COMPUTATIONAL INTELLIGENCE

(INTRODUCTION TO MACHINE LEARNING) SS17

Lecture 6:

- k-NN
- Cross-validation
- Regularization

LEARNING METHODS

Lazy vs eager learning

- **Eager learning –** generalizes training data before evaluation (e.g. Neural networks)
  - Fast prediction evaluation
  - Summarize training set (noise reduction)

- **Lazy learning** – wait a prediction query to generalize (e.g. k-NN)
  - Local approximation
  - Quick adaptation to variation of the training set
  - Require storage of the full training set
  - Slow evaluation

Instance based learning

- Type of lazy learning

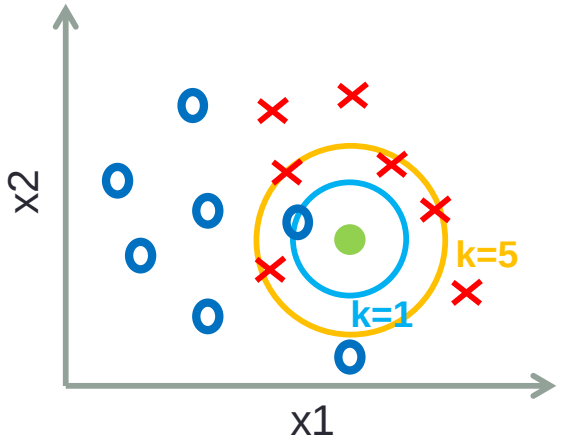
- Store in memory the training set
- Compare a test sample to the samples memory

K-NEAREST NEIGHBORS (K-NN)

k-NN

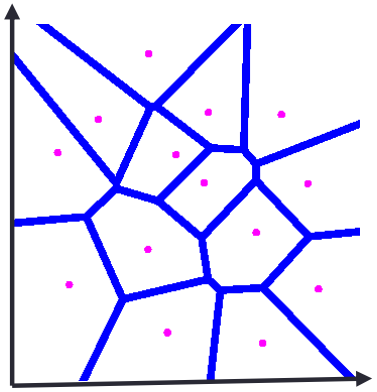
- Simple
- Non-differentiable
- Lazy learning

- The main idea:
  - Find the ***k*** closest samples (for instance with Euclidean distance)
  - Assign the most frequent class occurring on those ***k*** samples

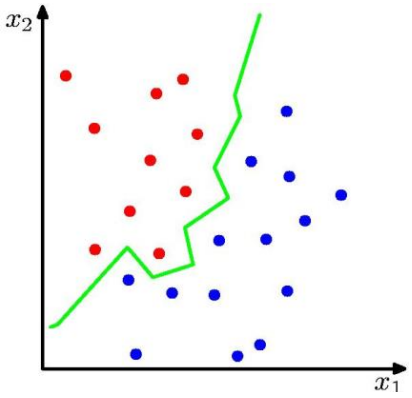


1-NN: Nearest Neighbor

- No computation of the explicit decision boundary
- The decision boundary form a subset of the Voronoi diagram
- Decision boundaries are irregular



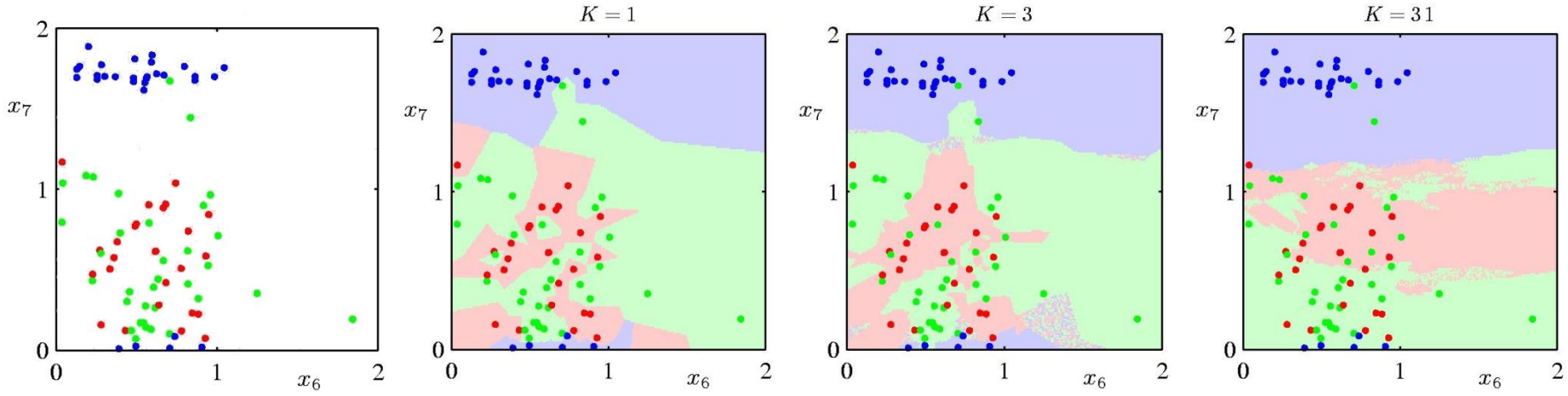
Voronoi diagram



Decision boundary

The number of neighbors influence

- The best ***k*** is data dependent
- Larger values of ***k*** : robustness to noise but fuzzy boundaries
- Model selection (validation set) is the best heuristic to optimize ***k***



Variants

- **Training:**
  - Save only preprocessed input
    (feature extraction and dimensionality reduction)

- **Testing**:
  - **Classification**:
    - Majority of votes of its ***k*** nearest neighbors
  - **Regression**:
    - Average of its ***k*** nearest neighbors.

Pros and cons

Pros:

- Easy to implement/understand
- No training
- Learn very complex decision boundaries
- No information loss (all samples are kept)

Cons:

- Require storage of all the data samples
- Slow at query time
- Bad performance if metric or feature vector is bad

Simple concepts are never deprecated

- **Memory Networks** (Weston et al. Facebook 2015) made tremendous progress in text processing and artificial reasoning:
  - For each input x
    - Find memory instance m most similar to x
    - Return a function f(x,m) and update the stored memories
- Differentiable version of these simple algorithms can be designed to use back-prop
  - Differentiable Neural Computer (Graves et al. Google 2016)
  - End-to-End Memory Networks (Sukbaathar et al. Facebook 2016)

Application tips

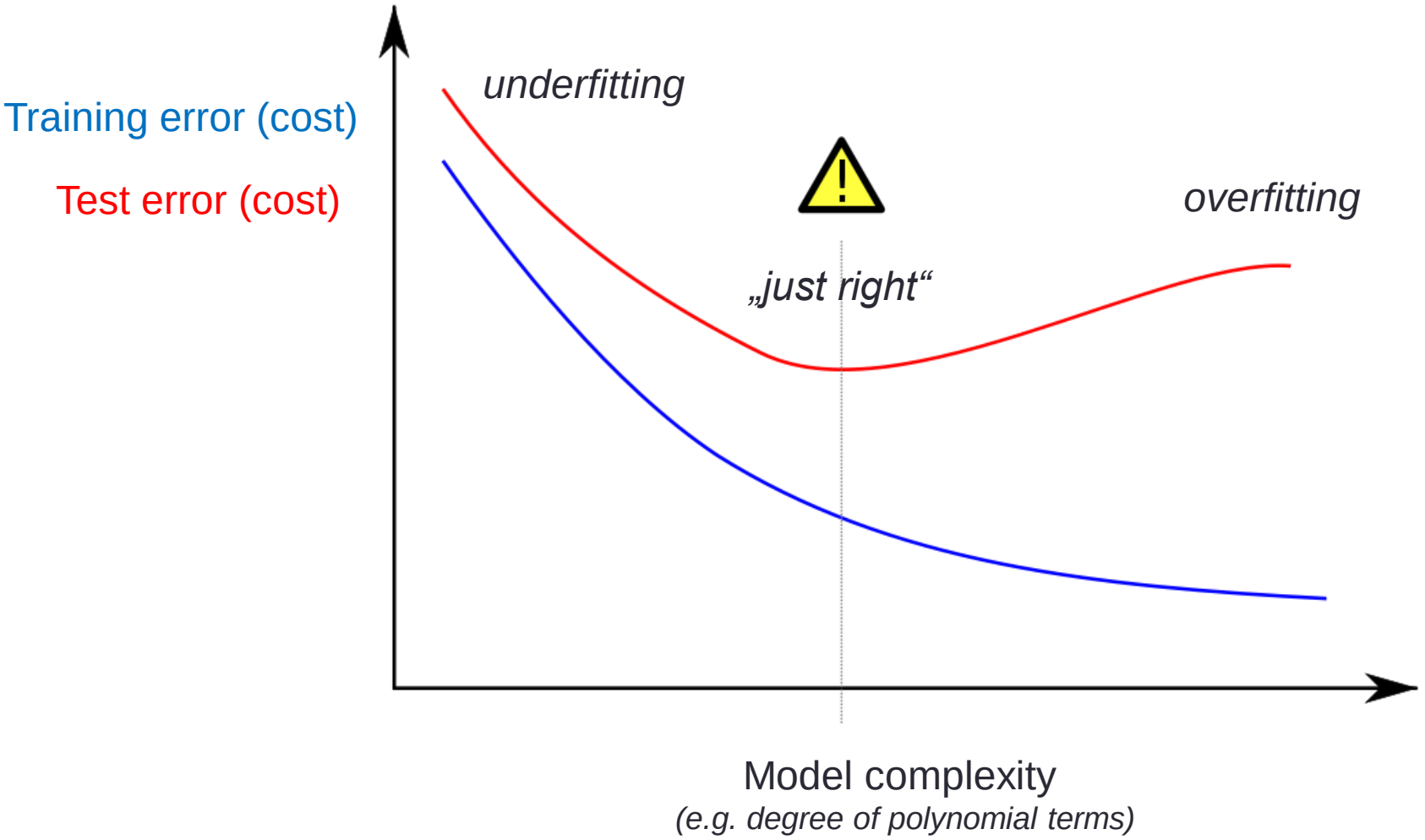
- When to use k-NN:
  - Lots of data is available
  - Small number of features

- What if the classes are not evenly represented?
  - In that case a more frequent class tend to dominate the prediction of the new example

  - Weighting heuristics

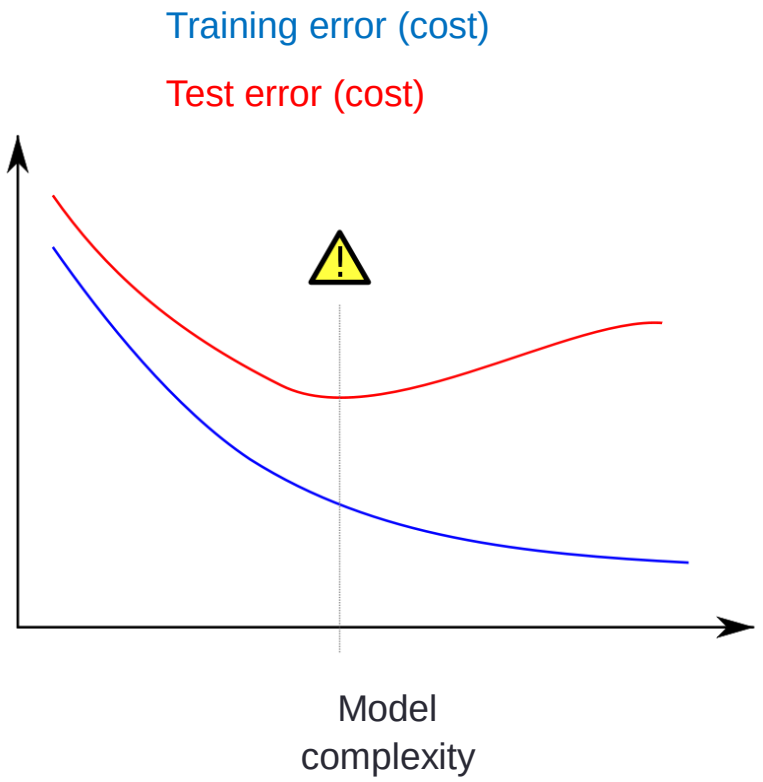
UNDERFITTING AND OVERFITTING - RECAP

Under-/ and Overfitting



Under- and Overfitting

- Underfitting:
  - Model is **too simple**
  - **High training error, high test error**
- Overfitting:
  - Model is **too complex** (often: too many parameters relative to number of training examples)
  - Low training error, **high test error**
- In between „just right“
  - Moderate training error
  - **Lowest test error**

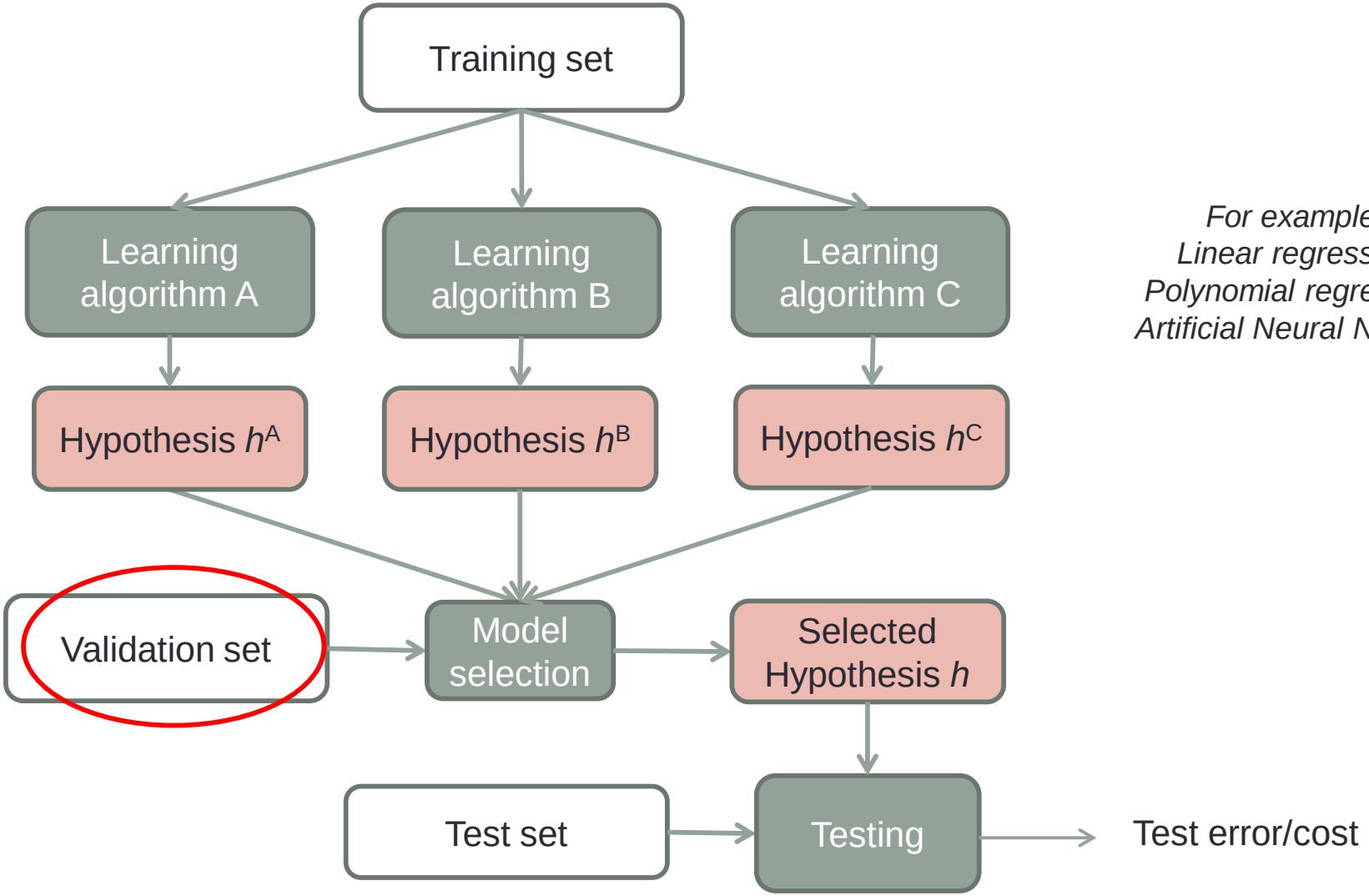


How to deal with overfitting

- Use **model selection** to automatically select the right model complexity
- Use **regularization** to keep parameters small

- Collect more data
  (often not possible or inefficient)
- Manually throw out features which are unlikely to contribute
  (often hard to guess which ones, potentially throwing out the wrong ones)
- Pre-processing, change the feature vector or perform dimension reduction
  (endless effort, often not possible or inefficient)

Model selection: Training/Validation/Test set workflow



For example:
Linear regression,
Polynomial regression,
Artificial Neural Network

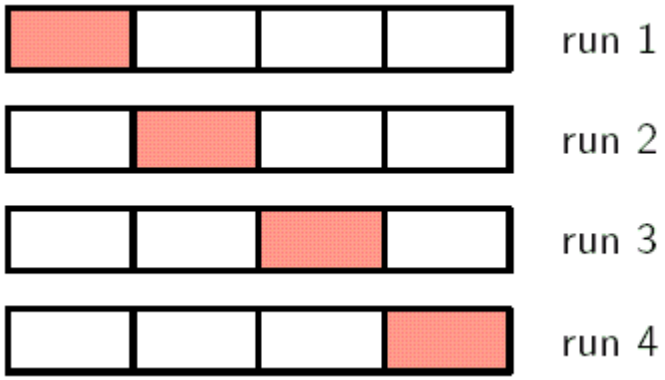
CROSS-VALIDATION

Cross-validation

- **The goal:**
  Define a **validation** set to **“pre-test"** in the **training** phase.

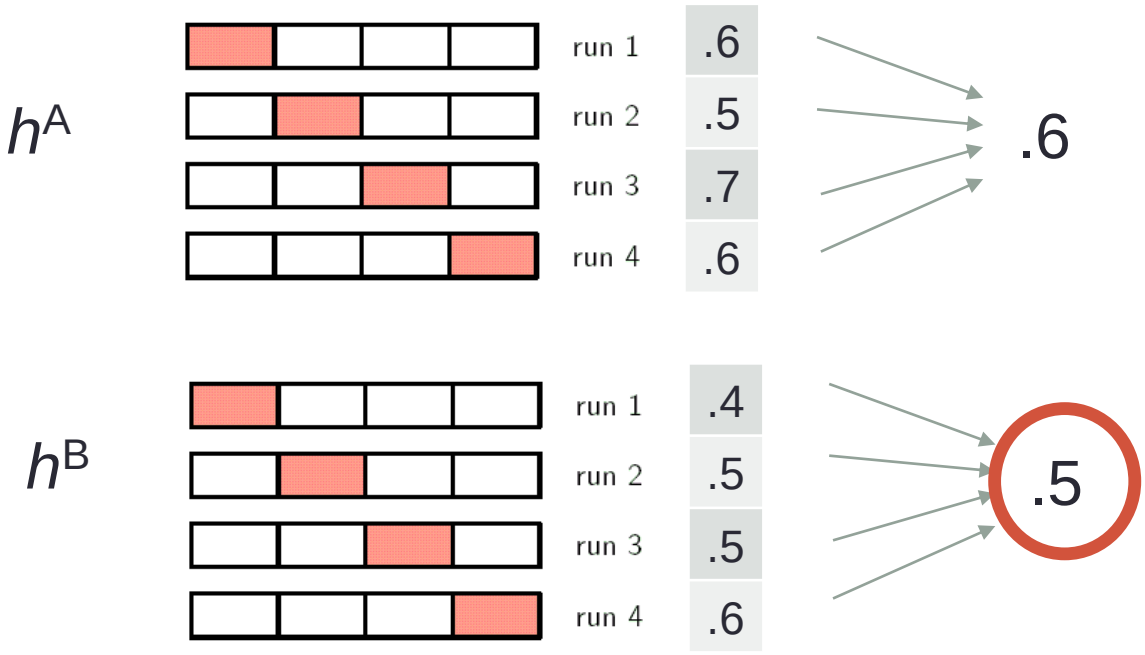
- **Why to use it:**
  Limit overfitting: keep track of the predictive power

- **The trick:**
  Recycle the data by using different training/validation partitions



Model selection with Cross-validation

1. Compute averaged cross-validated error (CV) for each model



2. Choose the model with smallest CV

Cross-validation approaches

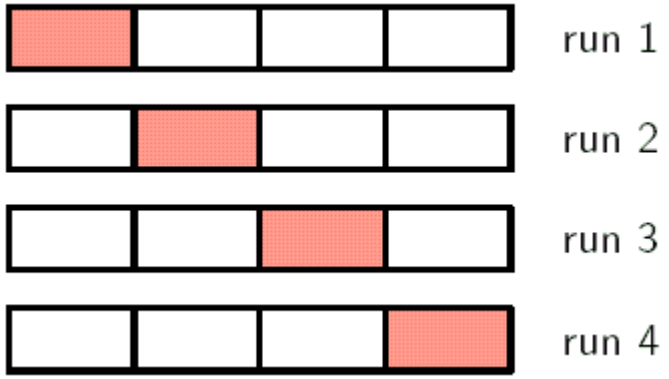
- Disadvantage of a single validation set:
  - Little training data - the function is poorly fitted
  - Little validation data - the true error is poorly estimated

- Tricks and warnings
  - Beware if **the variance of the error** over partitions is large
  - Train the best class over full data after selection
  - Use the same partitions for all hypothesis

- Common types of partitioning:
  - k-fold
  - 2-fold
  - Leave-one-out
  - Repeated random sub-sampling

K-fold cross-validation

- Useful when training dataset is small
- Steps:
  - Split the data into ***k*** equal folds
  - Repeat ***k*** times cross-validation process: each of the folds should be used once as a validation set and the rest as a training set
  - Calculate the mean and the variance of ***k*** runs



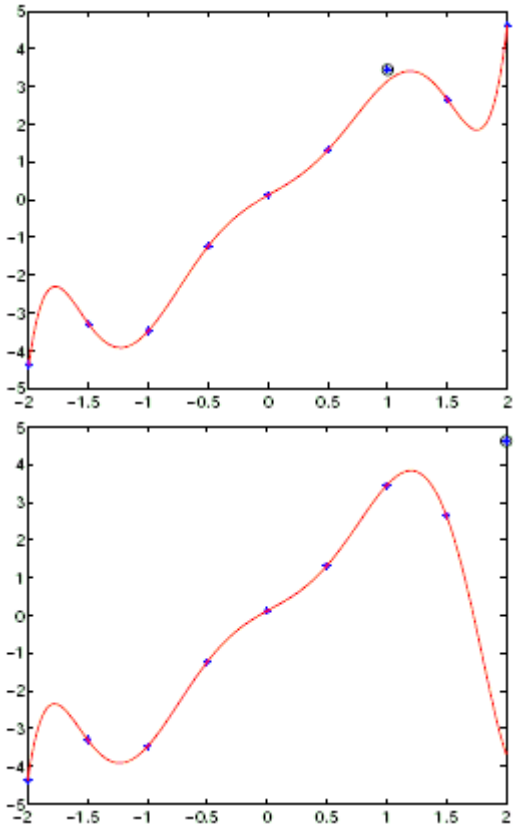
- Disadvantage:
  - It requires ***k*** runs of algorithm which means ***k*** times as much computation

2-fold cross-validation

- The simplest approach, also called holdout method
- Idea:
  - Split randomly the whole training data into 2 equal folds (***k***=2)
  - Train on the first fold and validate on the second, and vice verse
- Advantage:
  - Both training and validation sets are fairly large
  - Each data point is used for both training and validation on each fold

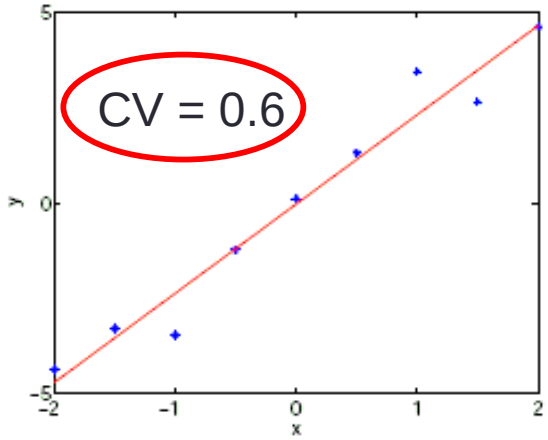
Leave-one-out cross-validation

- This is a special case where ***k*** equals the number of samples in the training set
- Idea:
  - Use a single sample as a validation set and all the rest as training set (***k*** times)
- Used in the case of really small training set

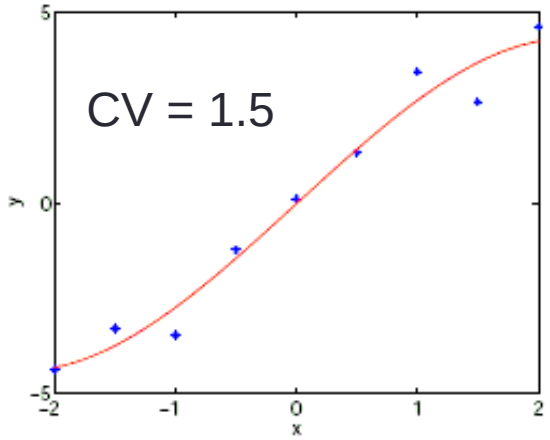


Leave-one-out cross-validation example

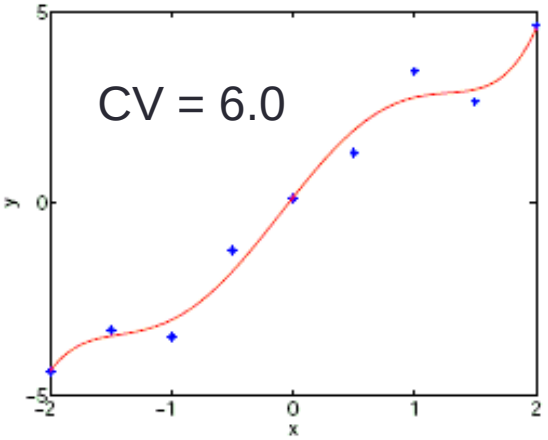
1st order



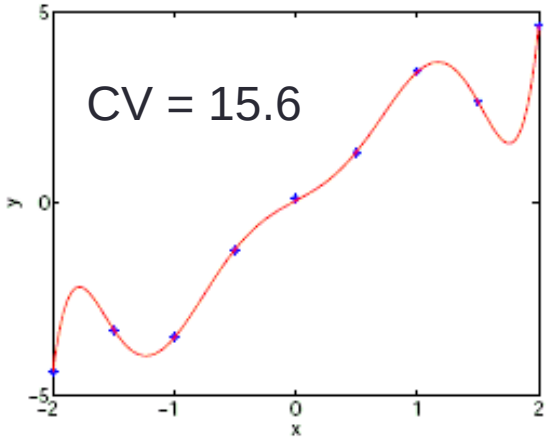
3rd order



5th order



7th order



Repeated random sub-sampling validation

- Idea:
  - Randomly split the dataset into training and validation sets ***k*** times
- Advantage:
  - Choose independently how large each validation set is and how many trials you average over
- Disadvantage:
  - Validation subsets may overlap (some sample may never be selected)

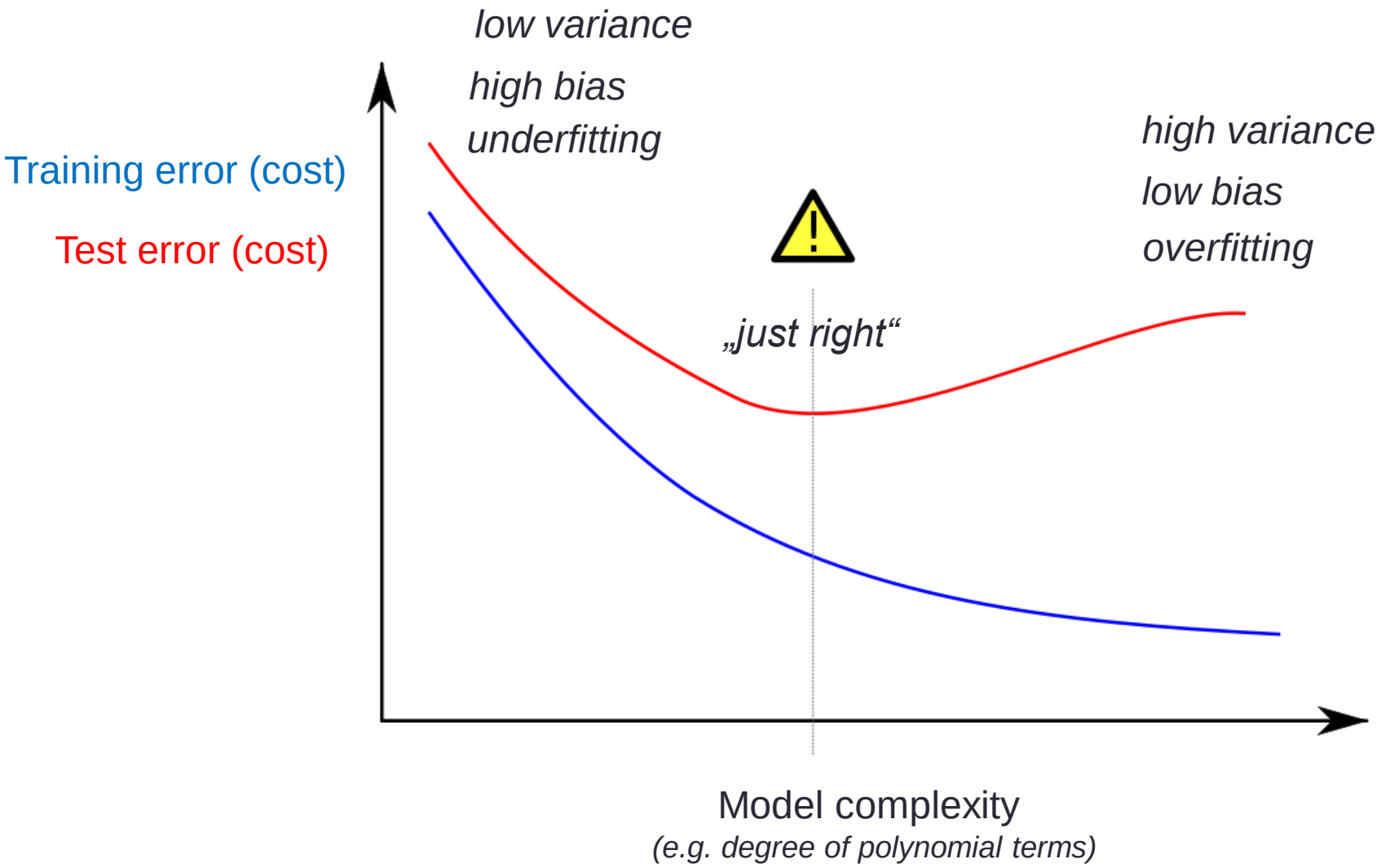
REGULARIZATION

Bias-variance dilemma (tradeoff)

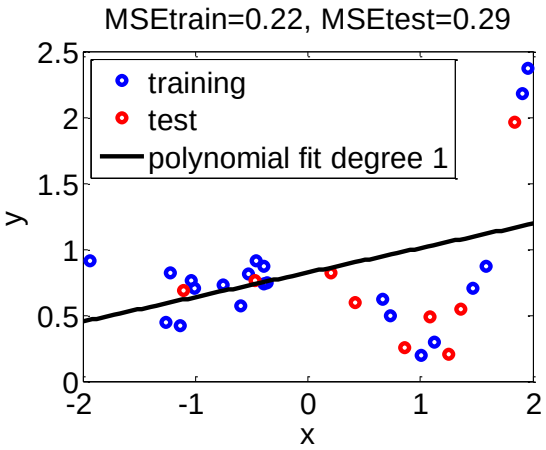
- error = Variance + Bias^2
- Variance – coherence across samples
- Bias – distance to target

- **Regularization** provides technics to reduce the Variance

Under-/ and Overfitting



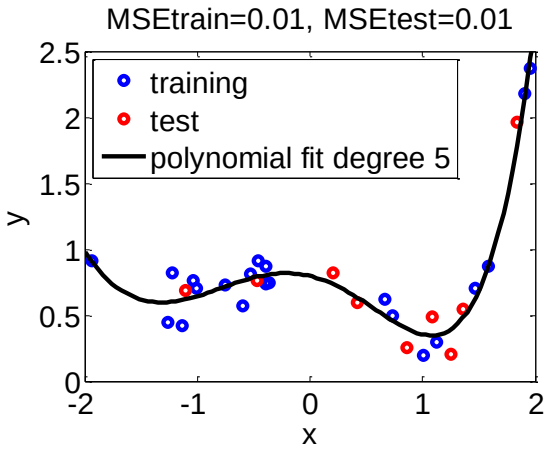
Polynomial regression under-/overfitting



underfitting

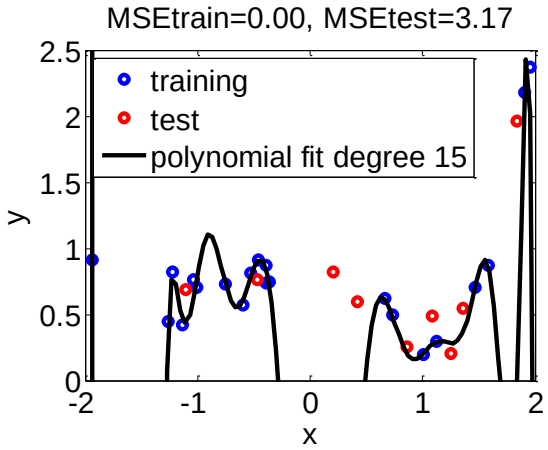
high bias

$$h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 \cdot x$$



„just right“

$$h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 \cdot x + \cdots + \theta_5 \cdot x^5$$



overfitting

high variance

$$h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 \cdot x + \cdots + \theta_5 \cdot x^5 + \theta_6 \cdot x^6 + \cdots + \theta_{15} \cdot x^{15}$$

$$\theta_6 \approx 0 \quad \ldots \quad \theta_{15} \approx 0$$

$$J(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^2 + 1000 \cdot \theta_6^2 + \cdots + 1000 \cdot \theta_{15}^2$$

suppose we penalize $\theta_6 \ldots \theta_{15}$

Regularization

- Prefer simple models
- Exclude extreme models

- How to do it:
  - Instead of minimizing the original problem $J(\boldsymbol{\theta})$ minimize $J(\boldsymbol{\theta}) + \lambda||\boldsymbol{\theta}||^2$ where $||\boldsymbol{\theta}||$ is L_2 norm (Euclidean norm)

- Large λ leads to underfitting (high bias)
- Low λ to overfitting (high variance)

Regularized linear regression

- Regularized cost function:

$$J(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2 + \frac{\lambda}{m}\sum_{j}\theta_j^2$$

$$J(\boldsymbol{\theta}) = \frac{1}{m}||\boldsymbol{X\theta} - \boldsymbol{y}||^2 + \frac{\lambda}{m}||\theta||^2$$

- Analytical solution:

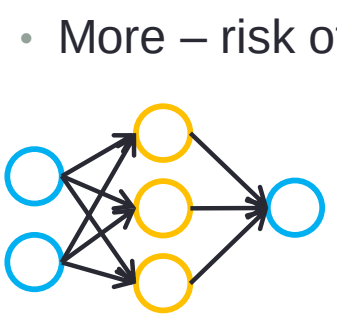
$$\boldsymbol{\theta}^* = \left(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

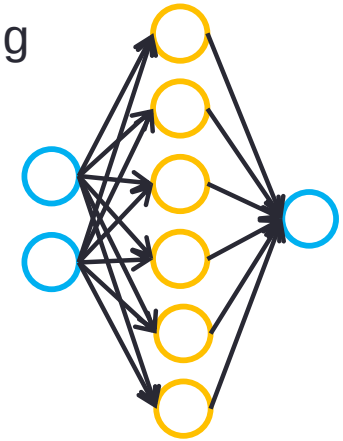
- Gradient descent solution:

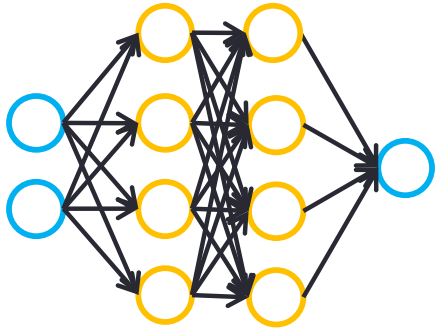
$$\theta_j := \theta_j(1 - 2\eta\frac{\lambda}{m}) - 2\eta\cdot\frac{1}{m}\sum_{i=1}^{m}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)\cdot x_j^{(i)}$$

Regularization of NN

- How many hidden layers and how many neurons ?
  - Fewer – risk of underfitting
  - More – risk of overfitting







- Reduce the complexity (reduce Variance)
  - Weight decay
  - Network structure (weight sharing)

- Keep track of predictive power (reduce Error directly)
  - Early stopping

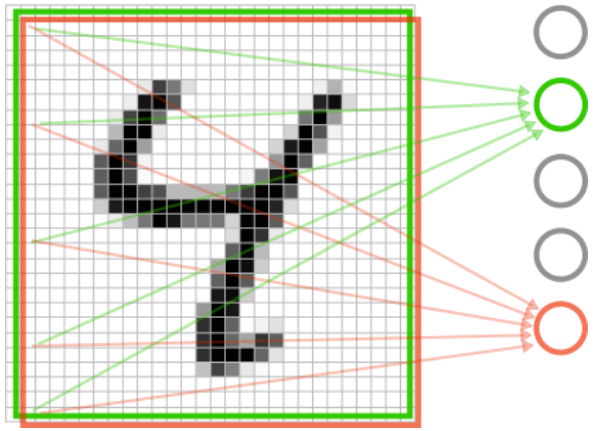
Weight decay

- "Weight decay" is a L_2 norm regularization for Neural networks
- The weights of a NN will be an additional term in an Error function:

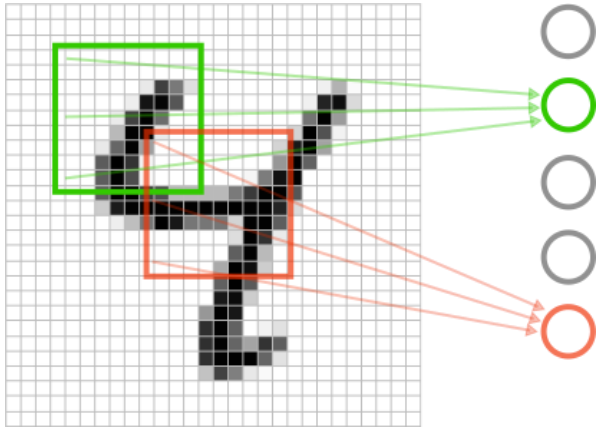
$$E(\boldsymbol{w}) = MSE(\boldsymbol{w}) + \frac{\lambda}{2}||\boldsymbol{w}||^2$$

Sparse structure

- Weights: 32 x 32 x K_{hidden}



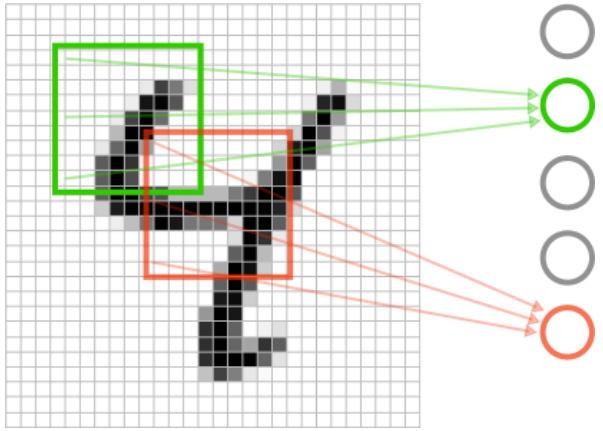
- Weights: 8 x 8 x K_{hidden}
- Different role between hidden units



Sparse = many weights set to null

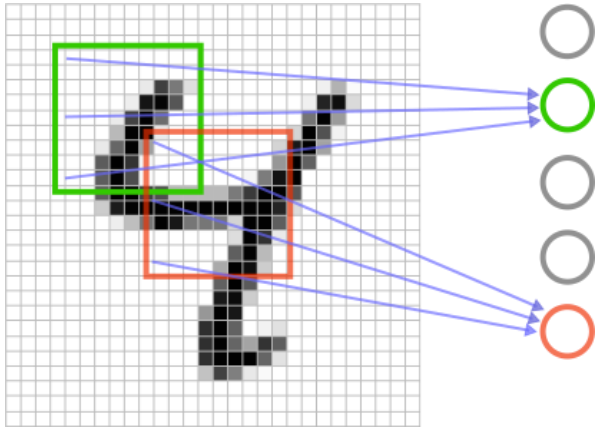
Weight sharing

- Weights: 8 x 8 x K_{hidden}



- $W_i = W_j = W_0$
- Weights: 8 x 8
- Spatial **invariance**

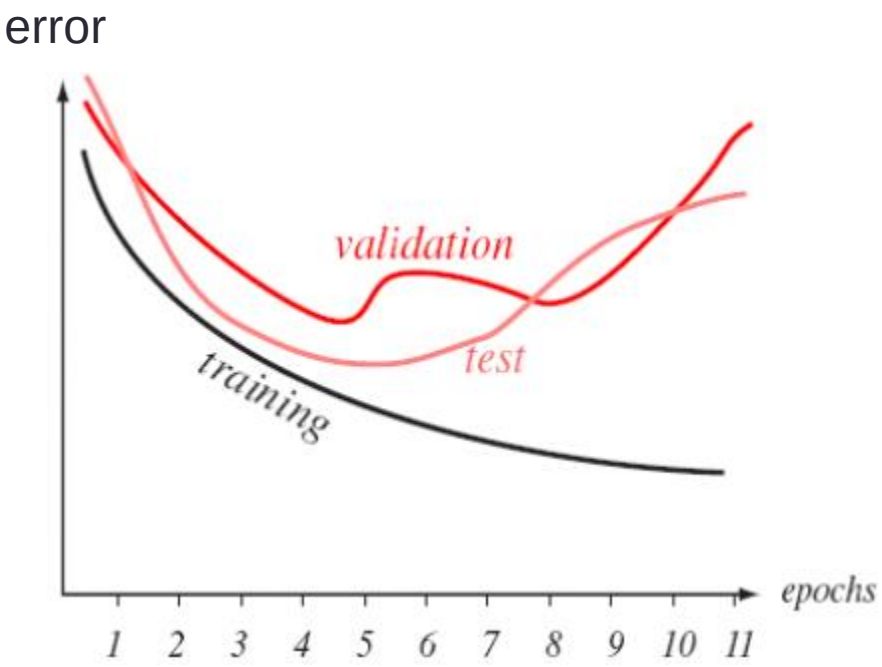
Even positions were pixels are always 0 may learn to recognize some shapes



Early stopping

- A form of regularization based on the scheme of model selection

- Steps:
  - The weights are initialized to small values
  - Stop when the error on validation data increases



PROBABILISTIC MODELS

Basics of probability theory

- The **random variable** X takes the value x with the probability p.

Is given by the probability density function (X is omitted by abuse of notations) $p(x) := p(X = x)$

- A random variable is well defined if $\forall x, p(x) \in [0, 1]$

$$\sum_x p(x) = 1$$

- The **conditional** probability is defined by $p(y|x) = \frac{p(y, x)}{p(x)}$

- If X and Y and independent : $p(y|x) = p(y)$ $p(x, y) = p(x)p(y)$

- The **expectation** is defined by $\mathbb{E}[f(x)] = \sum_x f(x)p(x)$

Linear Regression

- Model assumption:
  1) All samples are independent

$$\forall(i,j), p(x^{(i)}, y^{(i)}, x^{(j)}, y^{(j)}) = p(x^{(i)}, y^{(i)})p(x^{(j)}, y^{(j)})$$

  2) Y is a noisy observation of a linear combination of the feature vector X

$$y_{pred} = \sum_i w_i x_i$$

$$p_w(y|x) = \mathcal{N}(y_{pred}, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_{pred} - y)^2}{\sigma^2}\right)$$

  3) The probability of X does not depend on the parameters w

- Fit the model to the data, i.e. maximize the probability of observing the data under the model assumptions, i.e. maximizing the **likelihood** (or its log)

$$\max_w \mathcal{L} = p_w(y^{(1)}, x^{(1)}, \ldots y^{(n)}, x^{(n)}) \qquad \max_w \log \mathcal{L}$$

(Demo on the blackboard that this is equivalent to solve linear Regression, i.e: show that this new objective function is proportional to mean square error)

Regularization as a Prior

- New assumption: the parameters are in the neighborhood of zero (**Prior** knowledge about preferred parameters)

$$p(w) = \mathcal{N}(0, \sigma_w)$$

- The parameters are now **a random variable**

$$\max_w \log p(\text{data}, w) = \log \underbrace{p(\text{data}|w)}_{\text{Likelihood}} + \log \underbrace{p(w)}_{\text{Prior}}$$

(Demo on the blackboard that it leads to L2 regularization of w)

SUMMARY (QUESTIONS)

Some questions…

- Difference between lazy and eager learning?
- What is Instance based learning?
- Training and testing procedure for k-NN?
- Is k-NN better than linear classifiers for high-dimensional inputs ?

- What is overfitting and how to deal with it?
- What is validation set?
- What is cross-validation?
- Types of partitioning in cross-validation?

- What is the bias-variance tradeoff?
- What is regularization and how is it used?
- What are regularization methods for NN?