CS 2750 Machine Learning

Lecture 2

Machine Learning

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

2. Model selection:

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

  E.g. $y = ax + b$

3. Choose the objective function

- **Squared error** $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$

4. Learning:

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

5. Testing:

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

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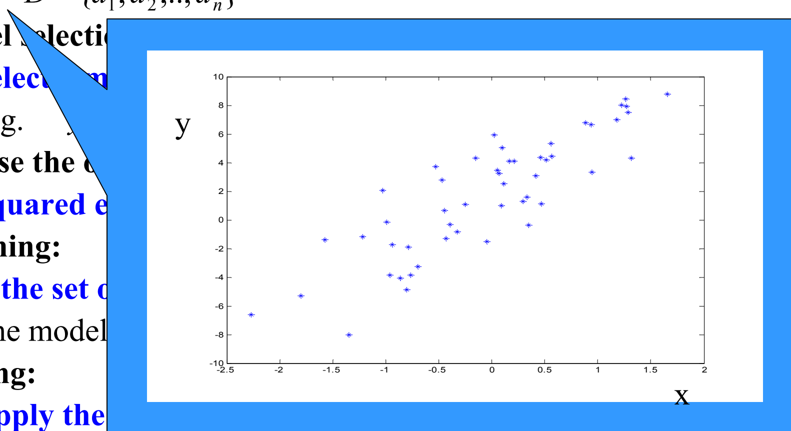

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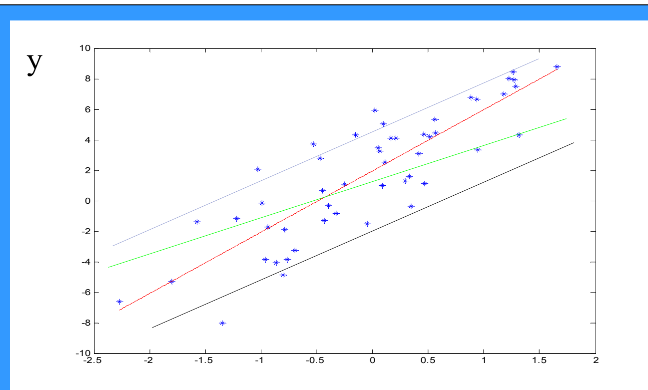

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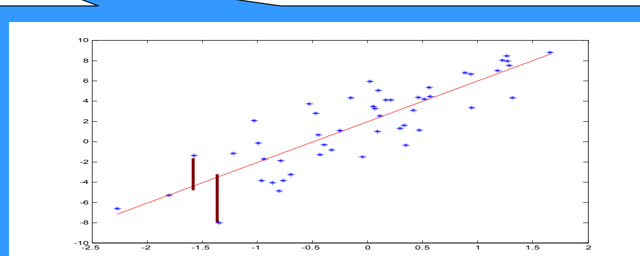


A learning system: basic cycle

1. Data: $D =$

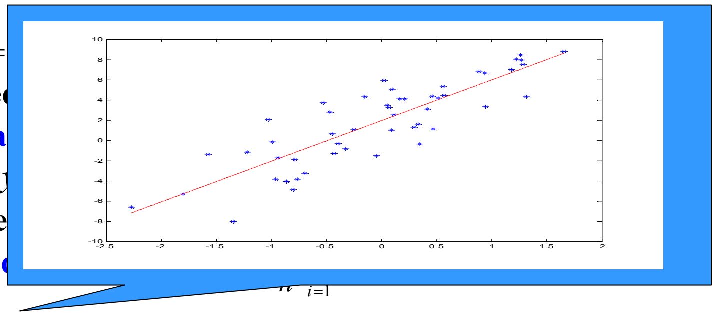
2. Model selec

– **Select a**

E.g. y

3. Choose the

– **Square**



$n \quad i=1$

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- **Find the set of parameters optimizing the error function**
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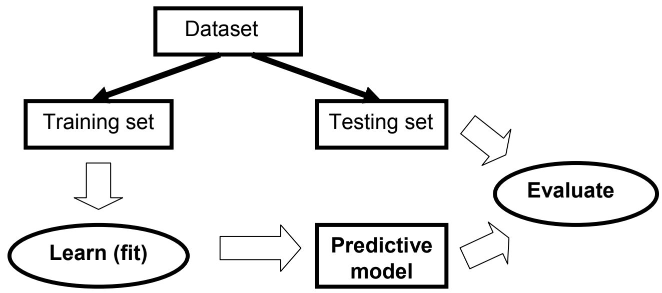
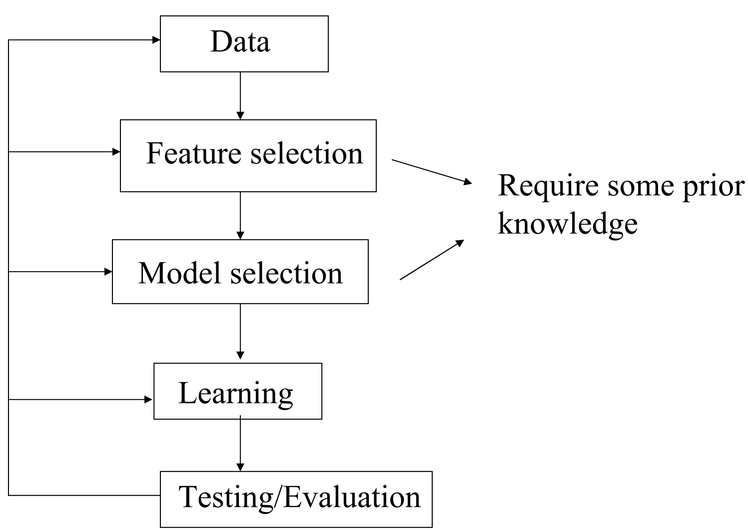
Testing of learning models

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

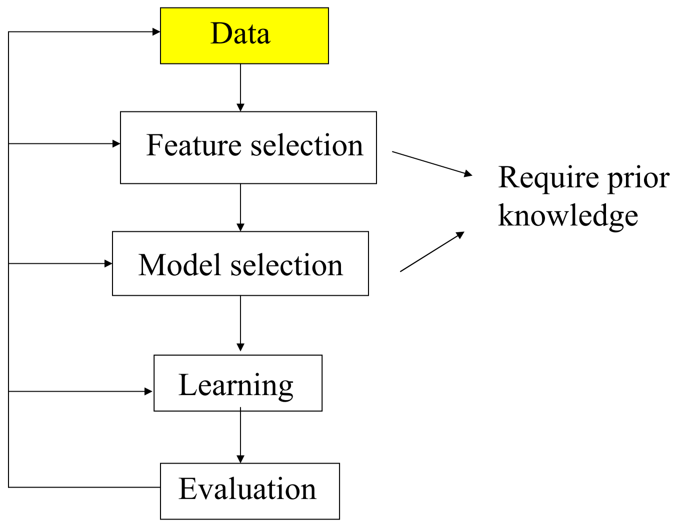


  - Typically 2/3 training and 1/3 testing

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**

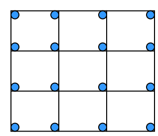
Data preprocessing

- **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

- **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
  - 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 biased data do not hold in general !!!**

Data biases

Example 1: Risks in pregnancy study

- Sponsored by DARPA at military hospitals

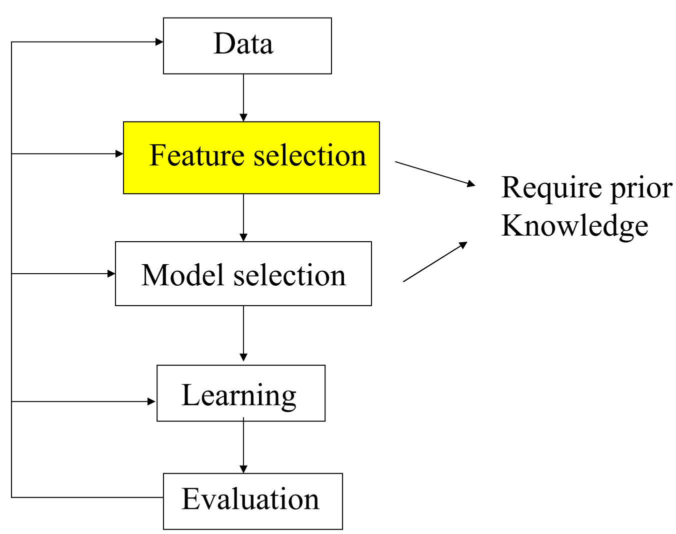
- Study of a large sample of pregnant woman who visited military hospitals
- **Conclusion:** the factor with the largest impact on reducing risks during pregnancy (statistically significant) is a pregnant woman being single
- a woman that is single → the smallest risk
- What is wrong?

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

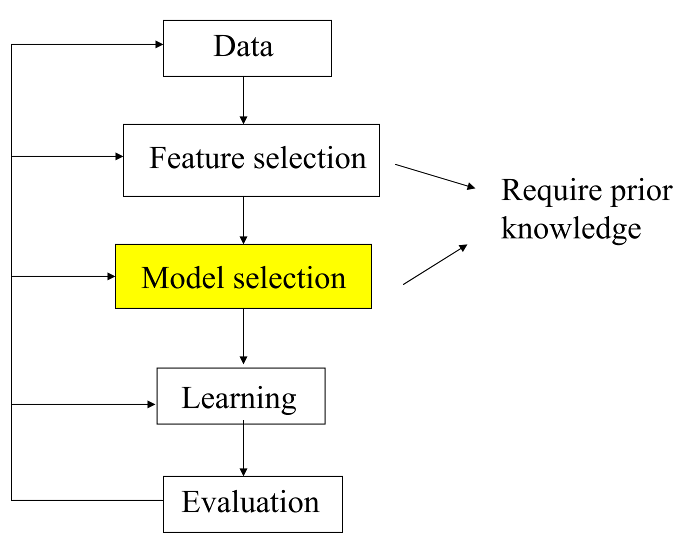


Feature selection

- **The size (dimensionality) of a sample** can be enormous
  $x_i = (x_i^1, x_i^2, .., x_i^d)$ $\quad d$ - 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

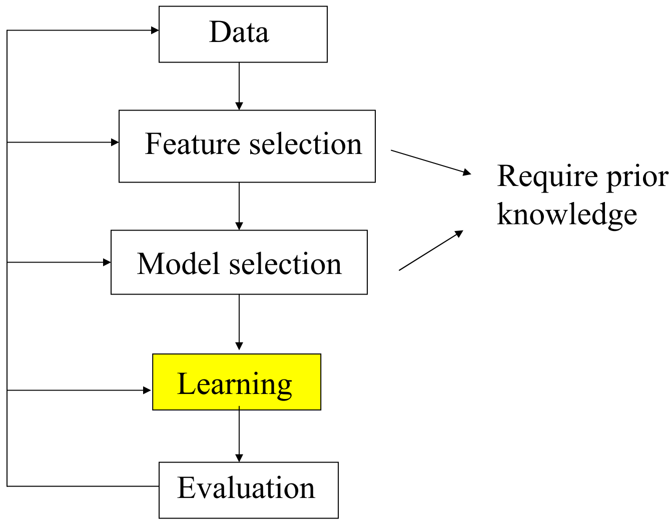
- **What is the right model to learn?**
  - A prior knowledge helps a lot, but still a lot of guessing
  - Initial data analysis and visualization
    - We can make a good guess about the form of the distribution, shape of the function
  - Independences and correlations
- **Overfitting problem**
  - 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 (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 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)

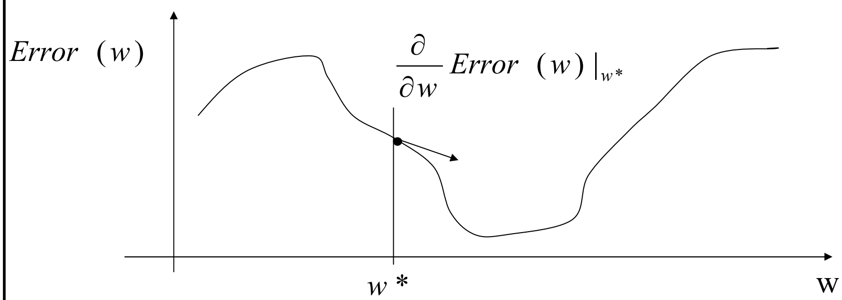
  Goal: $\mathbf{w}^* = \arg\min_{\mathbf{w}} f(\mathbf{w})$

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

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

Gradient descent method

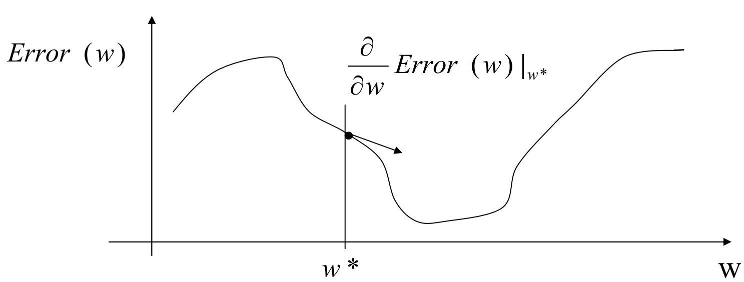
- Descend to the minimum of the function using the gradient information



- Change the parameter value of w according to the gradient

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

Gradient descent method



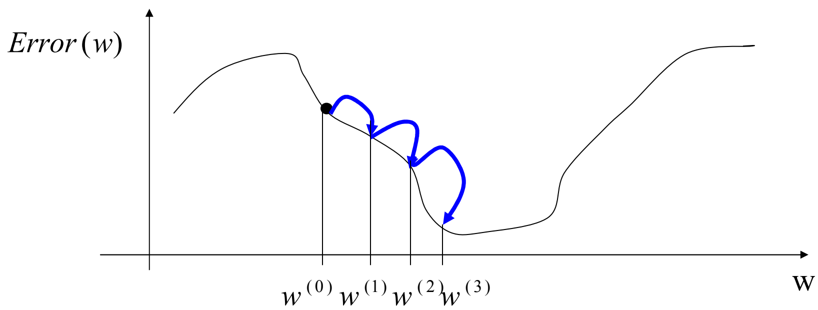
- New value of the parameter

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

$\alpha > 0$ - 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)

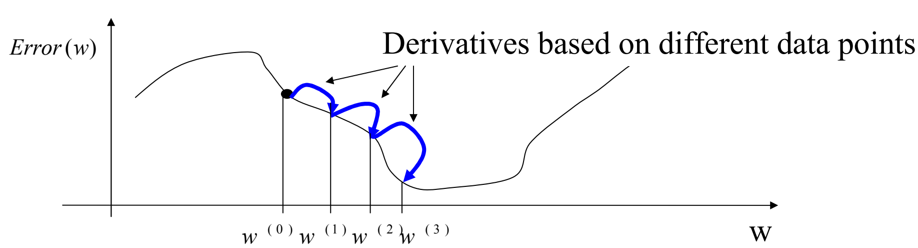
- Error function looks at all data points at the same time

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

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

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

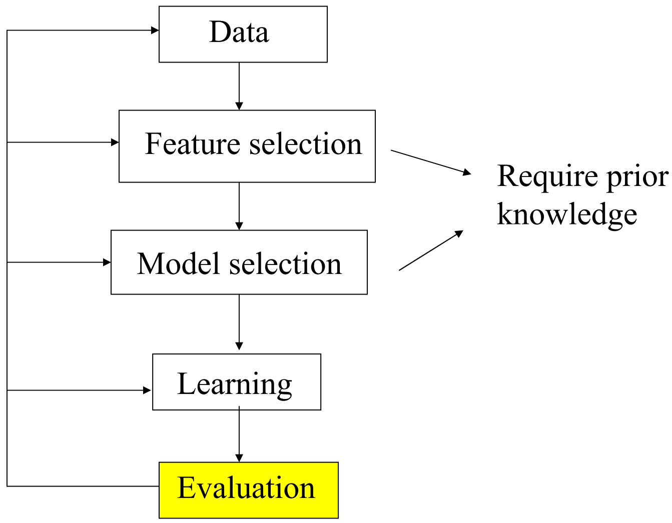
- **Example: On-line gradient descent**



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

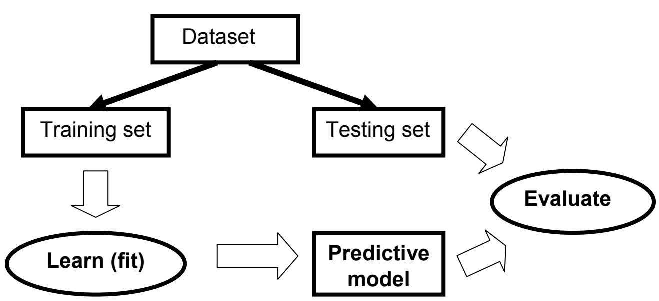
  2. no need to store data (on-line data streams)

Design cycle



Evaluation of learning models

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

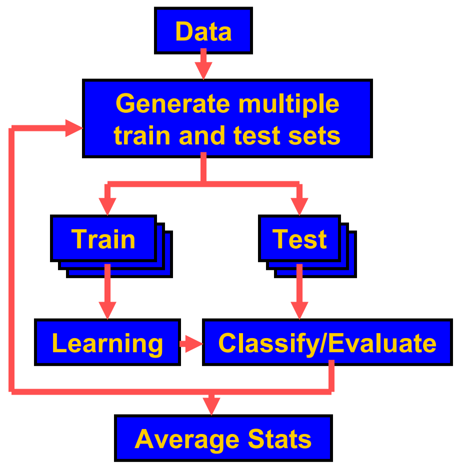


  - Typically 2/3 training and 1/3 testing

Evaluation

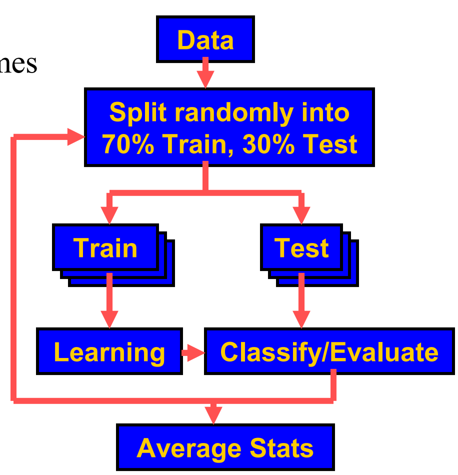
Other more complex methods

- 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

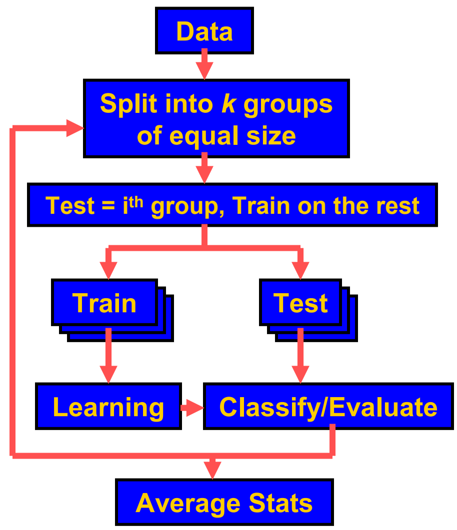


Evaluation

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

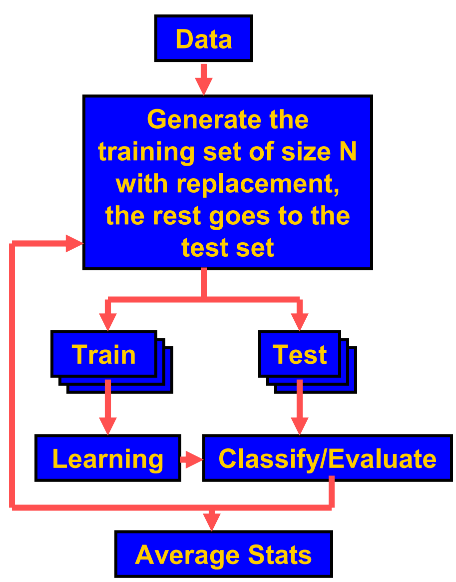
  (k = size of the data D)



Evaluation

Bootstrap

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



Evaluation

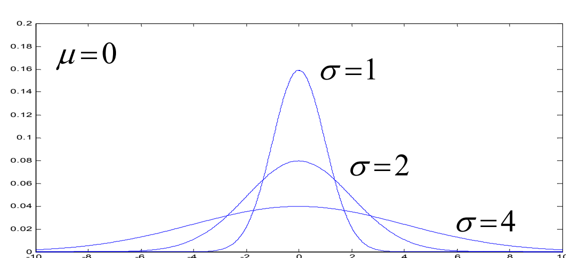
- What if we want to compare the predictive performance on a classification or a regression problem for two different learning methods?
- **Solution:** compare the error results on the test data set or the average statistics on the same training/testing data splits
- **Answer**: the method with better (smaller) testing error gives a better generalization error.
- But we need to use statistics to validate the choice

Evaluation

- **Problem:** we cannot be 100 % sure about generalization errors
- **Solution:** test the statistical significance of the result
- **Central limit theorem:**

  Let random variables $X_1, X_2, \cdots X_n$ form a random sample from a distribution with mean μ and variance σ, then if the sample n is large, the distribution

$$\sum_{i=1}^{n} X_i \approx N(n\mu, n\sigma^2) \quad \text{or} \quad \frac{1}{n}\sum_{i=1}^{n} X_i \approx N(\mu, \sigma^2 / n)$$



Statistical significance test

- **Sample mean:** $\frac{1}{n}\sum_{i=1}^{n} X_i$

$$\frac{1}{n}\sum_{i=1}^{n} X_i \approx N(\mu, \sigma^2 / n) \qquad X_i \text{ - Is a random variable}$$

- **Assume:**

  Regression learner 1 uses function $f_1(\mathbf{x})$ to predict ys

  Regression learner 2 uses function $f_2(\mathbf{x})$ to predict ys

$$Error_1 = \frac{1}{n}\sum_{i=1}^{n}(y_i - f_1(\mathbf{x}_i))^2 \quad Error_2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - f_2(\mathbf{x}_i))^2$$

$$\Delta Error = \frac{1}{n}\sum_{i=1}^{n}\left[(y_i - f_1(\mathbf{x}_i))^2 - (y_i - f_2(\mathbf{x}_i))^2\right]$$

$$X_i \to (y_i - f_1(\mathbf{x}_i))^2 - (y_i - f_2(\mathbf{x}_i))^2$$

Statistical significance test

- **Two learners are the same in terms of the generalization error when**

$$E_{(\mathbf{x},y)}(y - f_1(\mathbf{x}))^2 = E_{(\mathbf{x},y)}(y - f_2(\mathbf{x}))^2$$

$$E_{(\mathbf{x},y)}\left[(y - f_1(\mathbf{x}))^2 - (y - f_2(\mathbf{x}))^2\right] = \mu_{diff} = 0$$

- **Sample mean** (estimate of the last quantity)

$$\Delta Error = \frac{1}{n}\sum_{i=1}^{n}\left[(y_i - f_1(\mathbf{x}_i))^2 - (y_i - f_2(\mathbf{x}_i))^2\right]$$

$$\Delta Error \approx N(\mu_{diff}, \sigma_{diff}^2 / n)$$

- **Statistical tests for the mean**
  - **H0 (null hypothesis)** $\mu_{diff}^0 = 0$
  - **H1 (alternative hypothesis)** $\mu_{diff}^0 \neq 0$

Statistical significance test

- **Statistical tests for the mean**
  - **H0 (null hypothesis)** $\mu^0_{diff} = 0$
  - **H1 (alternative hypothesis)** $\mu^0_{diff} \neq 0$
- **Basic idea:**
  we use the sample mean and check how probable it is to occur given that the true mean is 0

$$E_{(\mathbf{x},y)}\left[(y - f_1(\mathbf{x}))^2 - (y - f_2(\mathbf{x}))^2\right] = \mu_{diff} = 0$$

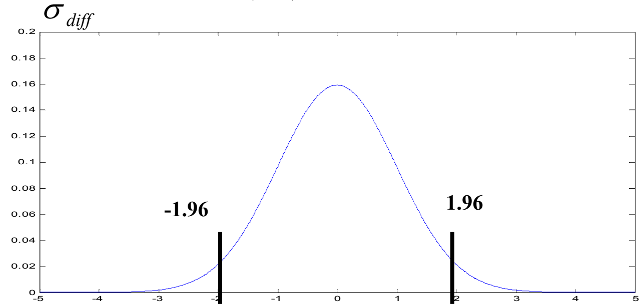
$$\Delta Error = \overline{X} = \frac{1}{n}\sum_{i=1}^{n}\left[(y_i - f_1(\mathbf{x}_i))^2 - (y_i - f_2(\mathbf{x}_i))^2\right]$$

If the probability that $\Delta Error$ comes from the normal distribution with mean 0 is small – we reject the null hypothesis on that probability level

Statistical significance test

- **Statistical tests for the mean**
  - **H0 (null hypothesis)** $\mu^0_{diff} = 0$
  - **H1 (alternative hypothesis)** $\mu^0_{diff} \neq 0$
- **Assume we know standard deviation** σ_{diff}

$$z = \frac{\overline{X} - \mu^0_{diff}}{\sigma_{diff}}\sqrt{n} \approx N(0,1) \quad \text{with} \quad \text{P=0.95} \quad z \in [-1.96, 1.96]$$

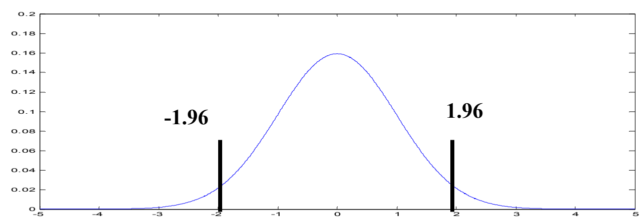


Statistical significance test

- Statistical tests for the mean
  - H0 (null hypothesis) $\mu_{diff}^{0} = 0$
- Assume we know standard deviation σ_{diff}

$$z = \frac{\bar{X} - \mu_{diff}^{0}}{\sigma_{diff}} \sqrt{n} \approx N(0,1) \qquad \text{with} \qquad \text{P=0.95} \qquad z \in [-1.96, 1.96]$$

- Z-test: If z is outside of the interval – reject the null hypothesis at significance level 5 %



Statistical significance test

- Statistical tests for the mean
  - H0 (null hypothesis) $\mu_{diff}^{0} = 0$
- Problem: we do not know the standard deviation σ_{diff}
- Solution:

$$t = \frac{\bar{X} - \mu_{diff}^{0}}{s_{diff}} \sqrt{n} \approx \text{t} - \text{distribution} \qquad \text{(Student distribution)}$$

$$s_{diff} = \sqrt{\frac{\sum_{i=1}^{n} (X_i - \bar{X})^2}{n-1}} \qquad \text{- Estimate of the standard deviation}$$

- T-test: If t is outside of the tabulated interval reject the null hypothesis at the corresponding significance level