CS 2750 Machine Learning

Lecture 1

Machine Learning

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Administration

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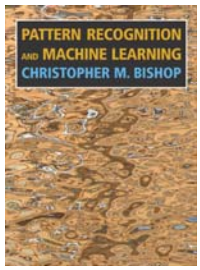
Study material

- **Handouts, your notes and course readings**
- **Primary textbook:**



  – Chris. Bishop. Pattern Recognition and Machine Learning. Springer, 2006.

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Study material

- **Other books:**
  – Friedman, Hastie, Tibshirani. Elements of statistical learning. Springer, 2001.
  – Duda, Hart, Stork. Pattern classification. 2nd edition. J Wiley and Sons, 2000.
  – C. Bishop. Neural networks for pattern recognition. Oxford U. Press, 1996.
  – T. Mitchell. Machine Learning. McGraw Hill, 1997
  – J. Han, M. Kamber. Data Mining. Morgan Kauffman, 2001.

Administration

- **Homeworks: weekly**
  - **Programming tool**: Matlab (CSSD machines and labs)
  - **Matlab Tutorial:** next week
- **Exams:**
  - **Midterm** (March)
  - **Final** (April 18-22)
- **Final project:**
  - **Written report + Oral presentation** (April 25-30)
- **Lectures:**
  - **Attendance and Activity**

Tentative topics

- Introduction to Machine Learning
- **Density estimation.**
- **Supervised Learning.**
  - Linear models for regression and classification.
  - Multi-layer neural networks.
  - Support vector machines. Kernel methods.
- **Unsupervised Learning.**
  - Learning Bayesian networks.
  - Latent variable models. Expectation maximization.
  - Clustering.

Tentative topics (cont)

- **Dimensionality reduction.**
  - Feature extraction.
  - Principal component analysis (PCA)
- **Ensemble methods.**
  - Mixture models.
  - Bagging and boosting.
- **Hidden Markov models.**
- **Reinforcement learning**

Machine Learning

- The field of **machine learning** studies the design of computer programs (agents) capable of learning from past experience or adapting to changes in the environment

- The need for building agents capable of learning is everywhere
  - predictions in medicine,
  - text and web page classification,
  - speech recognition,
  - image/text retrieval,
  - commercial software

Learning

Learning process:

Learner (a computer program) processes data ***D*** representing past experiences and tries to either develop an appropriate response to future data, or describe in some meaningful way the data seen

Example:

Learner sees a set of patient cases (patient records) with corresponding diagnoses. It can either try:

- to predict the presence of a disease for future patients
- describe the dependencies between diseases, symptoms

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, Active learning**

Supervised learning

Data: $D = \{d_1, d_2, .., d_n\}$ **a set of *n* examples**

$d_i = < \mathbf{x}_i, y_i >$

$\mathbf{x}_i$ is input vector, and y is desired output (given by a teacher)

Objective: learn the mapping $f : X \rightarrow Y$

s.t. $y_i \approx f(x_i)$ for all $i = 1, .., n$

Two types of problems:

- **Regression:** X discrete or continuous $\rightarrow$ Y is **continuous**
- **Classification:** X discrete or continuous $\rightarrow$ Y is **discrete**

Supervised learning examples

- **Regression:** Y is **continuous**

Debt/equity
Earnings
Future product orders

$\longrightarrow$ company stock price

- **Classification:** Y is **discrete**

```
# ######
      ##
     ##
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      ###
#      ##
# ##   ##
  #######
```

$\longrightarrow$ Label “3”

Handwritten digit (array of 0,1s)

Unsupervised learning

- **Data:** $D = \{d_1, d_2, .., d_n\}$
  $d_i = \mathbf{x}_i$ vector of values
  No target value (output) y

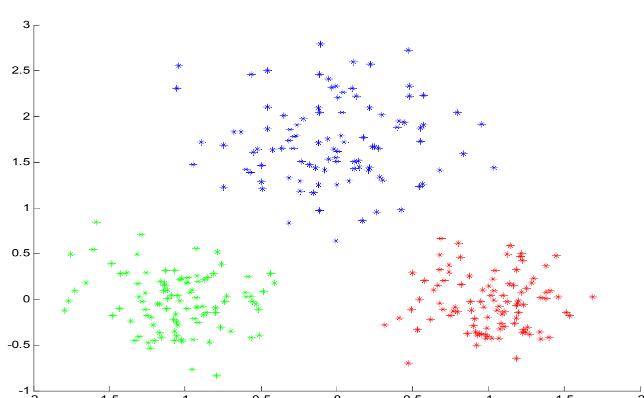
- **Objective:**
  – learn relations between samples, components of samples

Types of problems:

- **Clustering**
  Group together "similar" examples, e.g. patient cases
- **Density estimation**
  – Model probabilistically the population of samples

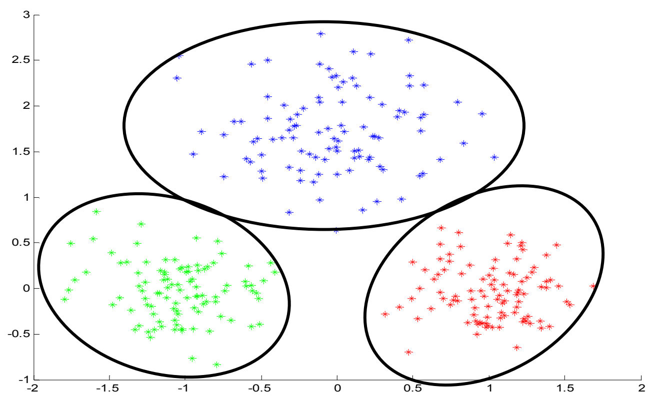
Unsupervised learning example

- **Clustering.** Group together similar examples $d_i = \mathbf{x}_i$



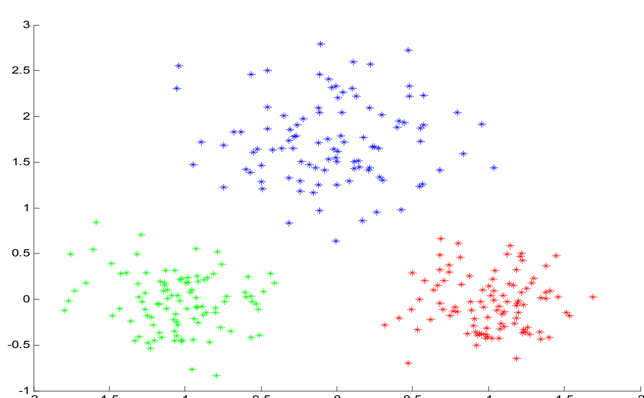
Unsupervised learning example

- **Clustering.** Group together similar examples $d_i = \mathbf{x}_i$



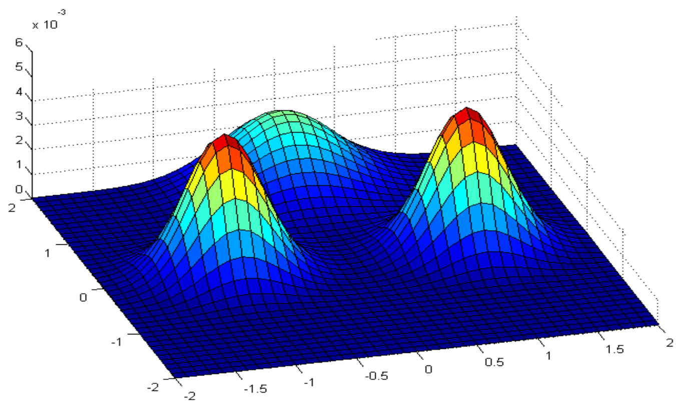
Unsupervised learning example

- **Density estimation.** We want to build the probability model P($\mathbf{x}$) of a population from which we draw examples $d_i = \mathbf{x}_i$



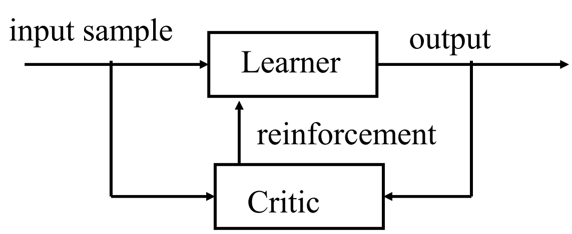
Unsupervised learning. Density estimation

- A probability density of a point in the two dimensional space
  - Model used here: **Mixture of Gaussians**



Reinforcement learning

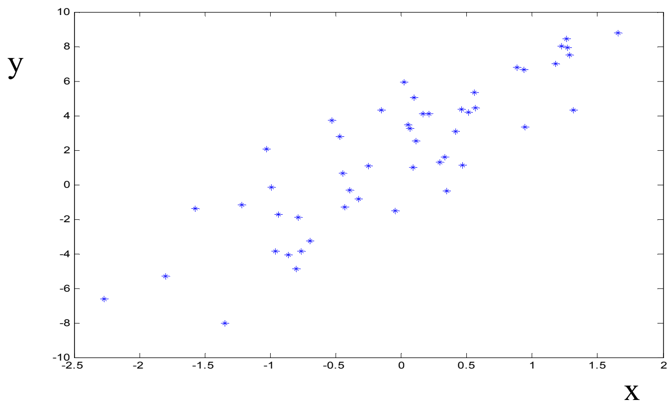
- We want to learn: $f : X \to Y$
- We see samples of **x** but not y
- Instead of y we get a feedback (reinforcement) from a **critic** about how good our output was



- The goal is to select outputs that lead to the best reinforcement

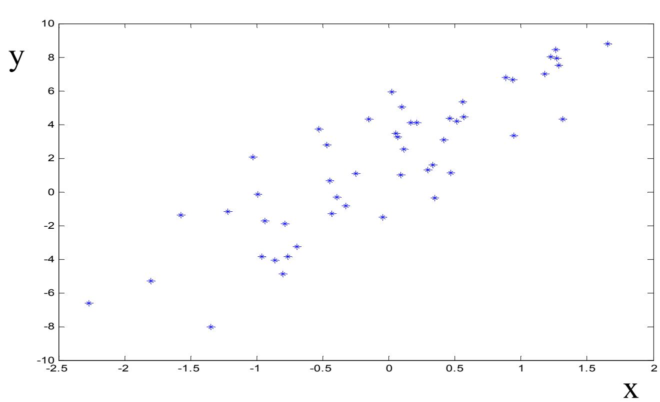
Learning: first look

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



Learning: first look

- **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!



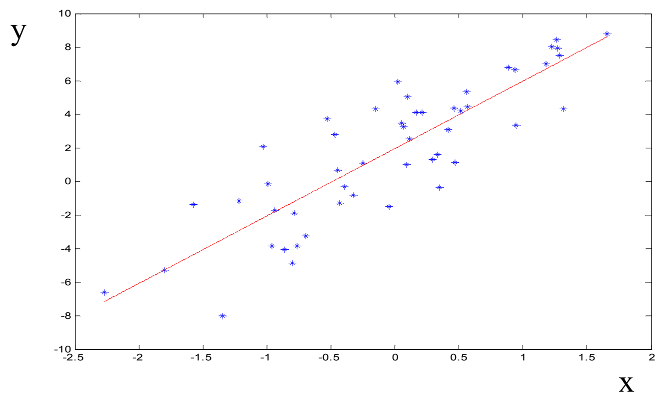
Learning: first look

- **Solution:** make an assumption about the model, say,

$$f(x) = ax + b + \varepsilon$$

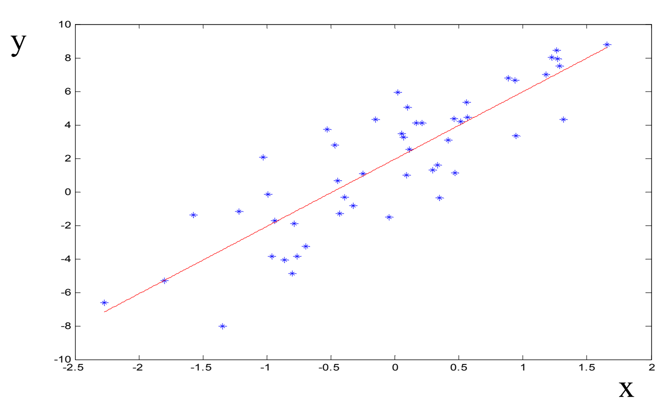
$\varepsilon = N(0,\sigma)$ - random (normally distributed) noise

- Restriction to a linear model is an example of learning bias



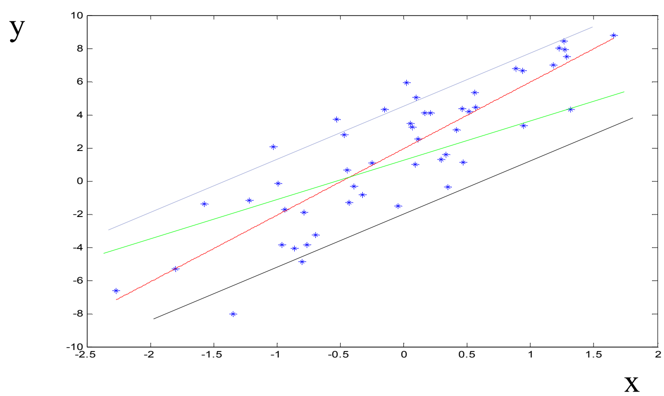
Learning: first look

- **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: first look

- Choosing a parametric model or a set of models is not enough
  Still too many functions $f(x) = ax + b + \varepsilon \quad \varepsilon = N(0,\sigma)$
  - One for every pair of parameters *a, b*



Fitting the data to the model

- We want the **best set** of model parameters

Objective: Find parameters that:

- reduce the misfit between the model **M** and observed data ***D***
- Or, (in other words) explain the data the best

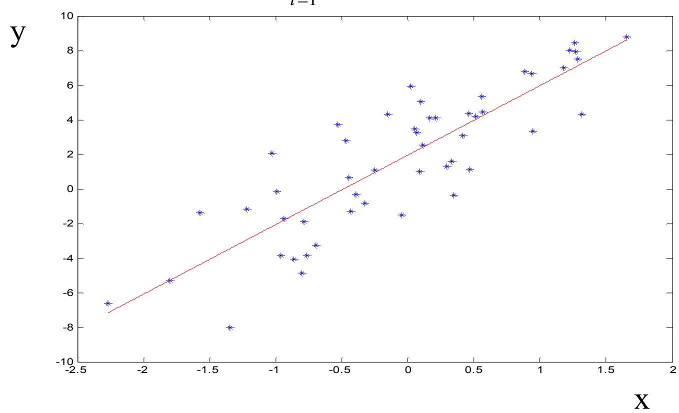
Objective function:

- **Error function: Measures the misfit between *D* and M**
- **Examples of error functions:**
  - Average Square 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 problem**
  - Minimizes the squared error function for the linear model
  - minimizes $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$



Learning: summary

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 ?

Learning

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):

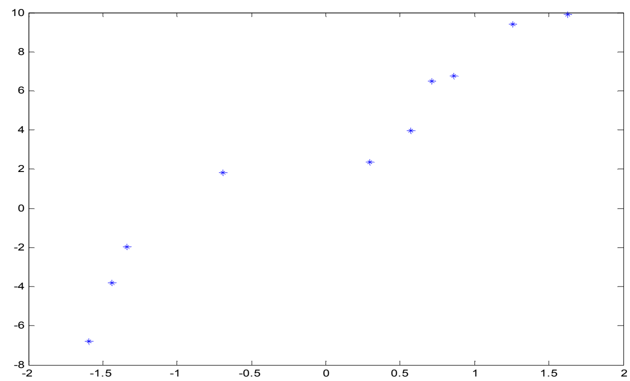
$$E_{(x,y)}[(y - f(x))^2] \quad \text{Mean squared error}$$

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

Does a good training error imply a good generalization error ?

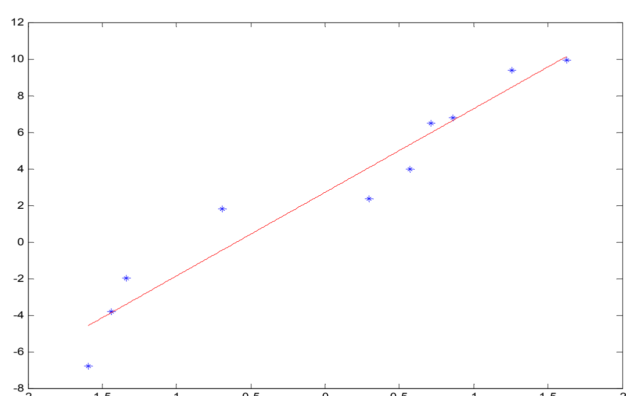
Overfitting

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



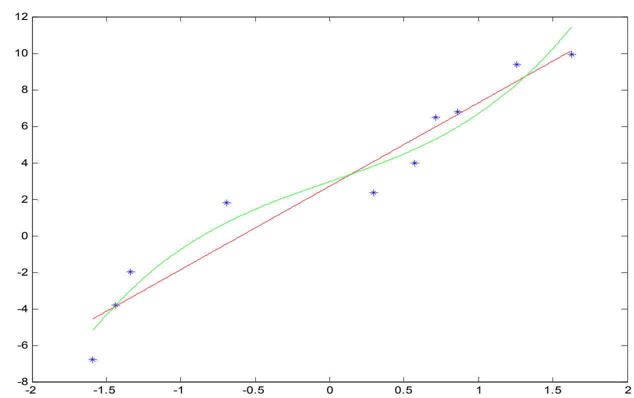
Overfitting

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



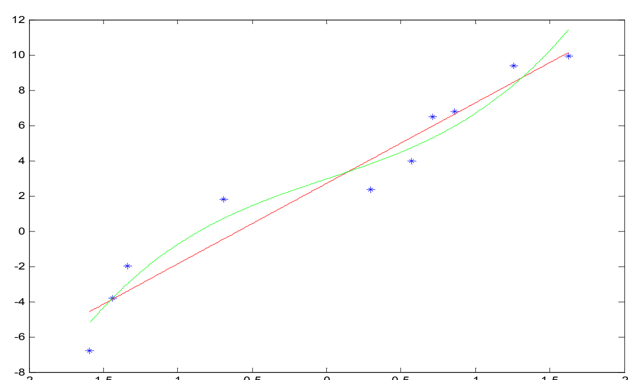
Overfitting

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



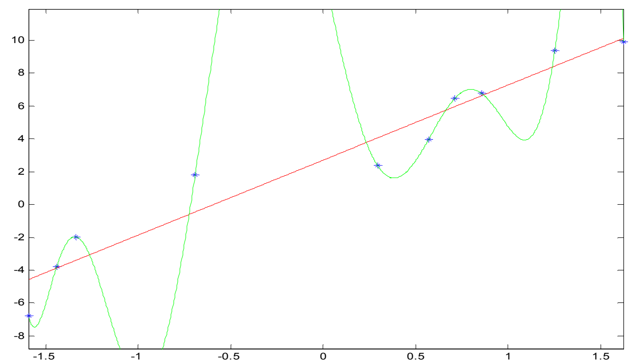
Overfitting

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



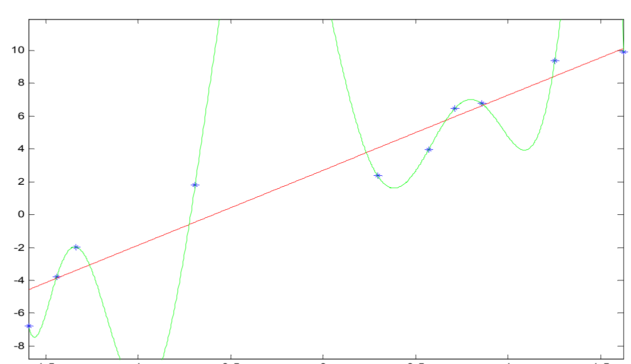
Overfitting

- 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

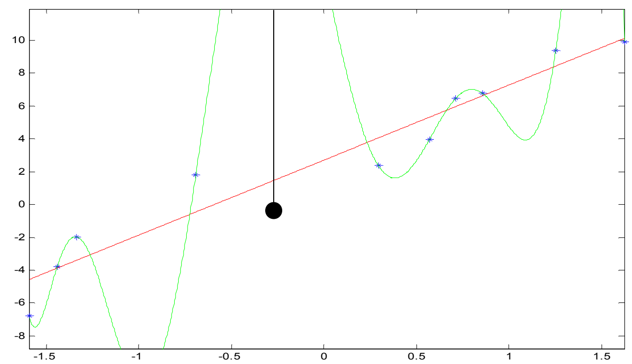
- For 10 data points, degree 9 polynomial gives a perfect fit (Lagrange interpolation). Error is zero.
- Is it always good to minimize the training error? NO !!
- **More important:** How do we perform on the unseen data?



Overfitting

Situation when the training error is low and the generalization error is high. Causes of the 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** $\frac{1}{m} \sum_{j=1,..m} (y_j - f(x_j))^2$

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