RESAMPLING METHODS

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Outline

- Cross Validation
  - The Validation Set Approach
  - Leave-One-Out Cross Validation
  - K-fold Cross Validation
  - Bias-Variance Trade-off for k-fold Cross Validation
  - Cross Validation on Classification Problems
- Bootstrap

What are resampling methods?

- Tools that involves repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain more information about the fitted model
  - Model Assessment: estimate test error rates
  - Model Selection: select the appropriate level of model flexibility
- They are computationally expensive! But these days we have powerful computers ☺
- Two resampling methods:
  - Cross Validation
  - Bootstrapping

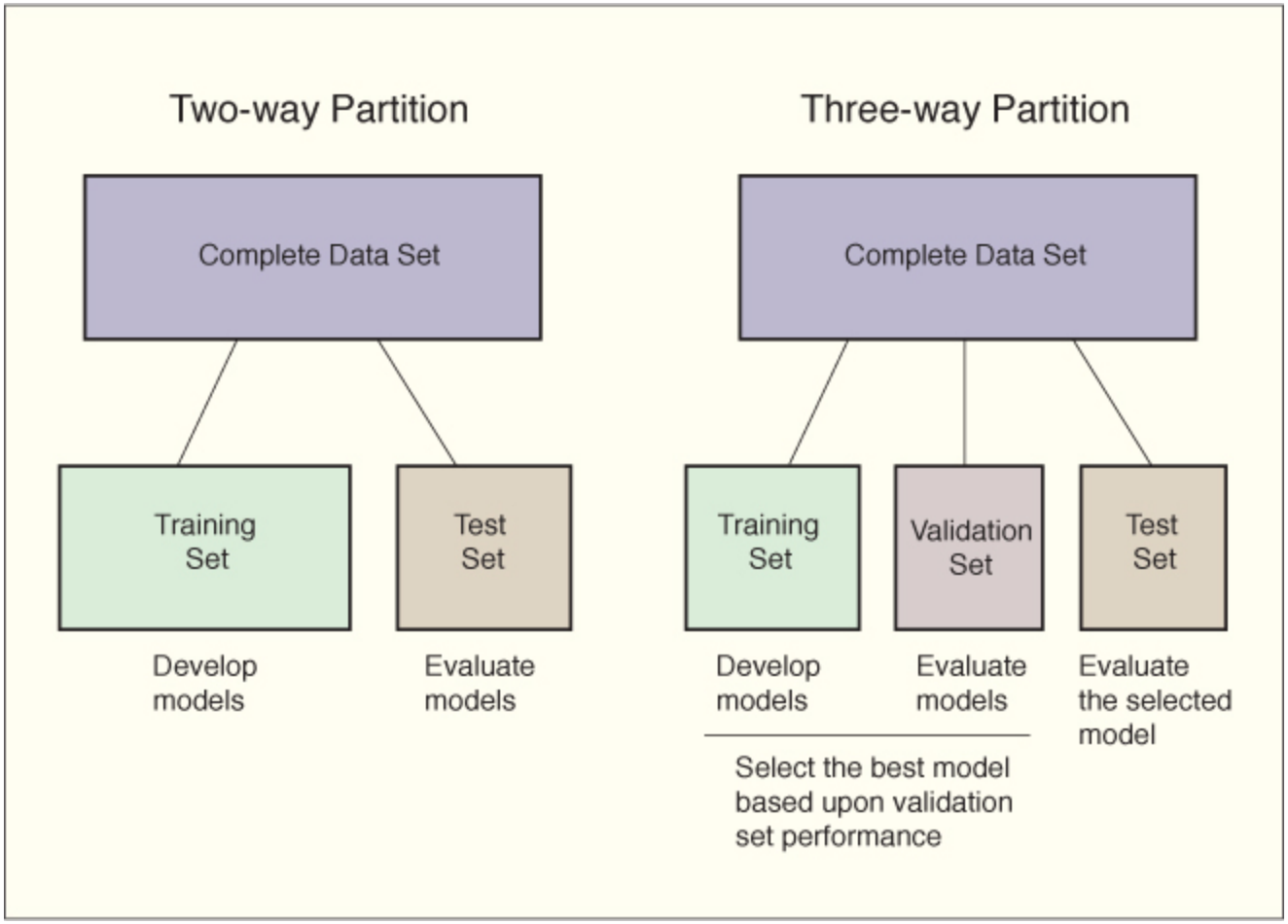
Machine Learning Phases

- Training phase
  - train your model, by pairing the input with expected output.
- Validation/Test phase
  - estimate how well your model has been trained
  - estimate model properties (mean error for numeric predictors, classification errors for classifiers, recall and precision for IR-models etc.)
- Application phase
  - apply your freshly-developed model to the real-world data and get the results.

Validation/Test phase

- The validation phase is often split into two parts:
  - first you look at your models and select the best performing approach using the validation data (=validation)
  - Then you estimate the accuracy of the selected approach (=test)
- Validation dataset and test dataset are used interchangeably in this class.

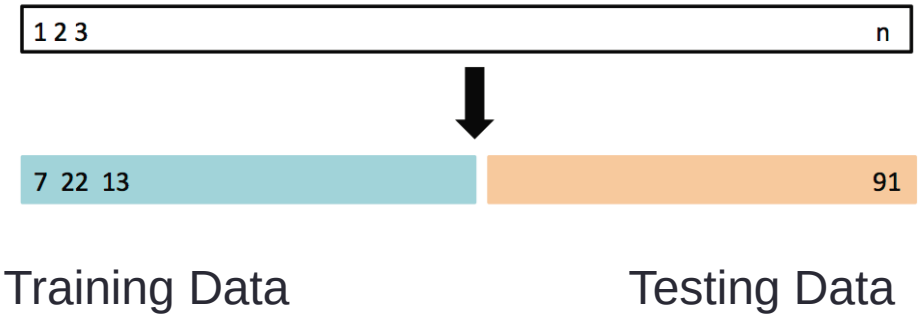
Dataset Partition



- Source of figure: Modeling Techniques in Predictive Analytics with Python and R: A Guide to Data Science by Thomas W. Miller

5.1.1 Typical Approach: The Validation Set Approach

- Suppose that we would like to find a set of variables that give the lowest test (not training) error rate
- If we have a large data set, we can achieve this goal by randomly splitting the data into training and validation(testing) parts
- We would then use the training part to build each possible model (i.e. the different combinations of variables) and choose the model that gave the lowest error rate when applied to the validation data

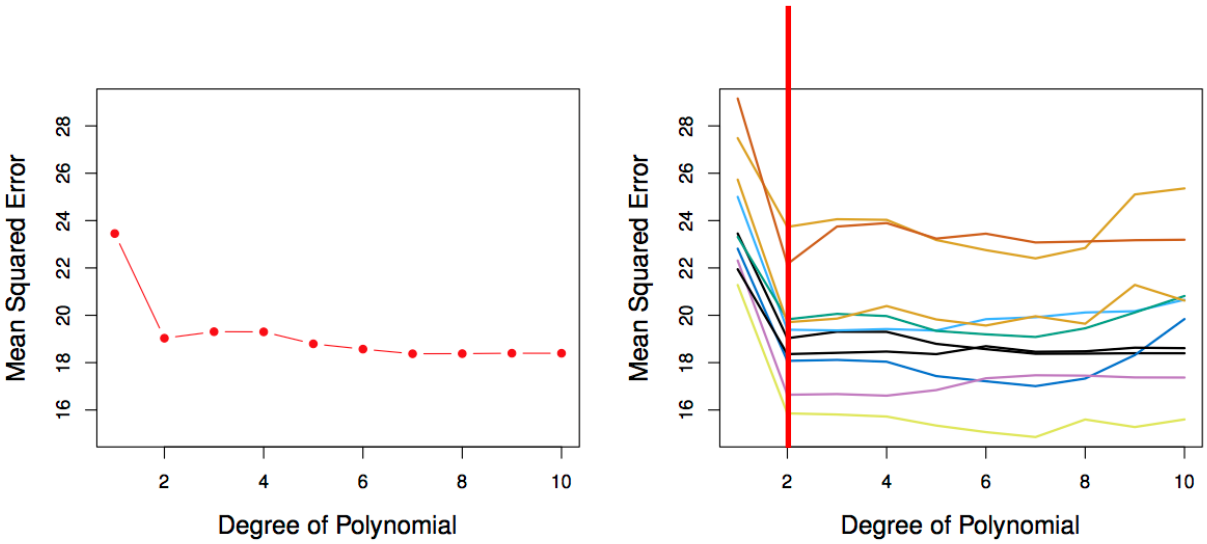


Example: Auto Data

- Suppose that we want to predict mpg from horsepower
- Two models:
  - mpg ~ horsepower
  - mpg ~ horsepower + horspower^2
- Which model gives a better fit?
  - Randomly split Auto data set into training (196 obs.) and validation data (196 obs.)
  - Fit both models using the training data set
  - Then, evaluate both models using the validation data set
  - The model with the lowest validation (testing) MSE is the winner!

Results: Auto Data

- Left: Validation error rate for a single split
- Right: Validation method repeated 10 times, each time the split is done randomly!
- There is a lot of variability among the MSE's… Not good! We need more stable methods!



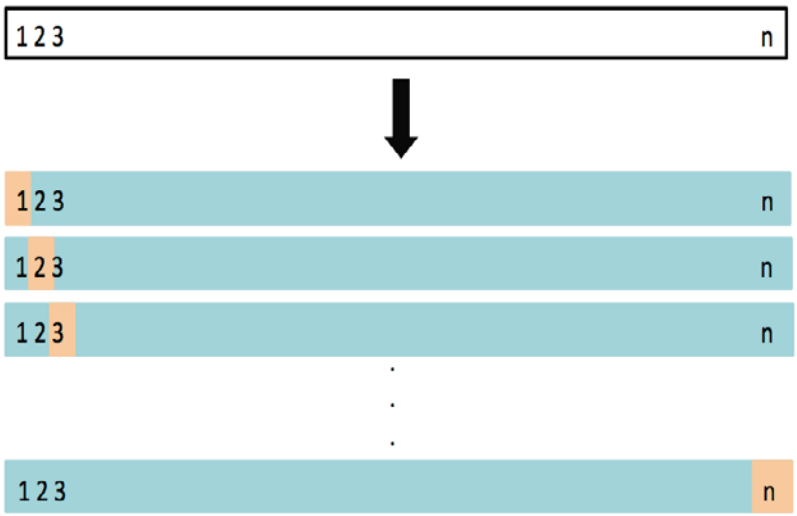
The Validation Set Approach

- Advantages:
  - Simple
  - Easy to implement

- Disadvantages:
  - The validation MSE can be highly variable
  - Only a subset of observations are used to fit the model (training data). Statistical methods tend to perform worse when trained on fewer observations

5.1.2 Leave-One-Out Cross Validation (LOOCV)

- This method is similar to the Validation Set Approach, but it tries to address the latter's disadvantages
- For each suggested model, do:
  - Split the data set of size n into
    - Training data set (blue) size: n -1
    - Validation data set (beige) size: 1
  - Fit the model using the training data
  - Validate model using the validation data, and compute the corresponding MSE
  - Repeat this process n times
  - The MSE for the model is computed as follows:



$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n} MSE_i .$$

LOOCV vs. the Validation Set Approach

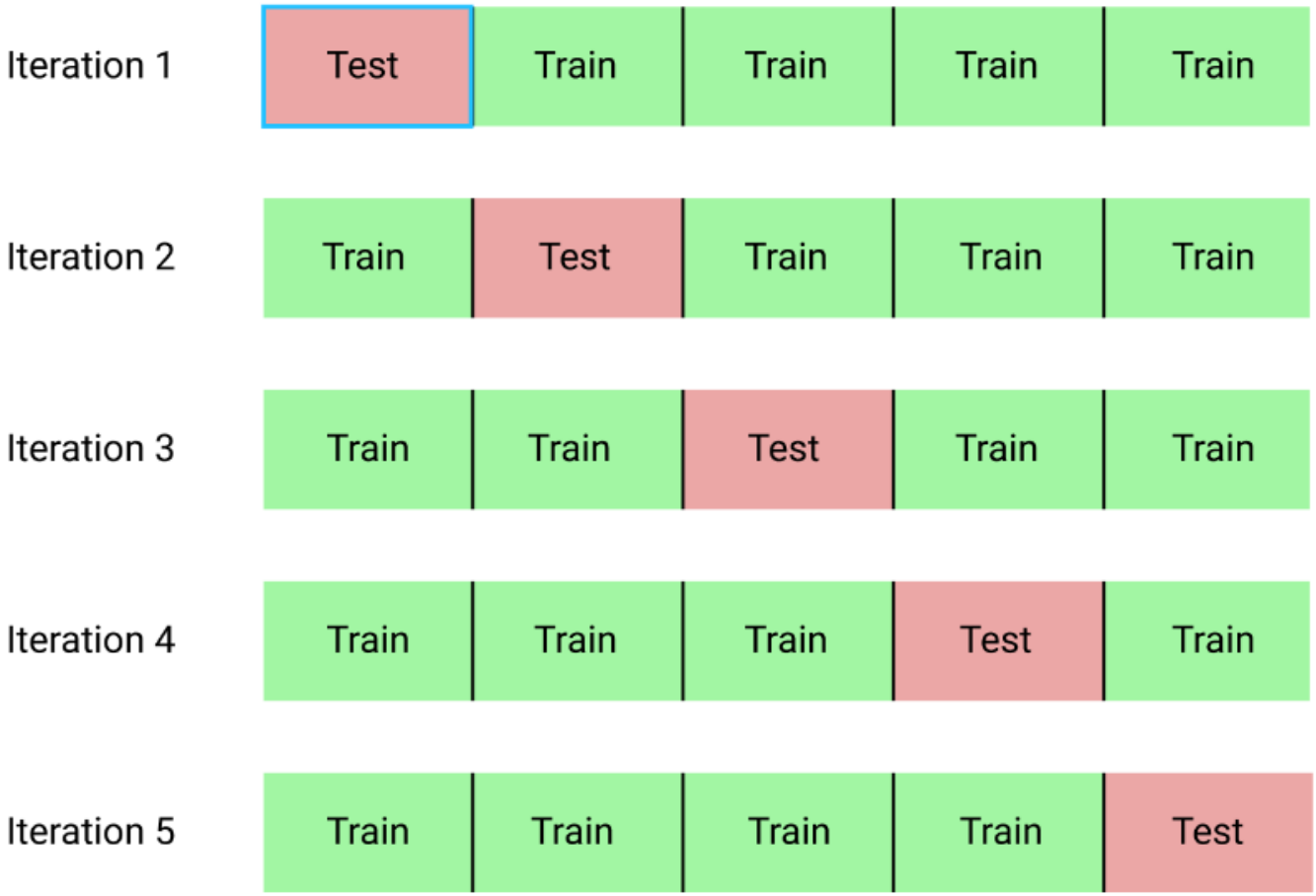
- LOOCV has less bias
  - We repeatedly fit the statistical learning method using training data that contains n-1 obs., i.e. almost all the data set is used
- LOOCV produces a less variable MSE
  - The validation approach produces different MSE when applied repeatedly due to randomness in the splitting process, while performing LOOCV multiple times will always yield the same results, because we split based on 1 obs. each time
- LOOCV is computationally intensive (disadvantage)
  - We fit the each model n times!

5.1.3 k-fold Cross Validation

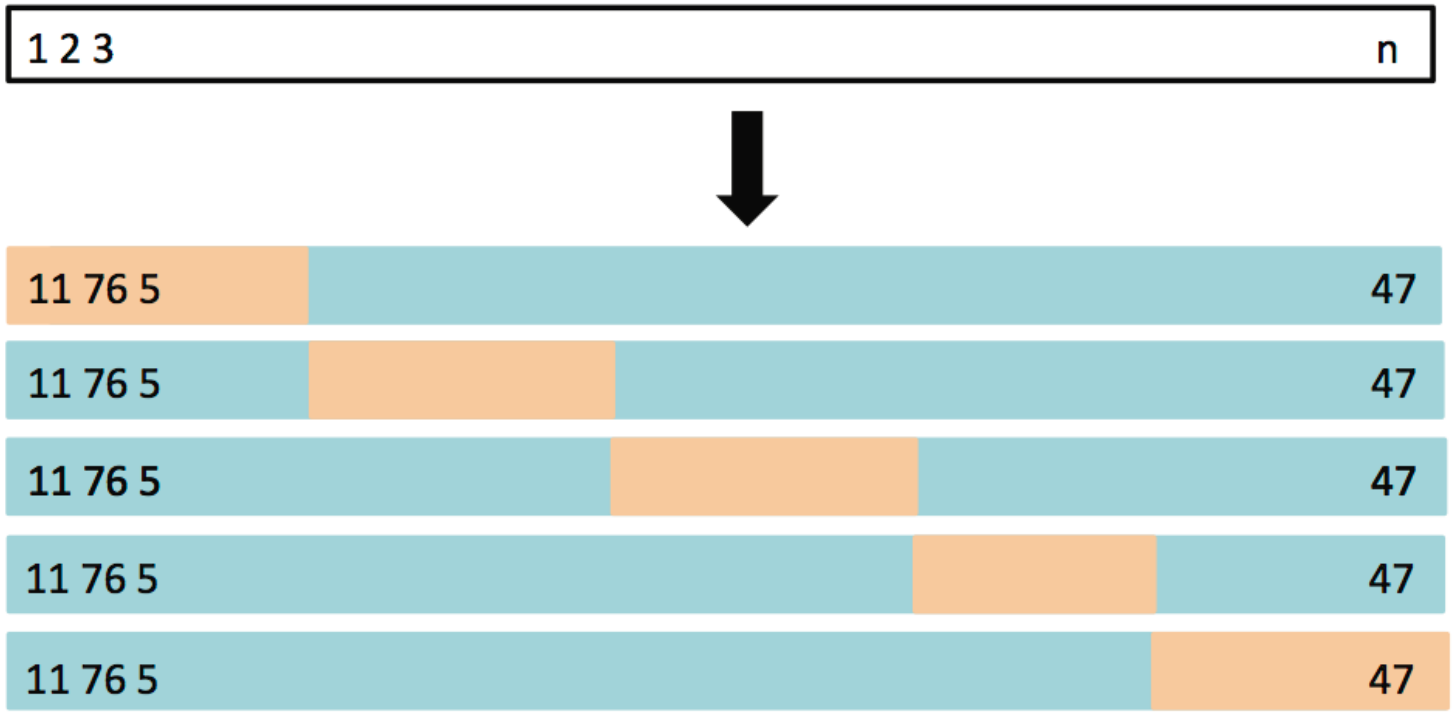
- LOOCV is computationally intensive, so we can run k-fold Cross Validation instead
- With k-fold Cross Validation, we divide the data set into K different parts (e.g. K = 5, or K = 10, etc.)
- We then remove the first part, fit the model on the remaining K-1 parts, and see how good the predictions are on the left out part (i.e. compute the MSE on the first part)
- We then repeat this K different times taking out a different part each time
- By averaging the K different MSE's we get an estimated validation (test) error rate for new observations

$$CV_{(k)} = \frac{1}{k}\sum_{i=1}^{k} MSE_i .$$

K-fold Cross Validation

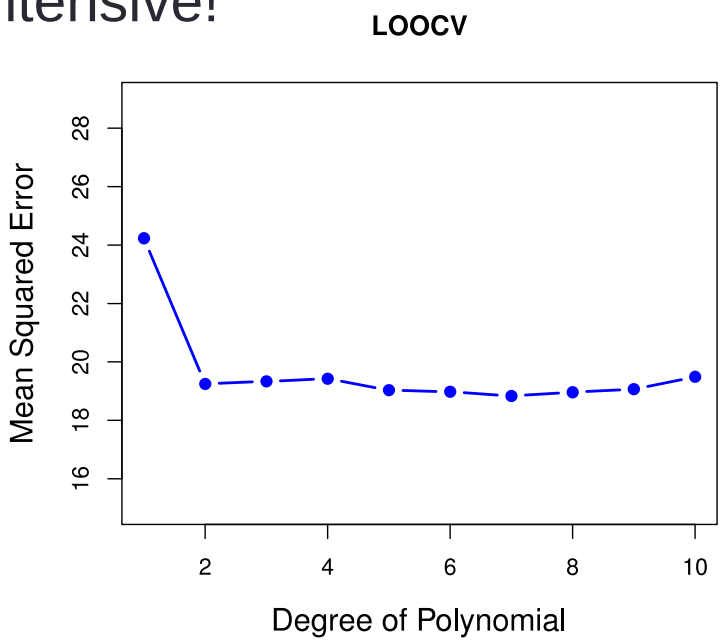


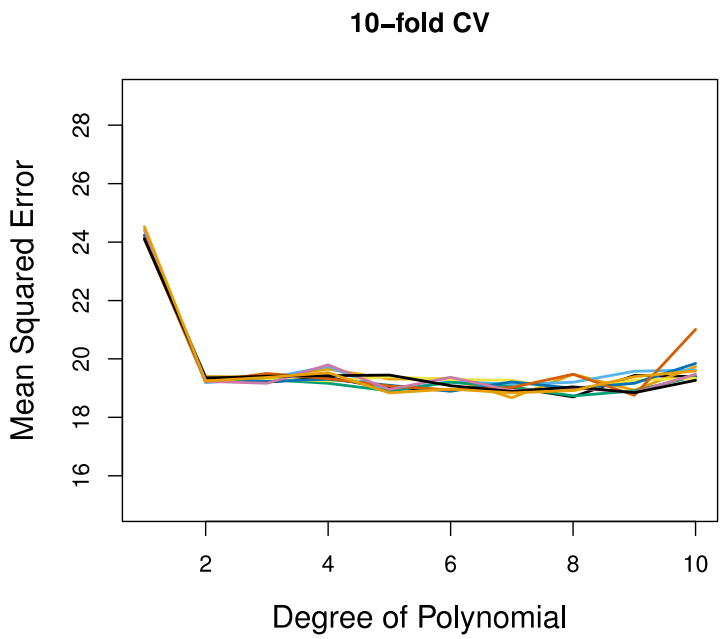
K-fold Cross Validation



Auto Data: LOOCV vs. K-fold CV

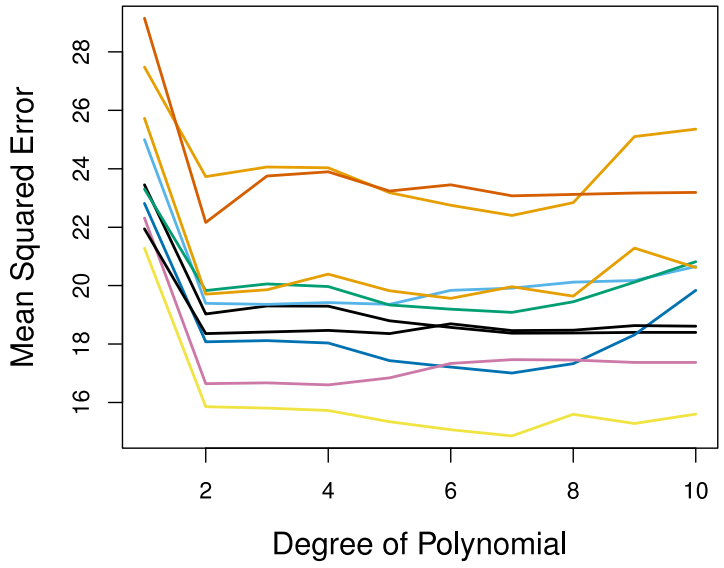
- Left: LOOCV error curve
- Right: 10-fold CV was run many times, and the figure shows the slightly different CV error rates
- LOOCV is a special case of k-fold, where k = n
- They are both stable, but LOOCV is more computationally intensive!

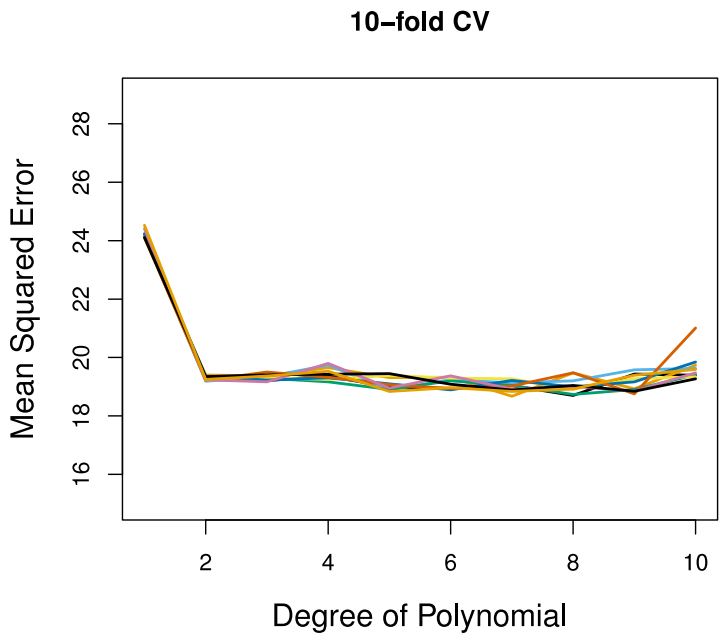




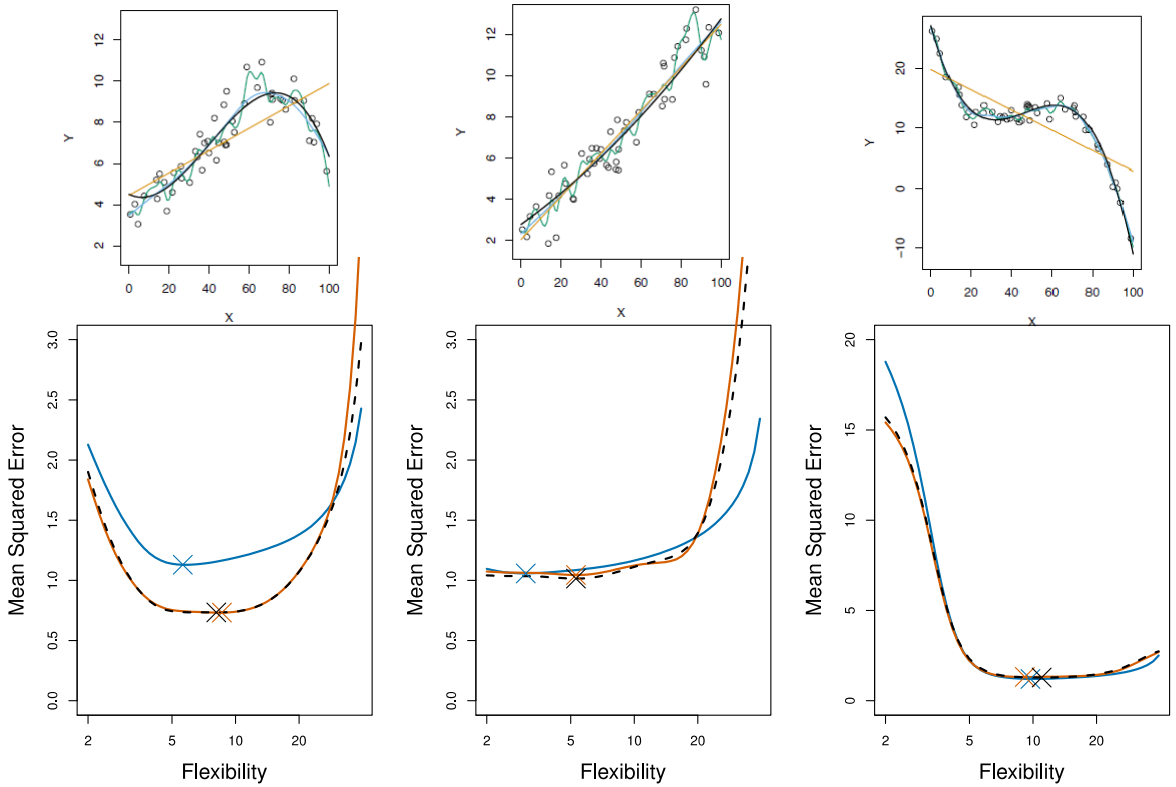
Auto Data: Validation Set Approach vs. K-fold CV Approach

- Left: Validation Set Approach
- Right: 10-fold Cross Validation Approach
- Indeed, 10-fold CV is more stable!





K-fold Cross Validation on Three Simulated Data



- Blue: True Test MSE
- Black: LOOCV MSE
- Orange: 10-fold MSE
- Refer to chapter 2 for the top graphs, Fig 2.9, 2.10, and 2.11

5.1.4 Bias- Variance Trade-off for k-fold CV

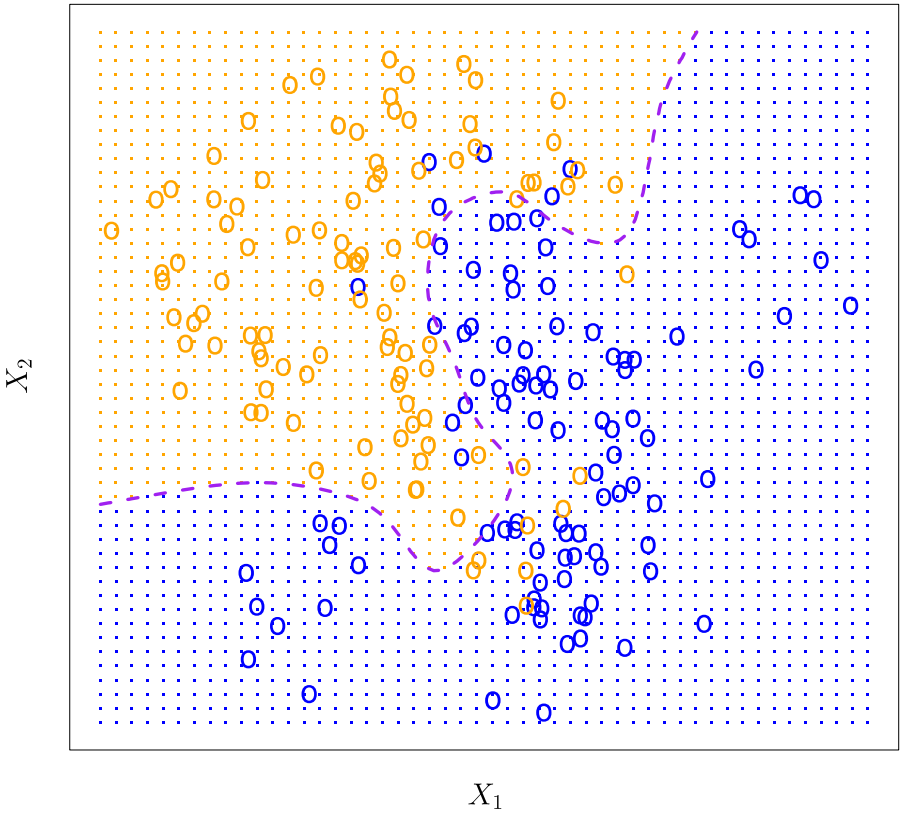
- Putting aside that LOOCV is more computationally intensive than k-fold CV… Which is better LOOCV or K-fold CV?
  - LOOCV is less bias than k-fold CV (when $k < n$)
  - But, LOOCV has higher variance than k-fold CV (when $k < n$)
  - Thus, there is a trade-off between what to use
- Conclusion:
  - We tend to use k-fold CV with ($K = 5$ and $K = 10$)
  - These are the magical K's ☺
  - It has been empirically shown that they yield test error rate estimates that suffer neither from excessively high bias, nor from very high variance

5.1.5 Cross Validation on Classification Problems

- So far, we have been dealing with CV on regression problems
- We can use cross validation in a classification situation in a similar manner
  - Divide data into K parts
  - Hold out one part, fit using the remaining data and compute the error rate on the hold out data
  - Repeat K times
  - CV error rate is the average over the K errors we have computed

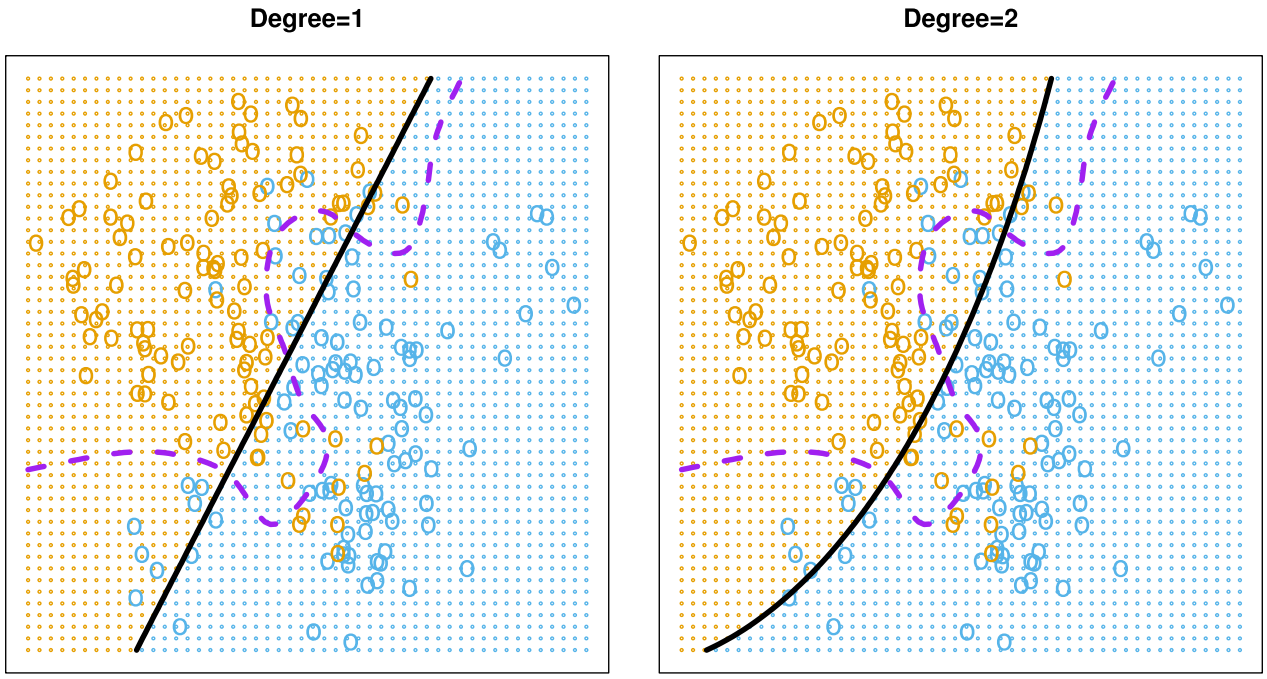
CV to Choose Order of Polynomial

- The data set used is simulated (refer to Fig 2.13)
- The purple dashed line is the Bayes' boundary



Bayes' Error Rate: 0.133

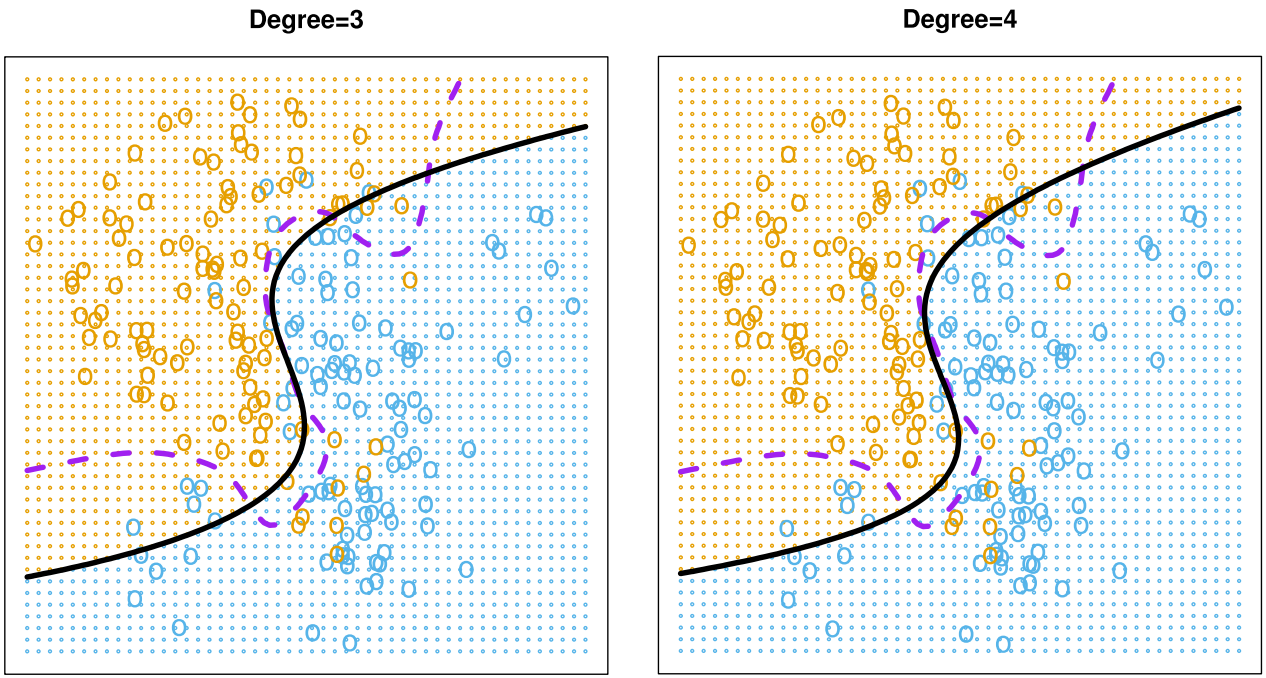
- Linear Logistic regression (Degree 1) is not able to fit the Bayes' decision boundary
- Quadratic Logistic regression does better than linear



Error Rate: 0.201

Error Rate: 0.197

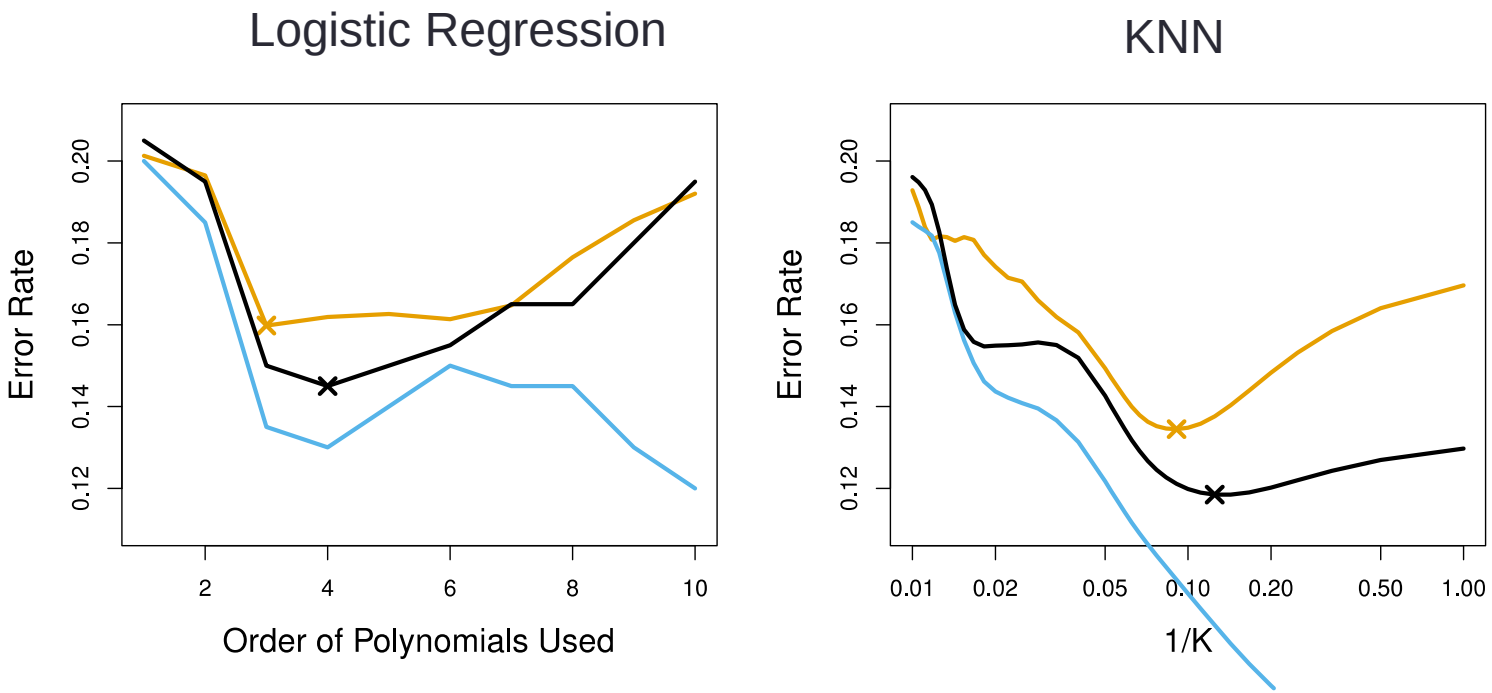
- Using cubic and quartic predictors, the accuracy of the model improves



Error Rate: 0.160

Error Rate: 0.162

CV to Choose the Order



- Brown: Test Error
- Blue: Training Error
- Black: 10-fold CV Error

Bootstrap

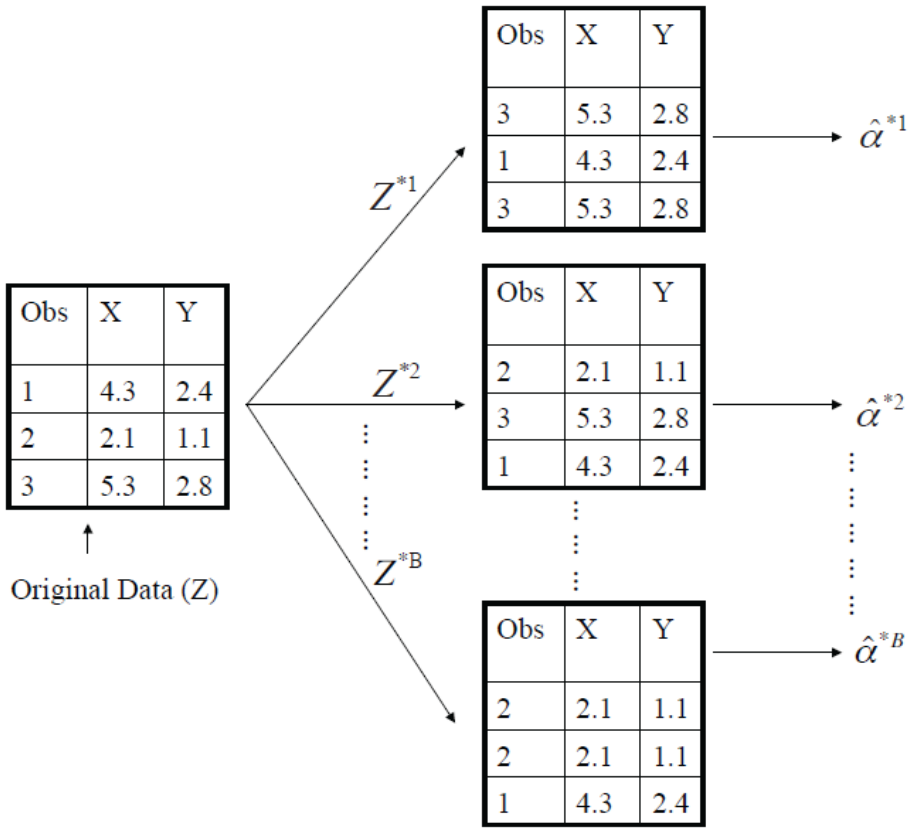
- The bootstrap is a flexible and powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.

- For example, it can provide an estimate of the standard error of a coefficient, or a confidence interval for that coefficient.

Where does the name came from?

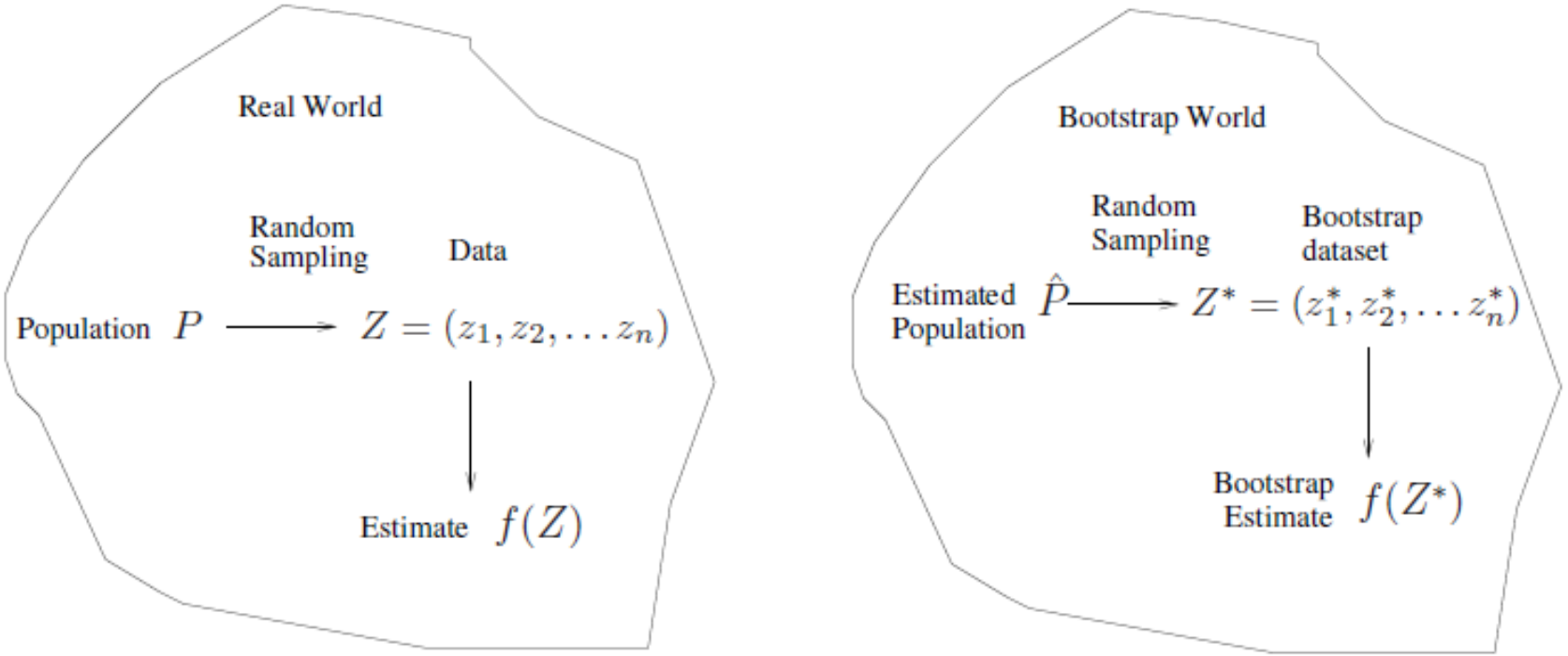
- The use of the term *bootstrap* derives from the phrase to pull oneself up by one's bootstraps, widely thought to be based on one of the eighteenth century fictions “The Surprising Adventures of Baron Munchausen" by Rudolph Erich Raspe:
- *The Baron had fallen to the bottom of a deep lake. Just when it looked like all was lost, he thought to pick himself up by his own bootstraps.*
- It is not the same as the term “bootstrap" used in computer science meaning to “boot" a computer from a set of core instructions, though the derivation is similar.

Example with just 3 observations



A graphical illustration of the bootstrap approach on a small sample containing n = 3 observations. Each bootstrap data set contains n observations, sampled with replacement from the original data set. Each bootstrap data set is used to obtain an estimate of alpha.

A general picture for the bootstrap



Reference

- James, Witten, Hastie, and Tibshirani. "*An Introduction to Statistical Learning*". Chapter 5.
- Tan, Pang-Ning et al. *Introduction to Data Mining*. (Section 3.6)