Lecture-2
Machine Learning

CS 277:
Machine Learning
and
Data Science

By:
Dr. Joydeep Chandra
Associate Professor
Dept. of CSE, IIT Patna

Types of learning

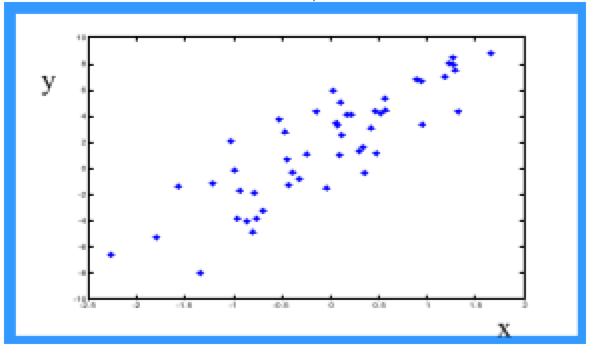
- **Supervised learning**
  - Learning mapping between input x and desired output y
  - Teacher gives me y's for the learning purposes
- **Unsupervised learning**
  - Learning relations between data components
  - No specific outputs given by a teacher
- **Reinforcement learning**
  - Learning mapping between input x and desired output y
  - Critic does not give me y's but instead a signal (reinforcement) of how good my answer was
- **Other types of learning:**
  - **Concept learning, explanation-based learning, etc.**

A learning system: basic cycle

1. **Data:** $D = \{d_1, d_2, \ldots, d_n\}$
2. **Model selection:**
   a. **Select a model** or a set of models (with parameters) E.g. $y = ax + b$
3. **Choose the objective function** $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
   a. **Squared error**
4. **Learning:**
   a. Find the set of parameters optimizing the error function
      i. The model and parameters with the smallest error

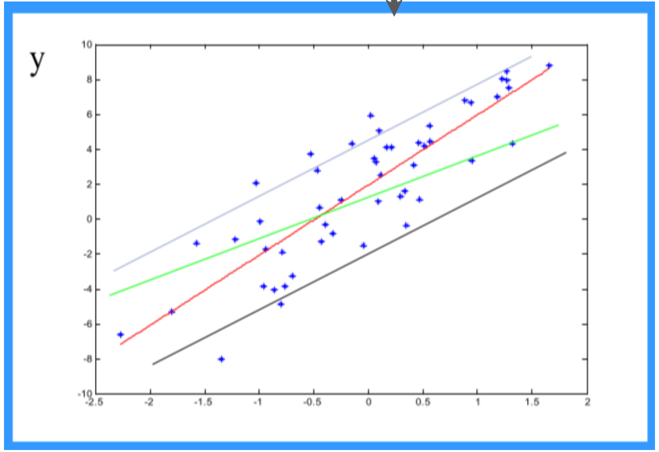
A learning system: basic cycle

1. **Data:** $D = \{d_1, d_2, \ldots, d_n\}$
2. **Model selection:**
   a. **Select a model** or a set of models (with parameters) E.g. *y =ax+ b*
3. **Choose the objective function** $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
   a. **Squared error**
4. **Learning:**
   a. Find the set of parameters optimizing the error function
      i. The model and parameters with the smallest error



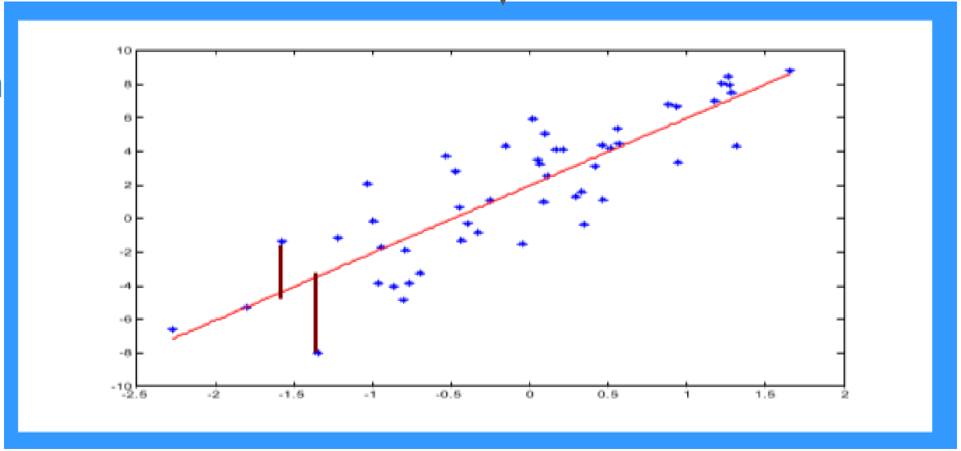
A learning system: basic cycle

1. **Data:** $D = \{d_1, d_2, \ldots, d_n\}$
2. **Model selection:**
   a. **Select a model** or a set of models (with parameters) E.g. $y = ax + b$
3. **Choose the objective function** $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
   a. **Squared error**
4. **Learning:**
   a. Find the set of parameters optimizing the error function
      i. The model and parameters with the smallest error



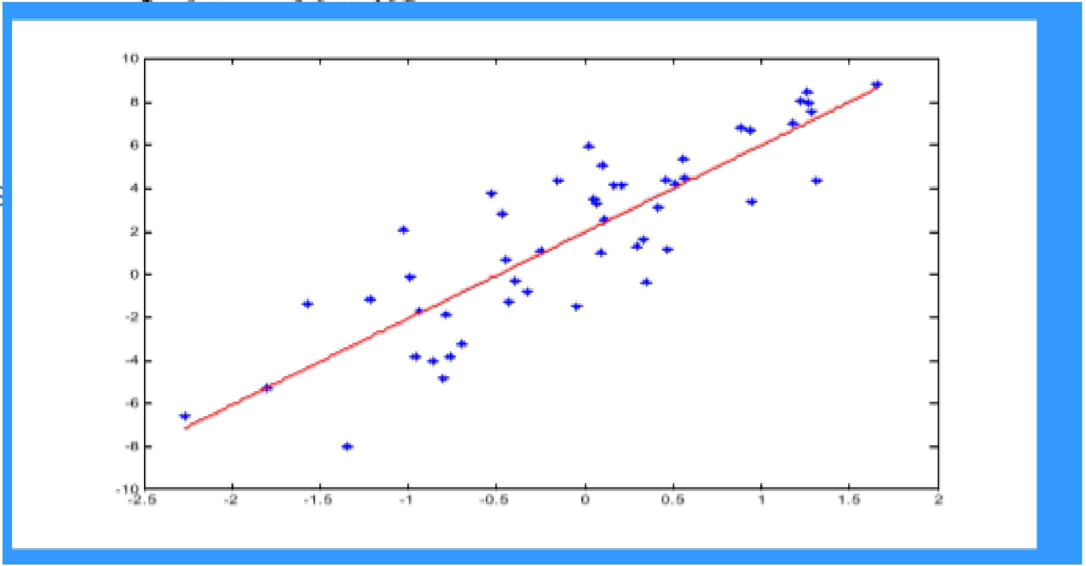
A learning system: basic cycle

1. **Data:** $D = \{d_1, d_2, \ldots, d_n\}$
2. **Model selection:**
   a. **Select a model** or a set of models (with parameters) E.g. $y = ax + b$
3. **Choose the objective function**
   a. **Squared error** $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
4. **Learning:**
   a. Find the set of parameters optimizing
      i. The model and parameters with



A learning system: basic cycle

1. **Data:** $D = \{d_1, d_2, \ldots, d_n\}$
2. **Model selection:**
    a. **Select a model** or a set of models (with parameters) E.g. *y =ax+ b*
3. **Choose the objective function**
    a. **Squared error**
4. **Learning:**
    a. Find the set of parameters optim
        i. The model and parameters



A learning system: basic cycle

1. **Data:** $D = \{d_1, d_2, \ldots, d_n\}$
2. **Model selection:**
   a. **Select a model** or a set of models (with parameters) E.g. $y = ax + b$
3. **Choose the objective function** $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
   a. **Squared error**
4. **Learning:**
   a. Find the set of parameters optimizing the error function
      i. The model and parameters with the smallest error

But there are problems one must be careful about …

Evaluation of the learned model

Problem

- We fit the model based on past examples observed in D
- But ultimately we are interested in learning the mapping that performs well on the whole population of examples

Training data: Data used to fit the parameters of the model

Training error:

$$Error(D, f) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$$

True (generalization) error (over the whole population):

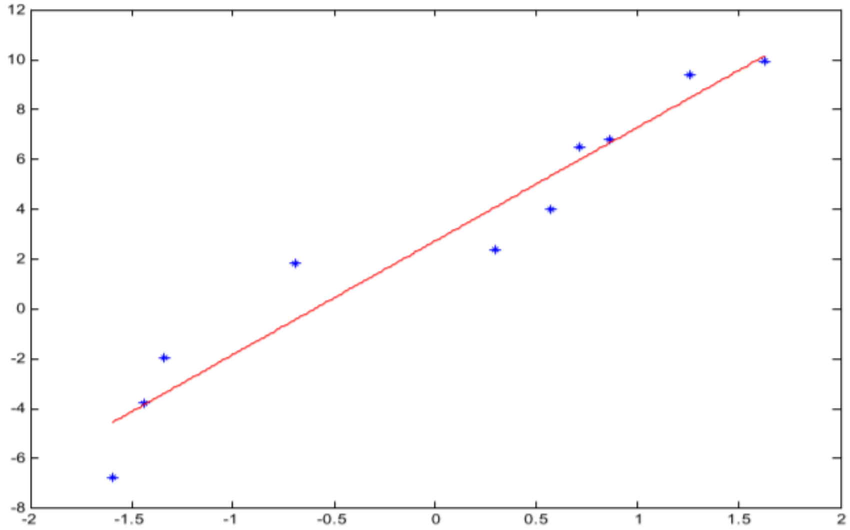
$$E_{(x,y)}[(y - f(x))^2]$$ Mean squared error

Training error tries to approximate the true error !!!!

Does a good training error imply a good generalization error ?

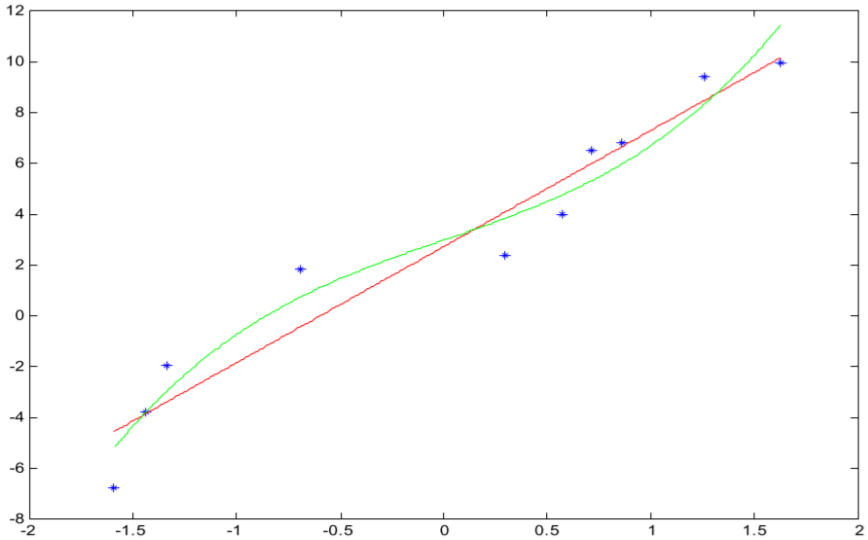
Overfitting

- Fitting a linear function with the square error
- Error is nonzero



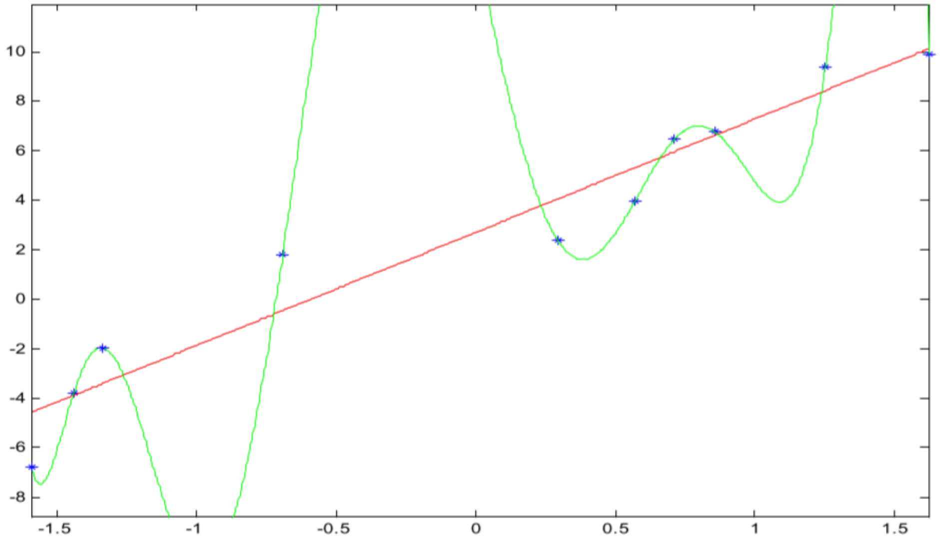
Overfitting

- Linear vs. cubic polynomial
- Higher order polynomial leads to a better fit, smaller error



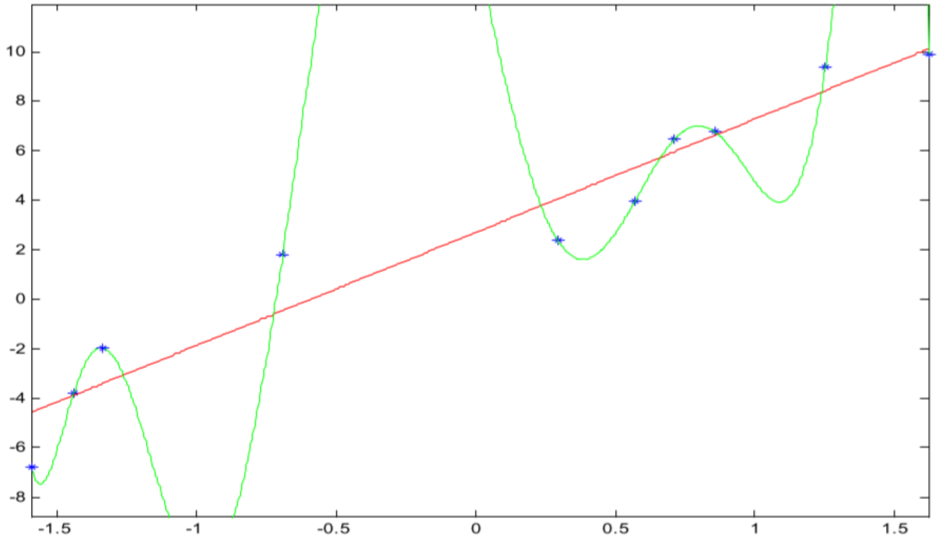
Overfitting

- For 10 data points, degree 9 polynomial gives a perfect fit (Lagrange interpolation). Error is zero.
- Is it always good to minimize the training error? NO !!



Overfitting

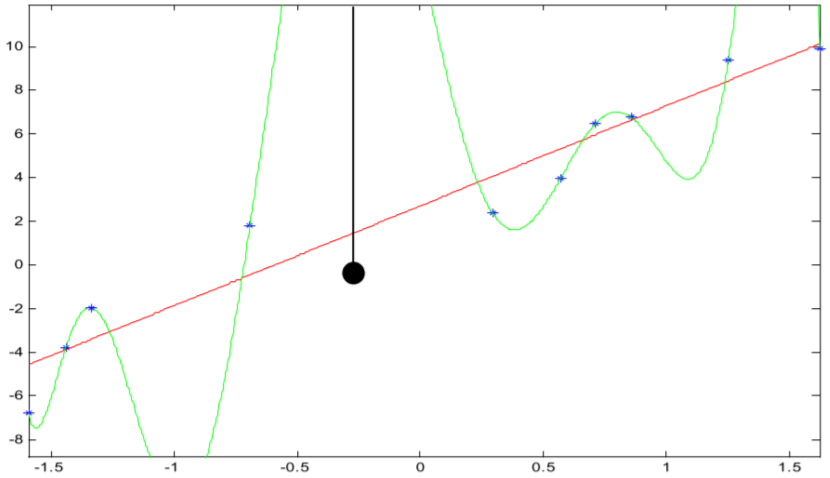
- For 10 data points, degree 9 polynomial gives a perfect fit (Lagrange interpolation). Error is zero.
- Is it always good to minimize the training error? NO !!
- **More important:** How do we perform on the unseen data?



Overfitting

Situation when the training error is low and the generalization error is high.
Causes of the phenomenon:

- Model with a large number of parameters (degrees of freedom)
- Small data size (as compared to the complexity of the model)



How to evaluate the learner’s performance?

- **Generalization error** is the true error for the population of examples we would like to optimize

$$E_{(x,y)}[(y - f(x))^2]$$

- But it cannot be computed exactly
- **Sample mean only approximates the true mean**
- **Optimizing (mean) training error can lead to the overfit,** i.e. training error may not reflect properly the generalization error

$$\frac{1}{n}\sum_{i=1,..n}(y_i - f(x_i))^2$$

- So how to test the generalization error?

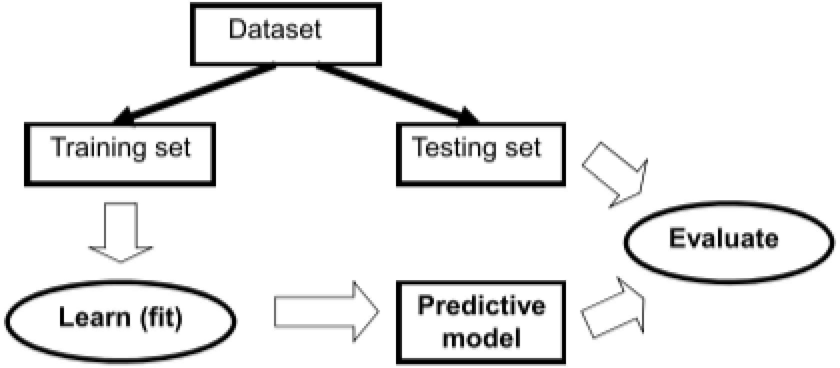
How to evaluate the learner's performance?

- **Generalization error** is the true error for the population of examples we would like to optimize
- Sample mean only approximates it
- Two ways to assess the generalization error is:
  - **Theoretical:** Law of Large numbers
    - statistical bounds on the difference between true and sample mean errors
  - **Practical:** Use a separate data set with m data samples to test the model •
    - **(Mean) test error**

$$\frac{1}{m}\sum_{j=1,..m}(y_j - f(x_j))^2$$

Testing of learning models

- Simple holdout method
  - Divide the data to the training and test data



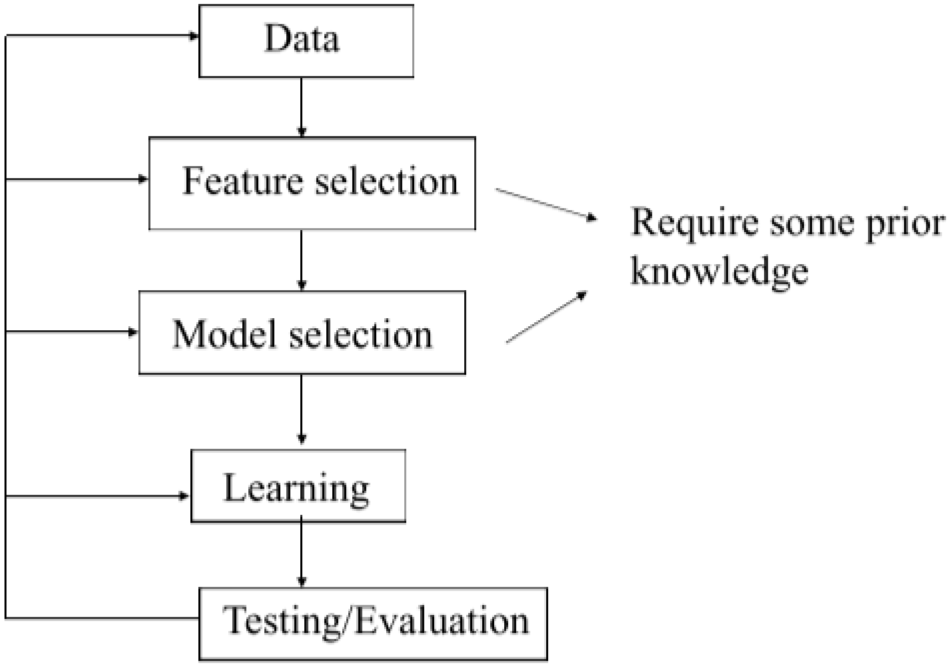
- Typically 2/3 training and 1/3 testing

Basic experimental setup to test the learner's performance

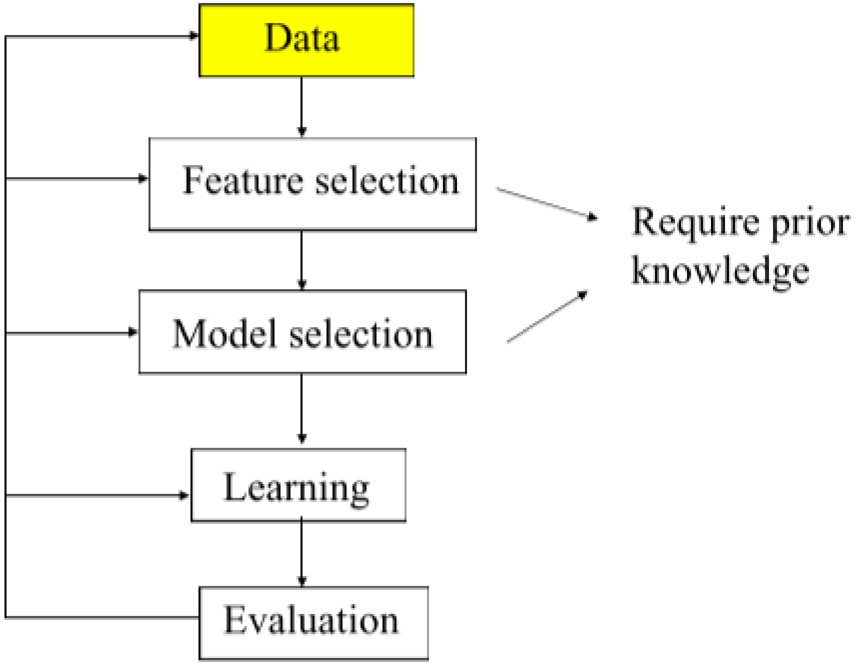
1. Take a dataset D and divide it into:
   a. Training data set
   b. Testing data set
2. Use the training set and your favorite ML algorithm to train the learner
3. Test (evaluate) the learner on the testing data set

The results on the testing set can be used to compare different learners powered with different models and learning algorithms

Design cycle



Design cycle



Data

Data may need a lot of:

- Cleaning
- Preprocessing (conversions)

Cleaning:

- ➔ Get rid of errors, noise
- ➔ Removal of redundancies

Preprocessing:

- ➔ Renaming
- ➔ Rescaling (normalization)
- ➔ Discretization
- ➔ Abstraction
- ➔ Aggregation
- ➔ New attributes

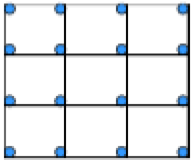
Data preprocessing

- **Renaming (relabeling)** categorical values to numbers
  - dangerous in conjunction with some learning methods
  - numbers will impose an order that is not warranted

High → 2 Normal → 1 Low → 0 √	True → 2 False → 1 Unknown → 0 ✗	Red → 2 Blue → 1 Green → 0 ✗

- **Rescaling (normalization):** continuous values transformed to some range, typically [-1, 1] or [0,1].

- **Discretizations (binning):** continuous values to a finite set of discrete values



- **Abstraction:** merge together categorical values
- **Aggregation:** summary or aggregation operations, such minimum value, maximum value, average etc.
- **New attributes:**
  - example: obesity-factor = weight/height

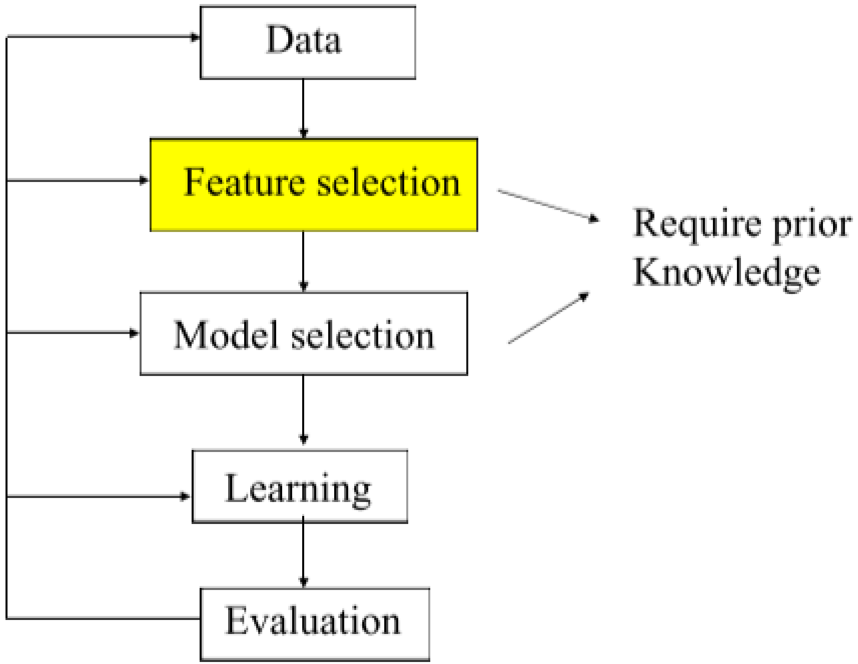
Data biases

- **Watch out for data biases:**
  - Try to understand the data source
  - Make sure the data we make conclusions on are the same as data we used in the analysis
  - It is very easy to derive "unexpected" results when data used for analysis and learning are biased (pre-selected)
- Results (conclusions) derived for a biased dataset do not hold in general !!!

Example 1: Risks in pregnancy study

- Sponsored by DARPA at military hospitals
- Study of a large sample of pregnant woman who visited military hospitals
- **Conclusion:** the factor with the largest impact on reducing risks during pregnancy (statistically significant) is a pregnant woman being single
- a woman that is single → the smallest risk
- What is wrong?

Design cycle



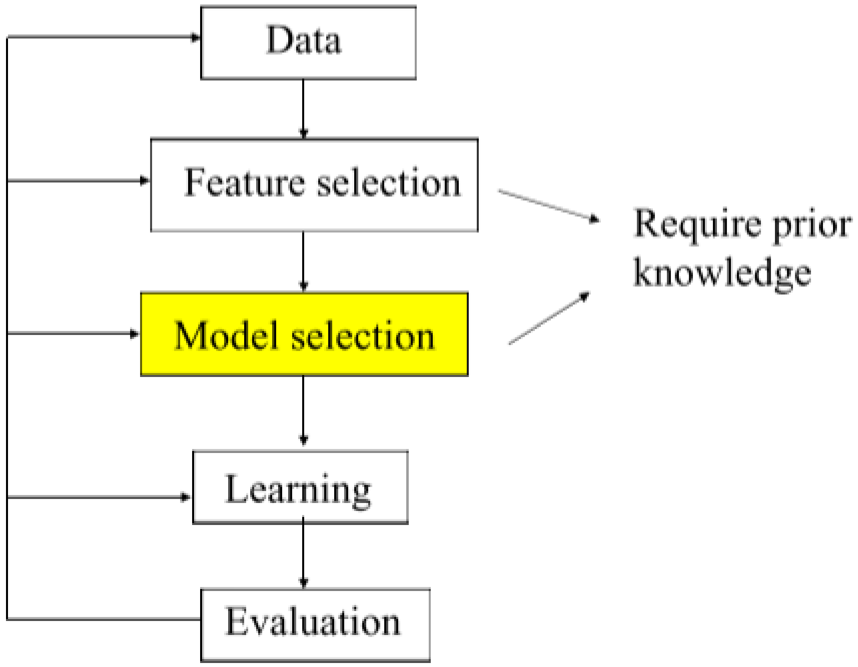
Feature selection

- **The size (dimensionality) of a sample** can be enormous d

  $x_i = (x_i^1, x_i^2, ..., x_i^d)$ d -very large

- **Example: document classification**
  - **thousands of documents**
  - 10,000 different words
  - **Features/Inputs:** counts of occurrences of different words
  - Overfit threat - too many parameters to learn, not enough samples to justify the estimates the parameters of the model
- **Feature selection: reduces the feature sets**
  - **Methods for removing input features**

Design cycle



Model selection

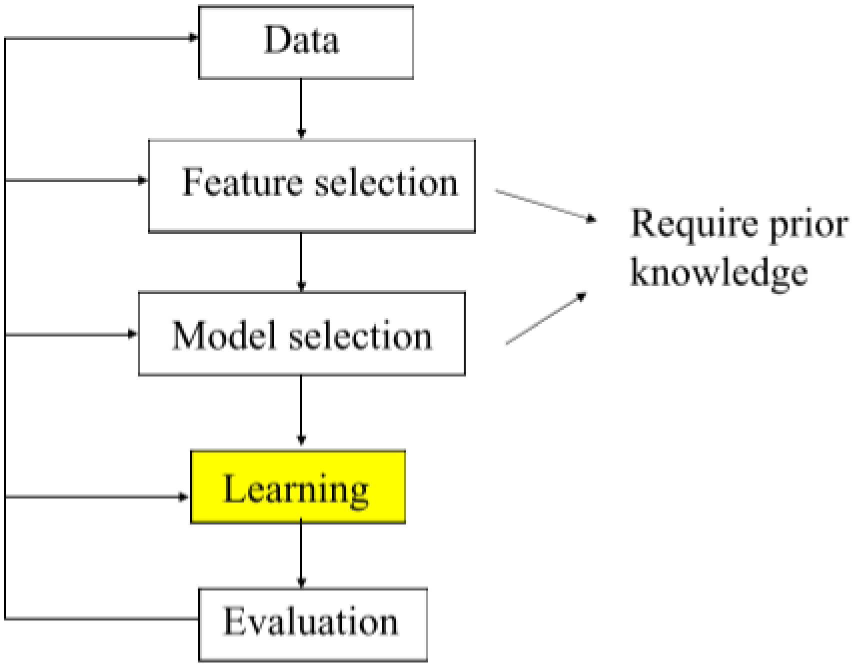
- **What is the right model to learn?**
  - A prior knowledge helps a lot, but still a lot of guessing
  - Initial data analysis and visualization
    - We can make a good guess about the form of the distribution, shape of the function
  - Independences and correlations
- • **Overfitting problem**
  - Take into account the **bias and variance** of error estimates
  - Simpler (more biased) model – parameters can be estimated more reliably (smaller variance of estimates)
  - Complex model with many parameters – parameter estimates are less reliable (large variance of the estimate)

Solutions for overfitting

How to make the learner avoid the overfit?

- **Assure sufficient number of samples** in the training set
  - May not be possible (small number of examples)
- **Hold some data out of the training set = validation set**
  - Train (fit) on the training set (w/o data held out);
  - Check for the generalization error on the validation set, choose the model based on the validation set error (random re-sampling validation techniques)
- **Regularization (Occam's Razor)**
  - Explicit preference towards simple models
  - Penalize for the model complexity (number of parameters) in the objective function

Design cycle



Learning

- **Learning = optimization problem**. Various criteria:
  - **Mean square error**

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} Error(\mathbf{w}) \qquad Error(\mathbf{w}) = \frac{1}{N} \sum_{i=1,..N} (y_i - f(x_i, \mathbf{w}))^2$$

  - **Maximum likelihood (ML) criterion**

$$\Theta^* = \arg\max_{\Theta} P(D \mid \Theta) \qquad Error(\Theta) = -\log P(D \mid \Theta)$$

  - **Maximum posterior probability (MAP)**

$$\Theta^* = \arg\max_{\Theta} P(\Theta \mid D) \qquad P(\Theta \mid D) = \frac{P(D \mid \Theta) P(\Theta)}{P(D)}$$

Learning

Learning = optimization problem

- Optimization problems can be hard to solve. Right choice of a model and an error function makes a difference.
- **Parameter optimizations (continuous space)**
  - Linear programming, Convex programming
  - Gradient methods: grad. descent, Conjugate gradient
  - Newton-Rhapson (2nd order method)
  - Levenberg-Marquard

  Some can be carried **on-line** on a sample by sample basis

- **Combinatorial optimizations (over discrete spaces):**
  - Hill-climbing
  - Simulated-annealing
  - Genetic algorithms

Parametric optimizations

- Sometimes can be solved directly but this depends on the objective function and the model
  - **Example:** squared error criterion for linear regression
- Very often the error function to be optimized is not that nice.

$$Error(\mathbf{w}) = f(\mathbf{w}) \qquad \mathbf{w} = (w_0, w_1, w_2 \ldots w_k)$$

- a complex function of weights (parameters)

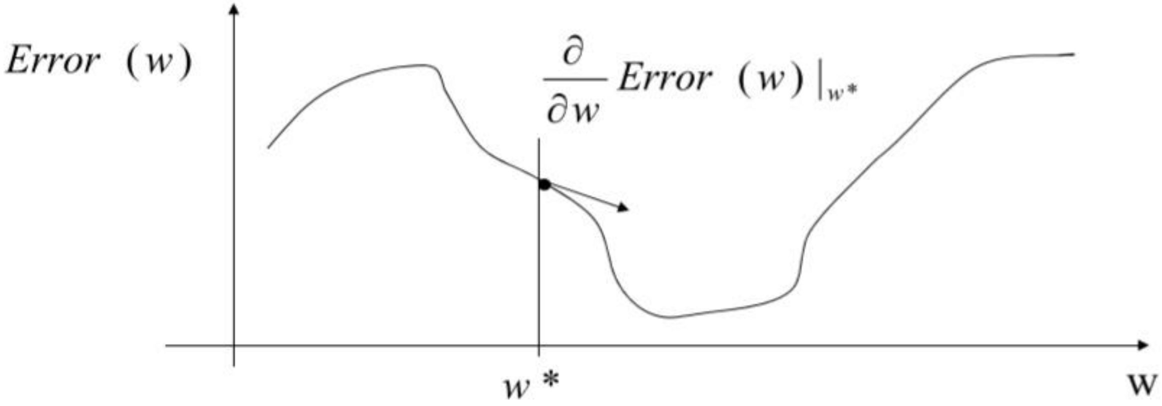
Goal: $\mathbf{w}^* = \arg\min_{\mathbf{w}} f(\mathbf{w})$

- **Example of a possible method: Gradient-descent method**

Idea: move the weights (free parameters) gradually in the error decreasing direction

Gradient descent method

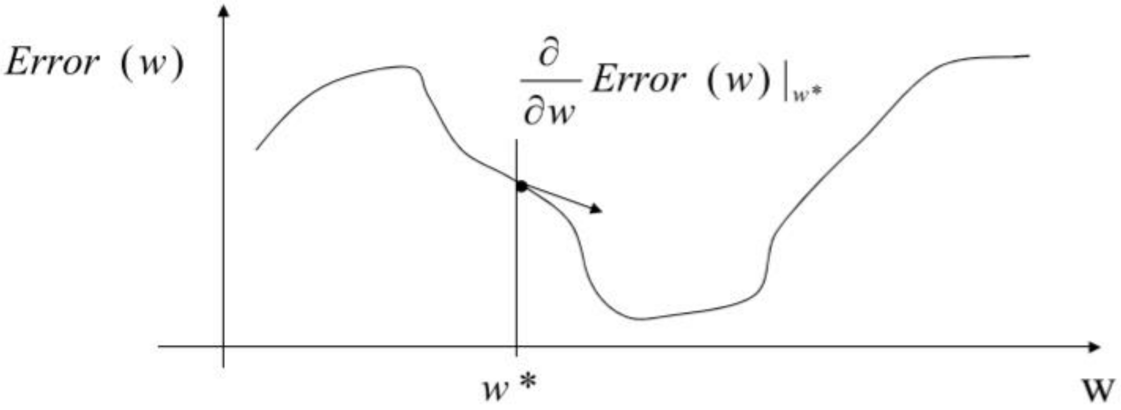
- Descend to the minimum of the function using the gradient information



- Change the parameter value of w according to the gradient

$$w \leftarrow w* - \alpha \frac{\partial}{\partial w} Error\ (w)|_{w*}$$

Gradient descent method



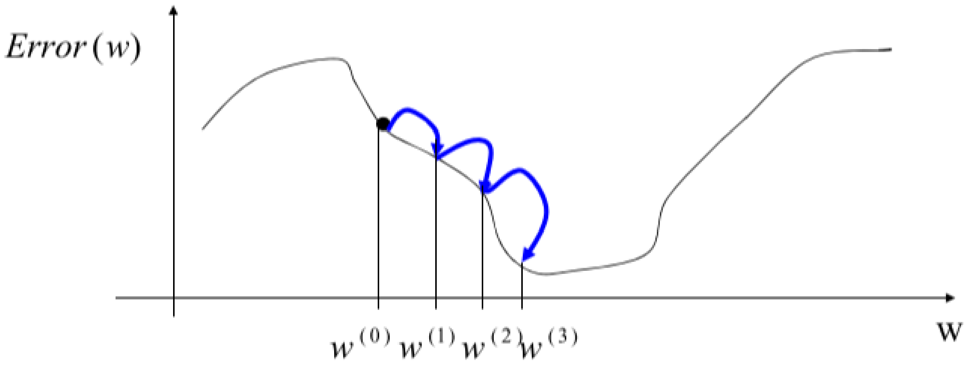
- New value of the parameter

$$w \leftarrow w^* - \alpha \frac{\partial}{\partial w} Error\ (w)|_{w*}$$

$\alpha > 0$ - a learning rate (scales the gradient changes)

Gradient descent method

- To get to the function minimum repeat (iterate) the gradient based update few times
- **Problems:** local optima, saddle points, slow convergence • More complex optimization techniques use additional
- information (e.g. second derivatives)



On-line learning (optimization)

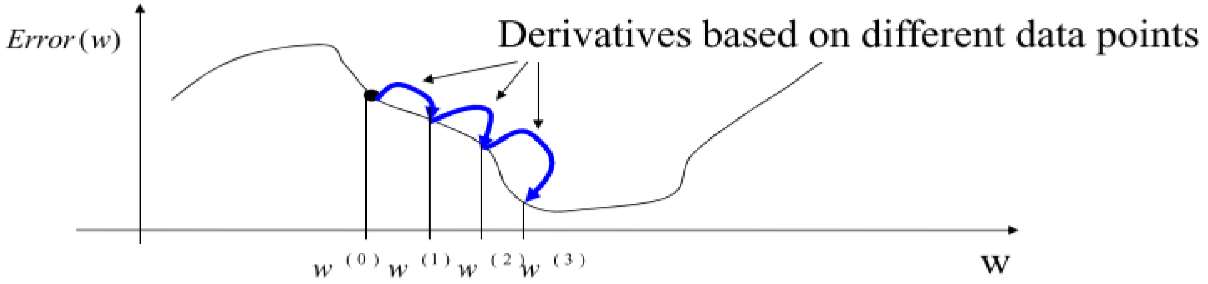
- Error function looks at all data points at the same time

$$\text{E.g.}\quad Error(\mathbf{w}) = \frac{1}{n}\sum_{i=1\dots n}(y_i - f(x_i,\mathbf{w}))^2$$

- **On-line error** - separates the contribution from a data point

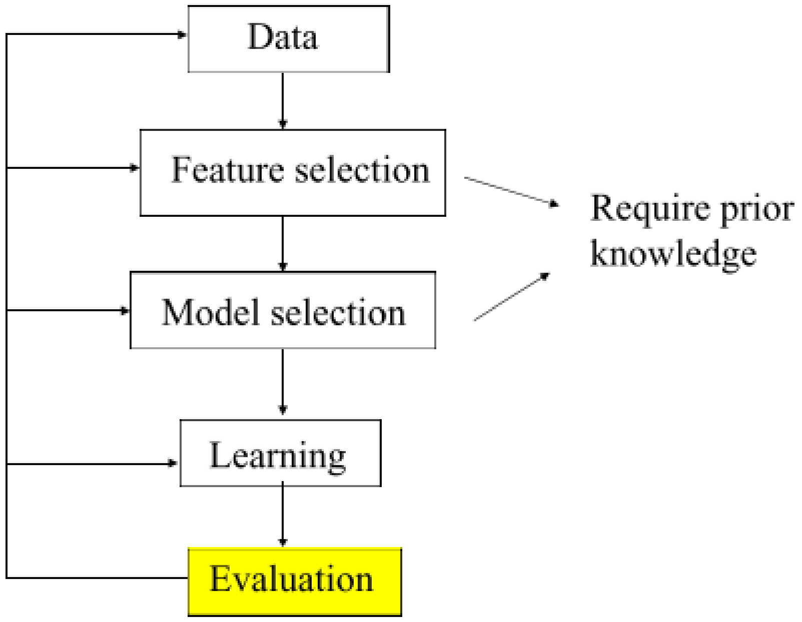
$$Error_{\text{ON-LINE}}(\mathbf{w}) = (y_i - f(x_i,\mathbf{w}))^2$$

- **Example: On-line gradient descent**



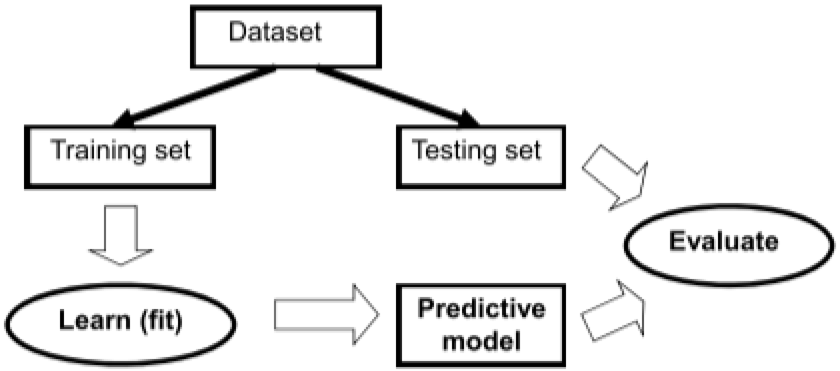
- **Advantages:**
  - **simple learning algorithm**
  - **no need to store data (on-line data streams)**

Design cycle



Evaluation of learning models

- Simple holdout method
    - Divide the data to the training and test data

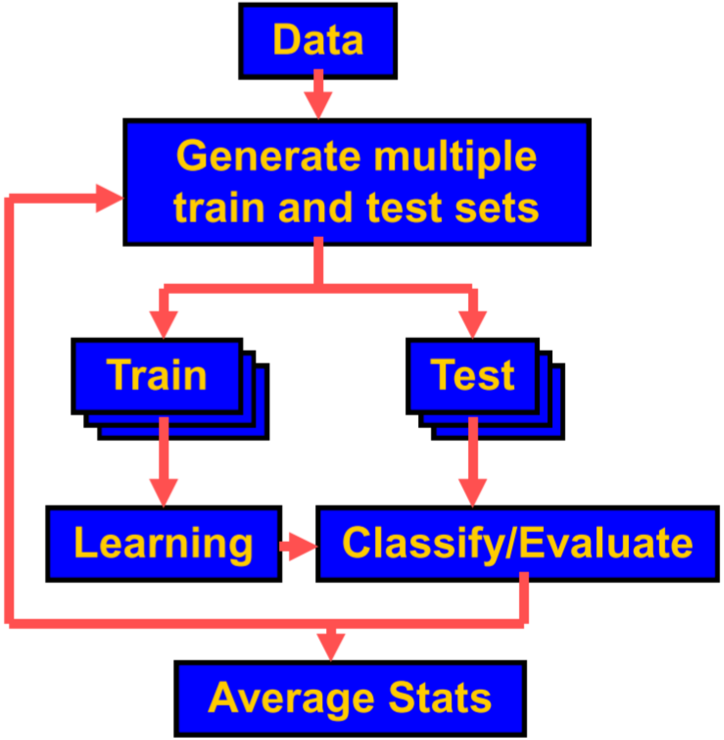


- Typically 2/3 training and 1/3 testing

Evaluation

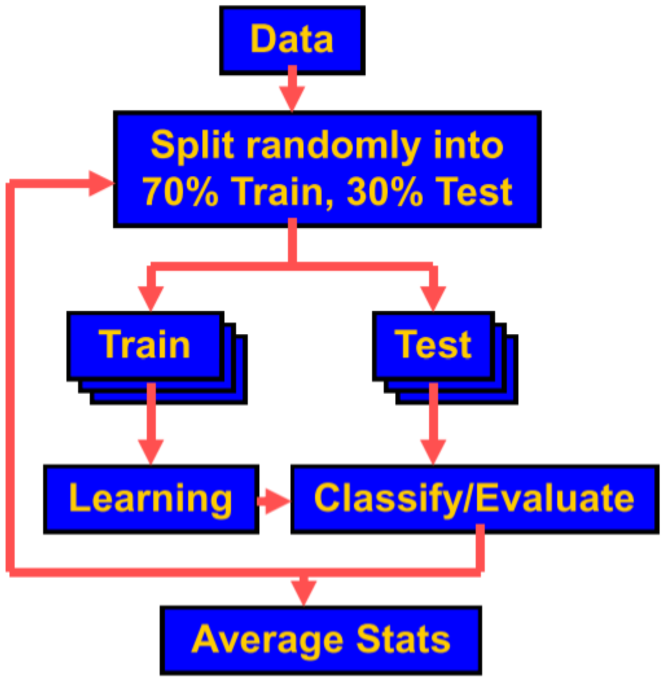
Other more complex methods

- Use multiple train/test sets
- Based on various random re-sampling schemes:
  - Random sub-sampling
  - Cross-validation
  - Bootstrap



Evaluation

- Random sub-sampling
  - Repeat a simple
  - holdout method k times

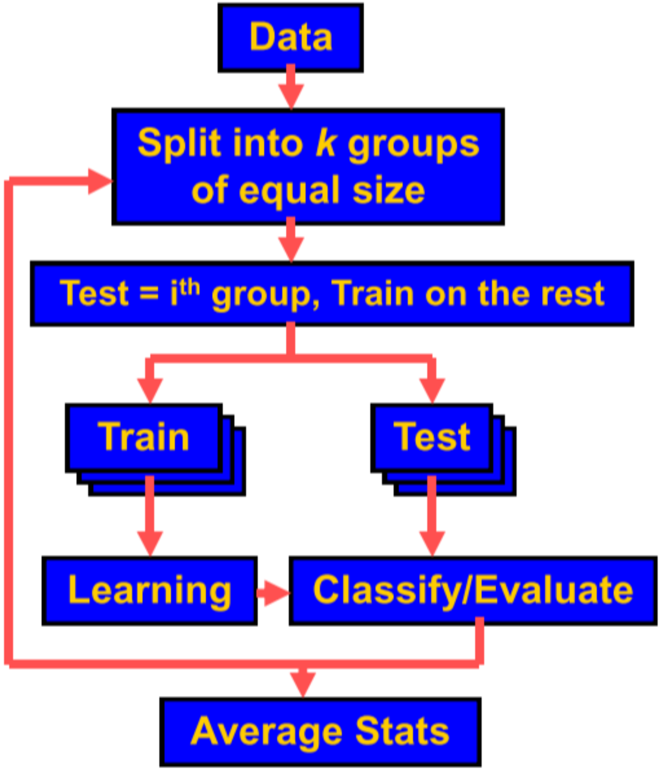


Evaluation

Cross-validation (k-fold)

- Divide data into k disjoint groups, test on k-th group/train on the rest
- Typically 10-fold cross-validation
- Leave one out cross-validation

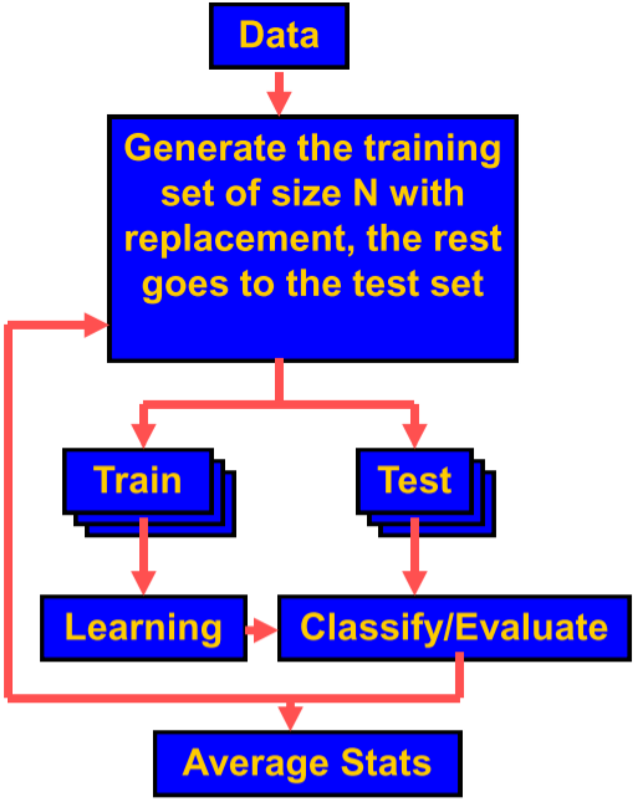
(k = size of the data D)



Evaluation

Bootstrap

- The training set of size N = size of the data D
- Sampling with the replacement



Any Questions??