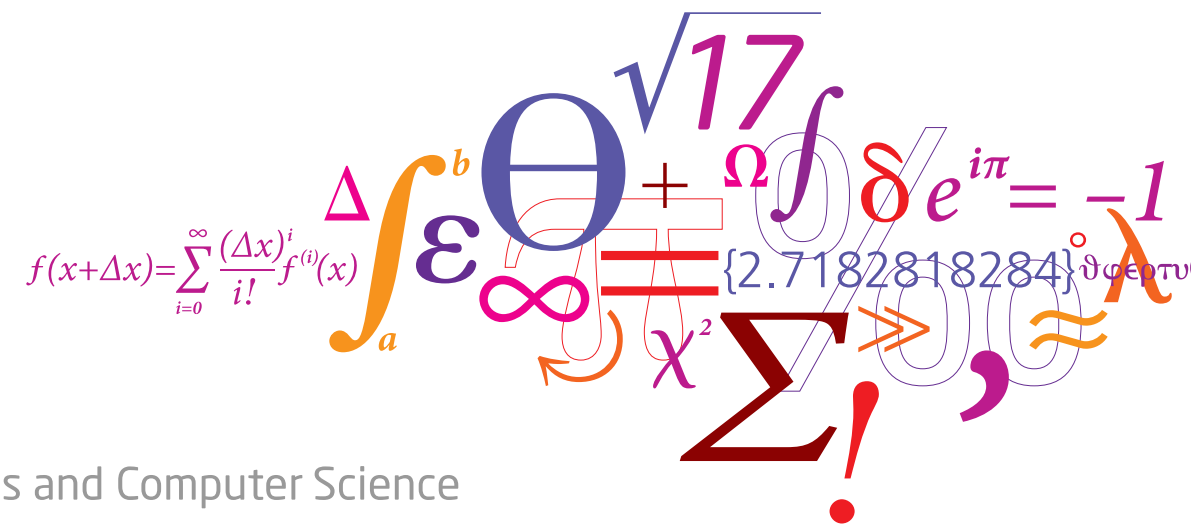
02450: Introduction to Machine Learning and Data Mining

Overfitting, cross-validation and Nearest Neighbor

Morten Mørup

DTU Compute, Technical University of Denmark (DTU)



DTU Compute
Department of Applied Mathematics and Computer Science

Lecture Schedule

1. Introduction
   7 October: C1

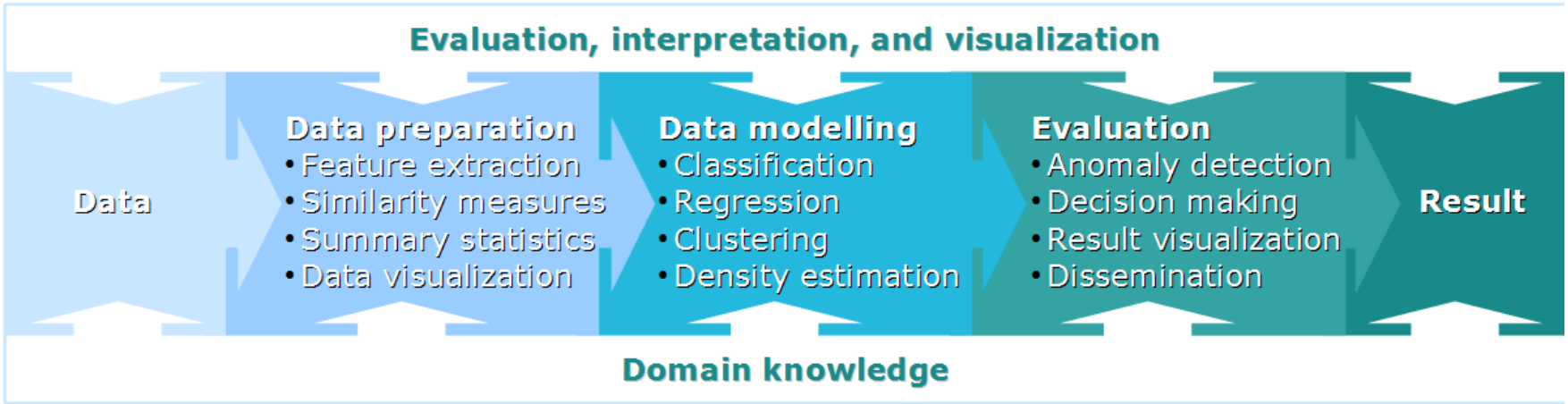
   Data: Feature extraction, and visualization
2. Data, feature extraction and PCA
   7 October: C2, C3
3. Measures of similarity, summary statistics and probabilities
   7 October: C4, C5
4. Probability densities and data Visualization
   7 October: C6, C7

   Supervised learning: Classification and regression
5. Decision trees and linear regression
   8 October: C8, C9
6. **Overfitting, cross-validation and Nearest Neighbor**
   8 October: C10, C12
7. Performance evaluation, Bayes, and Naive Bayes
   9 October: C11, C13
8. Artificial Neural Networks and Bias/Variance
   9 October: C14, C15
9. AUC and ensemble methods
   10 October: C16, C17

   Unsupervised learning: Clustering and density estimation
10. K-means and hierarchical clustering
    10 October: C18
11. Mixture models and density estimation
    11 October: C19, C20
12. Association mining
    11 October: C21

    Recap
13. Recap
    11 October: C1-C21

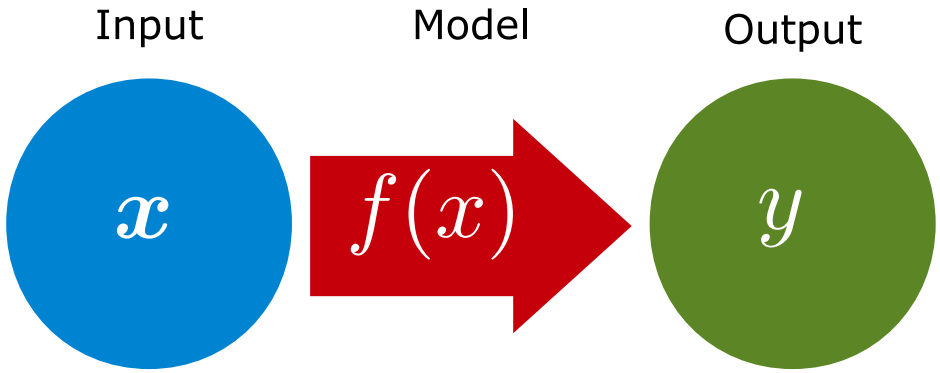
Piazza online help: `https://piazza.com/dtu.dk/fall2019/october2019`



Learning Objectives

- Explain the difference between training, test and generalization error
- Explain how cross-validation can be used for (i) performance evaluation (ii) model selection
- Apply forward and backward selection

Supervised learning



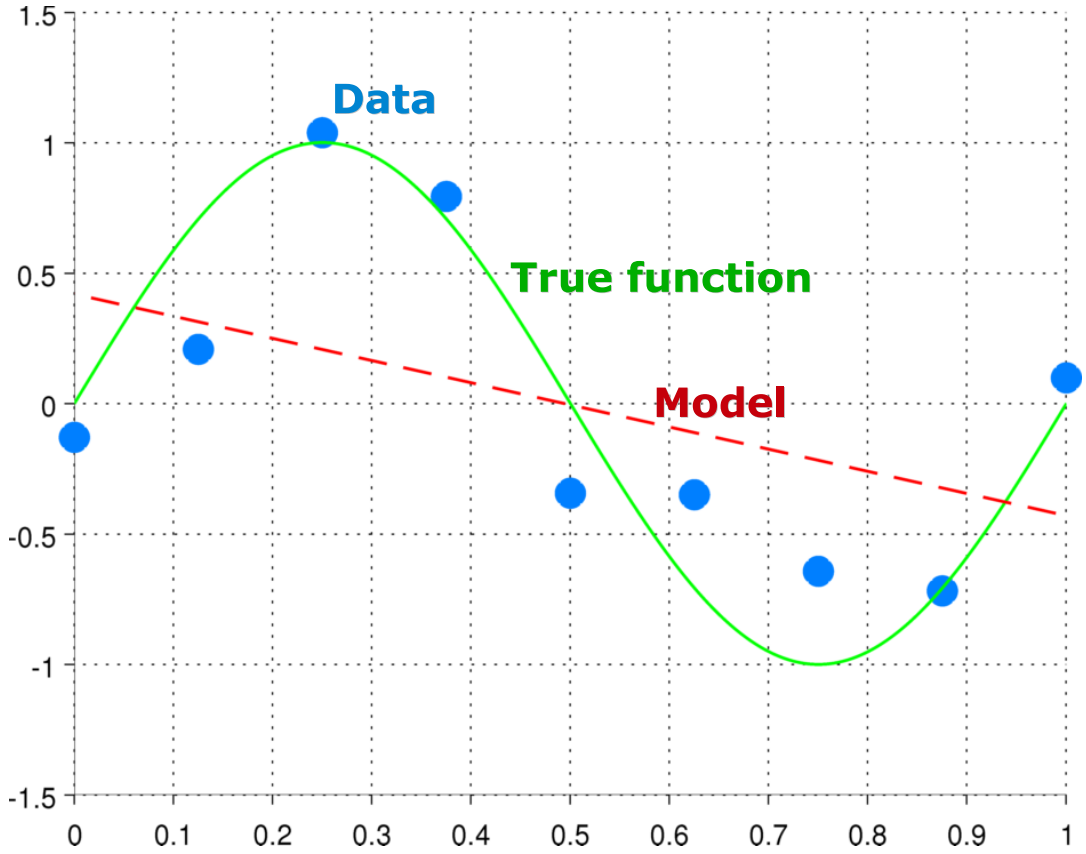
- **Mapping between domains**
  - Classification: Discrete output
  - Regression: Continuous output

Roadmap

- Introduce errors
  - Training error
  - Test error
  - Generalization error
- Introduce cross-validation
  - **Basic cross validation** for **performance evaluation**
  - **Cross-validation** for **model selection**
  - **Two-level cross-validation** for **model selection and performance evaluation**
- Statistical comparison of two classifiers

Why are there "multiple models"? Example: Linear regression

- Bad fit
- **Too simple model**



$$f(x) = w_0 + w_1 x$$

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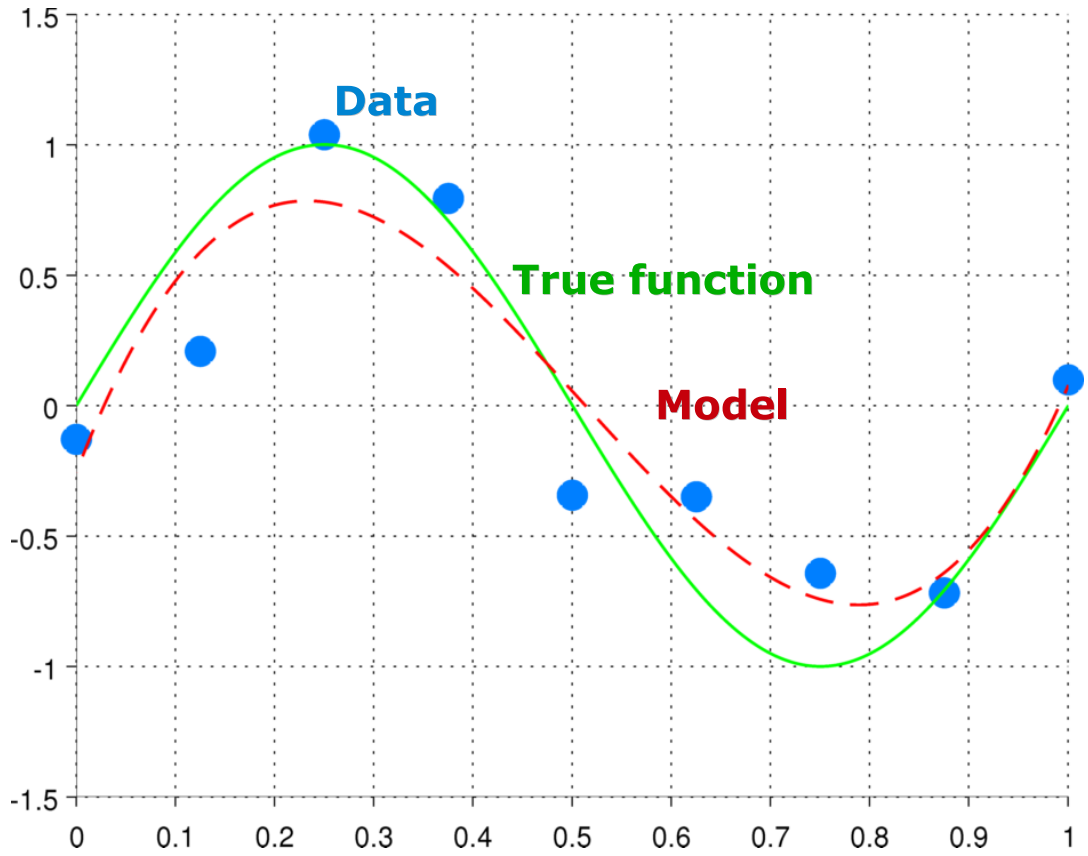

$$f(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

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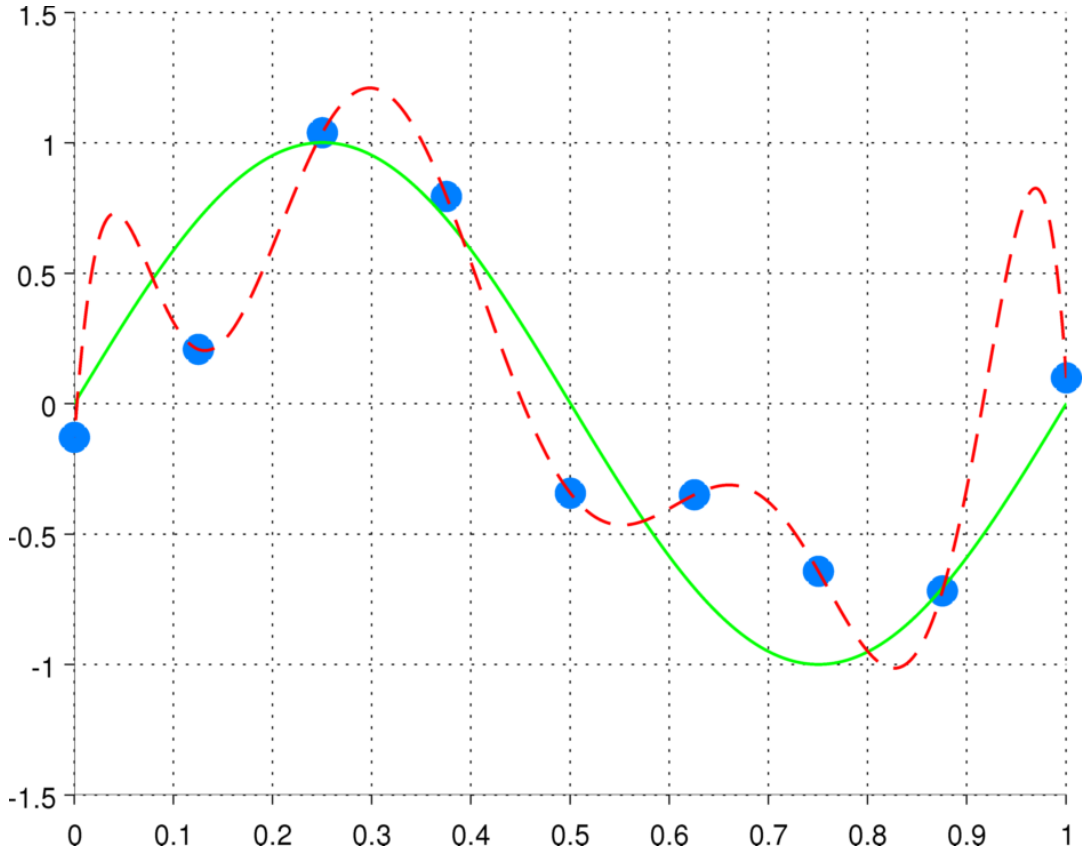
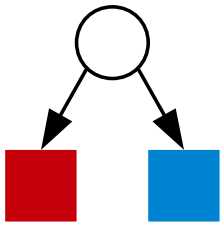
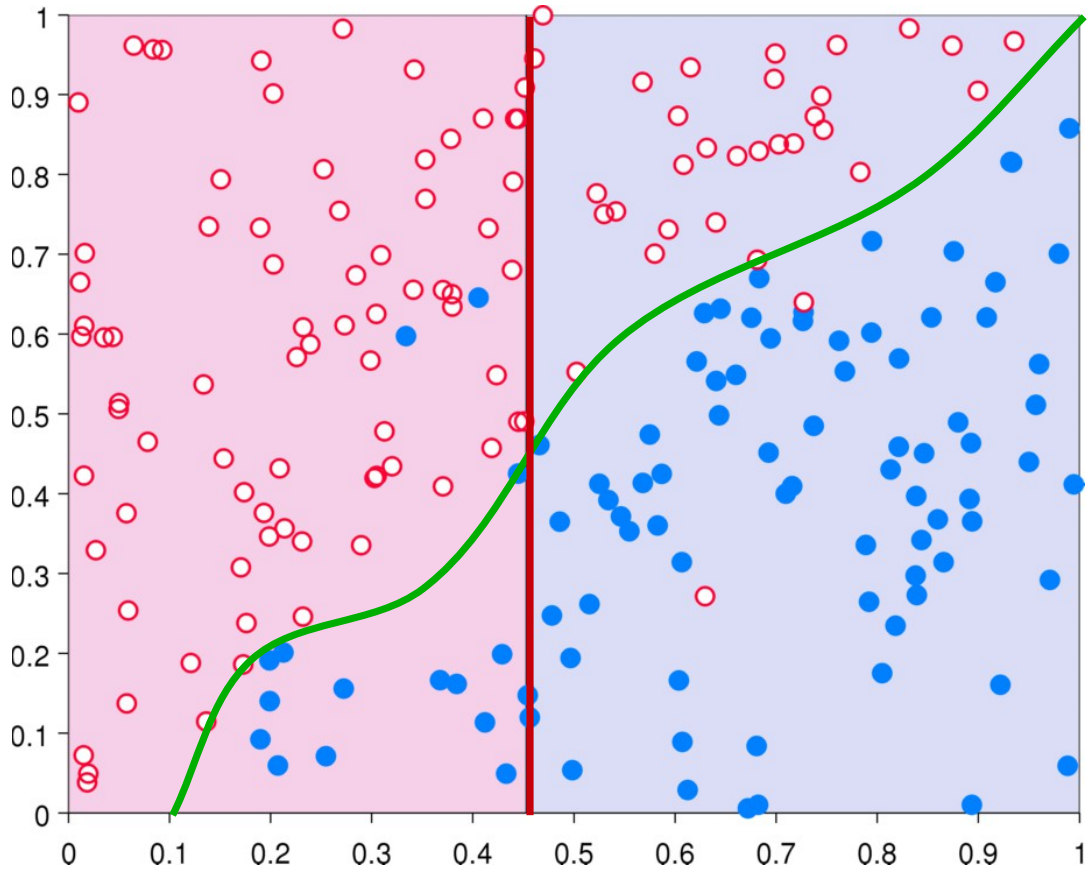


$$f(x) = w_0 + w_1 x + \cdots + w_8 x^8$$

Why are there "multiple models"? Example: Classification tree

- Bad fit
- **Too simple model**





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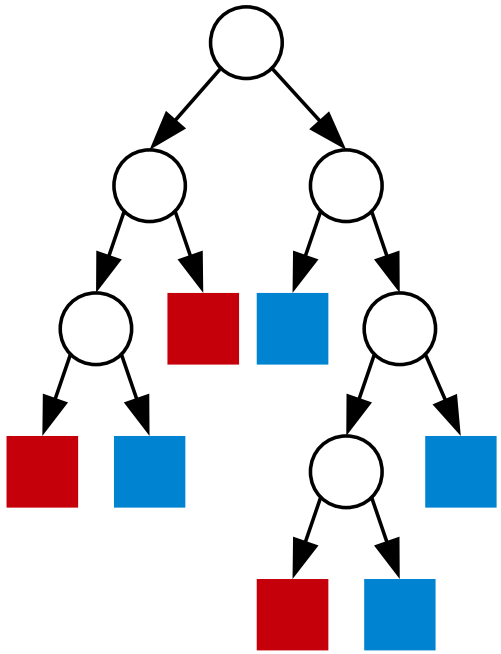

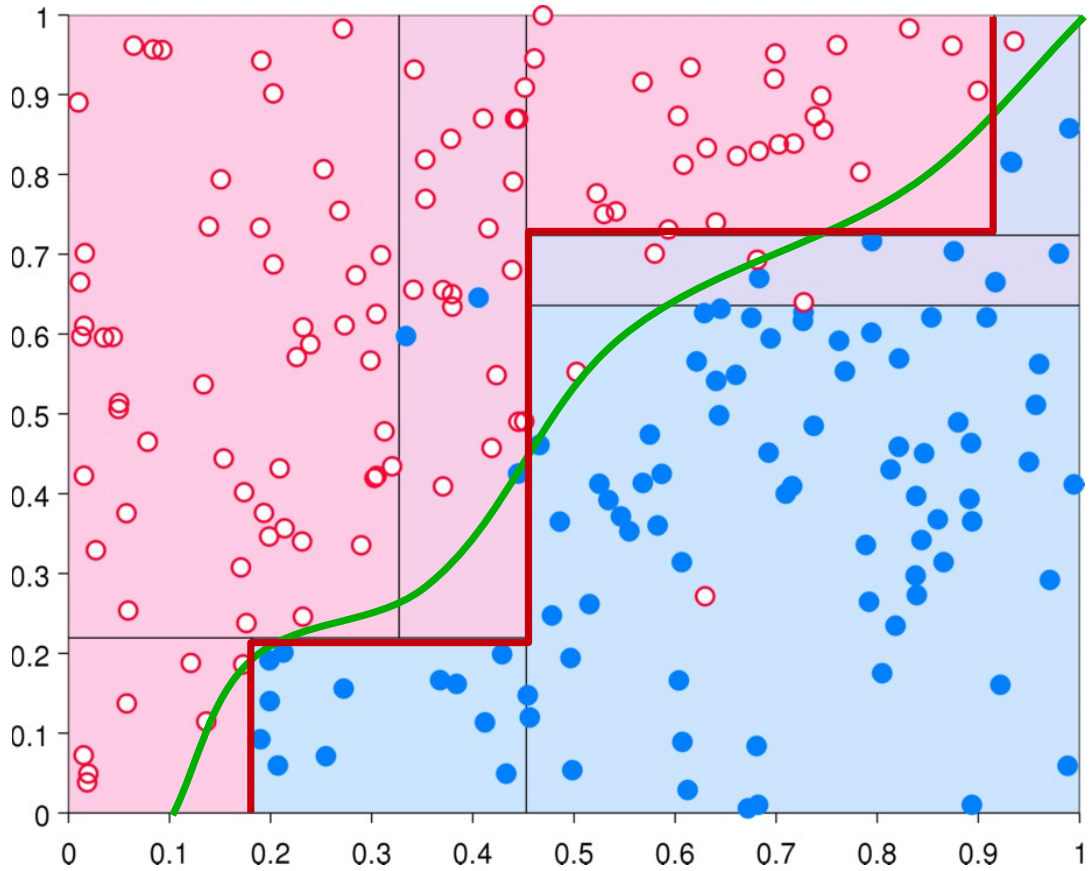

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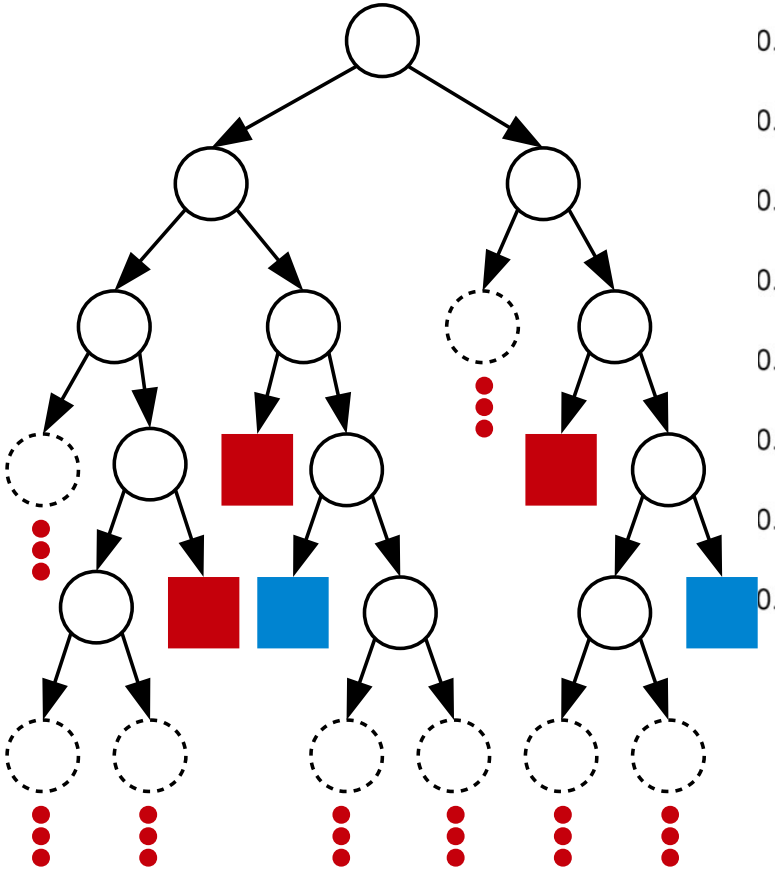
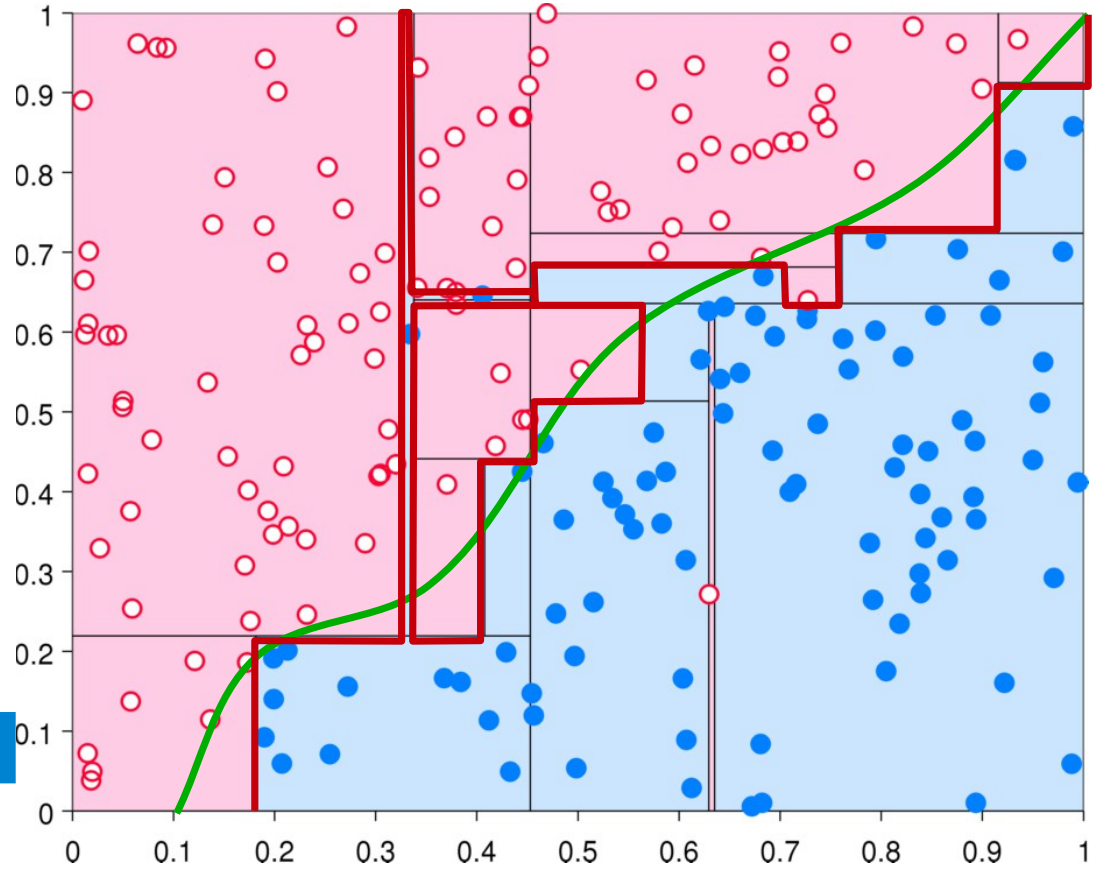
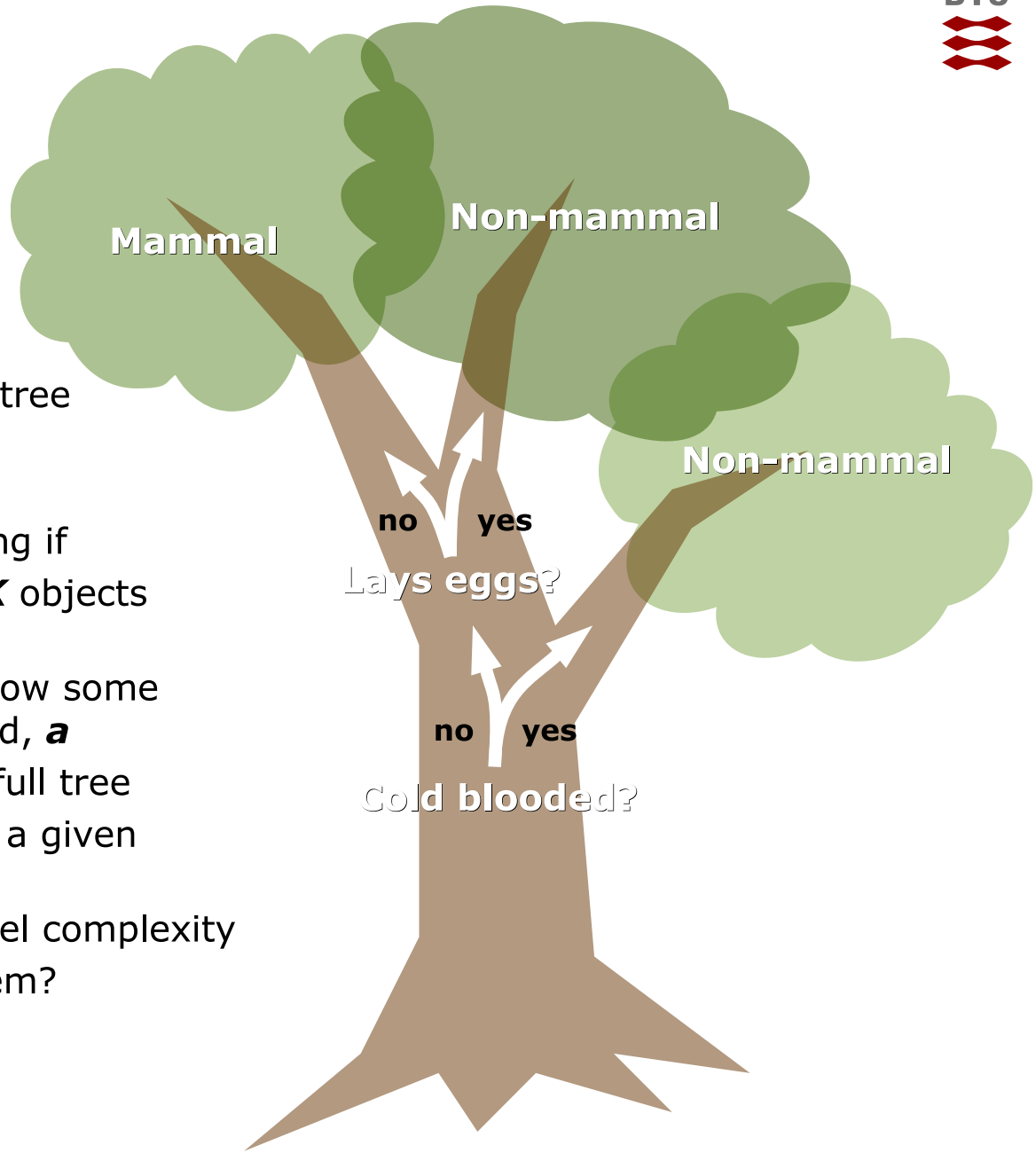


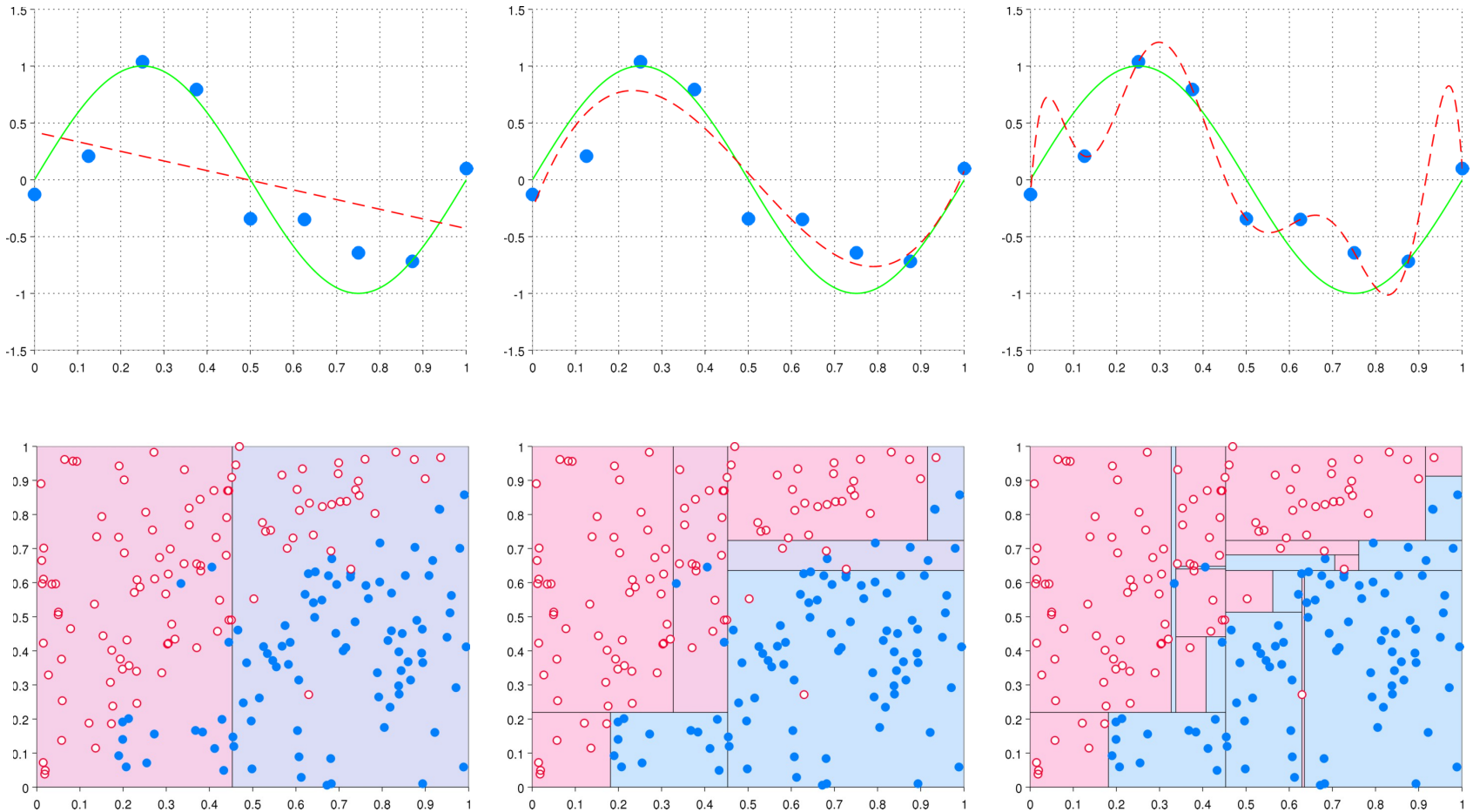


Decision trees

- Hunts algorithm
  - Continue splitting until each node is pure
  - Results in a very complex tree (overfitting)
- **Control complexity**
  - **Pre-pruning**: Stop splitting if
    - There is less than ***K*** objects on the branch
    - Impurity gain is below some predefined threshold, ***a***
  - **Post-pruning**: Generate full tree
    - Cut off branches to a given pruning level, ***c***
- ***K***, ***a***, and/or ***c*** determine model complexity
  - How should we choose them?

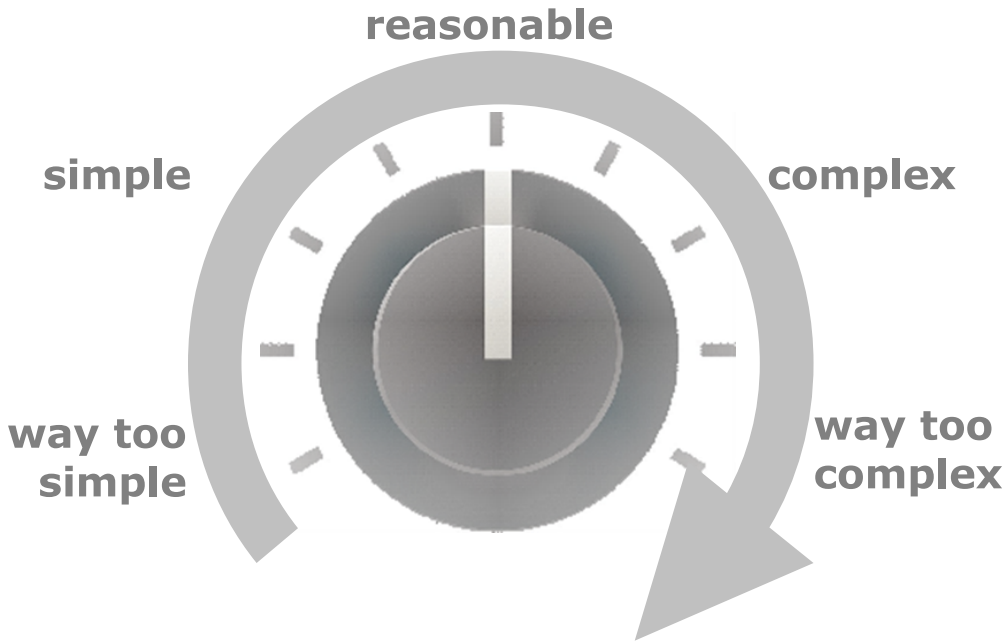


Model overfitting



Control the model complexity

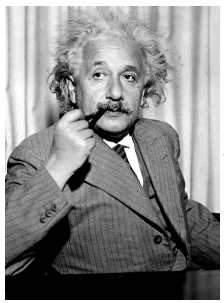
- Find **parameter** or **mechanism** in model that controls complexity



Lex Parsimoniae, Law of parsimony

Given two models with same predictive performance, the simpler model is preferred over the more complex model - William of Ockham (1288-1347) (paraphrased)

https://commons.wikimedia.org/wiki/File:William_of_Ockham.png



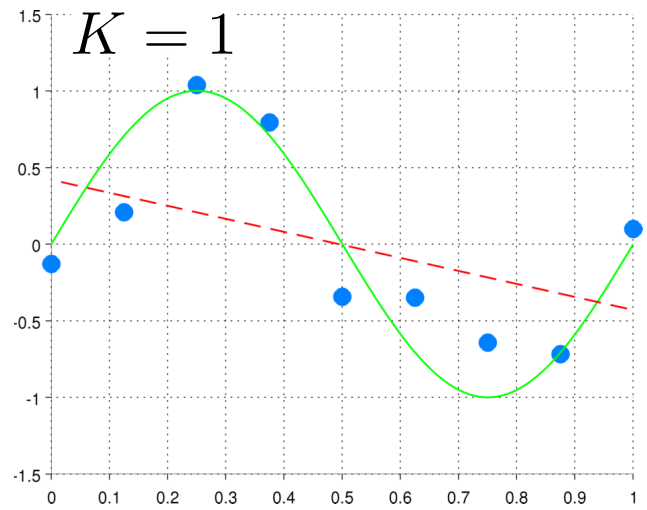
"Everything should be made as simple as possible, but not simpler" - Einstein

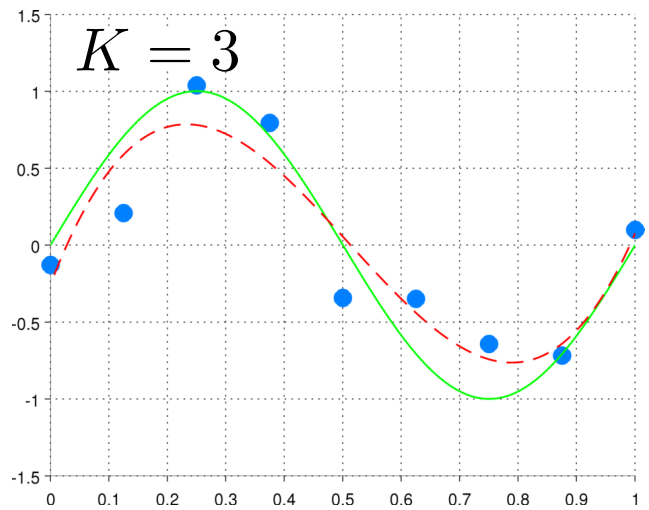
Linear regression

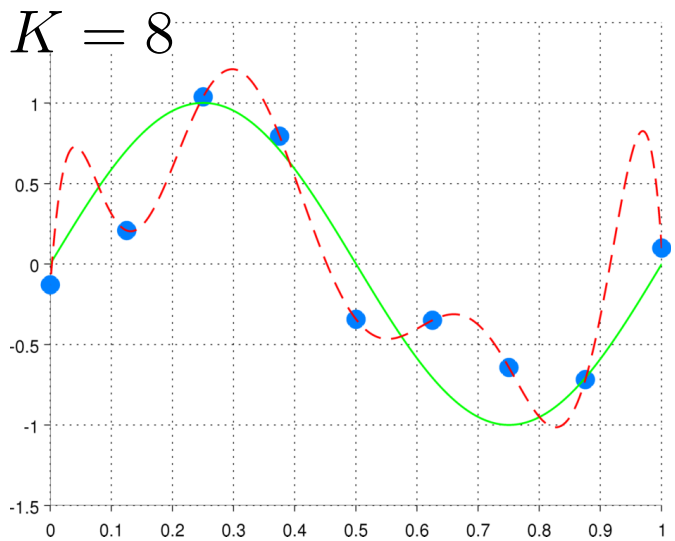
- Linear regression on non-linearly transformed inputs (polynomials)

$$f(x) = w_0 + w_1 x + \cdots + w_8 x^8$$

  - **Control complexity**: Choose a suitable value for *K*





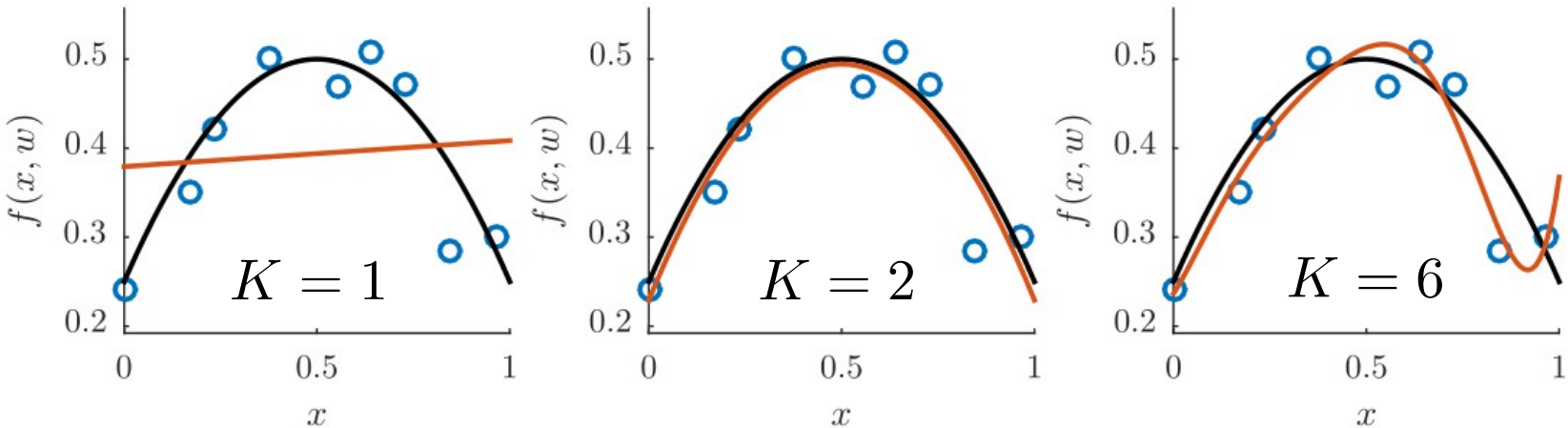


Solution:
Assess model performance correctly and select best model

Training error

- Suppose we train 3 models on a dataset of 9 observations

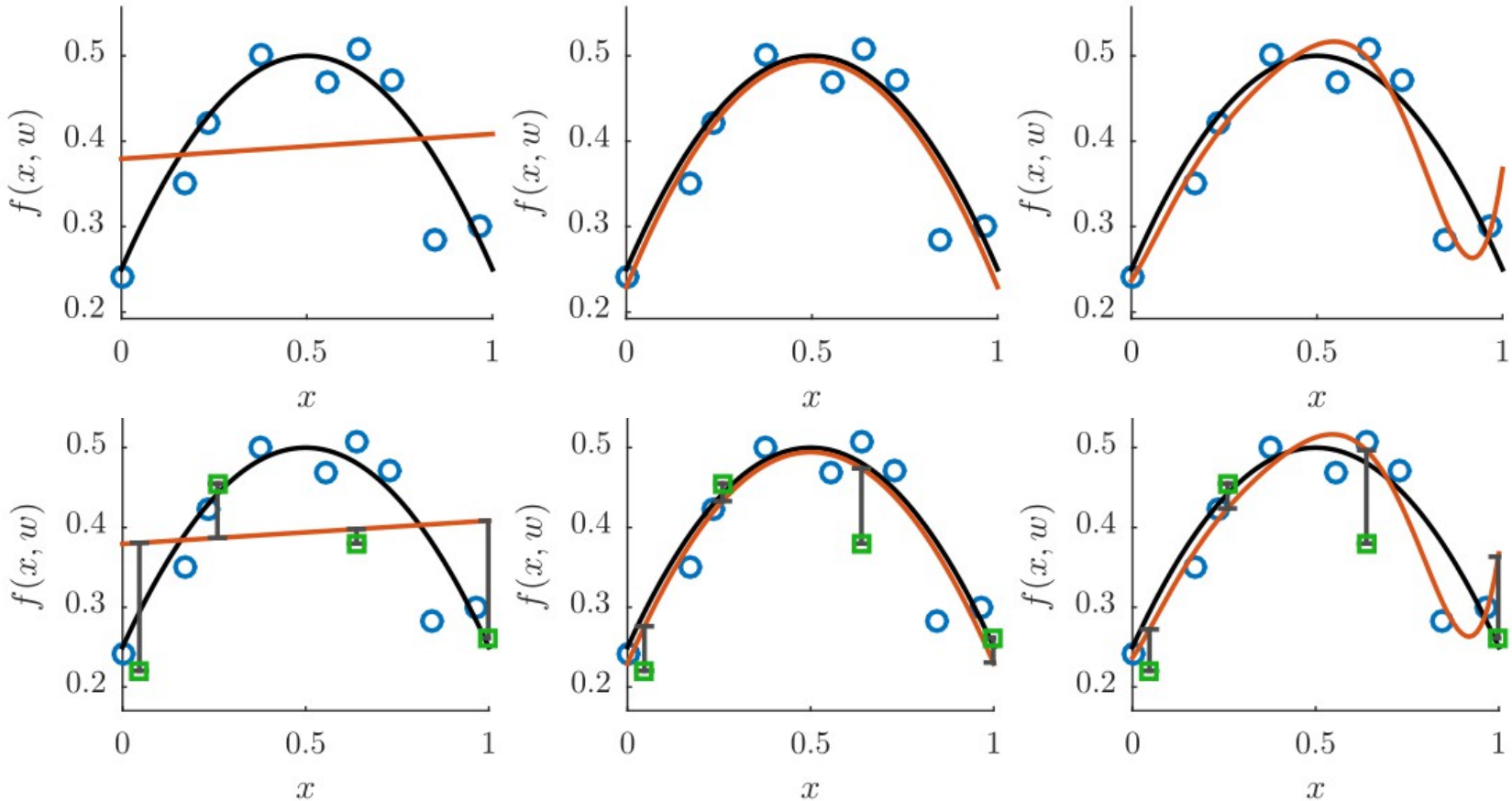
$$\mathcal{M}_1 = \{\text{1'st order polynomial}\}$$
$$\mathcal{M}_2 = \{\text{2'nd order polynomial}\}$$
$$\mathcal{M}_3 = \{\text{6'th order polynomial}\}$$



$$E^{\text{train}}_{\mathcal{M}_k} = \frac{1}{N^{\text{train}}} \sum_{i \in \mathcal{D}^{\text{train}}} (y_i - f_{\mathcal{M}_k}(x_i, \boldsymbol{w}))^2.$$

Test error error

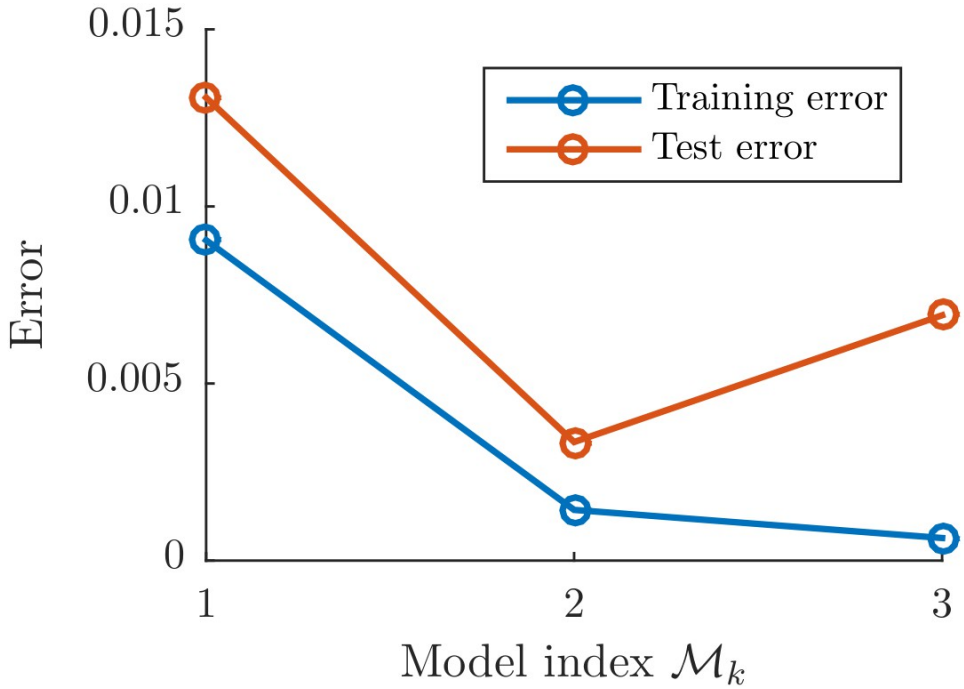
- Test error is obtaining by testing the trained models on new data



$$E_{\mathcal{M}_k}^{\text{train}} = \frac{1}{N^{\text{train}}} \sum_{i \in \mathcal{D}^{\text{train}}} (y_i - f_{\mathcal{M}_k}(x_i, \boldsymbol{w}))^2.$$

$$E_{\mathcal{M}_k}^{\text{test}} = \frac{1}{N^{\text{test}}} \sum_{i \in \mathcal{D}^{\text{test}}} (y_i - f_{\mathcal{M}_k}(x_i, \boldsymbol{w}))^2$$

Overfitting

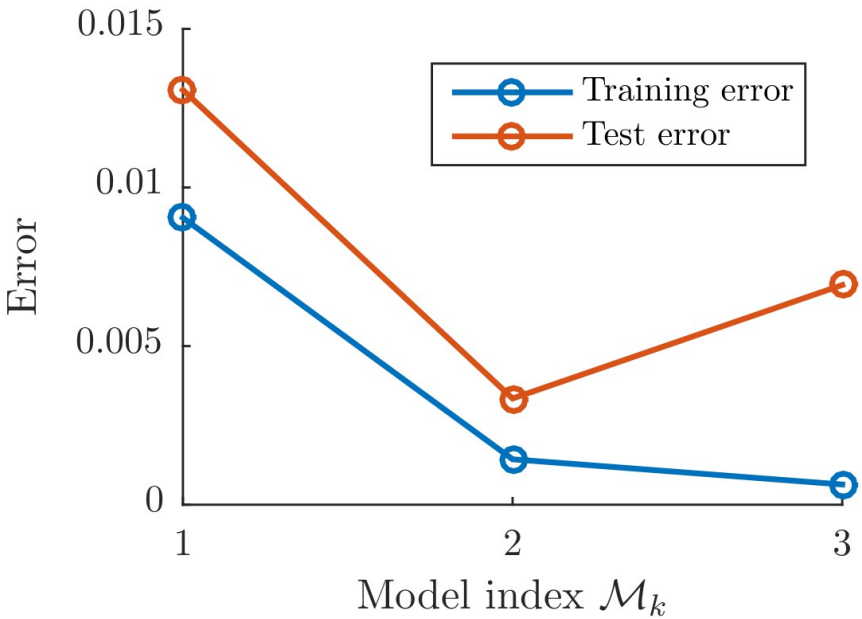


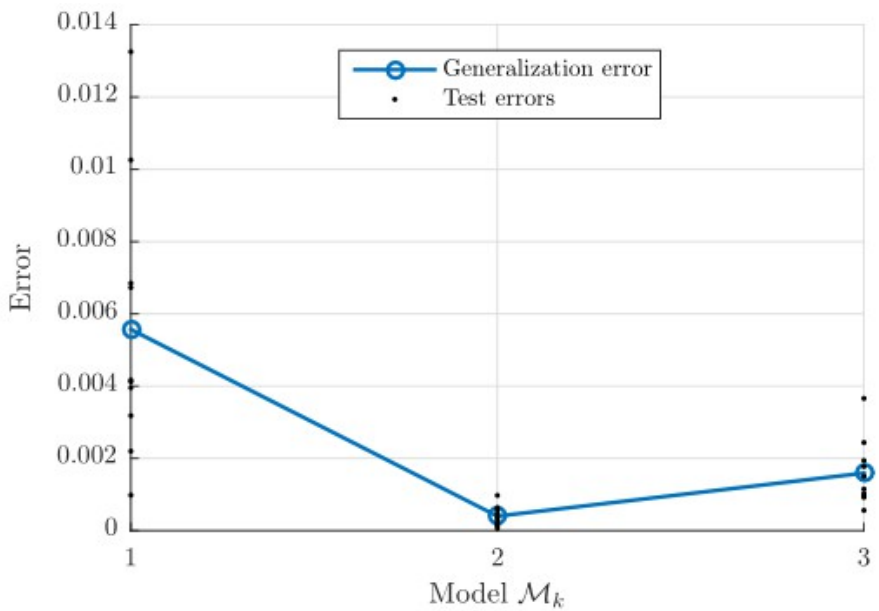
- **Overfitting** is that the training error usually decreases for overly complex models while the test error increases
- Test error is the more true error
- **Never, ever validate a model on the same data is was trained upon**

Generalization error

- The generalization error is the test error evaluated over an infinitely large test set
- The generalization error is the "true performance" of the trained model
  - Train model $\mathcal{M}$ on the available dataset $\mathcal{D}$ to get prediction rule $\boldsymbol{f}_{\mathcal{M}}$
  - Compute $E_{\mathcal{M}}^{\text{gen}} = \mathbb{E}_{(\boldsymbol{x},\boldsymbol{y})}\left[L(\boldsymbol{y}, \boldsymbol{f}_{\mathcal{M}}(\boldsymbol{x}))\right]$
- If we somehow had many test sets $\mathcal{D}_1, \ldots, \mathcal{D}_k$

$$E_{\mathcal{M}}^{\text{gen}} \approx \frac{1}{K} \sum_{k=1}^{K} E_{\mathcal{M},\mathcal{D}_k}^{\text{test}}$$





Basic cross-validation

- **Purpose: Estimate the generalization error**

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- 3 variants:
  - **Holdout:** Partitions dataset in two (training, test), approximate the generalization error based on the generated test set

$$\mathcal{D} = \mathcal{D}^{\text{train}} \bigcup \mathcal{D}^{\text{test}}$$

$$E_{\mathcal{M}}^{\text{gen}} \approx E_{\mathcal{M}}^{\text{test}}$$

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  - **K-fold:** Partitions dataset in K parts. Each part is a test set and the other K-1 training sets

$$\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_K$$
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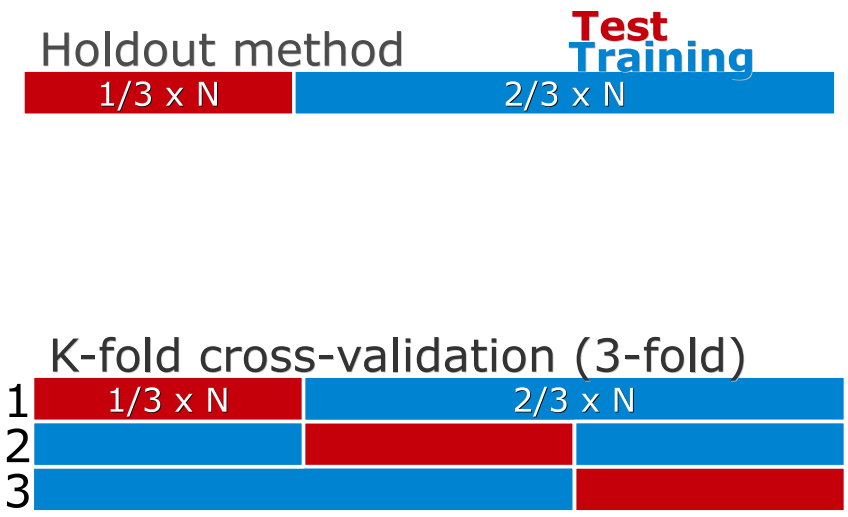

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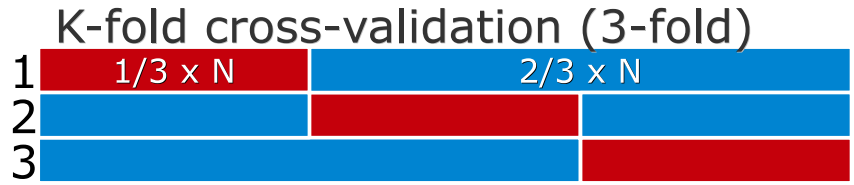
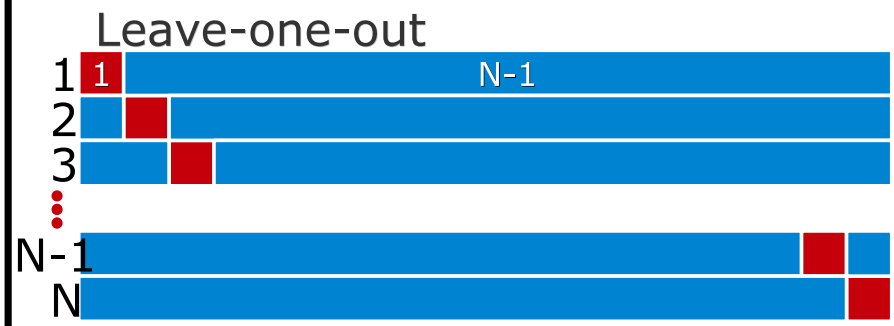
  - **Leave-one-out:** Partitions dataset into N parts. Let each observation be a test set and the other N-1 training sets (K-fold with K=N)

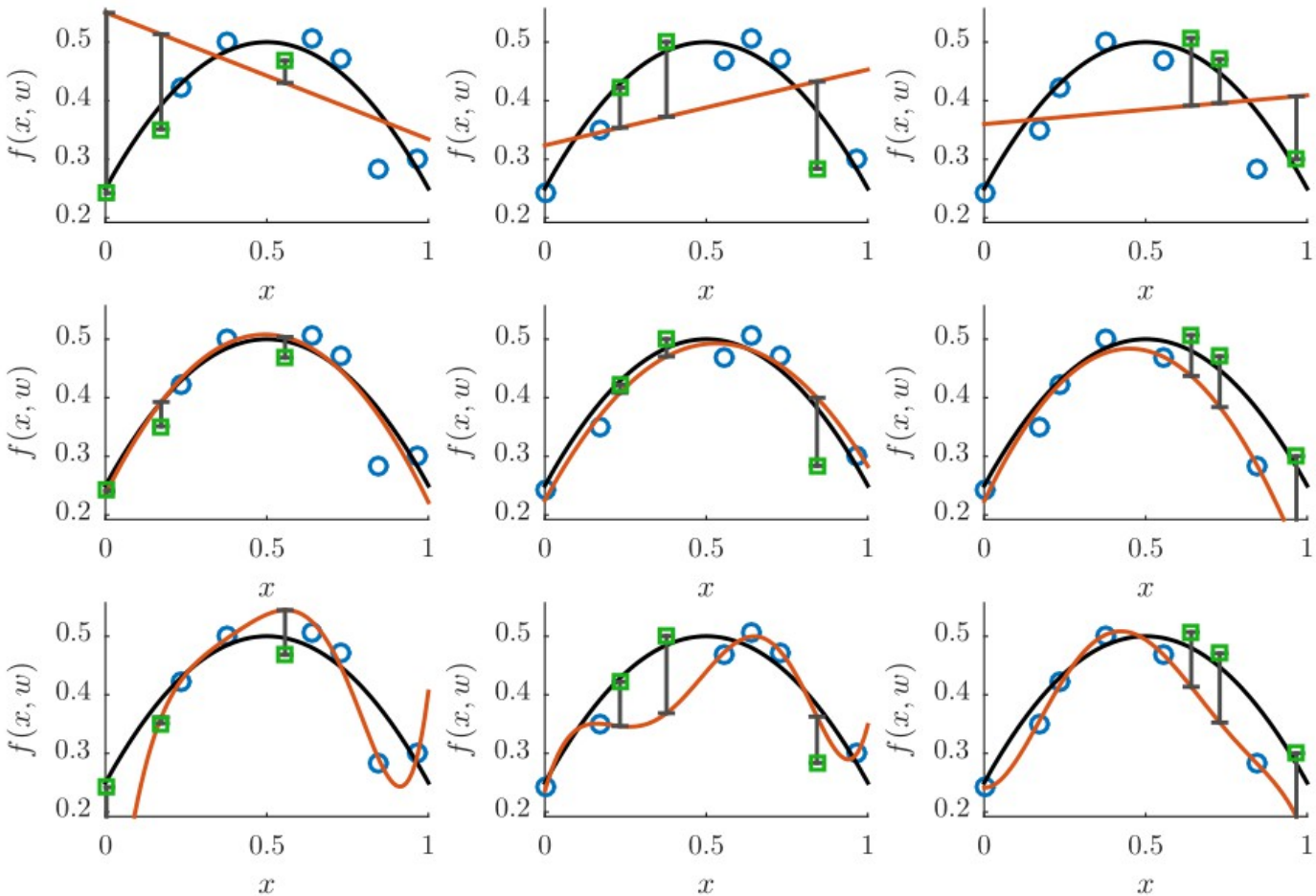
$$\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_N$$
$$E^{\text{gen}}_{\mathcal{M}} \approx \frac{1}{N} \sum_{k=1}^{N} E^{\text{test}}_{\mathcal{M},k}$$





Cross-validation (1-layer)

- **K=3 fold cross-validation for the three Linear-regression models**
  Vertically: The three models
  Horizontally: The three cross-validation folds



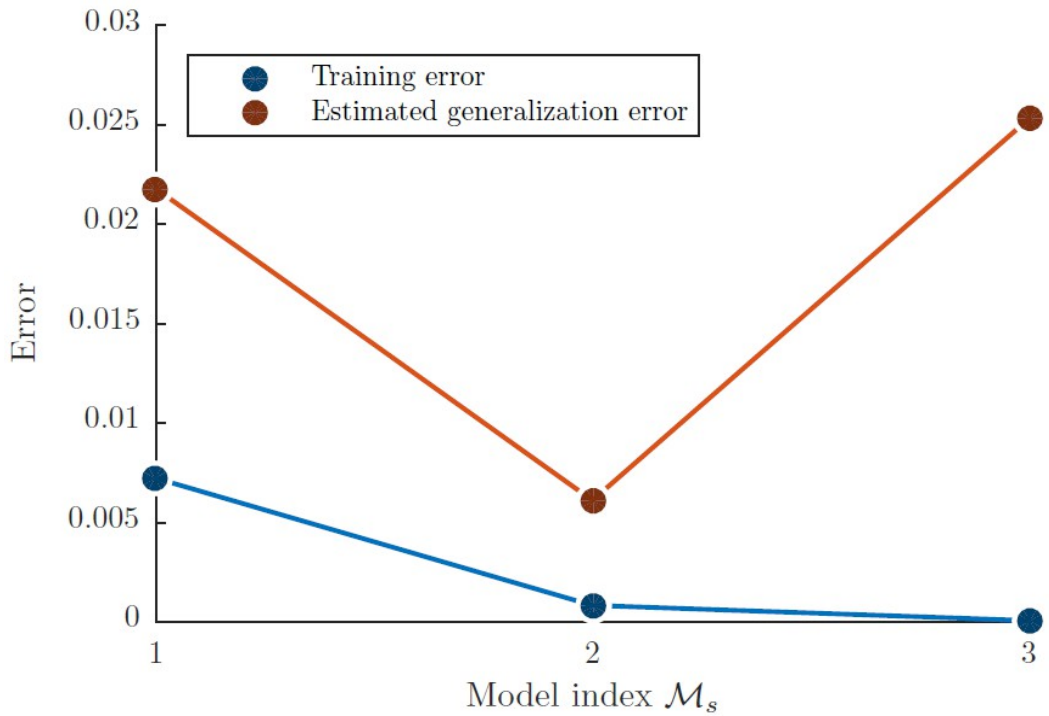
Cross-validation for model selection (1-layer)

- **Purpose: Select the best of S models**
- **The idea:**

- For each model, estimate the cross-validation error $\hat{E}^{\text{gen}}_{\mathcal{M}_1}, \ldots, \hat{E}^{\text{gen}}_{\mathcal{M}_S}$ using basic cross-validation.

- Select the optimal model $\mathcal{M}_{s^*}$ as that with the lowest error:

$$s^* = \arg\min_s \hat{E}^{\text{gen}}_{\mathcal{M}_s}$$



Cross-validation (1-layer)

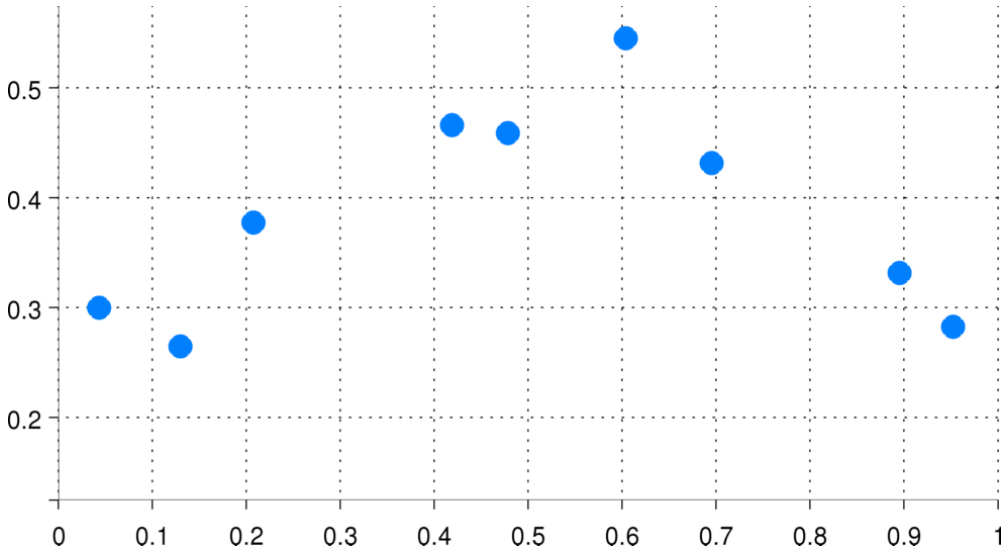
- **K-fold cross-validation for model selection, the algorithm**

Algorithm 4: K-fold cross-validation for model selection

Require: K, the number of folds in the cross-validation loop
Require: $\mathcal{M}_1, \ldots, \mathcal{M}_S$. The S different models to select between
Ensure: $\mathcal{M}_{s^*}$ the optimal model suggested by cross-validation
  for $k = 1, \ldots, K$ splits **do**
    Let $\mathcal{D}_k^{\text{train}}$, $\mathcal{D}_k^{\text{test}}$ the k'th split of $\mathcal{D}$
    for $s = 1, \ldots, S$ models **do**
      Train model $\mathcal{M}_s$ on the data $\mathcal{D}_k^{\text{train}}$
      Let $E_{\mathcal{M}_s,k}^{\text{test}}$ be the *test error* of the model $\mathcal{M}_s$ when it is *tested* on $\mathcal{D}_k^{\text{test}}$
    end for
  end for
  For each s compute: $\hat{E}_{\mathcal{M}_s}^{\text{gen}} = \sum_{k=1}^{K} \frac{N_k^{\text{test}}}{N} E_{\mathcal{M}_s,k}^{\text{test}}$
  Select the optimal model: $s^* = \arg\min_s \hat{E}_{\mathcal{M}_s}^{\text{gen}}$
  $\mathcal{M}_{s^*}$ is now the optimal model suggested by cross-validation

Holdout method

- Randomly choose a subset of data points to be in a **test set**
  - For example choose 1/3 of the points
- The rest is the **training set**



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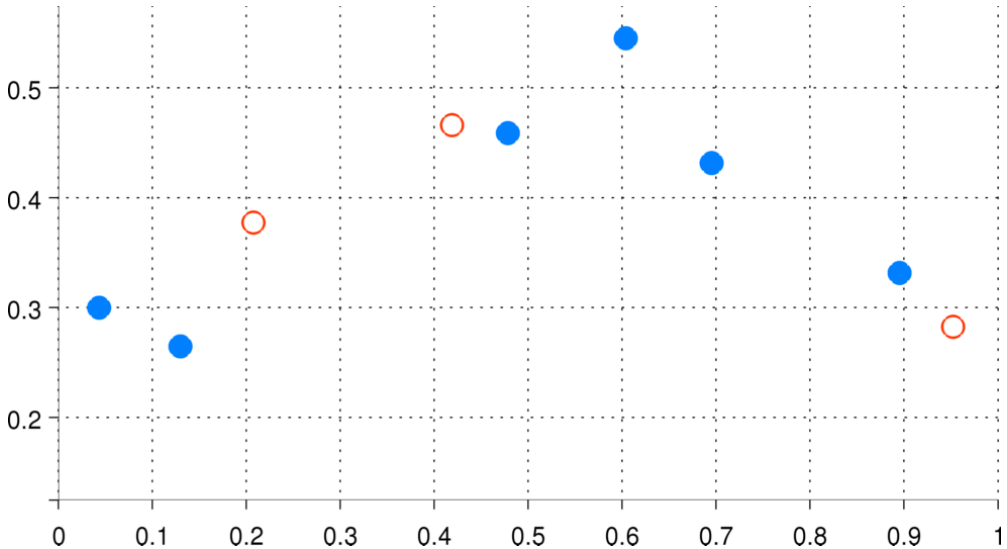
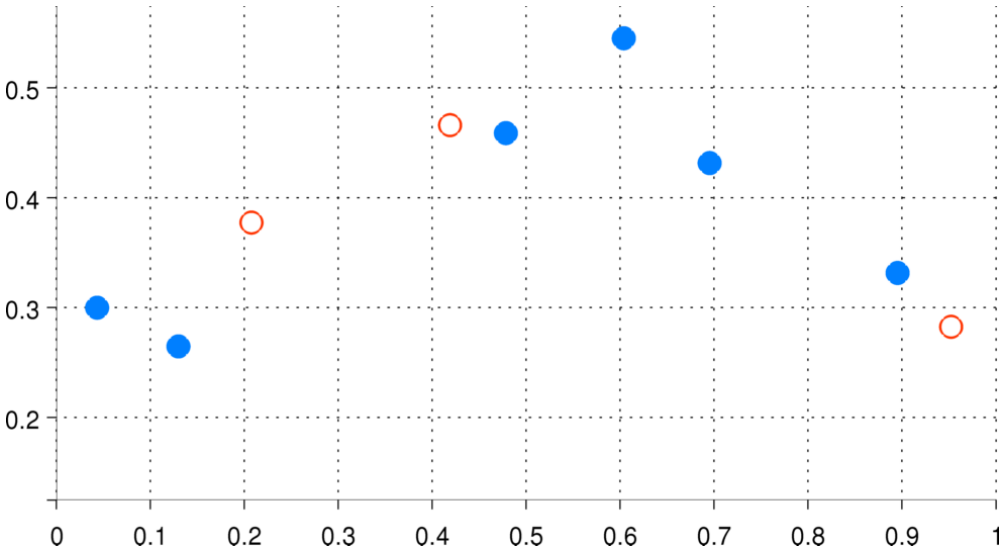
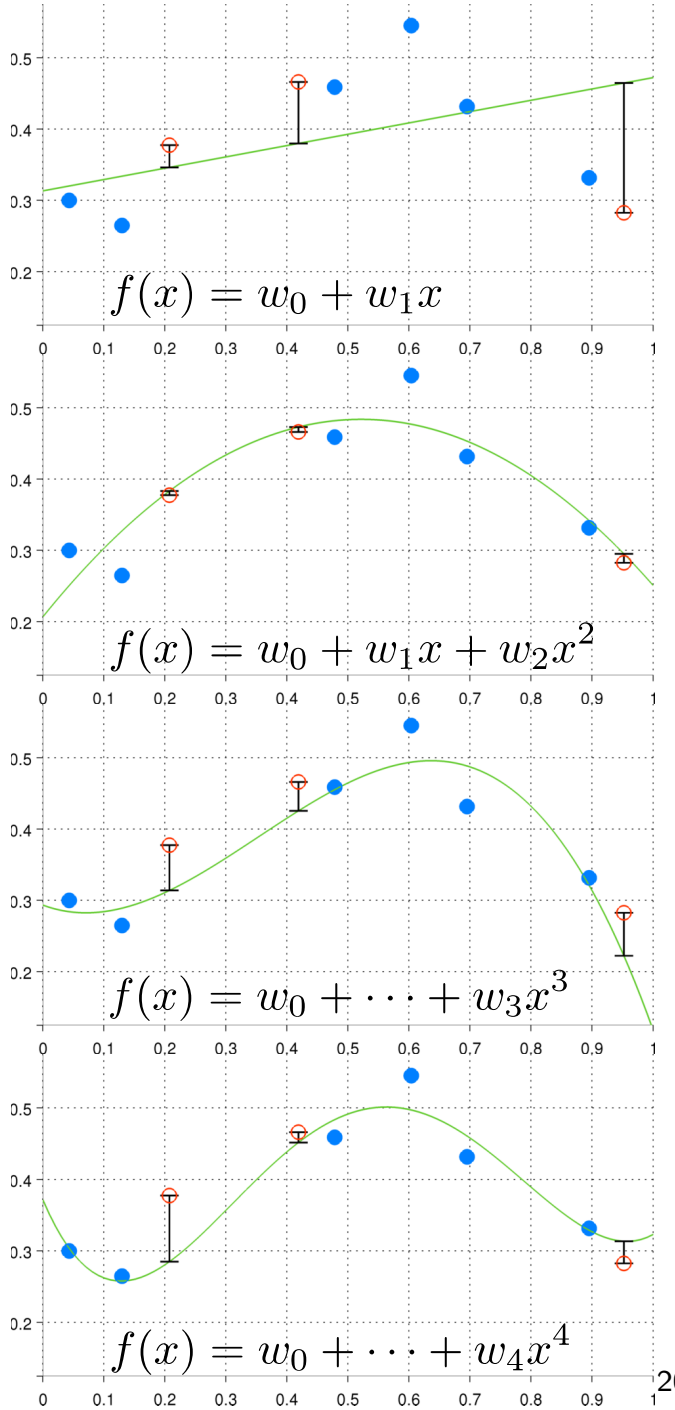


Holdout method

- Using the **training set**
  - Train the model for different complexities
- Using the **test set**
  - Compute the test error
- Choose the model with lowest **test error**





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  - Compute the test error
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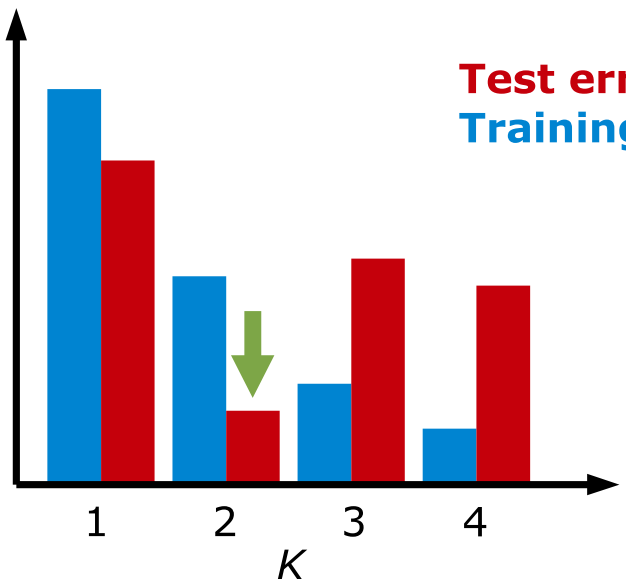
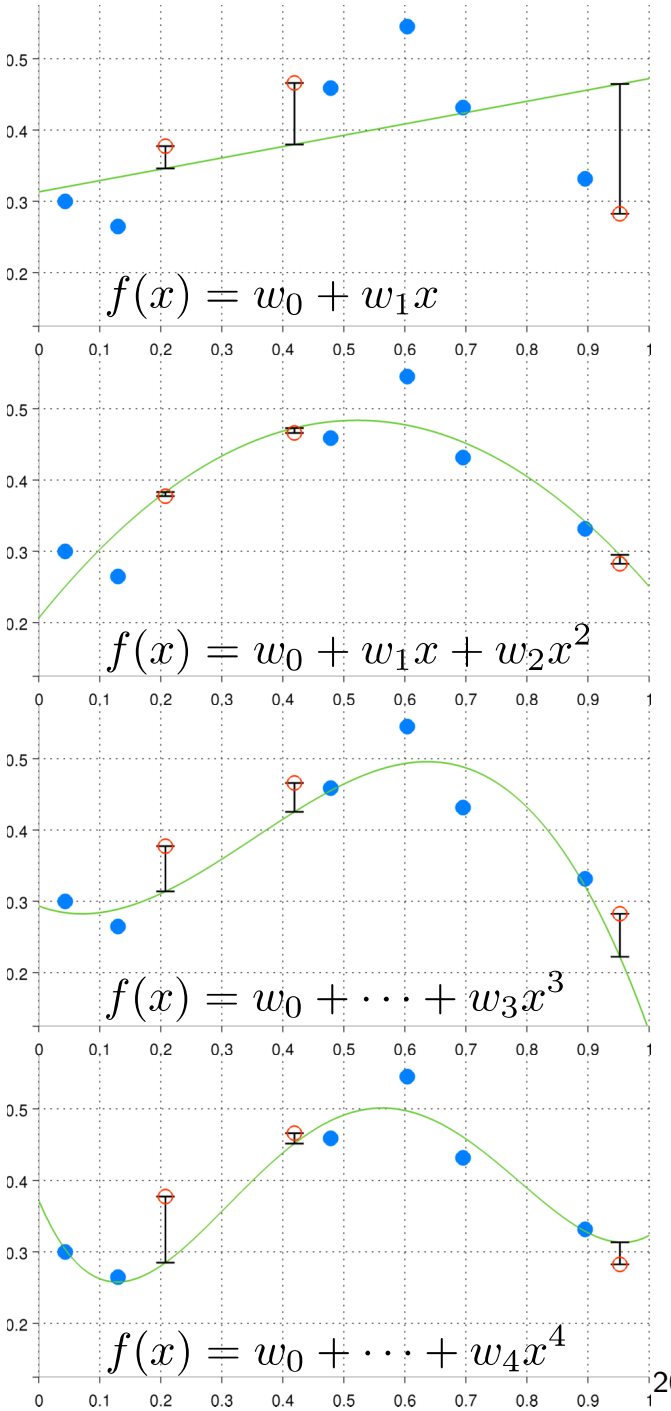
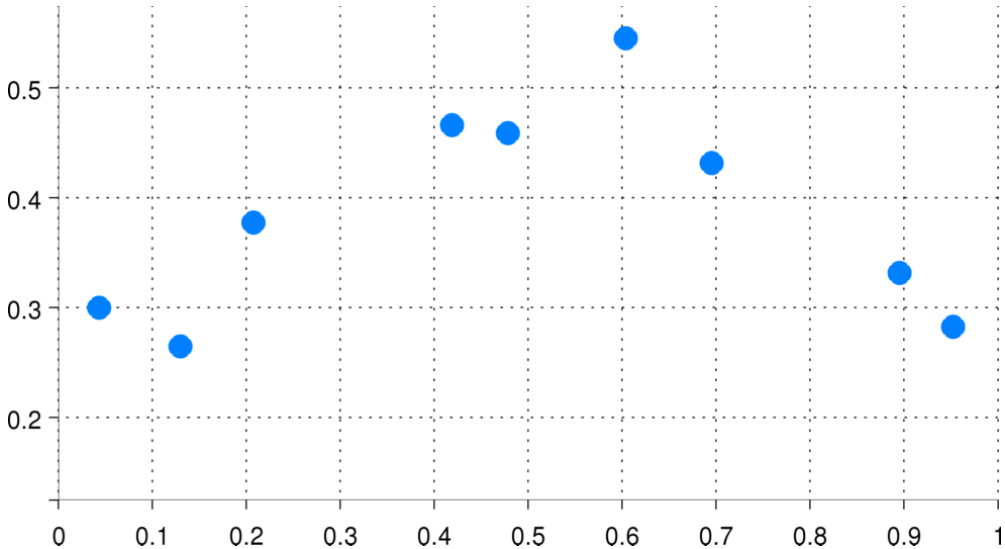




Leave-one-out

- Choose the first data point as a **test set**
- The rest is the **training set**



Leave-one-out

- Choose the first data point as a **test set**
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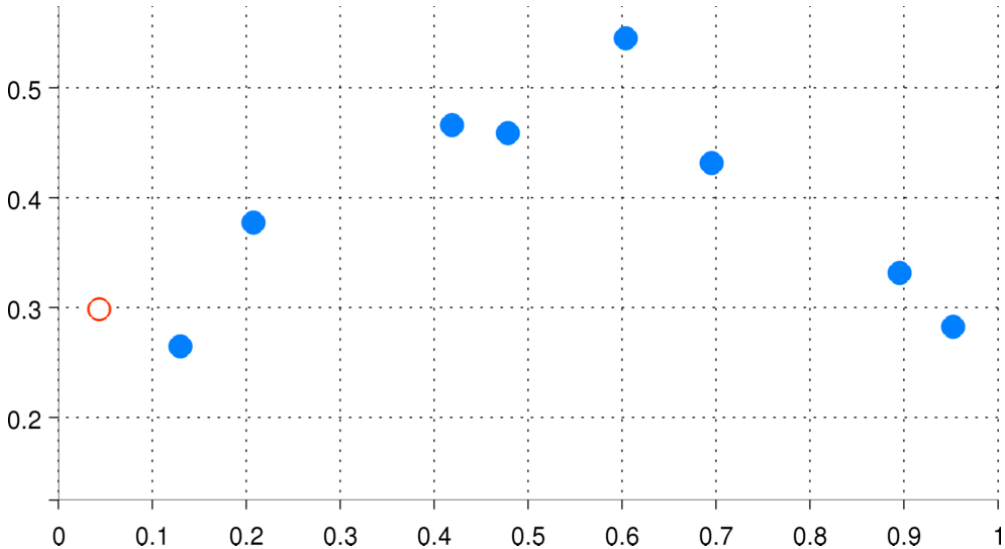
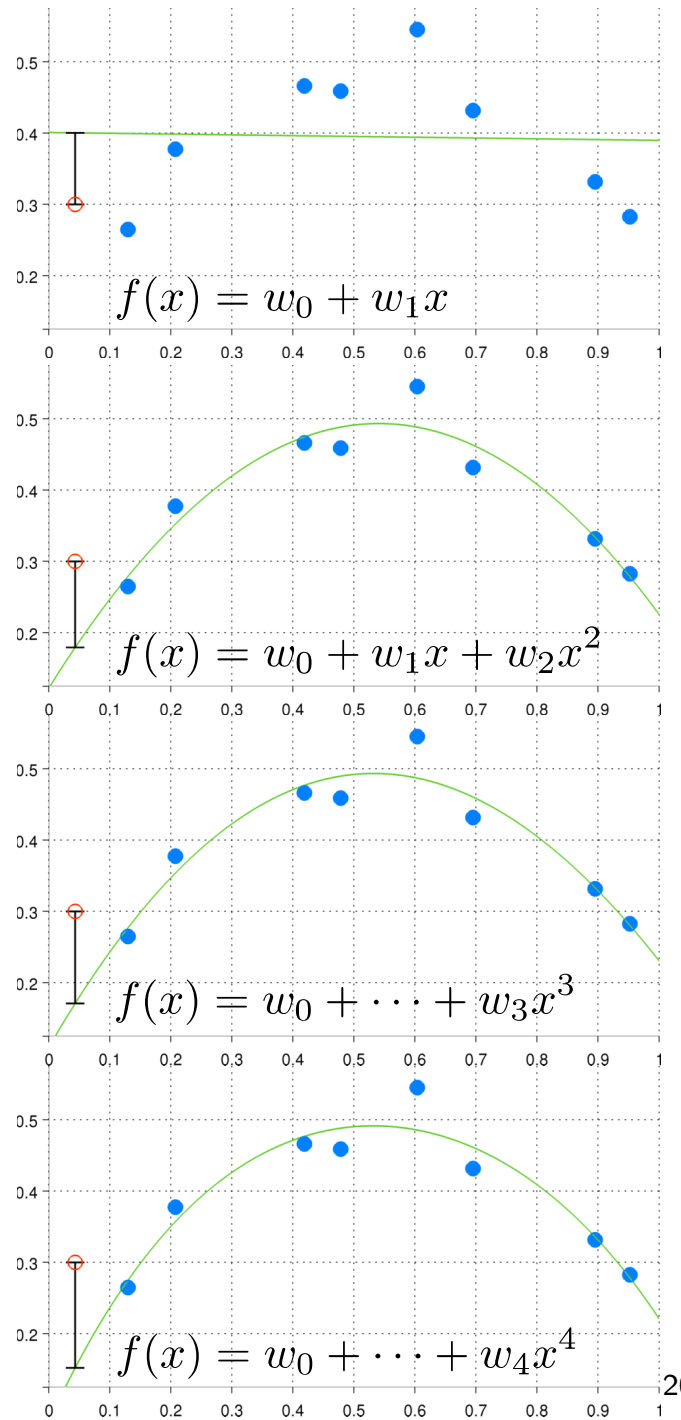
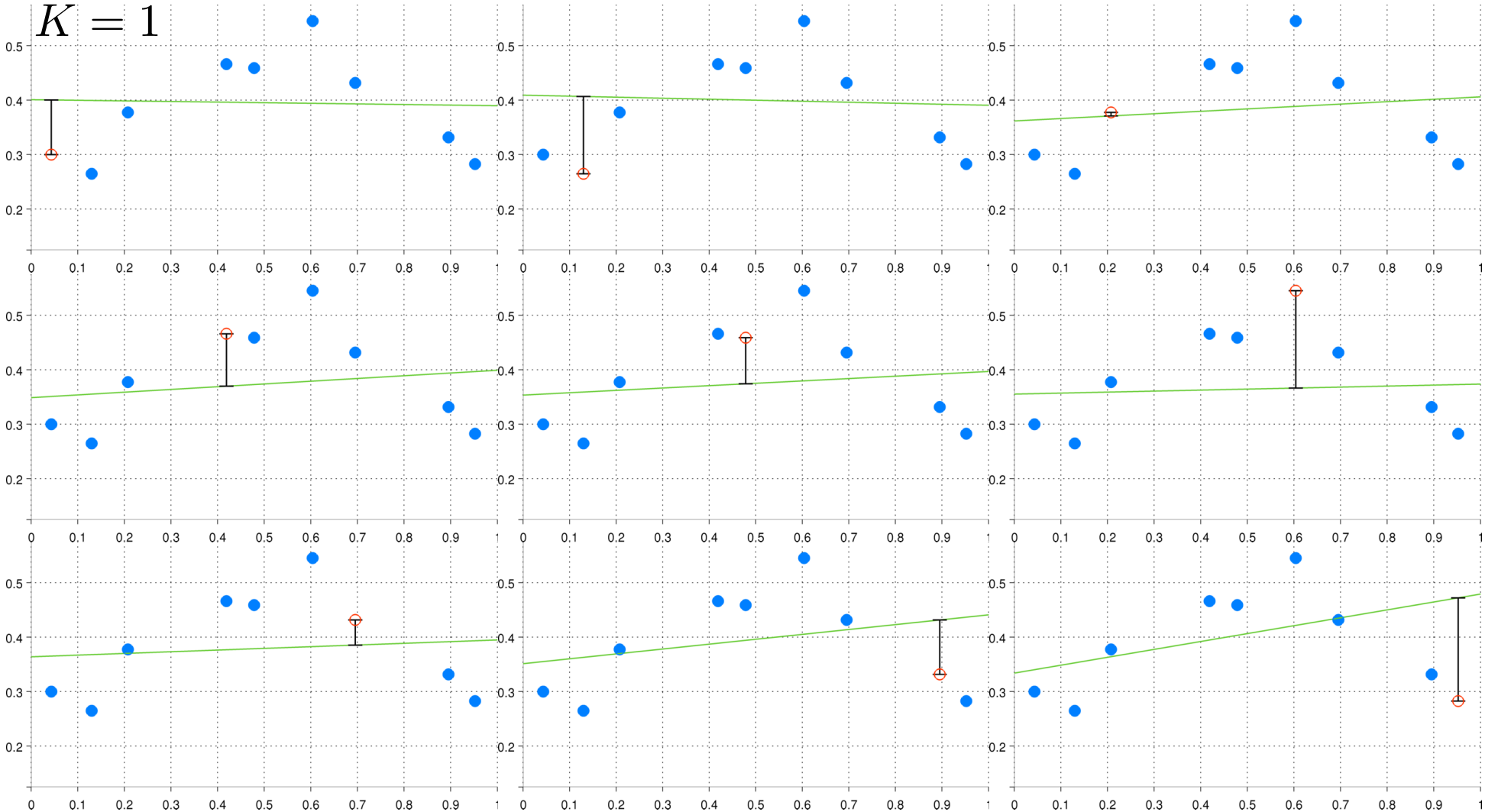


Leave-one-out

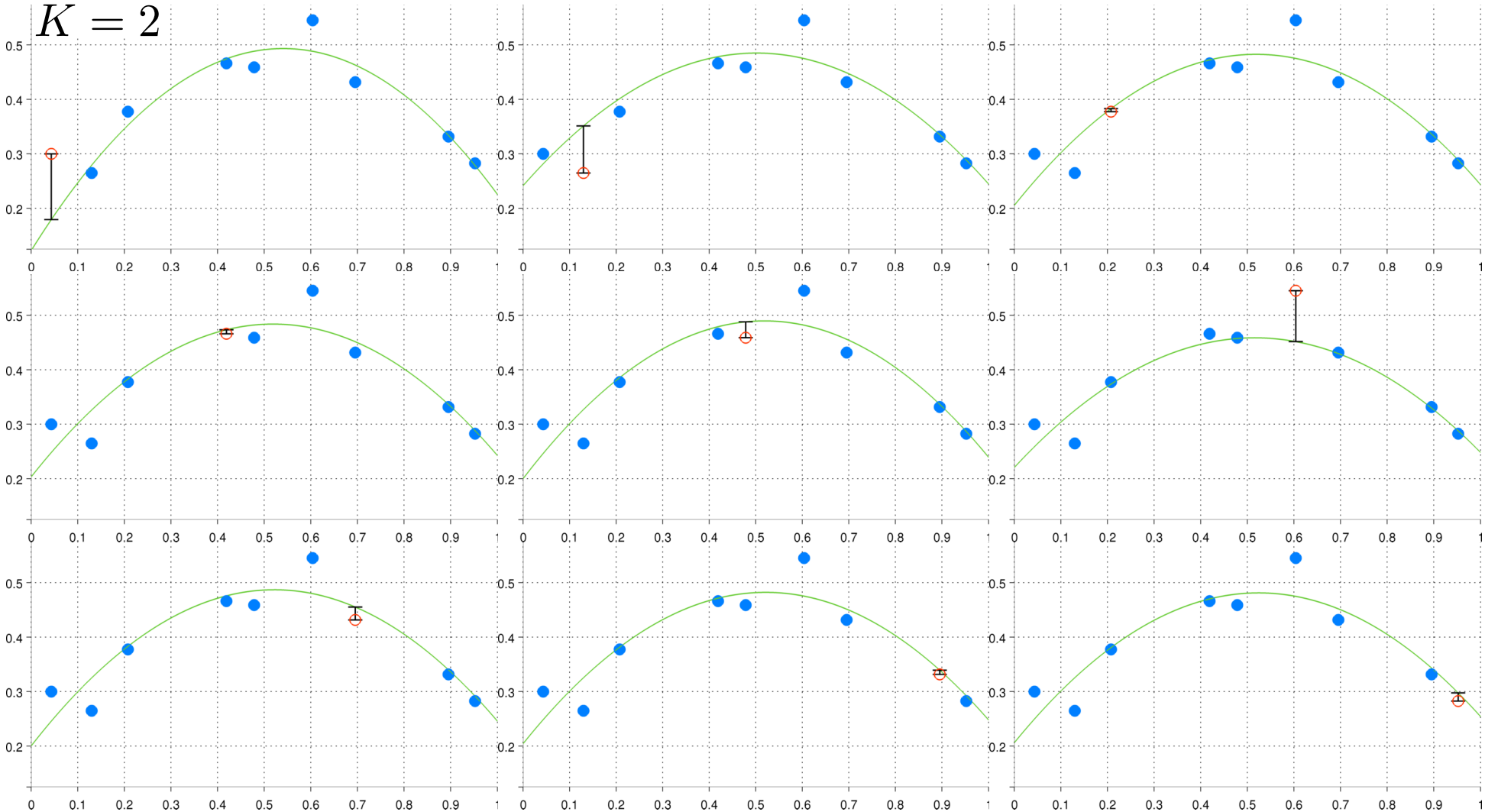
- Using the **training set**
  - Train the model for different complexities
- Using the **test set**
  - Compute the test error
- **Repeat for all data points**
  - All data points get to be test set
  - Compute **average test error**



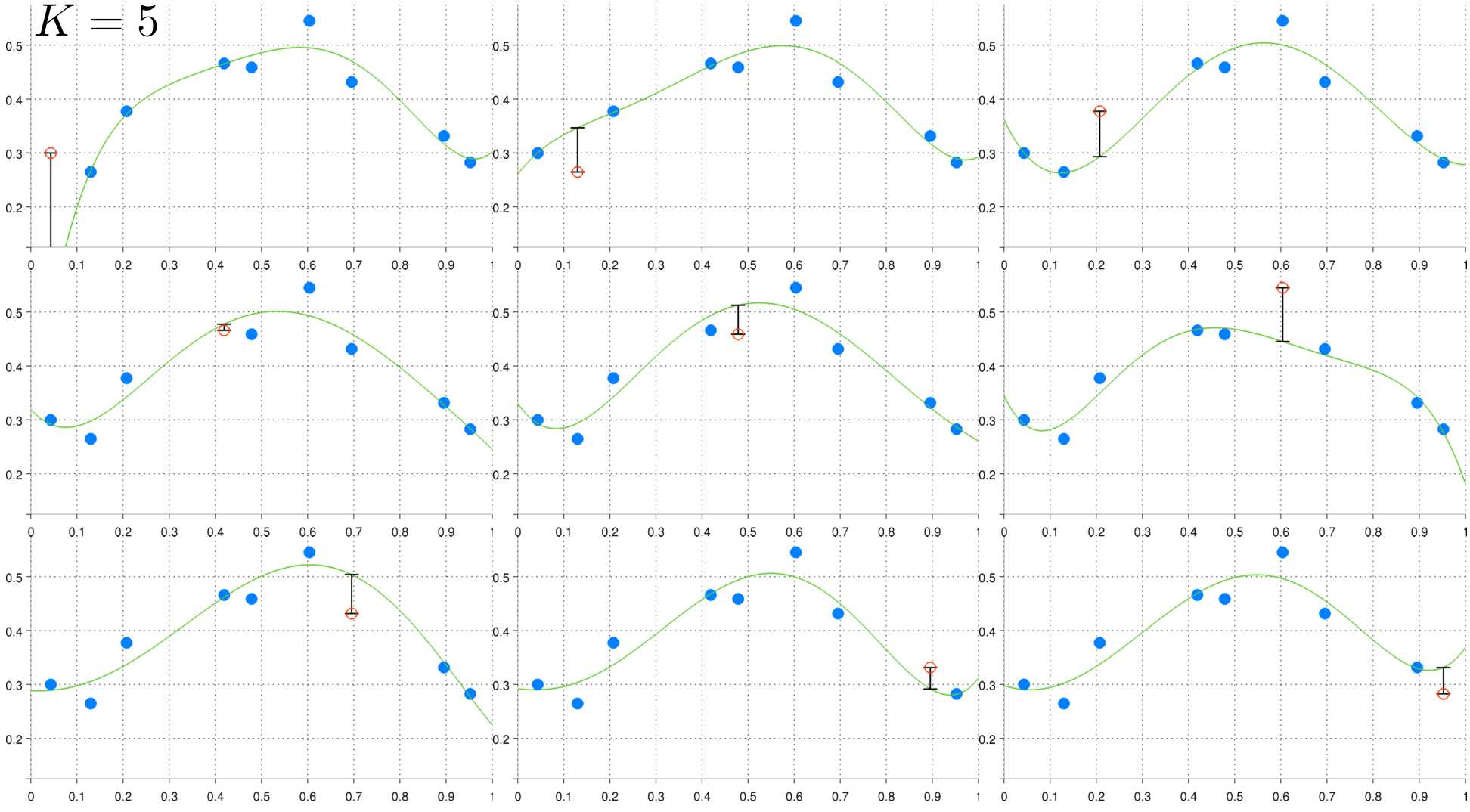
Leave-one-out



Leave-one-out



Leave-one-out cross-validation

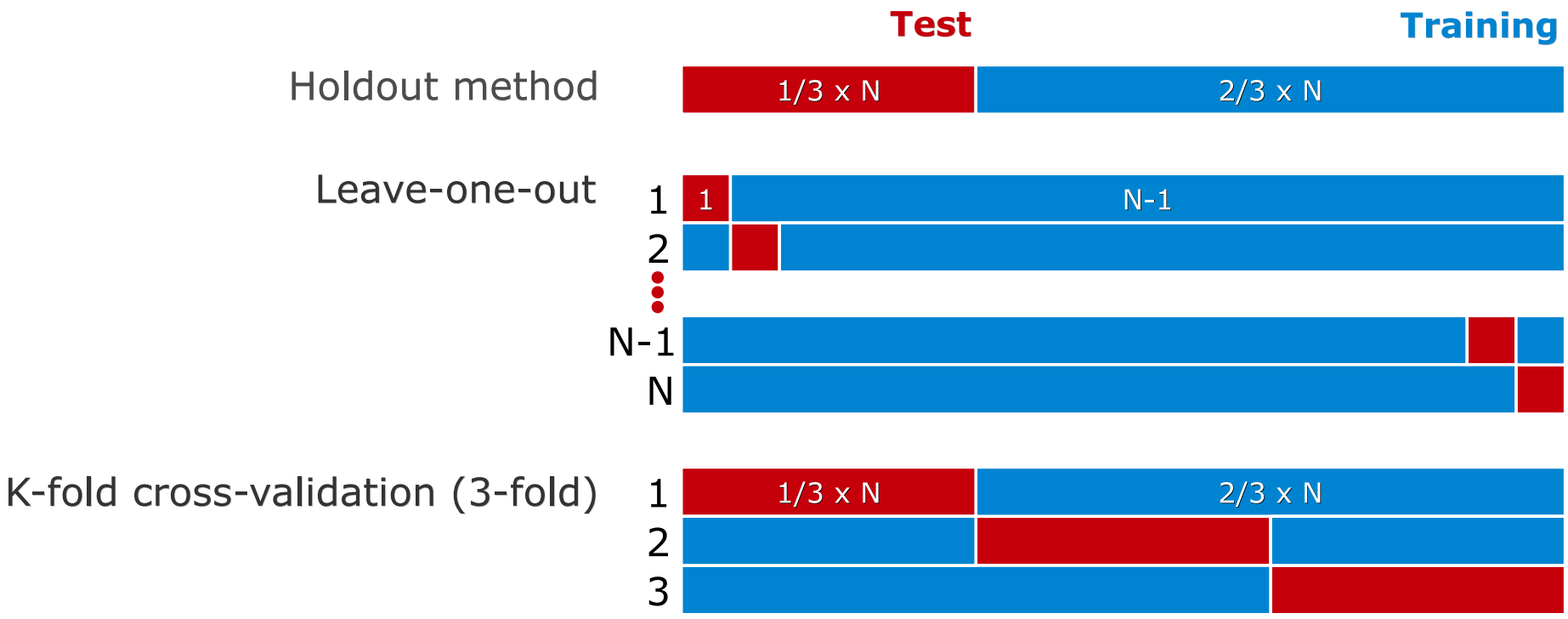


Leave-one-out

- Using the **training set**
  - Train the model for different complexities
- Using the **test set**
  - Compute the test error
- **Repeat for all data points**
  - All data points get to be test set
  - Compute **average test error**

So which method should I choose?

- Holdout is computationally least intensive, but not very data efficient
- Leave-one-out is very computationally intensive, and the estimates are highly correlated
- Recommendation: K-fold for $K = 5, 10$ or holdout if problem very large.



Quiz 1, Cross validation (Spring 2012)

Feature(s)	Training MSE	Test MSE
A	2.0	2.2
B	1.8	1.9
C	1.6	1.7
D	1.9	2.1
A and B	1.7	2.0
A and C	1.3	1.8
A and D	1.4	1.5
B and C	1.5	1.6
B and D	1.7	1.8
C and D	1.5	2.0
A and B and C	1.2	2.1
A and B and D	1.1	2.0
A and C and D	1.0	2.3
B and C and D	1.2	2.5
A and B and C and D	0.9	2.8

Question 1. Consider a neural network regression problem with four attributes denoted A, B, C and D. A neural network with two hidden units is trained using different combinations of the attributes. The neural network is trained on 50% of the data and tested on the remaining 50% of the data using the hold-out method. In the table is given the training and test performance of the neural network for the different combinations of attributes. Which of the following statements is *incorrect*

A. Hold-out 50% of the data is more computationally efficient than 5 fold cross-validation.

B. Leave one-out cross-validation gives a poor estimate of the generalization error as only one observation is part of the test set at a time.

C. The size of the training set in 10 fold cross-validation is larger than the size of the training set in 5 fold cross-validation.

D. Not all observations are used for testing using the hold-out method.

E. Don't know.

In the hold-out method a given percentage, here 50% are removed for testing and the data trained on the remaining 100%-50%=50% of the data. This is more computationally efficient than 5 fold cross-validation as we only need to estimate one model for each combination of attributes. Leave-one-out cross-validation would however give a more precise estimate of the generalization error as all observations are used in the test set once while keeping as many observations as possible for training, thus, second answer is incorrect. The size of the training set is larger in 10 fold cross-validation as 10 % of data is removed for testing whereas 20% of data is removed for testing for each fold of 5 fold cross-validation.

Forward selection

$$f(x) = w_0$$
$$f(x) = w_0 + w_1 x_1 + w_2 x_{27} + w_3 x_{88}$$
$$f(x) = w_0 + w_1 x_{19} + w_2 x_{76}$$
$$f(x) = w_0 + w_1 x_{19} + w_2 x_{76} + w_3 x_{88}$$
$$f(x) = w_0 + w_1 x_1 + w_2 x_{27} + w_3 x_{19}$$
$$f(x) = w_0 + w_1 x_{27} + w_2 x_{88}$$

- Suppose we want to do linear regression
- As usual, we have M attributes

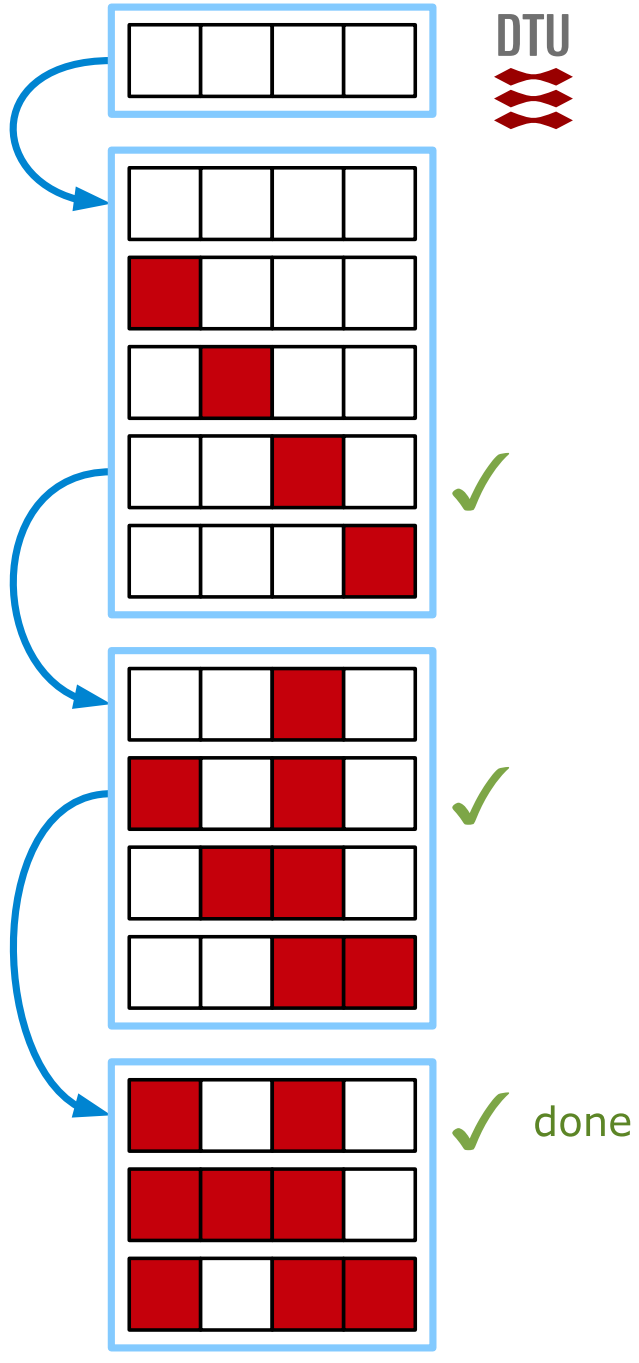
$$x_1, x_2, \ldots, x_M$$

- We can control model complexity by using a subset of attributes
  - Large subset: Complex model; hard to interpret
  - Small subset: Too simple model
- In general, we can construct 2^M models; often far too many
- Sequential feature selection allow us to efficiently search the model space

Sequential feature selection

Forward selection

- Start with no features
- Compute **cross-validation error** for
  - Current feature subset
  - All subsets equal to the current + one added feature
- Choose best subset
- Repeat until no further improvement



Sequential feature selection

Forward selection

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  - All subsets equal to the current + one added feature
- Choose best subset
- Repeat until no further improvement

$f(x) = w_0$

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$f(x) = w_0 + w_1 x_1$

$f(x) = w_0 + w_1 x_2$

$f(x) = w_0 + w_1 x_3$

$f(x) = w_0 + w_1 x_4$

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$f(x) = w_0 + w_1 x_3 + w_2 x_4$

$f(x) = w_0 + w_1 x_3 + w_2 x_1$

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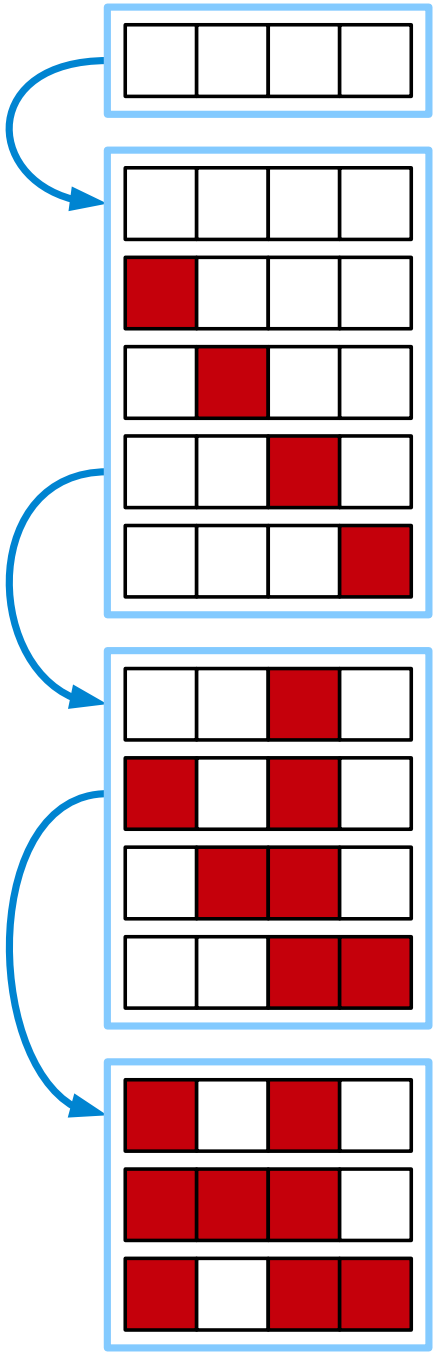
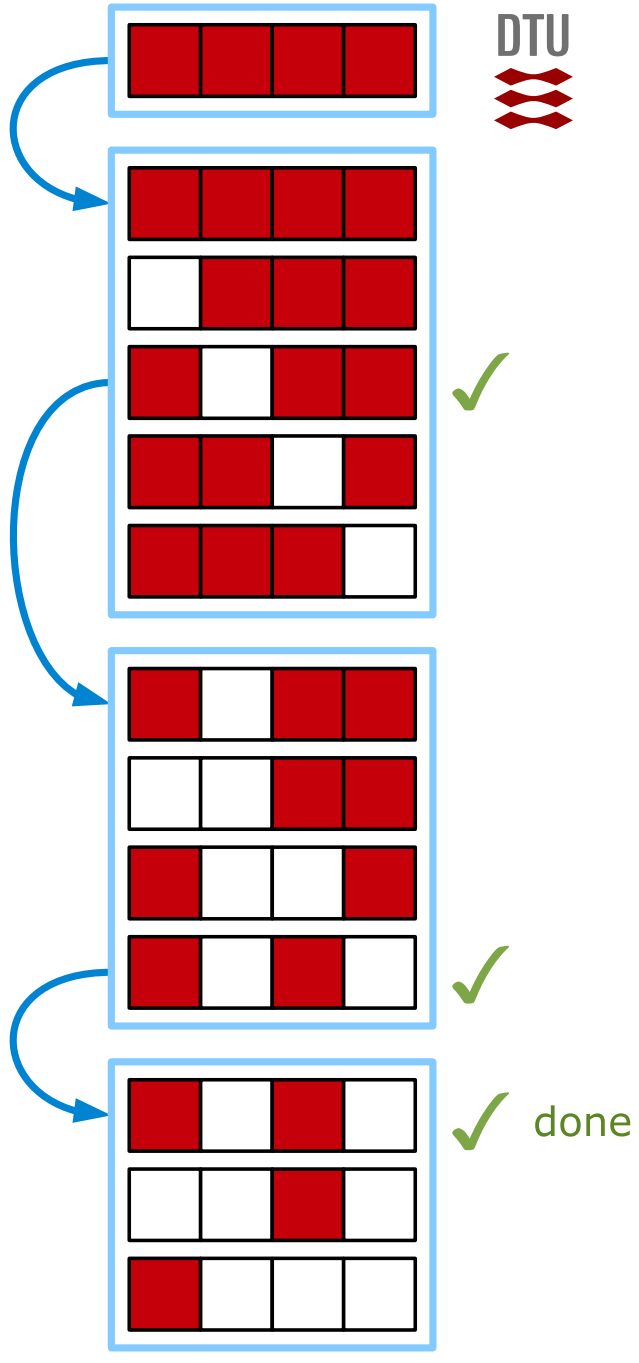
$f(x) = w_0 + w_1 x_3 + w_2 x_1 + w_3 x_4$



Sequential feature selection

Backward selection

- Start with all features
- Compute **cross-validation error** for
  - Current feature subset
  - All subsets equal to the current - one removed feature
- Choose best subset
- Repeat until no further improvement



Quiz 2, Forward selection (Spring 2012)

Feature(s)	Training MSE	Test MSE
A	2.0	2.2
B	1.8	1.9
C	1.6	1.7
D	1.9	2.1
A and B	1.7	2.0
A and C	1.3	1.8
A and D	1.4	1.5
B and C	1.5	1.6
B and D	1.7	1.8
C and D	1.5	2.0
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A and C and D	1.0	2.3
B and C and D	1.2	2.5
A and B and C and D	0.9	2.8

Consider a neural network regression problem with four attributes denoted A, B, C and D where a neural network with two hidden units is trained using different combinations of the attributes. The table gives the training and test performance of the neural network for different combinations of attributes. Which of the following statements is *correct*?

A. Using a forward selection strategy feature B and C would be selected as the optimal model.

B. Using a forward selection strategy features A and D would be selected as the optimal model.

C. Using a forward selection strategy features A and C and D would be selected as the optimal model.

D. Using a forward selection strategy features A and B and C would be selected as the optimal model.

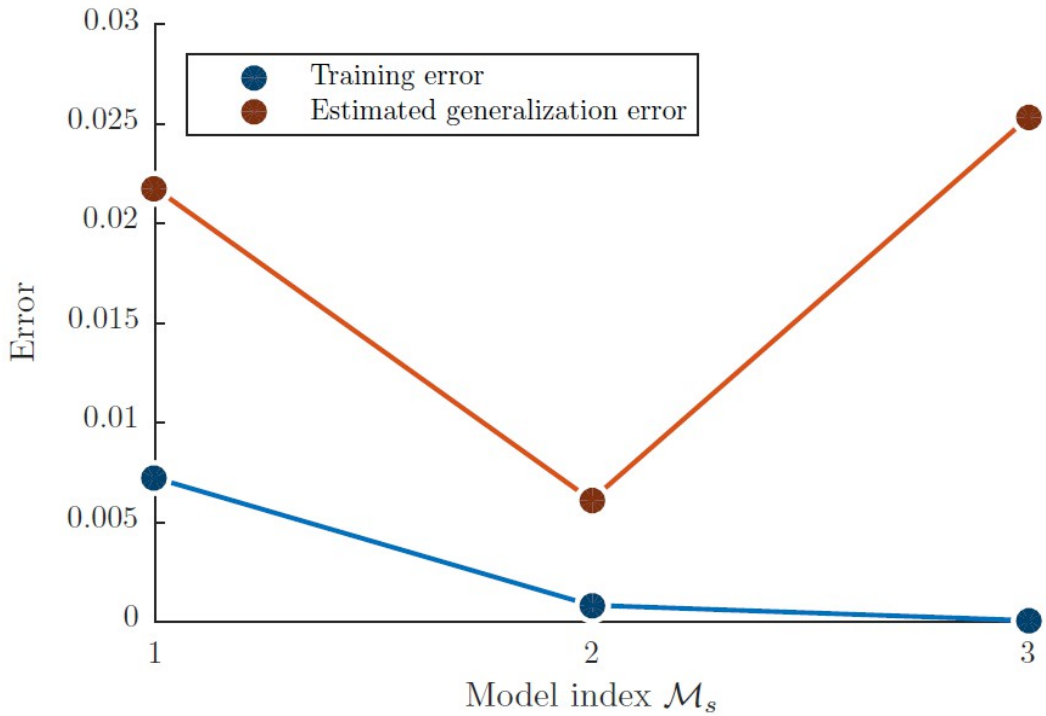
E. Don't know.

Using forward selection we would like to minimize the test error. Thus, the Forward selection would first select C and subsequently B terminating at the solution B and C. Selecting additional attributes will not improve on the test error.

A problem with 1 level cross-validation?

- For each model, estimate the cross-validation error $\hat{E}^{\text{gen}}_{\mathcal{M}_1}, \ldots, \hat{E}^{\text{gen}}_{\mathcal{M}_S}$ using basic cross-validation.
- Select the optimal model $\mathcal{M}_{s^*}$ as that with the lowest error:

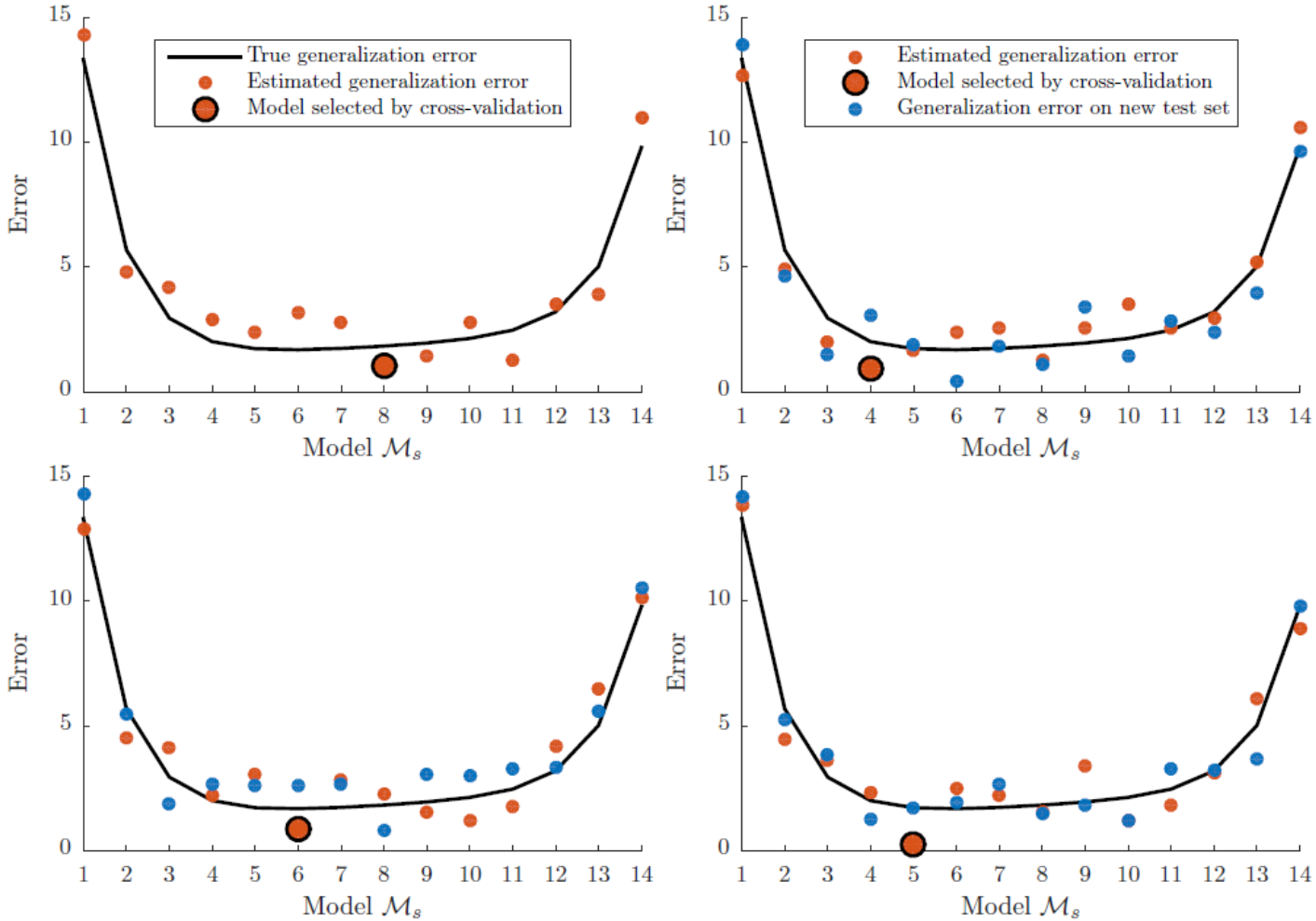
$$s^* = \arg\min_s \hat{E}^{\text{gen}}_{\mathcal{M}_s}$$



- **Is the generalization error the selected model (k=2) about 0.007?**

A problem with 1 level cross-validation?

- **Same as before, just with more models. Is the error of the red dot a fair estimate of the generalization error?**



Two-layer cross-validation

- **Purpose: Select optimal model and estimate generalization error of optimal model**

Two-layer cross-validation

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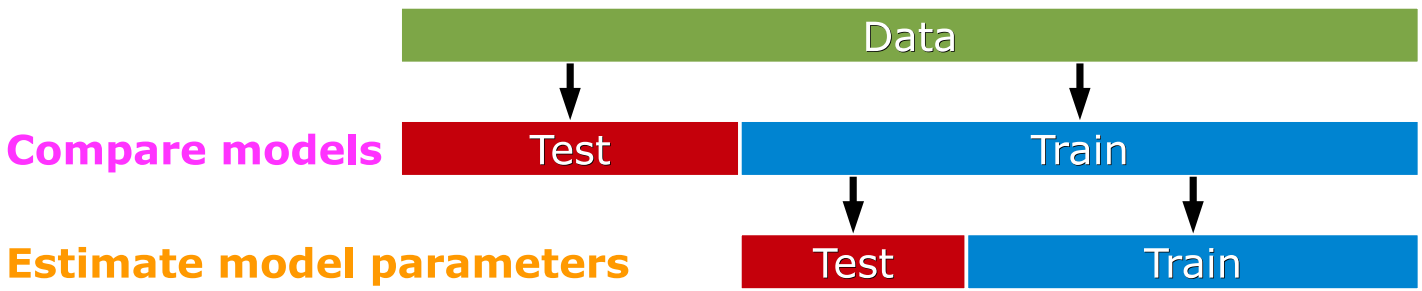
- **How?**
  - Recall ***"one layer cross-validation for model selection"***
  - This method returns a model (the best model)
  - We can consider **"one-layer cross-validation for model selection"** as a single model

Two-layer cross-validation

- **Purpose: Select optimal model and estimate generalization error of optimal model**
- **How?**
  - Recall ***"one layer cross-validation for model selection"***
  - This method returns a model (the best model)
  - We can consider **"one-layer cross-validation for model selection"** as a single model
- **Recall:**
  - **"Basic cross-validation for performance evaluation"** estimates the generalization error of a model

Two-layer cross-validation

- **Purpose: Select optimal model and estimate generalization error of optimal model**
- **How?**
  - Recall ***"one layer cross-validation for model selection"***
  - This method returns a model (the best model)
  - We can consider **"one-layer cross-validation for model selection"** as a single model
- **Recall:**
  - **"Basic cross-validation for performance evaluation"** estimates the generalization error of a model
- **Idea:** Apply **"basic cross-validation for performance evaluation"** on the **"one-layer cross-validation for model selection"**-model to estimate it's generalization error

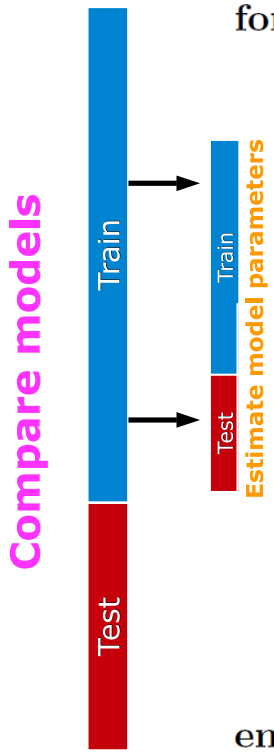


Cross-validation (2-layer)

- **Two-layer cross-validation, the algorithm**

Algorithm 5: Two-level cross-validation

Require: K_1, K_2, folds in outer, and inner cross-validation loop respectively
Require: $\mathcal{M}_1, \ldots, \mathcal{M}_S$: The S different models to cross-validate
Ensure: $\hat{E}^{\text{gen}}$, the estimate of the generalization error
for $i = 1, \ldots, K_1$ **do**
Outer cross-validation loop. First make the outer split into K_1 folds
Let $\mathcal{D}_i^{\text{par}}$, $\mathcal{D}_i^{\text{test}}$ be the i'th split of $\mathcal{D}$
for $j = 1, \ldots, K_2$ **do**
Inner cross-validation loop. Use cross-validation to select optimal model
Let $\mathcal{D}_j^{\text{train}}$, $\mathcal{D}_j^{\text{val}}$ be the j'th split of $\mathcal{D}_i^{\text{par}}$
for $s = 1, \ldots, S$ **do**
Train $\mathcal{M}_s$ on $\mathcal{D}_j^{\text{train}}$
Let $E_{\mathcal{M}_s,j}^{\text{val}}$ be the *validation error* of the model $\mathcal{M}_s$ when it is *tested* on $\mathcal{D}_j^{\text{val}}$
end for
end for
For each s compute: $\hat{E}_s^{\text{gen}} = \sum_{j=1}^{K_2} \frac{|\mathcal{D}_j^{\text{val}}|}{|\mathcal{D}_i^{\text{par}}|} E_{\mathcal{M}_s,j}^{\text{val}}$
Select the optimal model $\mathcal{M}^* = \mathcal{M}_{s^*}$ where $s^* = \arg\min_s \hat{E}_s^{\text{gen}}$
Train $\mathcal{M}^*$ on $\mathcal{D}_i^{\text{par}}$
Let E_i^{test} be the *test error* of the model $\mathcal{M}^*$ when it is *tested* on $\mathcal{D}_i^{\text{test}}$
end for
Compute the estimate of the generalization error: $\hat{E}^{\text{gen}} = \sum_{i=1}^{K_1} \frac{|\mathcal{D}_i^{\text{test}}|}{N} E_i^{\text{test}}$



Quiz 3, 2-level CV

Consider a classification tree model applied to a dataset of $N = 1000$ observations. Suppose we wish to both select the optimal pruning level and estimate the generalization error of the classification tree model by cross-validation. To simplify the problem, we only consider 3 possible pruning levels:

$$3, 4, 5.$$

We opt for a two-level cross-validation strategy in which we use an inner loop of $K_2 = 5$-fold cross-validation to estimate the optimal pruning level and an outer loop of $K_1 = 10$ fold cross-validation to estimate the generalization error. That is, for each of the K_1 outer folds, the dataset is divided into a validation set and a parameter estimation set on which K_2-fold cross-validation is used to select the optimal pruning level for this outer fold.

How many models do we *train* using 2-level cross-validation?

A. 50

B. 150

C. 160

D. 180

E. Don't know.

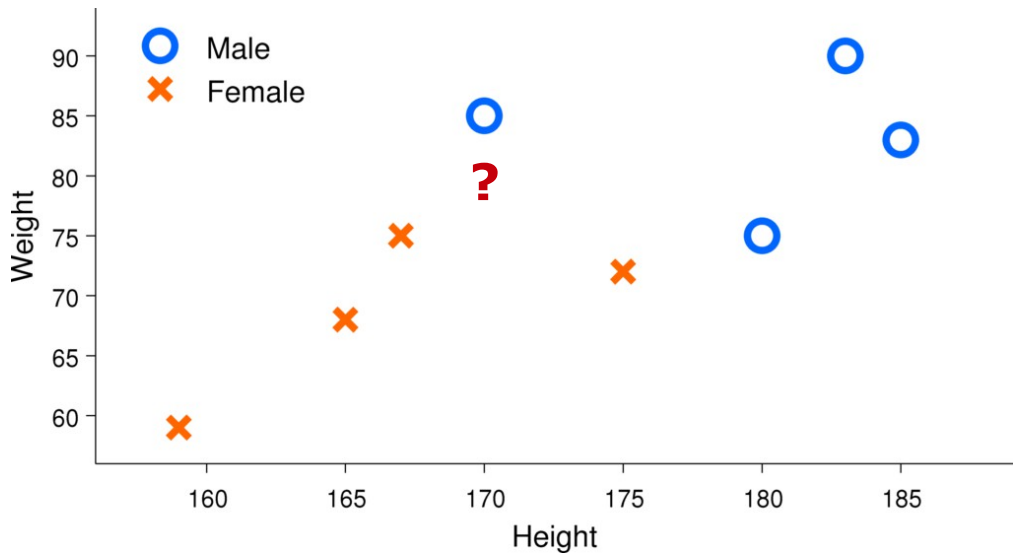
This can easily be obtained noting for each of the K_1 outer folds we must both (i) train K_2 models on the $L = 3$ different settings of pruning level (ii) train a single new model to estimate the generalization error for this fold. Accordingly the number of trained models is

$$K_1(K_2L + 1).$$

Therefore, option C is correct.

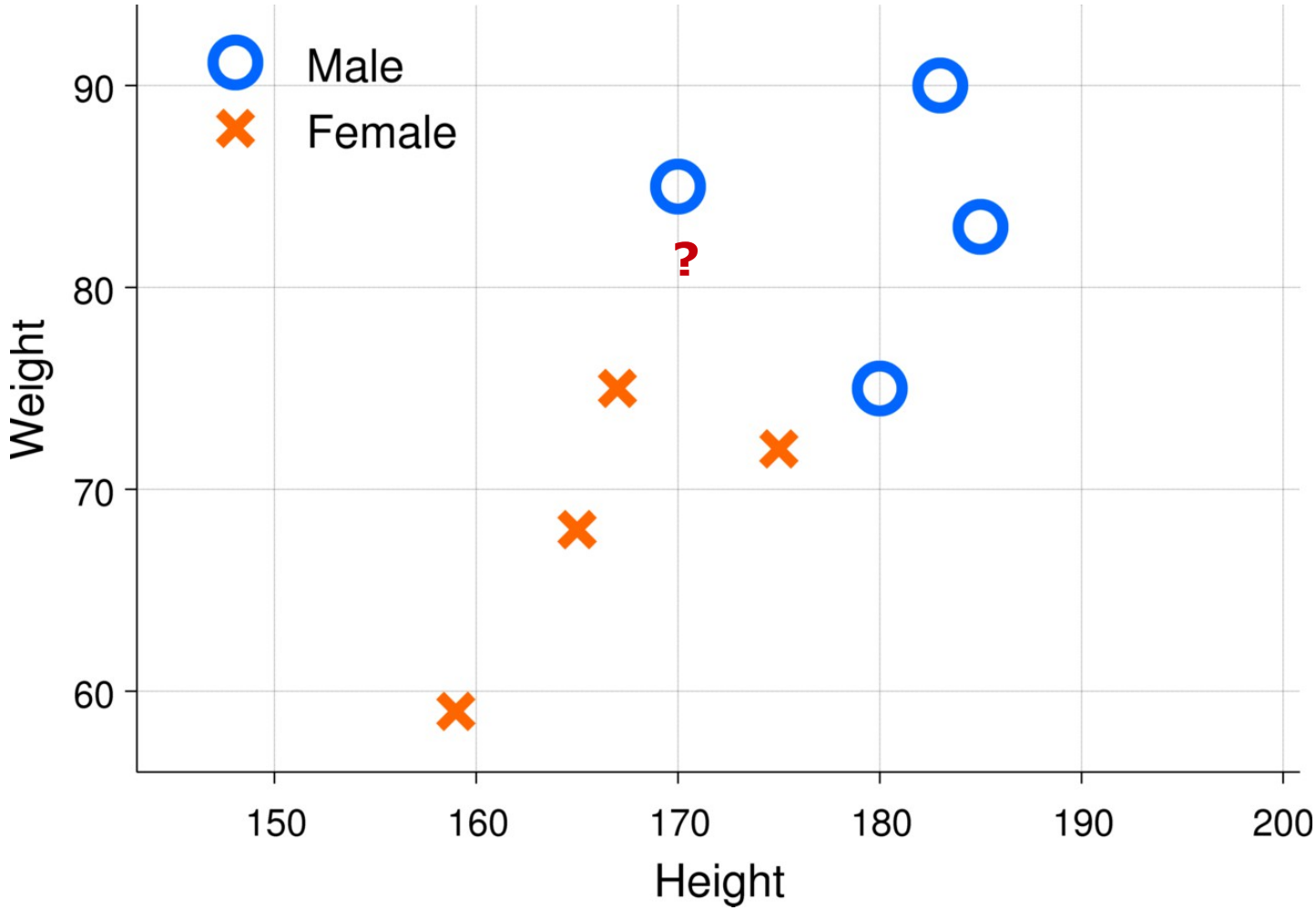
Classify gender based on height and weight

	Height	Weight	Gender
1	183	90	Male
2	180	75	Male
3	170	85	Male
4	185	83	Male
5	159	59	Female
6	167	75	Female
7	165	68	Female
8	175	72	Female
9	171	82	?



Nearest neighbor classifier

- 1 nearest neighbor



Nearest neighbor classifier

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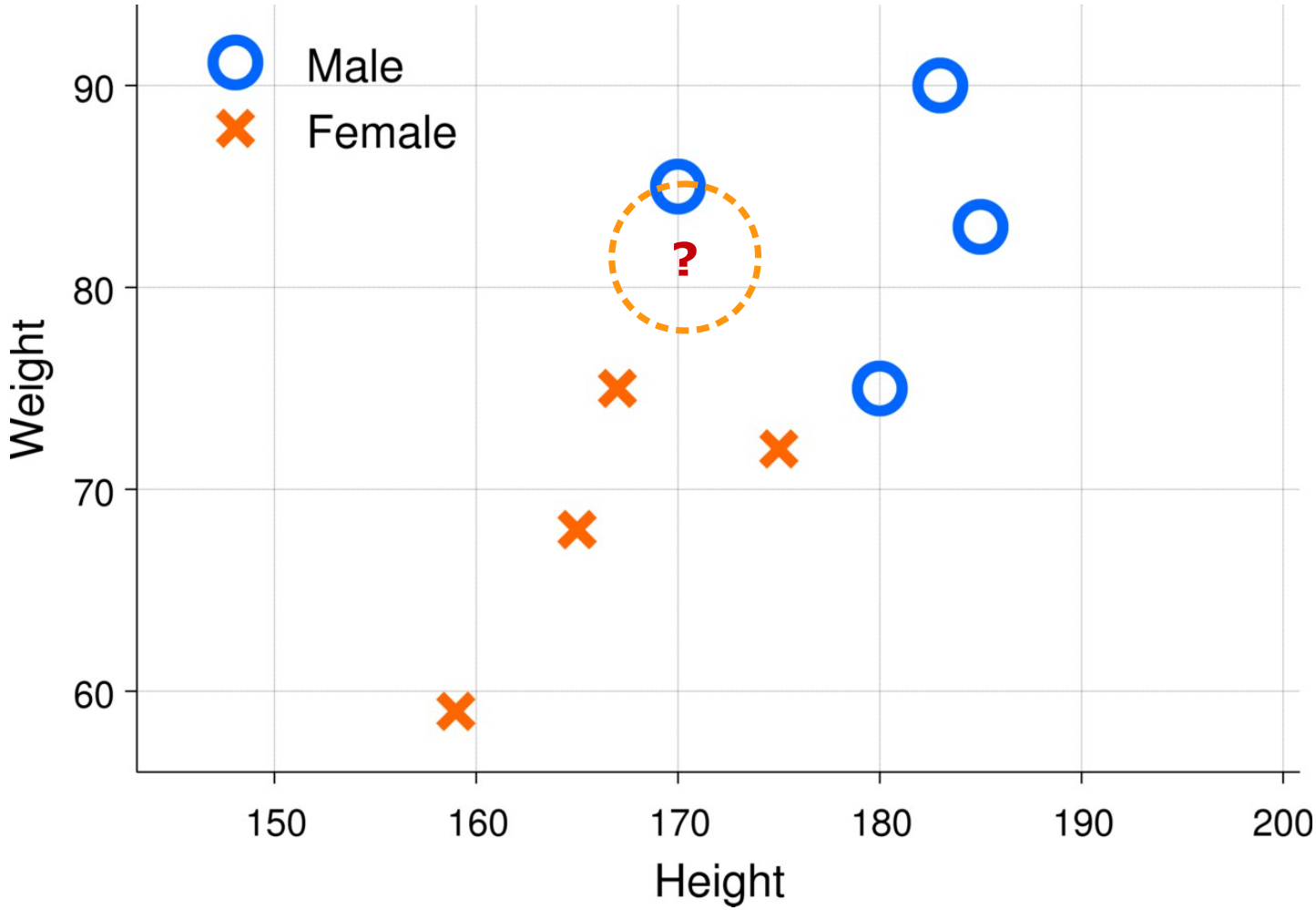
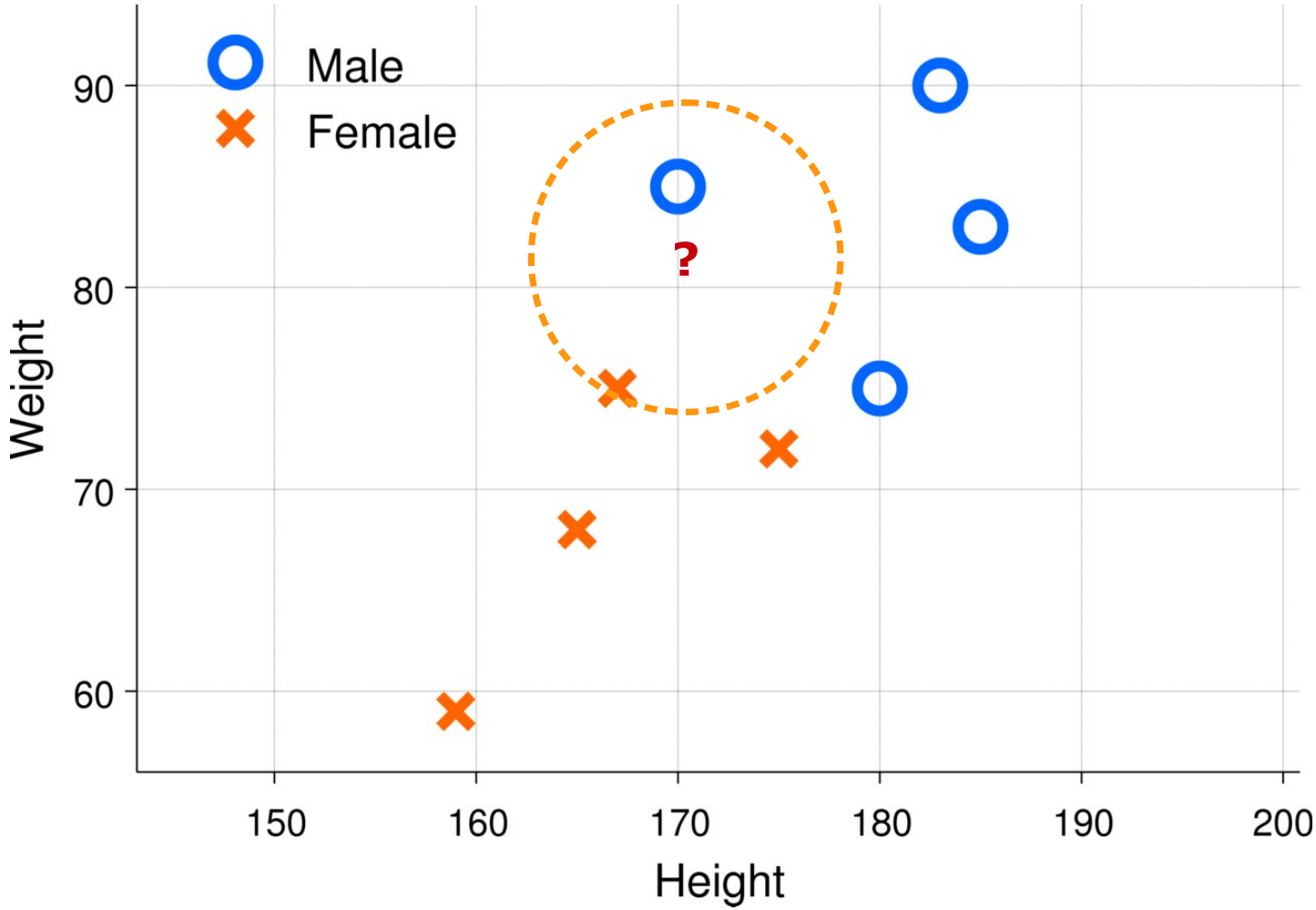


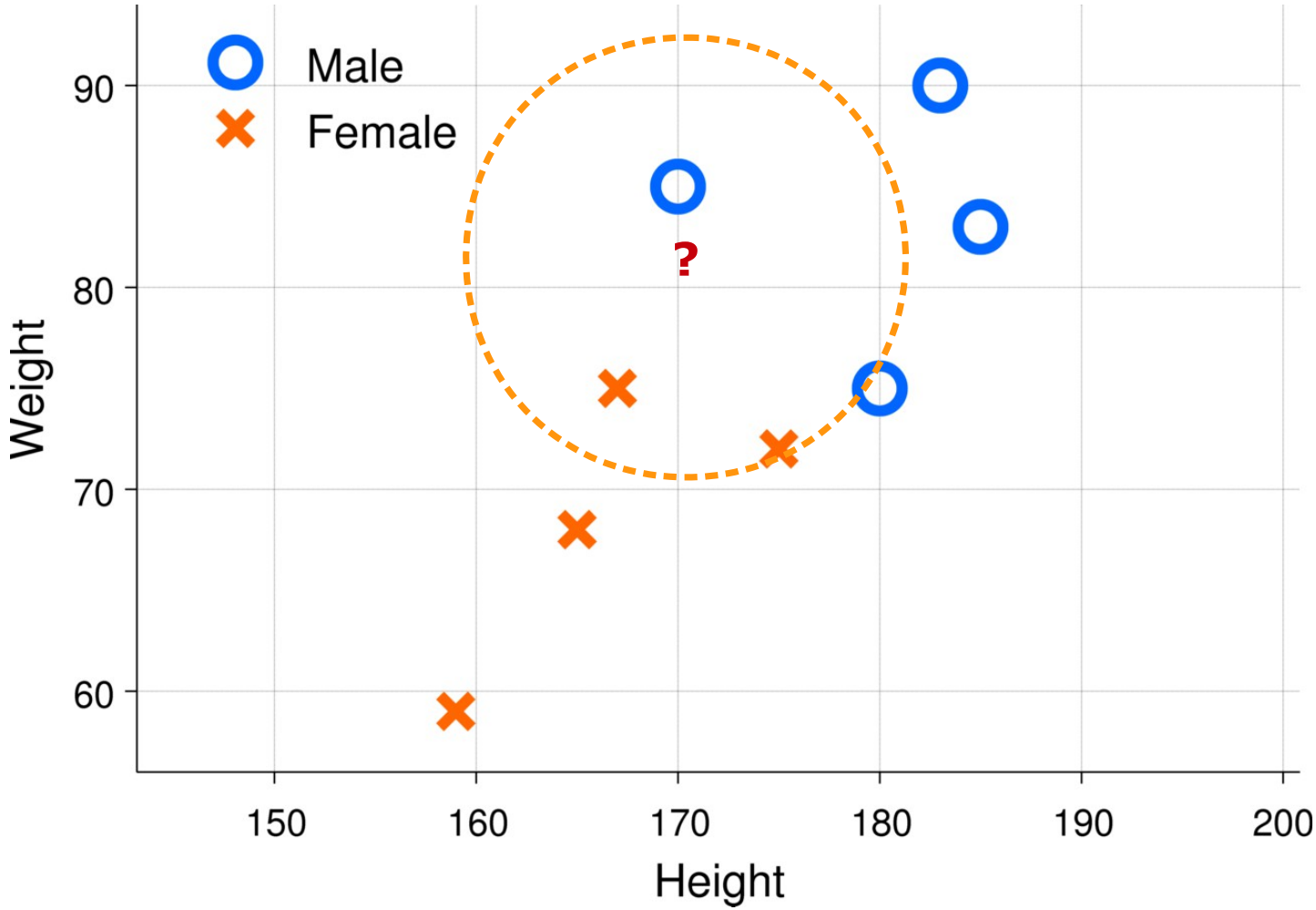
Nearest neighbor classifier

- 2 nearest neighbors



Nearest neighbor classifier

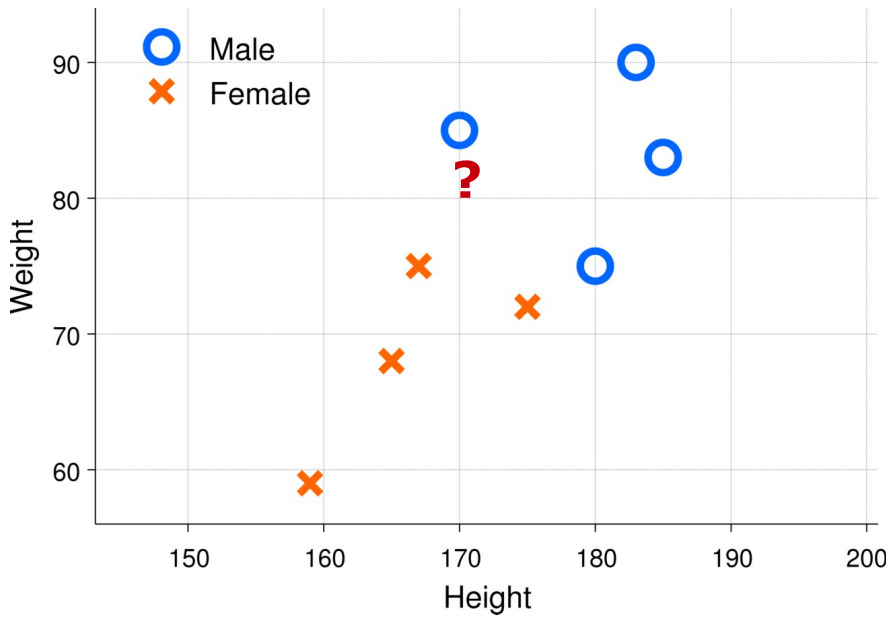
- 3 nearest neighbors



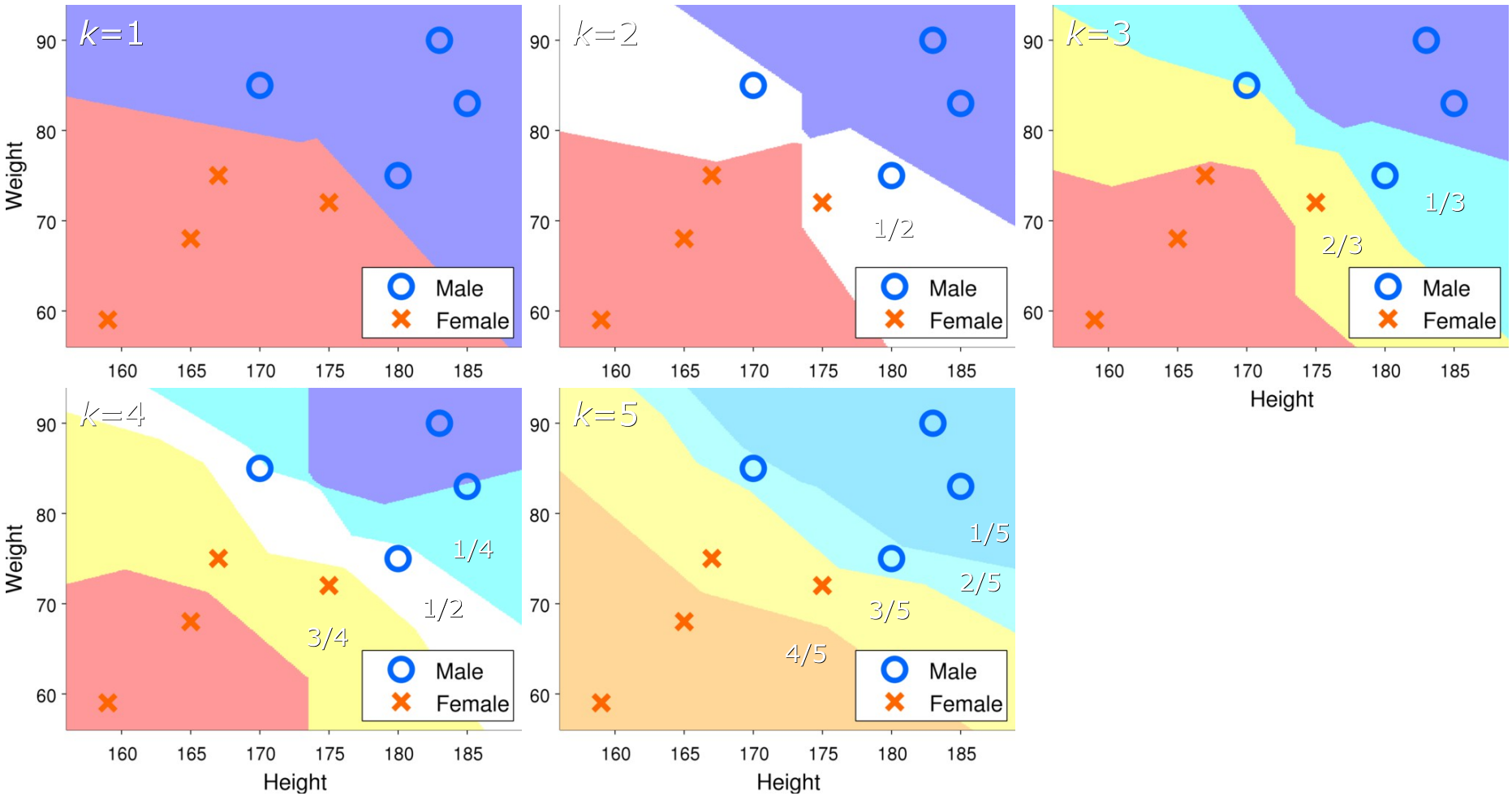
Nearest neighbor classifier

- Choose
  - The number of neighbors, k
  - A distance measure

1. Compute distance to all other data objects
2. Find the k nearest data objects
3. Classify according to majority of neighbors



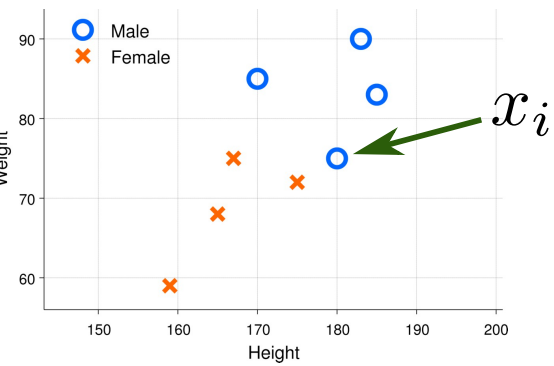
Nearest neighbor decision surface



KNN with leave-one-out CV

Leave-one-out CV is convenient with KNN

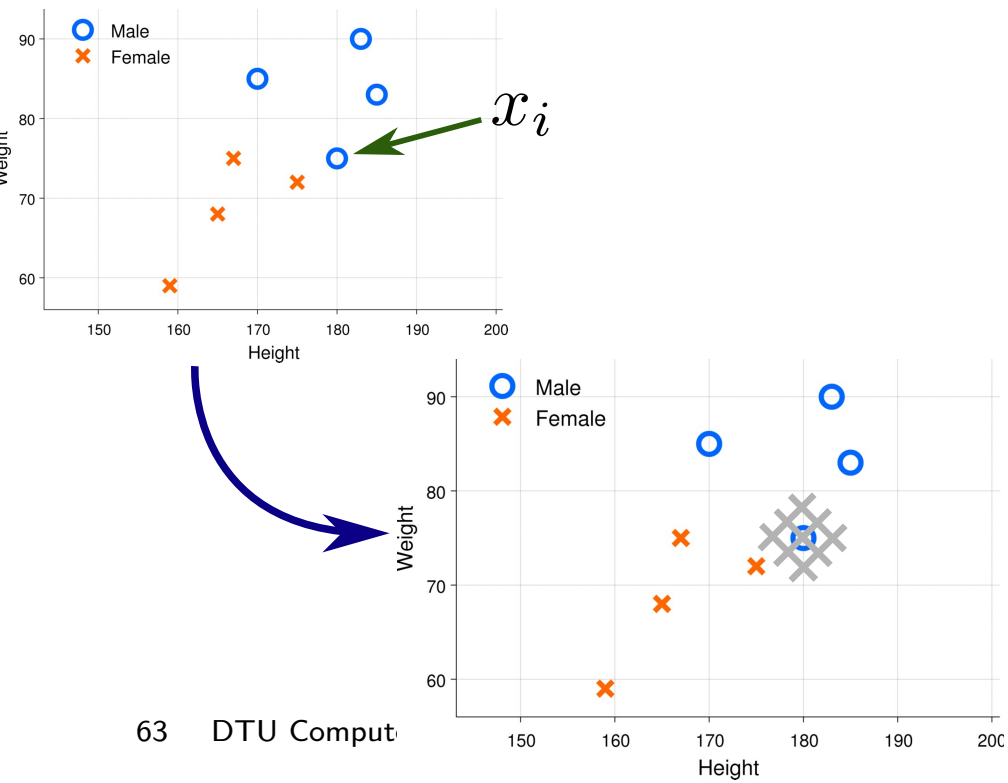
- For each observation x_i



KNN with leave-one-out CV

Leave-one-out CV is convenient with KNN

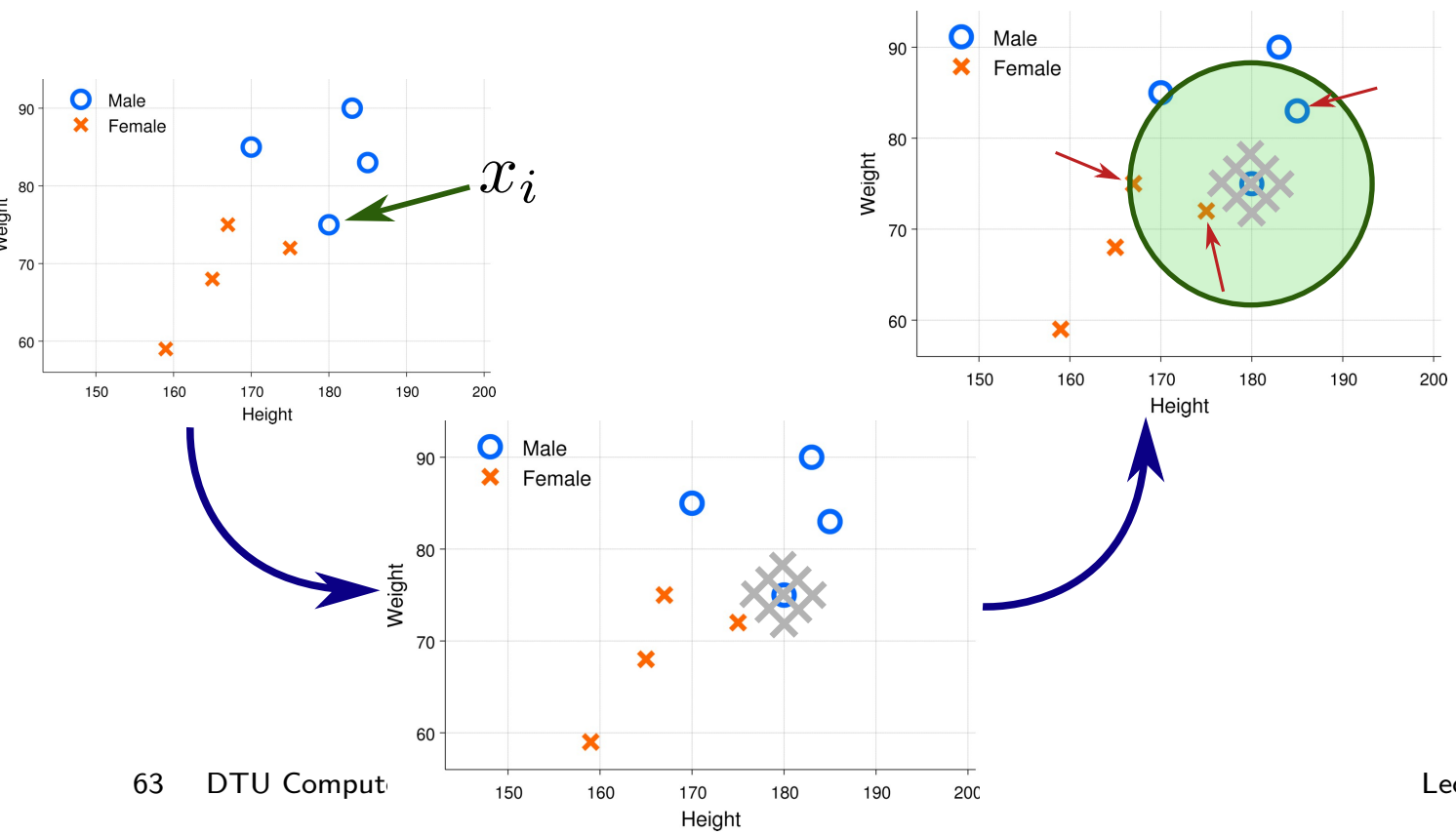
- For each observation x_i
  - Temporarily remove x_i



KNN with leave-one-out CV

Leave-one-out CV is convenient with KNN

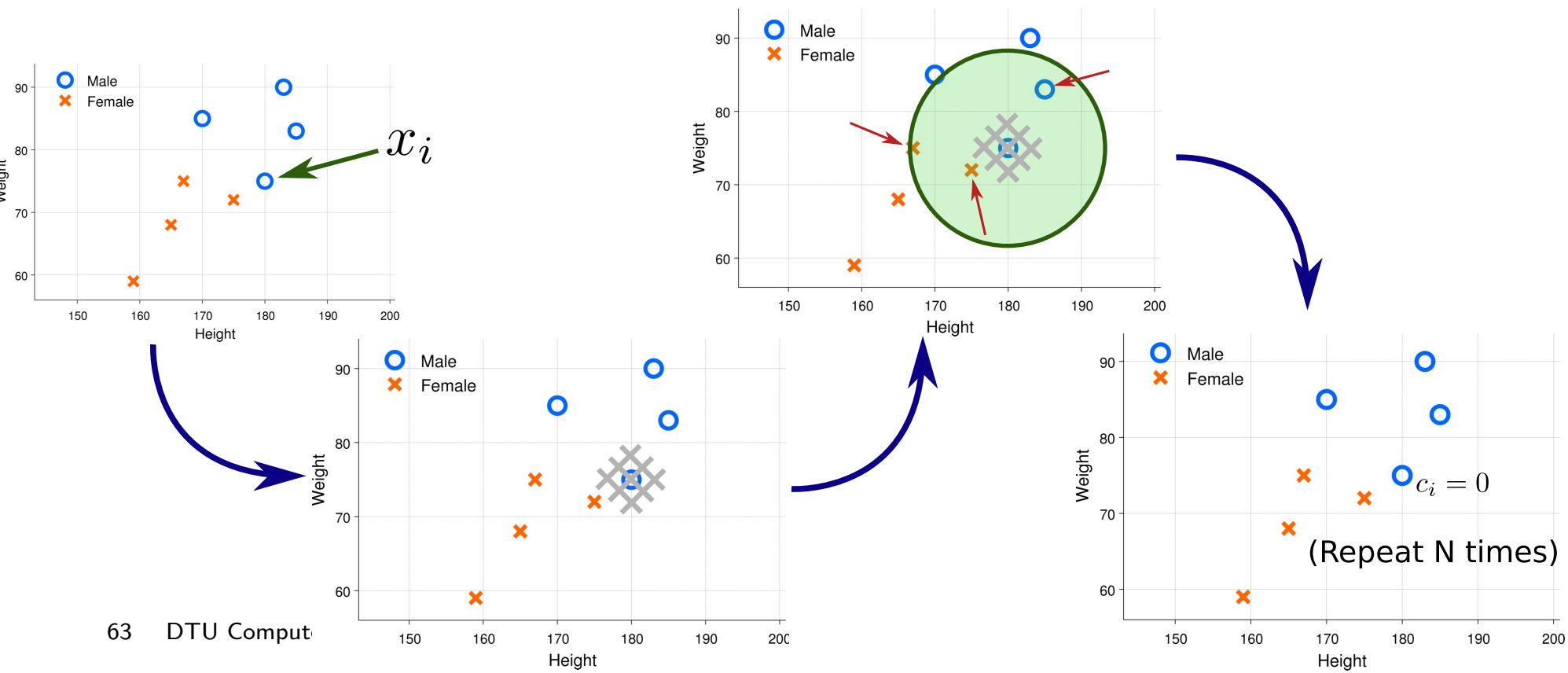
- For each observation x_i
  - Temporarily remove x_i
  - Find K nearest neighbors around x_i (not x_i itself)



KNN with leave-one-out CV

Leave-one-out CV is convenient with KNN

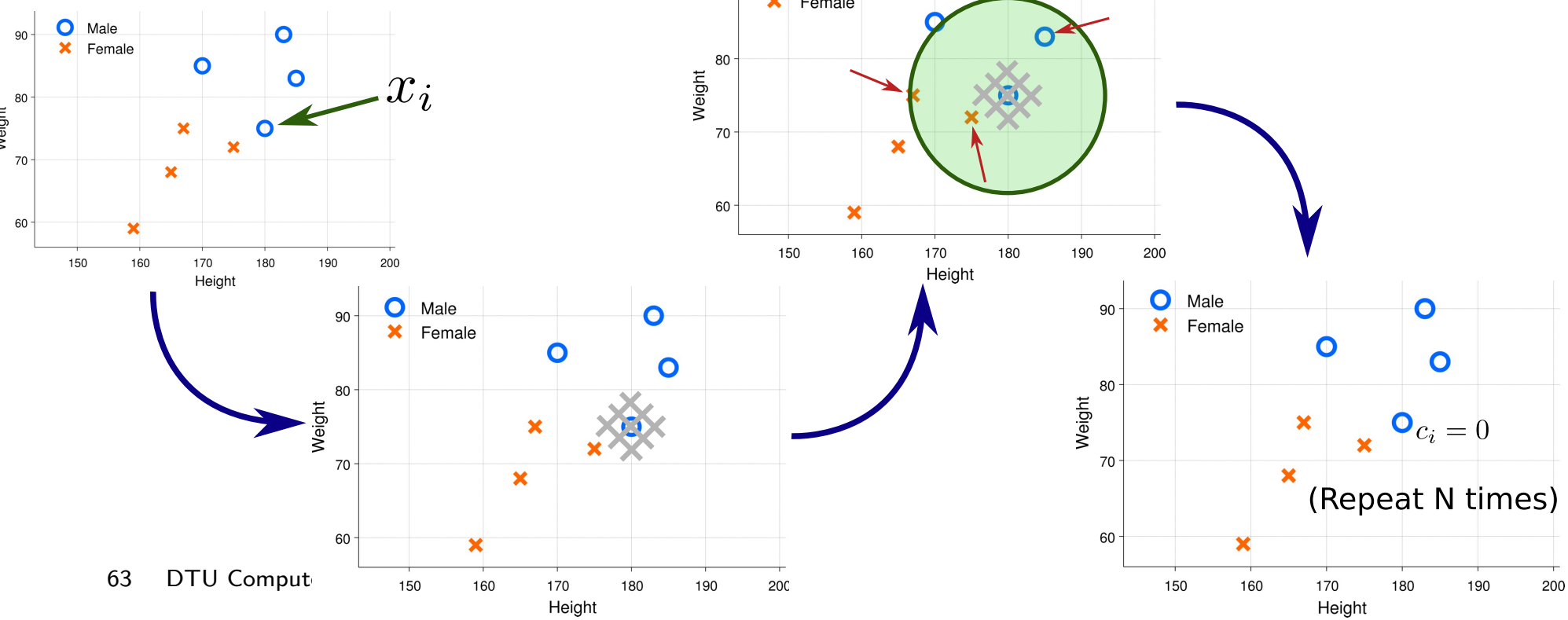
- For each observation x_i
  - Temporarily remove x_i
  - Find K nearest neighbors around x_i (not x_i itself)
  - Determine whether x_i is classified correctly based on this neighborhood, $c_i = 0, 1$

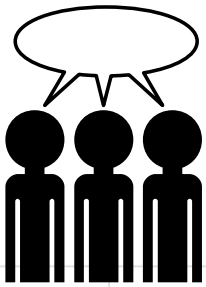


KNN with leave-one-out CV

Leave-one-out CV is convenient with KNN

- For each observation x_i
  - Temporarily remove x_i
  - Find K nearest neighbors around x_i (not x_i itself)
  - Determine whether x_i is classified correctly based on this neighborhood, $c_i = 0, 1$
- Compute accuracy as $\frac{1}{N}\sum_{i=1}^{N} c_i$



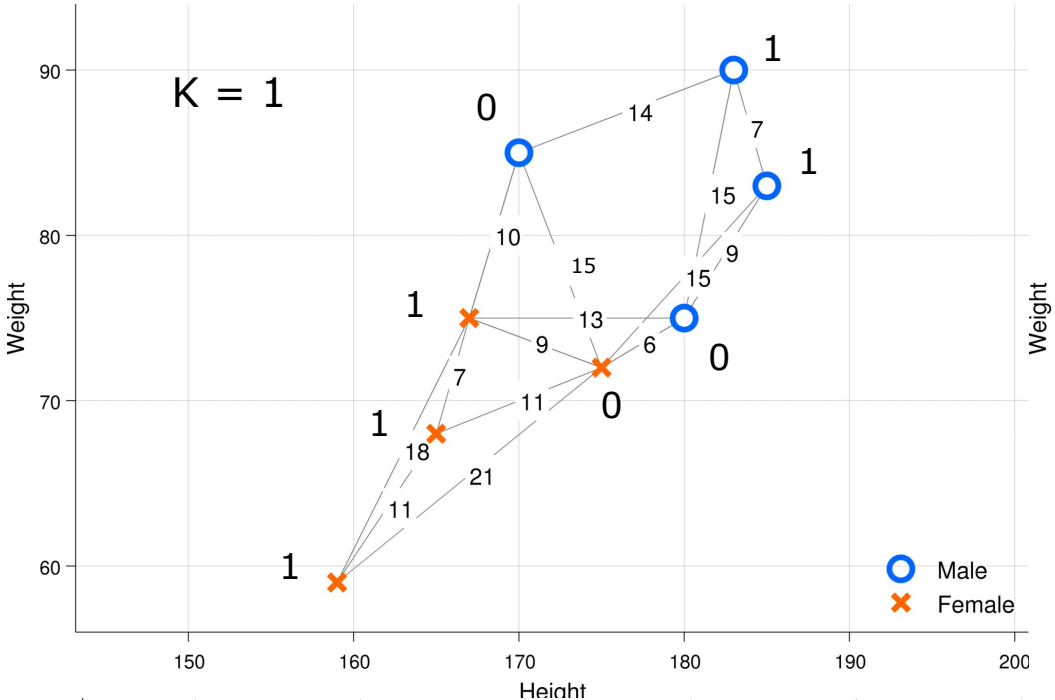


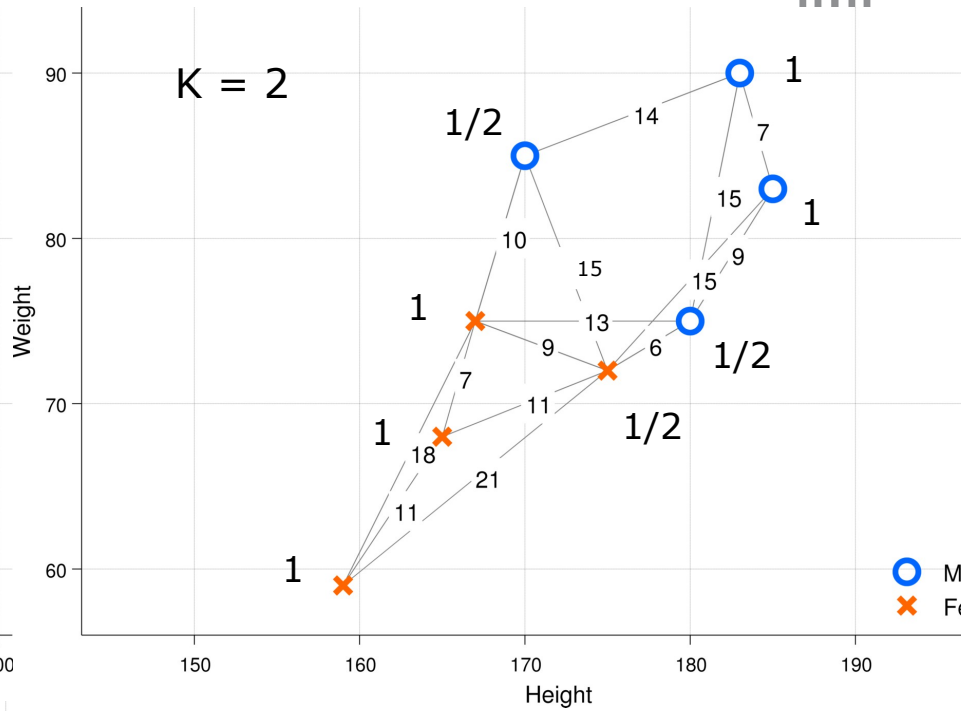
Group exercise

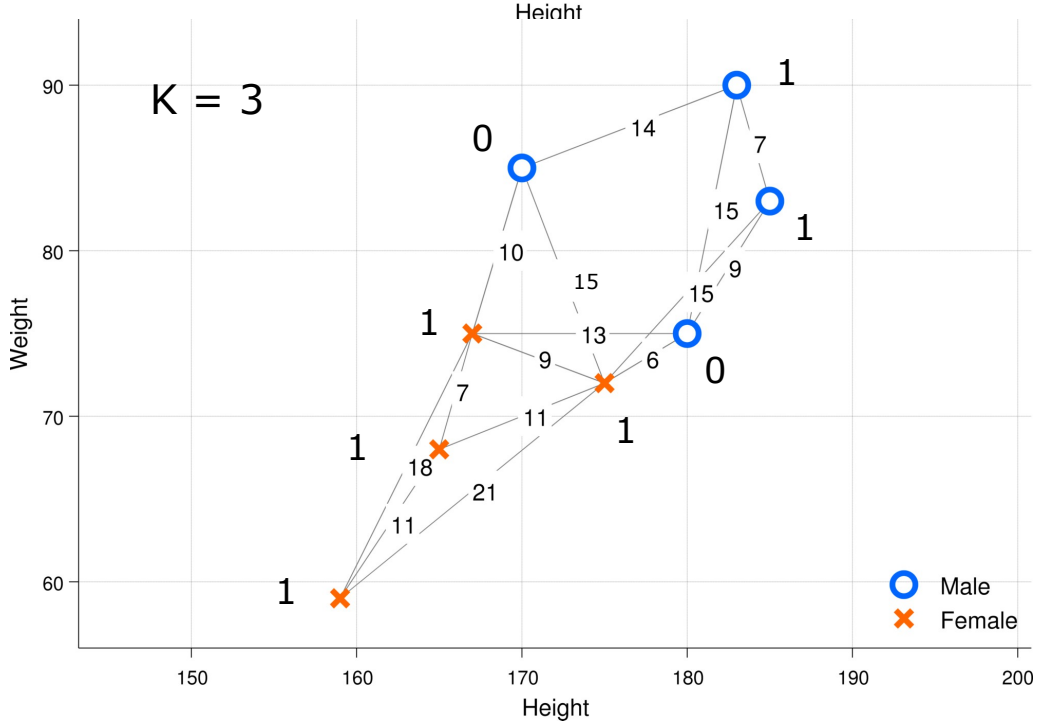
***k*-nearest neighbors**

- Choose $k \in \{1, 2, 3\}$ using leave-one-out cross-validation

Hint: For each data object, find the k nearest neighbors and count the number of correct classifications. Count ties as ½


K = 1
Weight
Height
Male
Female


K = 2
Weight
Height


K = 3
Weight
Height
Male
Female

Resources

https://towardsdatascience.com Alternative introduction to cross-validation

(https://towardsdatascience.com/

cross-validation-explained-evaluating-estimator-performance-e51e5430ff85)