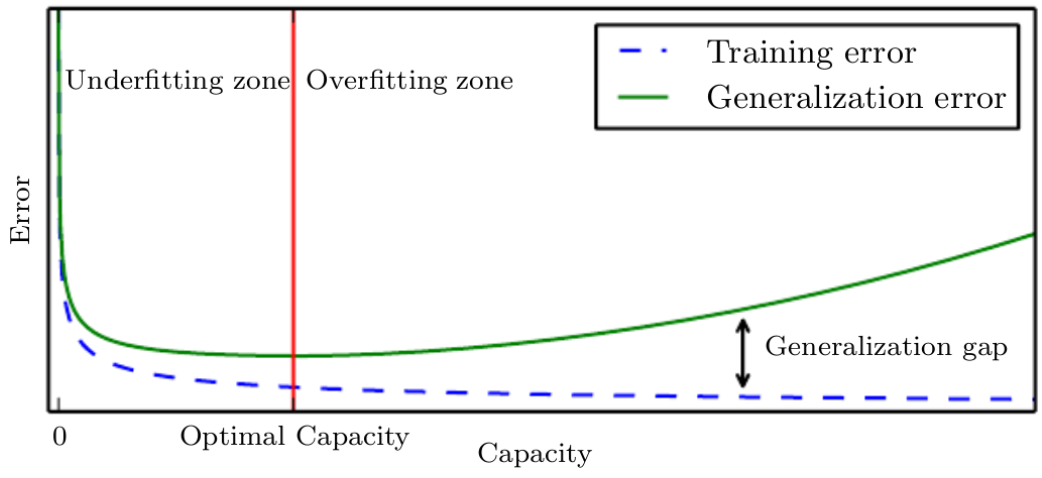
Exercise: `generalization_error.ipynb`

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

(capacity $\sim$ degree of poly)



(Figure 5.3 from [DL])



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."
>
> — Mitchell (1997).

Generalization Error

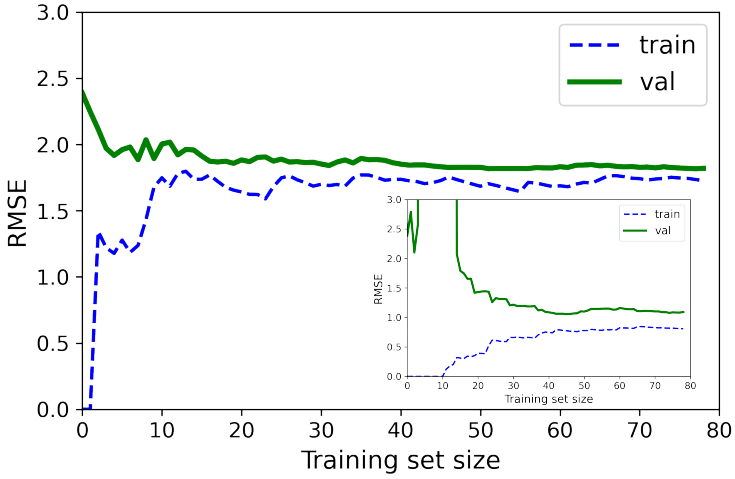
Exercise: `generalization_error.ipynb`

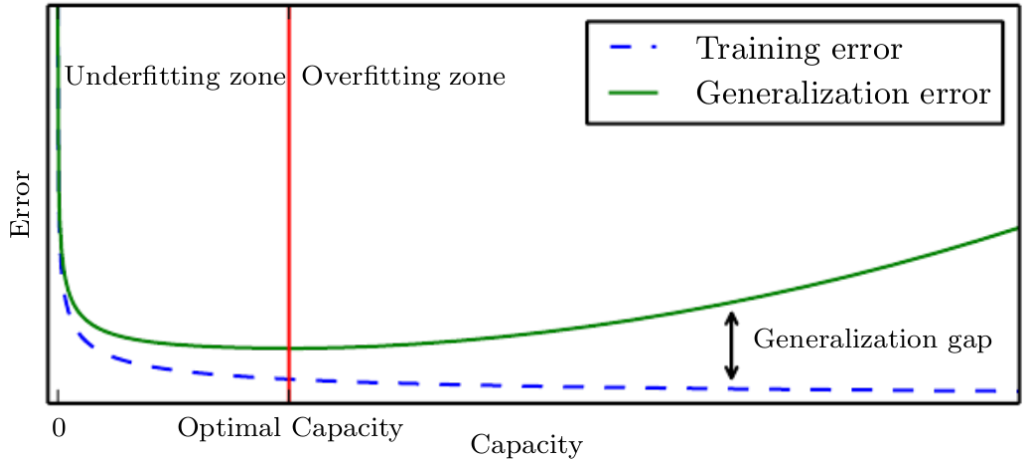
NOTE: three methods/plots:

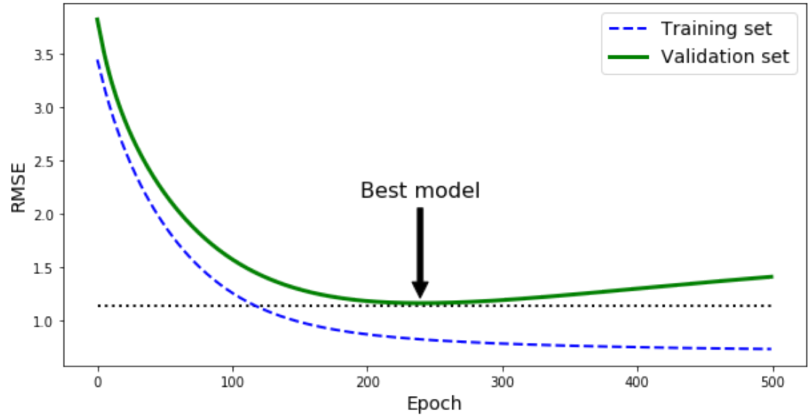
i) via **learning curves** as in [HOML],

ii) via an **error-capacity** plot as in [GITHOML] and [DL],

iii) via an **error-epoch** plot as in [GITHOML].







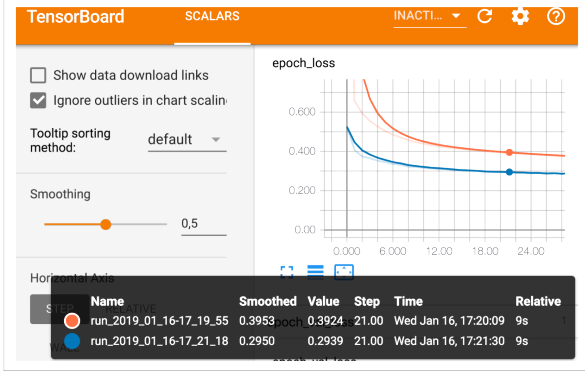


Figure 10-16. Visualizing Learning Curves with TensorBoard