COMPUTATIONAL INTELLIGENCE

(INTRODUCTION TO MACHINE LEARNING) SS16

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

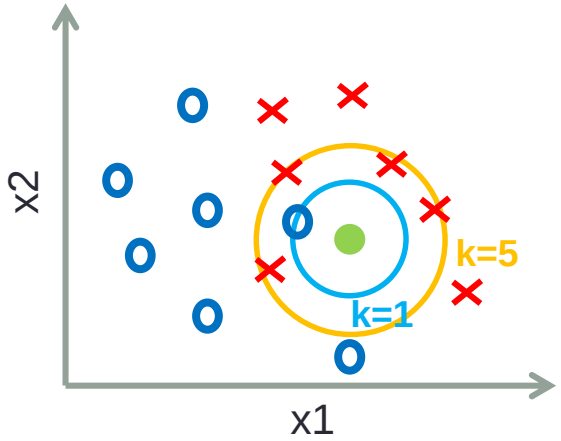
- Store in memory the training set
- Compare a test sample to the samples memory

K-NEAREST NEIGHBORS (K-NN)

k-NN

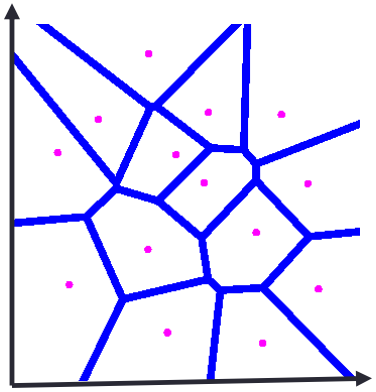
- Simple
- Non-differentiable
- Lazy learning

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

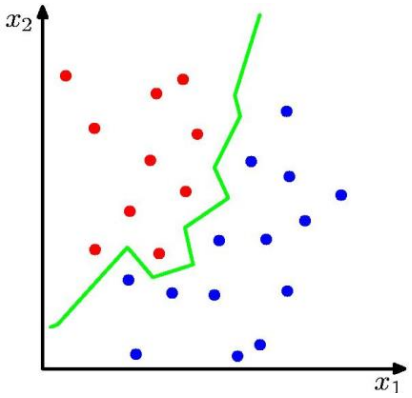


1-NN: Nearest Neighbor

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



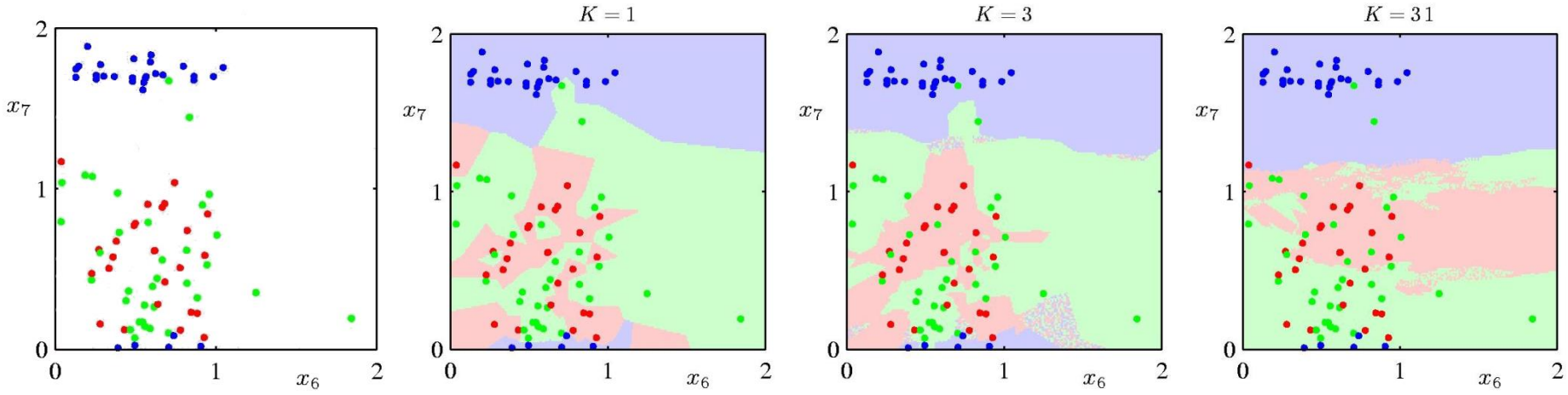
Voronoi diagram



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:**
  - Very fast (basically non-existing)
  - Only input preprocessing (feature extraction and dimensionality reduction)

- **Testing** (k-NN can be used for classification and regression):
  - **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

Application tips

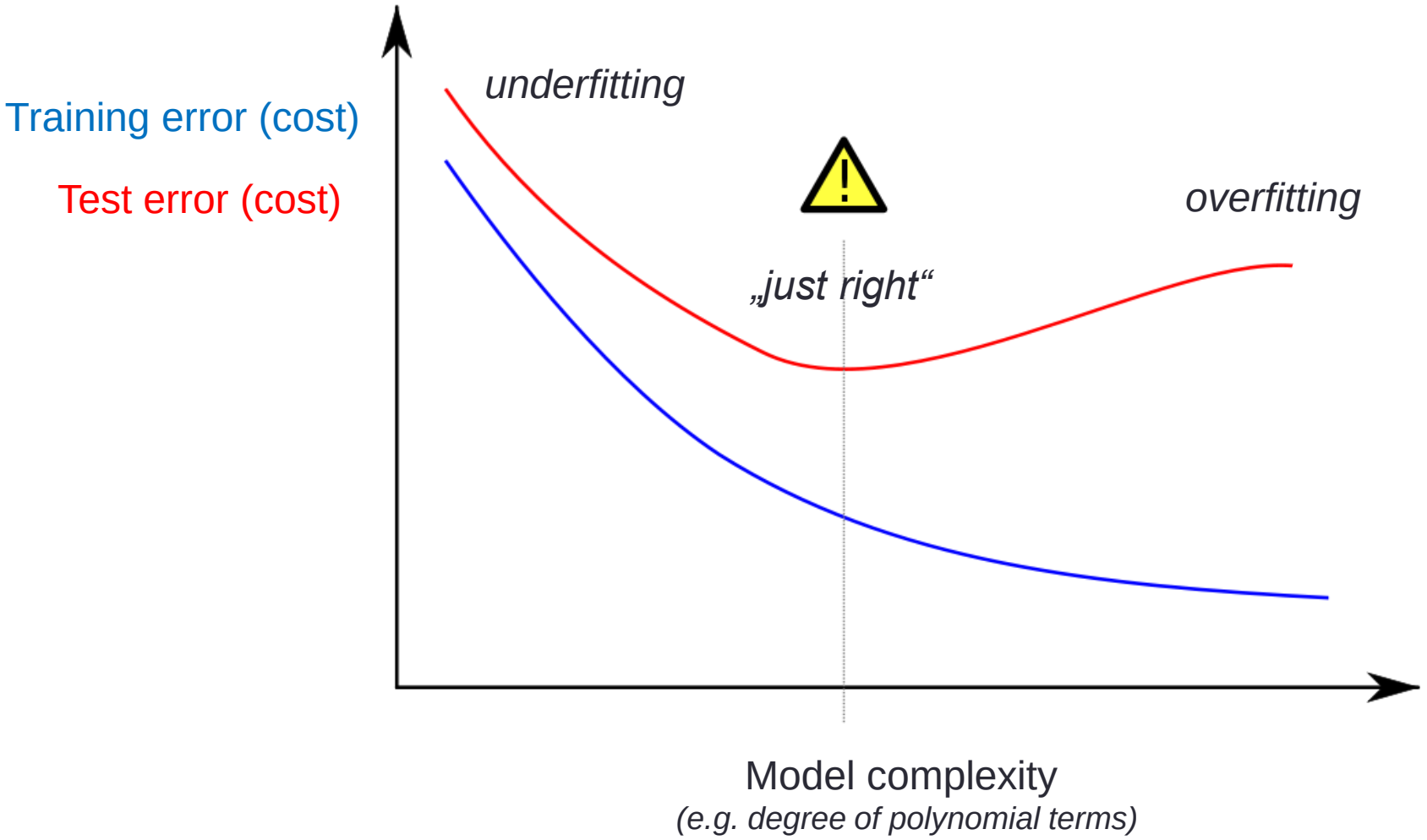
- When to use k-NN:
  - Lots of data is available
  - Small number of features

- 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

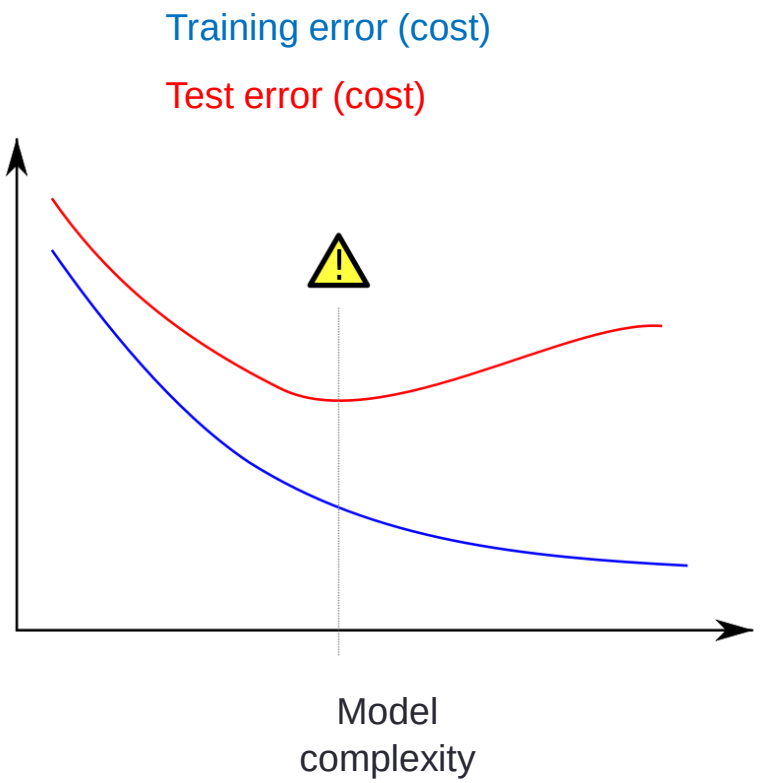
UNDERFITTING AND OVERFITTING - RECAP

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**

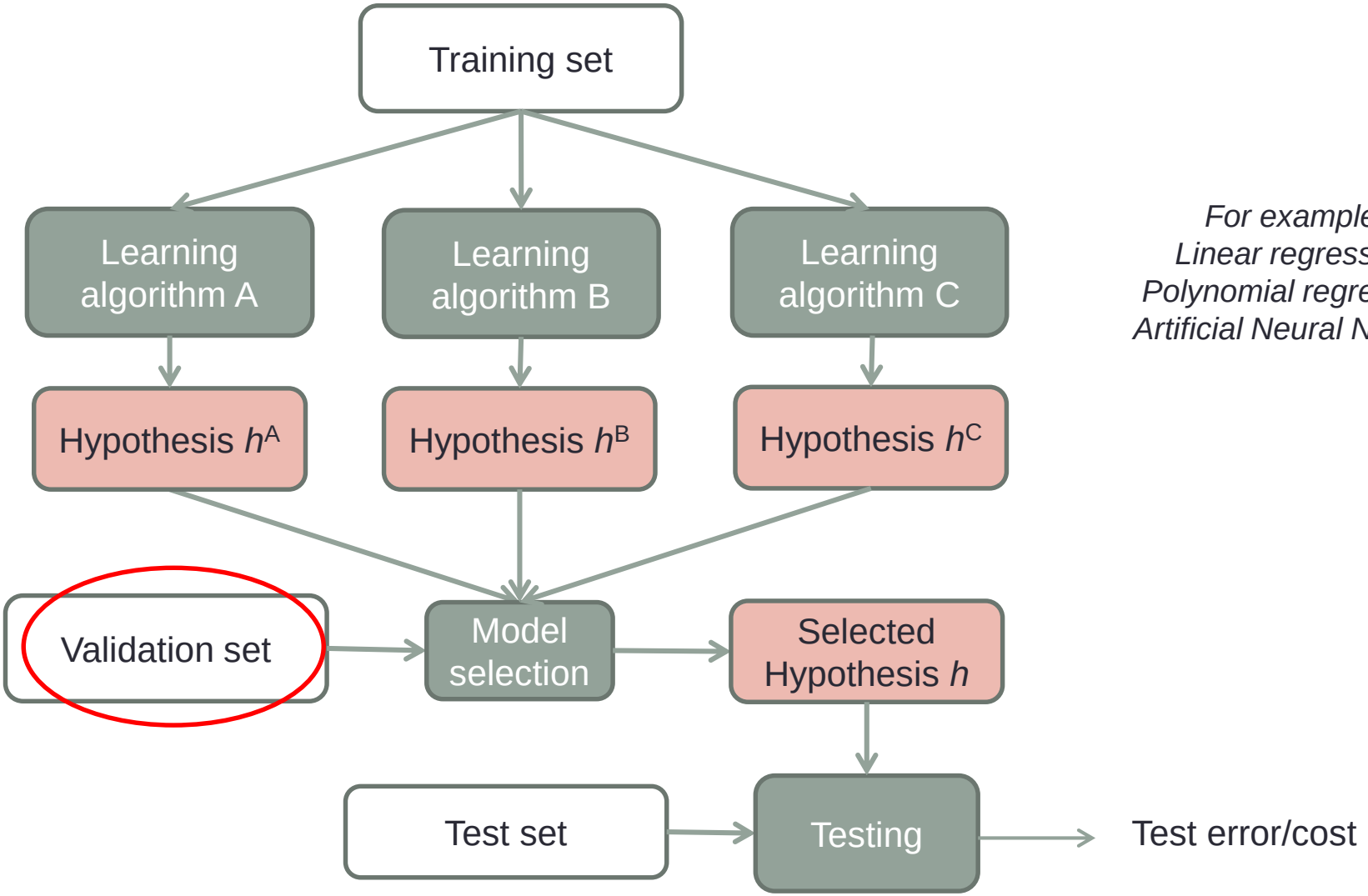


How to deal with overfitting

- 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

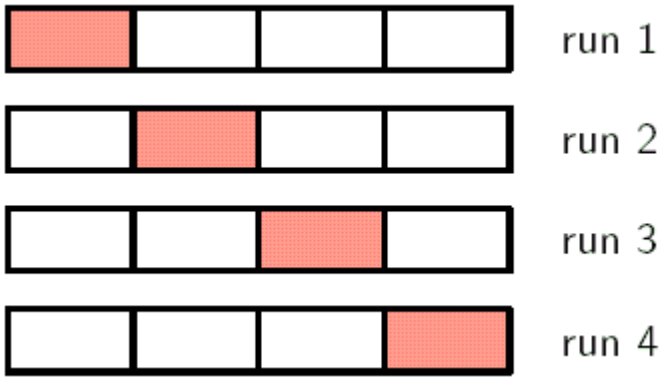
CROSS-VALIDATION

Cross-validation

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

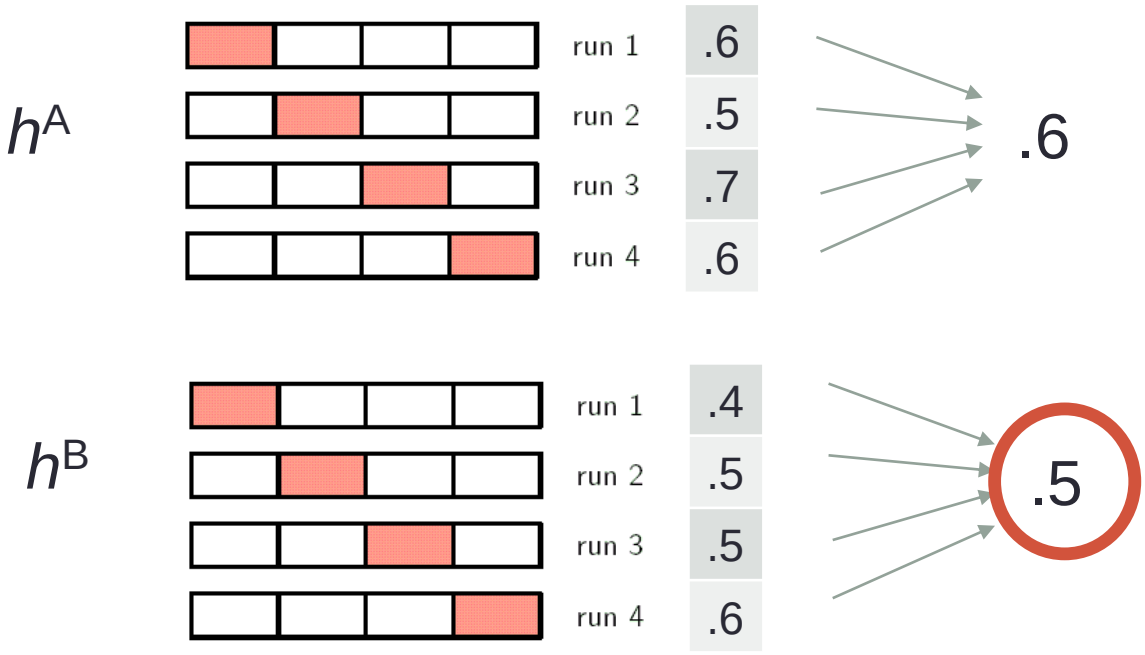
- **Why to use it:**
  Instead of training error keep track of the predictive power

- **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

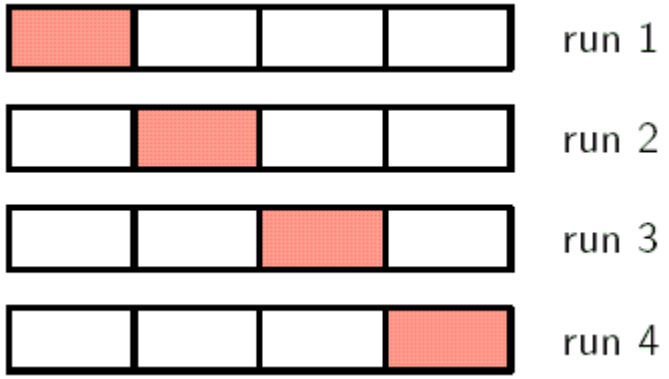
- Disadvantage of a single validation set:
  - Little training data - the function is poorly fitted
  - Little validation data - the true error is poorly estimated

- 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



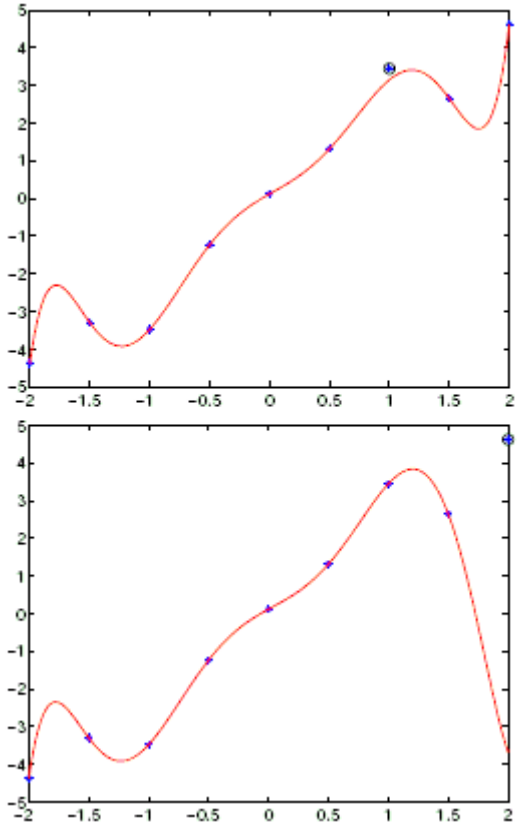
- Disadvantage:
  - It requires ***k*** runs of algorithm which means ***k*** times as much computation

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

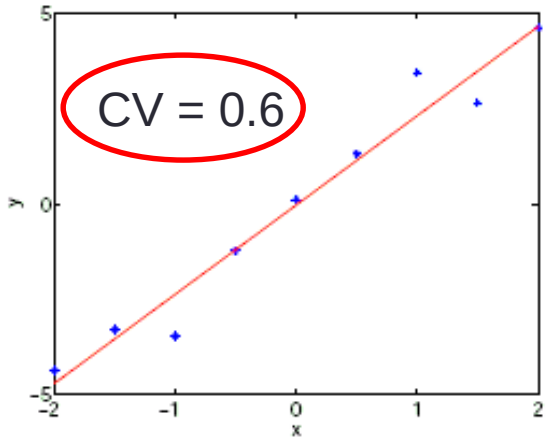
Leave-one-out cross-validation

- 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

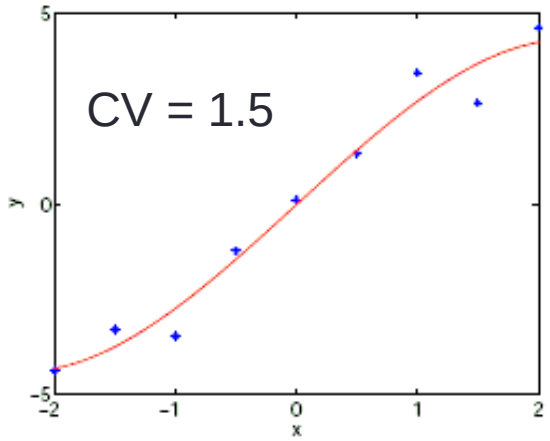


Leave-one-out cross-validation example

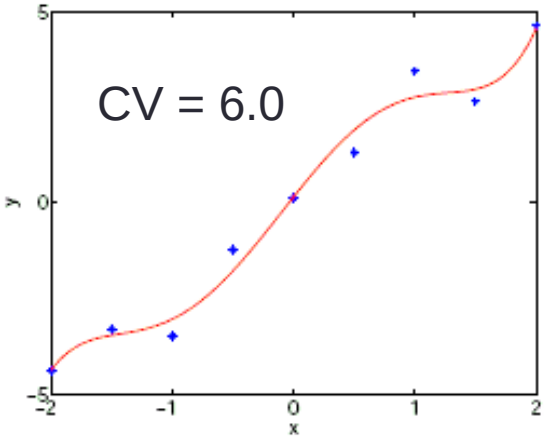
1st order



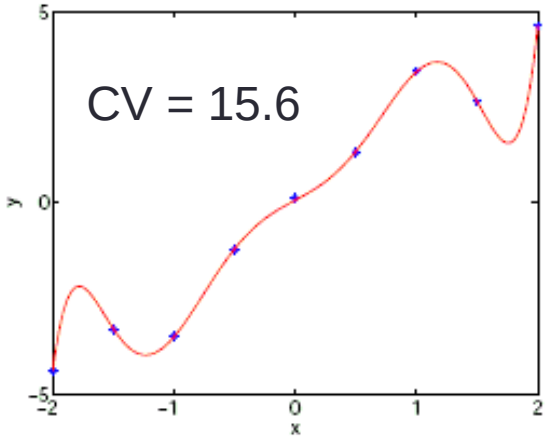
3rd order



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)

- Expected prediction error = Variance + Bias^2 + Noise

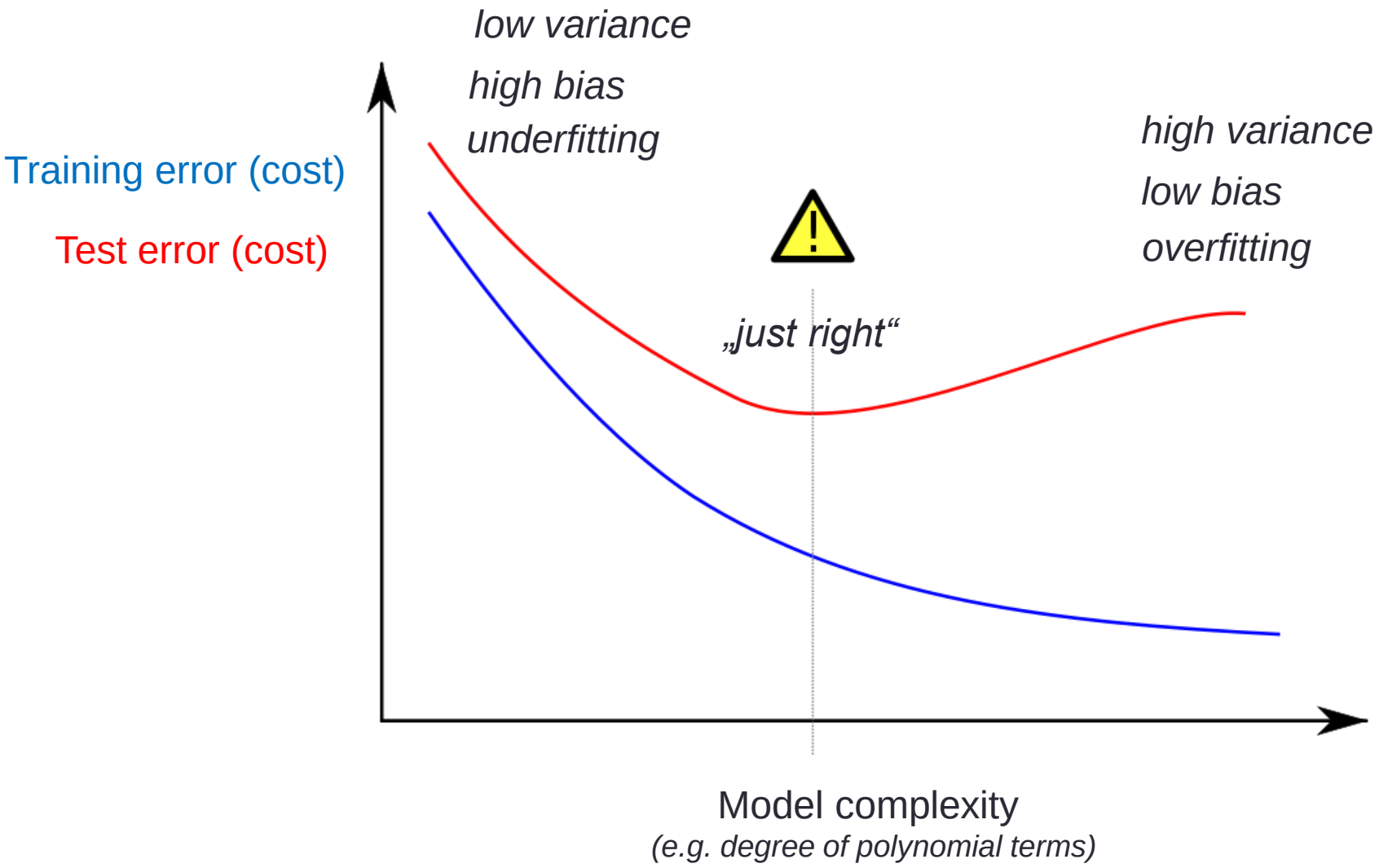
- The bias–variance dilemma (tradeoff) is the problem of simultaneously minimizing the bias and the variance of the model error

- Variance - how sensitive the model is to small changes in the training set
- Bias - how accurate a model is across different training sets

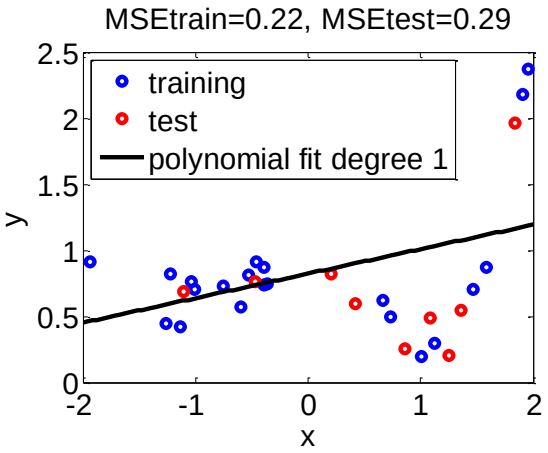
  - High bias -> underfitting (the model is too simple)
  - High variance -> overfitting (the model is too complex)

  - To achieve good performance on data outside the training set a tradeoff must be made!

Under-/ and Overfitting



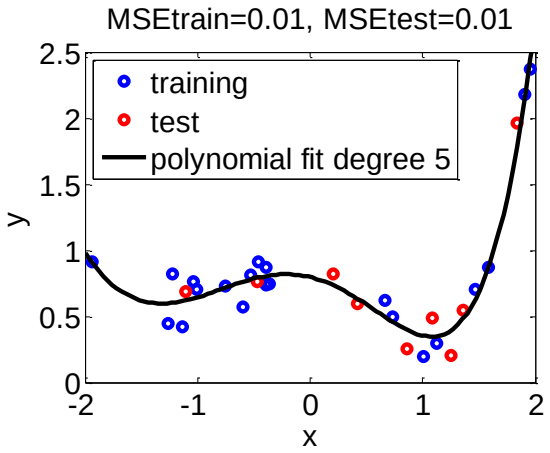
Polynomial regression under-/overfitting



underfitting

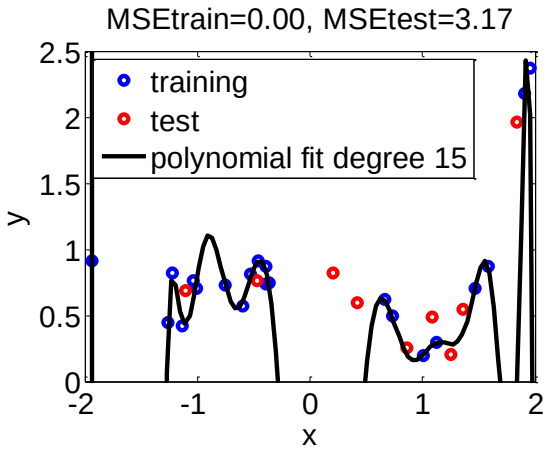
high bias

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



„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:

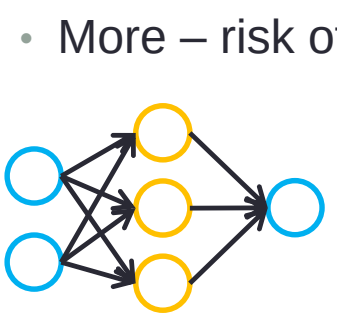
$$\boldsymbol{\theta}^* = \left(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

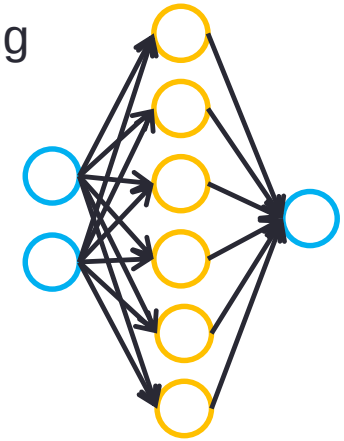
- Gradient descent solution:

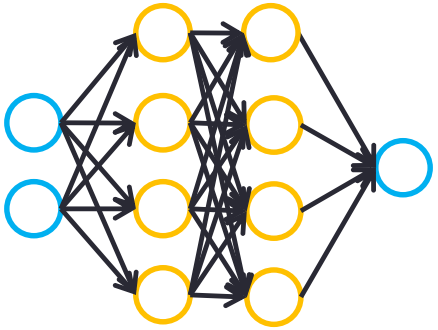
$$\theta_j := \theta_j(1 - 2\eta\frac{\lambda}{m}) - 2\eta\cdot\frac{1}{m}\sum_{i=1}^{m}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)\cdot x_j^{(i)}$$

Regularization of NN

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







- Reduce the parameter space:
  - Weight decay
  - Network structure (weight sharing)

- Keep track of predictive power:
  - Early stopping

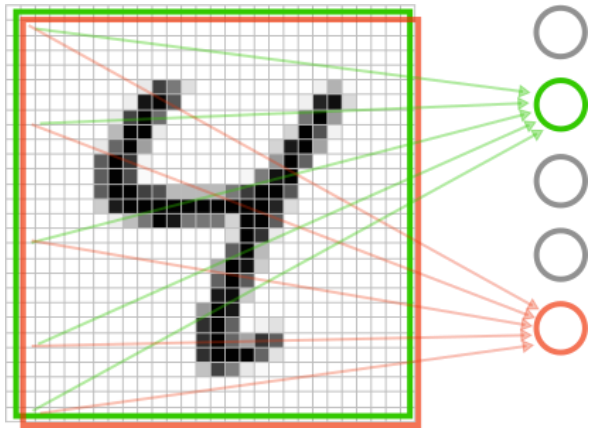
Weight decay

- “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:

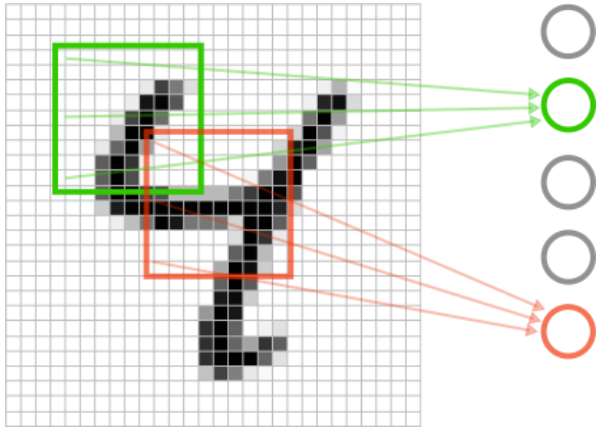
$$E(\boldsymbol{w}) = MSE(\boldsymbol{w}) + \frac{\lambda}{2}||\boldsymbol{w}||^2$$

Sparse structure

- Weights: 32 x 32 x K_{hidden}



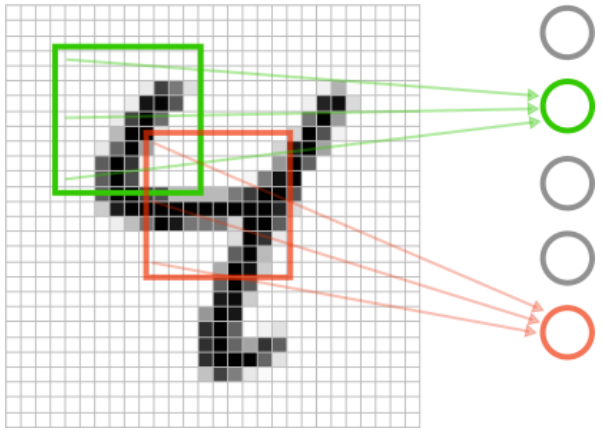
- Weights: 8 x 8 x K_{hidden}
- Different role between hidden units



Sparse = many weights set to null

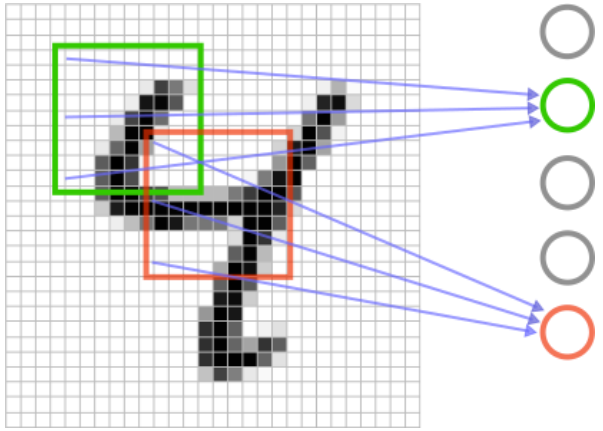
Weight sharing

- Weights: 8 x 8 x K_{hidden}



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

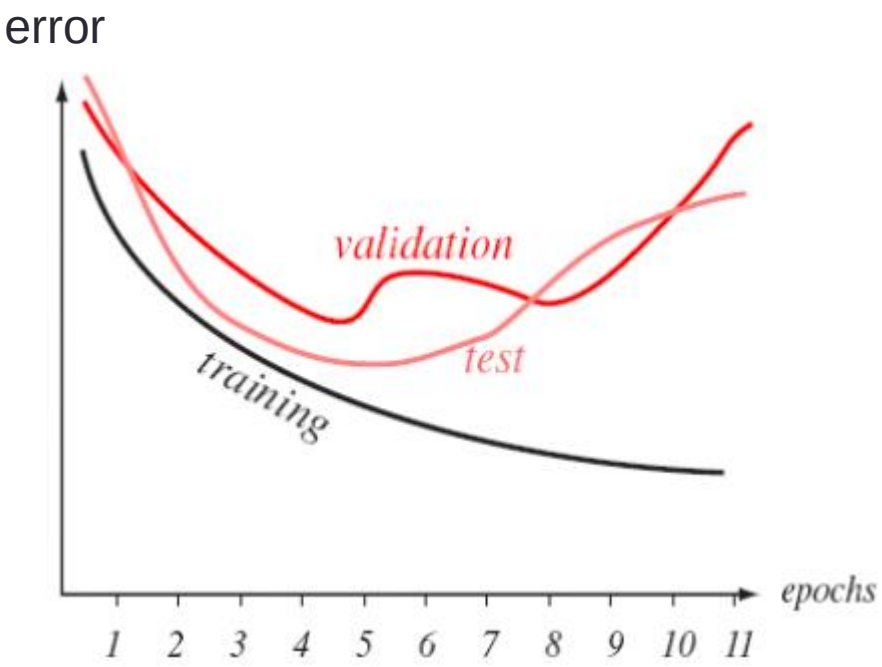
Even positions were pixels are always 0 may learn to recognize some shapes



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



SUMMARY (QUESTIONS)

Some questions…

- Difference between lazy and eager learning?
- What is Instance based learning?
- Training and testing procedure for k-NN?
- How does the number of neighbors influence k-NN?
- When to use k-NN and what are pros/cons?

- 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?