# CS 2750 Machine Learning

## Lecture 2

# Machine Learning

**Milos Hauskrecht**
milos@cs.pitt.edu
5329 Sennott Square, x4-8845

http://www.cs.pitt.edu/~milos/courses/cs2750/



# Administration

**Instructor:**

**Milos Hauskrecht**
milos@cs.pitt.edu
5329 Sennott Square, x4-8845

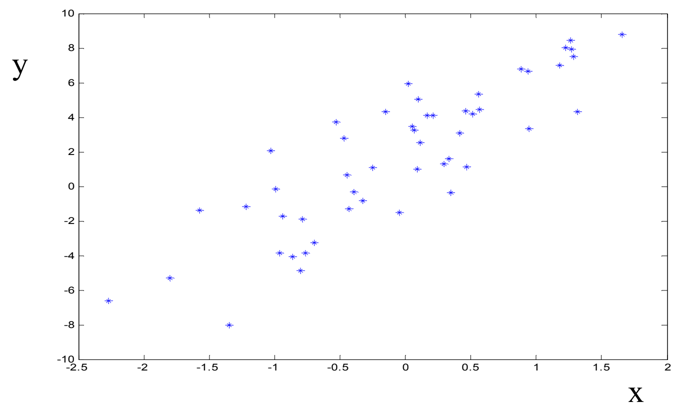
**TA:**

**Chenhai Xi**
chenhai@cs.pitt.edu
5503 Sennott Square,

**Office hours:** TBA

## Learning

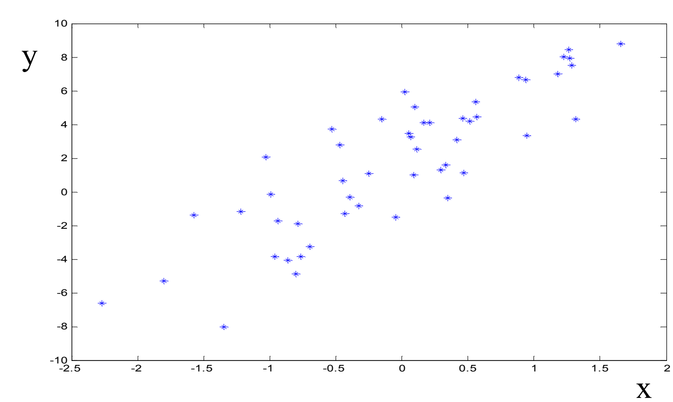
- Assume we see examples of pairs $(\mathbf{x}, y)$ and we want to learn the mapping $f: X \rightarrow Y$ to predict future ys for values of $\mathbf{x}$
- We get the data what should we do?





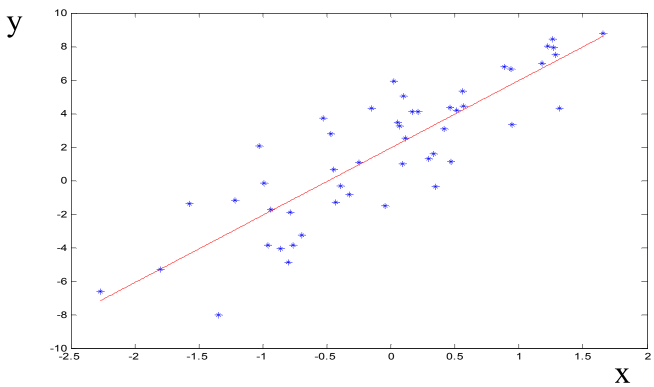

## Learning bias

- **Problem:** many possible functions $f: X \rightarrow Y$ exists for representing the mapping between **x** and y
- Which one to choose? Many examples still unseen!



# Learning bias

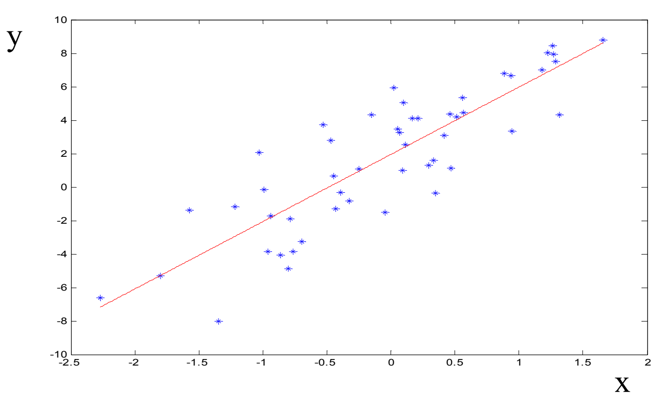
- Problem is easier when we make an assumption about the model, say, $f(x) = ax + b$
- Restriction to a linear model is an example of learning bias





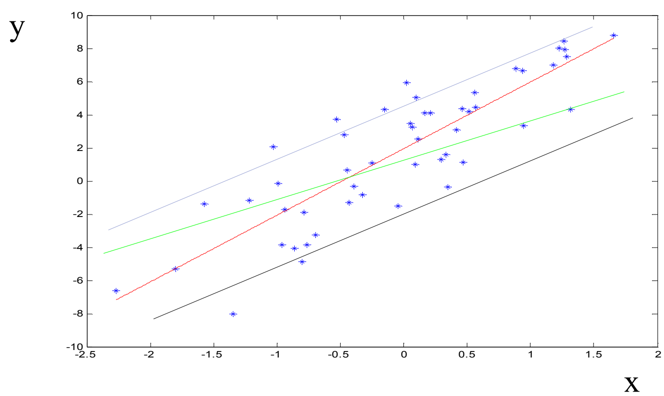

# Learning bias

- **Bias** provides the learner with some basis for choosing among possible representations of the function.
- **Forms of bias:** constraints, restrictions, model preferences
- **Important: There is no learning without a bias!**



# Learning bias

- Choosing a parametric model or a set of models is not enough
  Still too many functions $f(x) = ax + b$
  – One for every pair of parameters *a, b*






# Fitting the data to the model

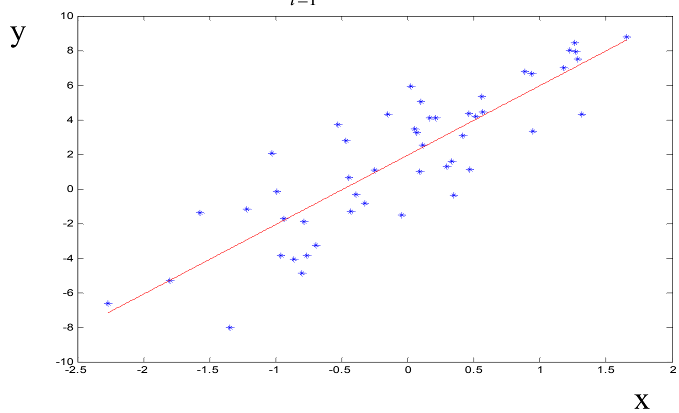
We are interested in finding the **best set** of model parameters

- **Objective: Find the set of parameters** that:
  – reduces the misfit between the model and observed data
  – Or, (in other words) that explain the data the best
- **Error function:**
  – **Measures of misfit between the data and the model**
- **Examples of error functions:**
  – Average squared error $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
  – Average misclassification error $\frac{1}{n}\sum_{i=1}^{n} 1_{y_i \neq f(x_i)}$

  Average # of misclassified cases

# Fitting the data to the model

- **Linear regression**
  – Least squares fit with the linear model
  – minimizes $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$






# Typical learning

**Three basic steps:**

- **Select a model** or a set of models (with parameters)
  E.g. $y = ax + b$
- **Select the error function** to be optimized
  E.g. $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
- **Find the set of parameters optimizing the error function**
  – The model and parameters with the smallest error represent the best fit of the model to the data

But there are problems one must be careful about …

# Learning

**Problem**

- We fit the model based on past experience (past examples seen)
- 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:** $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$

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

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

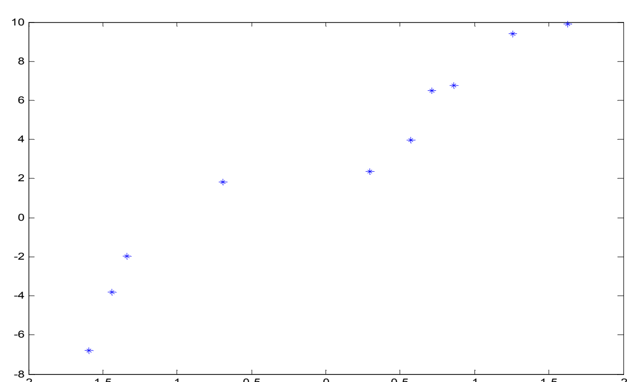
**Training error tries to approximate the true error !!!!**

Does a good training error imply a good generalization error ?



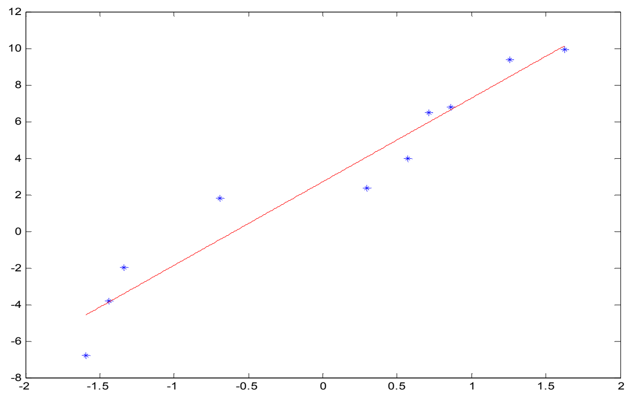
# Overfitting

- Assume we have a set of 10 points and we consider polynomial functions as our possible models



# Overfitting

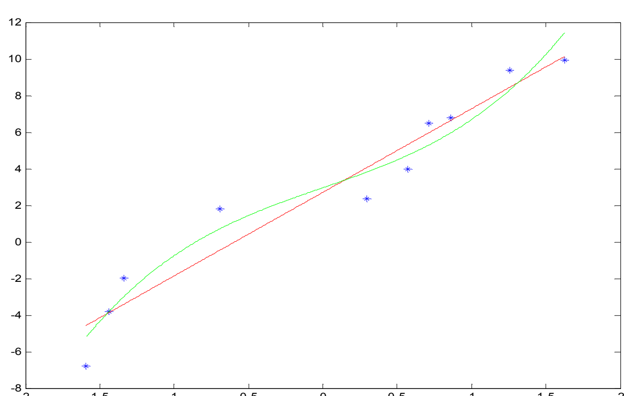
- Fitting a linear function with the square error
- Error is nonzero





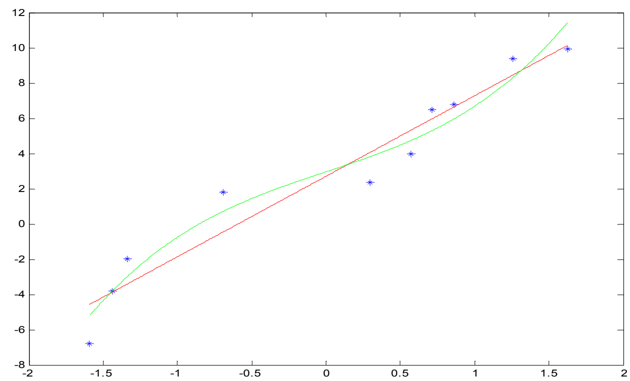

# Overfitting

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



# Overfitting

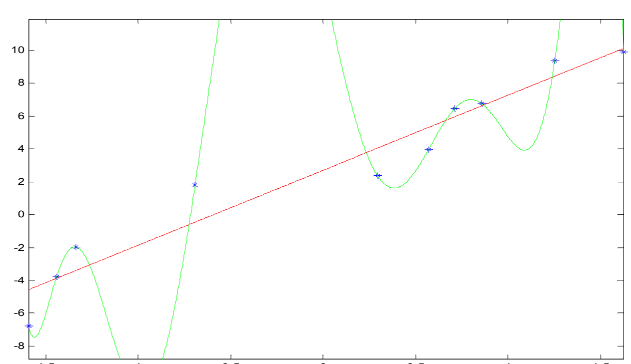
- Is it always good to minimize the error of the observed data?





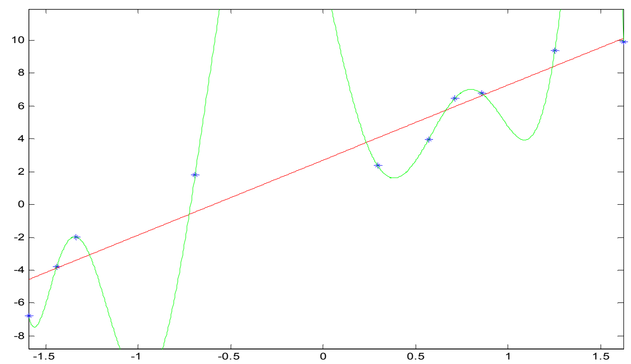

# Overfitting

- For 10 data points, the degree 9 polynomial gives a perfect fit (Lagrange interpolation). Error is zero.
- Is it always good to minimize the training 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 !!
- **More important:** How do we perform on the unseen data?

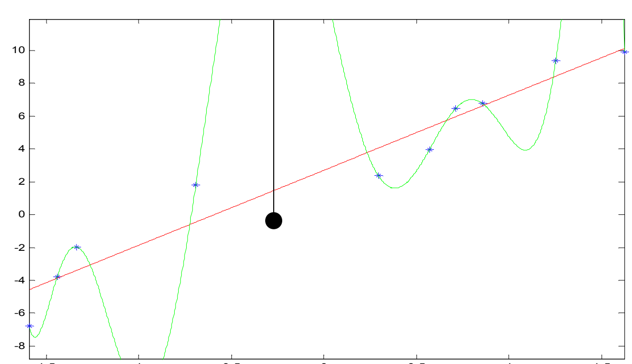





# Overfitting

**Situation** when the training error is low and the generalization error is high. Causes of the overfitting 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 the 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

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

- **Sample mean only approximates it**
- **Two ways to estimate generalization error:**
  - **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
    - **Test error** $\frac{1}{m}\sum_{j=1,..m}(y_j - f(x_j))^2$

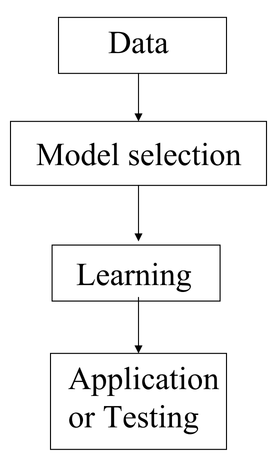
## Basic experimental setup to test the learner's performance

1. **Take a dataset D and divide it into:**
   - **Training data set**
   - **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 of a learning system (first view)



# Design of a learning system.

**1. Data:** $D = \{d_1, d_2, .., d_n\}$

**2. Model selection:**

- **Select a model** or a set of models (with parameters)

  E.g. $y = ax + b$

- **Select the error function** to be optimized

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

**3. Learning:**

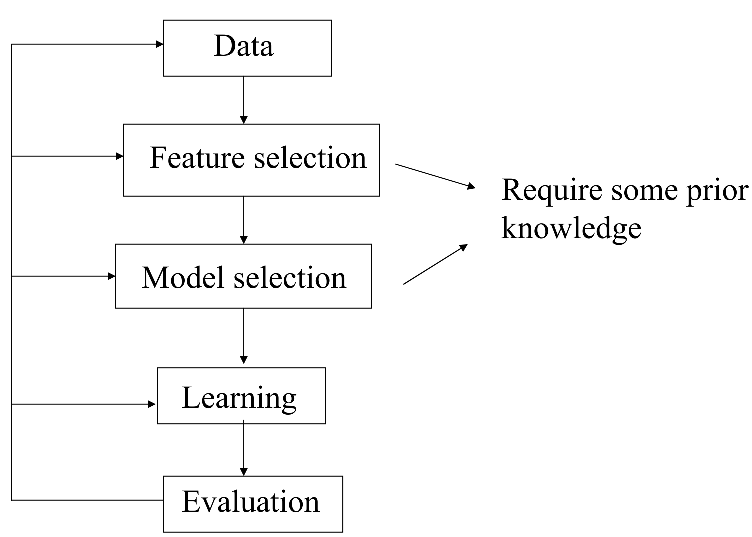
- **Find the set of parameters optimizing the error function**
  - The model and parameters with the smallest error

**4. Application:**

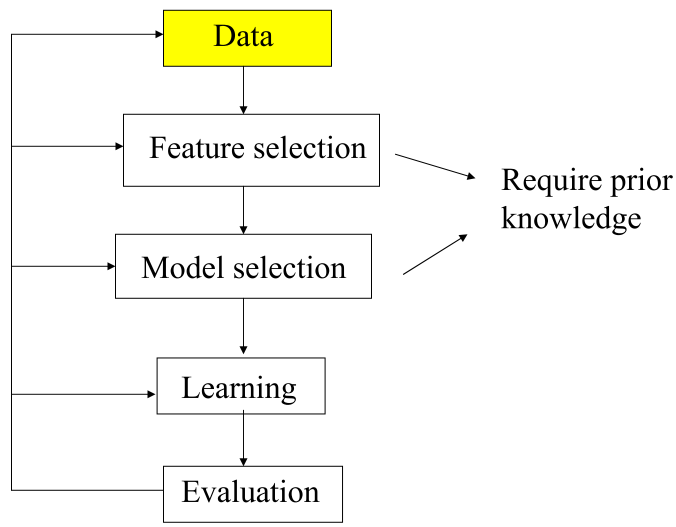
- **Apply the learned model**
  - E.g. predict ys for new inputs **x** using learned $f(\mathbf{x})$



# 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)**
- **Discretizations**
- **Abstraction**
- **Aggregation**
- **New attributes**

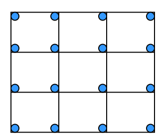
# Data preprocessing

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

High → 2
Normal → 1
Low → 0

True → 2
False → 1
Unknown → 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





# Data preprocessing

- **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
  - It is very easy to derive "unexpected" results when data used for analysis and learning are biased (pre-selected)

- **Results (conclusions) derived for pre-selected data do not hold in general !!!**



## Data biases

**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
- Single woman → the smallest risk
- What is wrong?

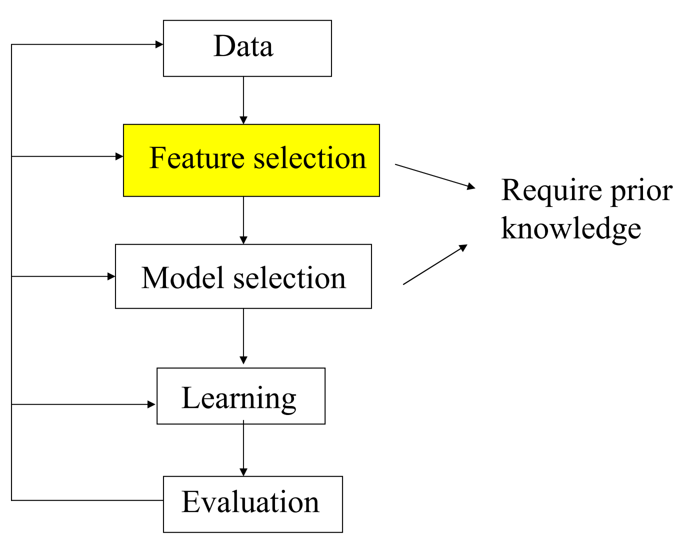
# Data

**Example 2: Stock market trading (example by Andrew Lo)**

– Data on stock performances of companies traded on stock market over past 25 year
– **Investment goal:** pick a stock to hold long term
– **Proposed strategy**: invest in a company stock with an IPO corresponding to a Carmichael number
- **Evaluation result:** excellent return over 25 years
- Where the magic comes from?



# Design cycle



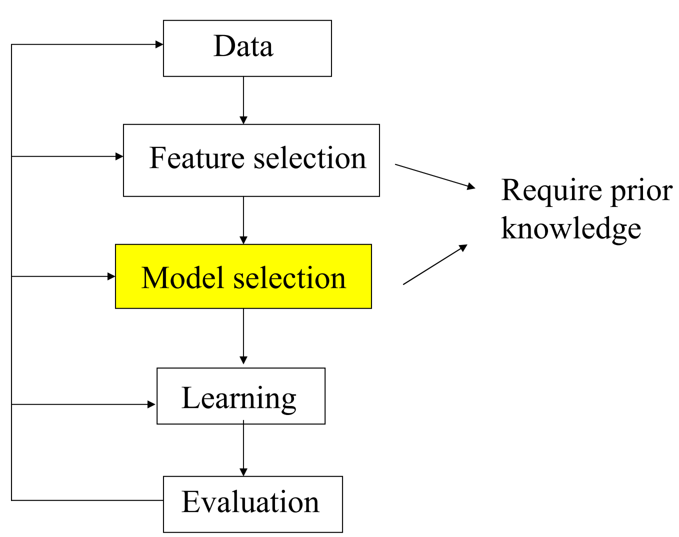
# Feature selection

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

  $x_i = (x_i^1, x_i^2, .., x_i^d)$ $d$ - very large
- **Example: document classification**
  - 10,000 different words
  - Inputs: counts of occurrences of different words
  - Too many parameters to learn (not enough samples to justify the estimates the parameters of the model)
- **Dimensionality reduction: replace inputs with features**
  - **Extract relevant inputs** (e.g. mutual information measure)
  - **PCA** – principal component analysis
  - **Group (cluster) similar words** (uses a similarity measure)
    - Replace with the group label



# 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)

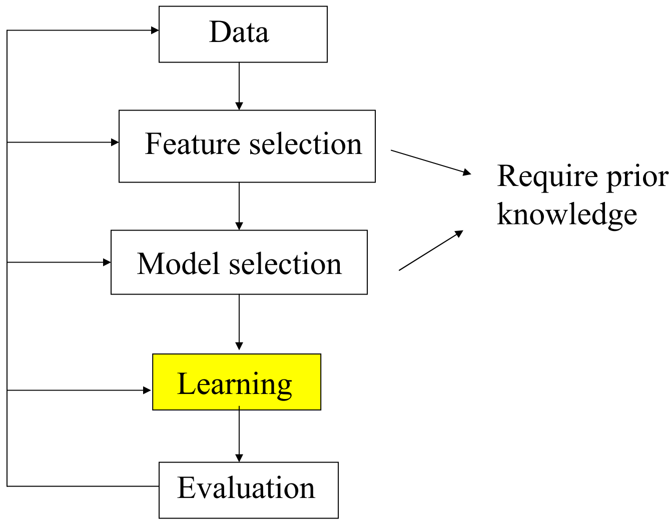


# Solutions for overfitting

**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 resampling validation techniques)
- **Regularization (Occam's Razor)**
  - Penalize for the model complexity (number of parameters)
  - Explicit preference towards simple models

# 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**
  - Gradient descent, Conjugate gradient ($1^{st}$ order method)
  - Newton-Rhapson ($2^{nd}$ 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 error function and the model
  - **Example:** squared error criterion for linear regression
- Very often the error function to be optimized is not that nice.

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

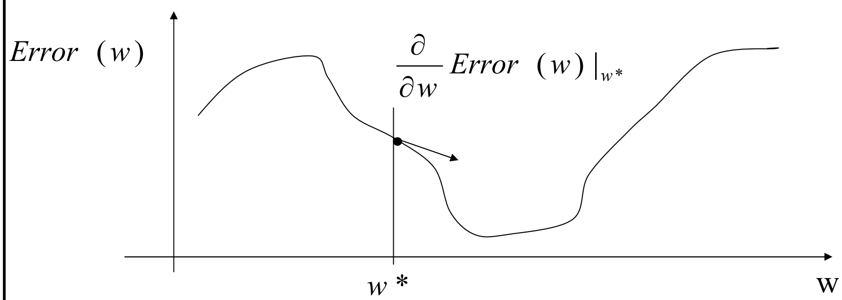
  - a complex function of weights (parameters)

  **Goal:** $\mathbf{w}^* = \arg\min_{\mathbf{w}} f(\mathbf{w})$
- One solution: **iterative optimization methods**
- **Example: 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

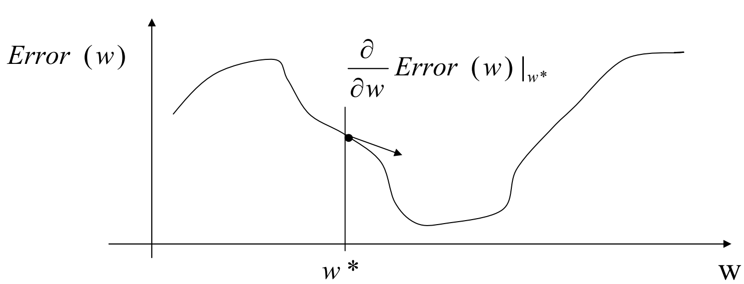



- Change the parameter value of w according to the gradient

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



# Gradient descent method



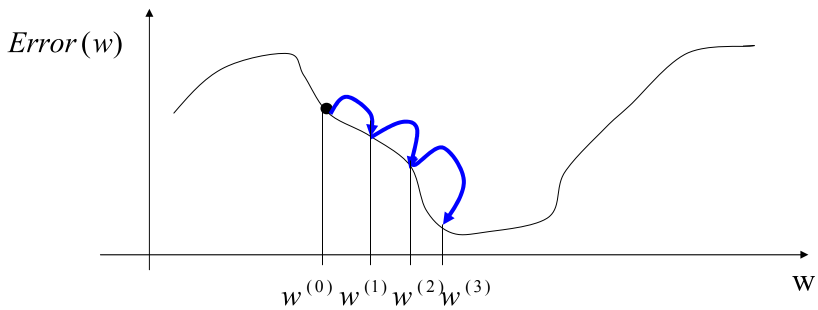

- New value of the parameter

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

$\alpha > 0$ - 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)

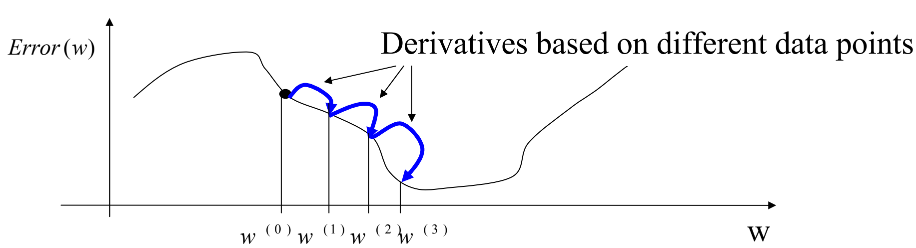
- Error function looks at all data points at the same time

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

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

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

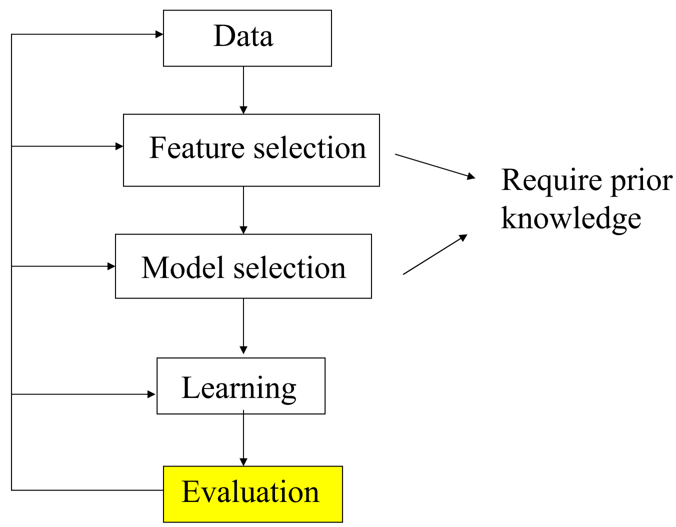
- **Example: On-line gradient descent**




- **Advantages: 1. simple learning algorithm**

  **2. no need to store data (on-line data streams)**

# Design cycle






# Evaluation.

- **Simple holdout method.**
  - Divide the data to the training and test data.
- **Other more complex methods**
  - Based on random re-sampling validation schemes:
    - cross-validation, random sub-sampling.
- What if we want to compare the predictive performance on a classification or a regression problem for two different learning methods?
- **Solution:** compare the error results on the test data set
- **Possible answer**: the method with better (smaller) testing error gives a better generalization error.
- But we need to use statistics to validate the choice