CS 2750 Machine Learning

Lecture 1

Machine Learning

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Administration

Study material

- **Handouts, your notes and course readings**
- **Primary textbook:**
  - Duda, Hart, Stork. Pattern classification. 2nd edition. J Wiley and Sons, 2000.
- **Recommended book:**
  - Friedman, Hastie, Tibshirani. Elements of statistical learning. Springer, 2001.
- **Other books:**
  - 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

- **Lectures:**
  - **Random** short quizzes testing the understanding of basic concepts from previous lectures
- **Homeworks: weekly**
  - **Programming tool**: Matlab (CSSD machines and labs)
  - **Matlab Tutorial:** next week
- **Exams:**
  - **Midterm** (March)
- **Final project:**
  - **Proposals** (early March)
  - **Written report + Oral presentation** (end of the semester)

Tentative topics

- Concept learning.
- Density estimation.
- Linear models for regression and classification.
- Multi-layer neural networks.
- Support vector machines. Kernel methods.
- Learning Bayesian networks.
- Clustering. Latent variable models.
- Dimensionality reduction. Feature extraction.
- 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:**
  - **explanation-based learning, etc.**

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	→	company stock price

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

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

→ 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

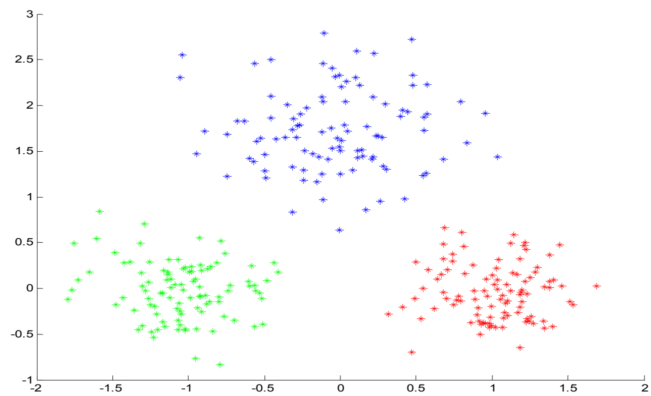
- **Objective:**
  – learn relations between samples, components of samples

Types of problems:

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

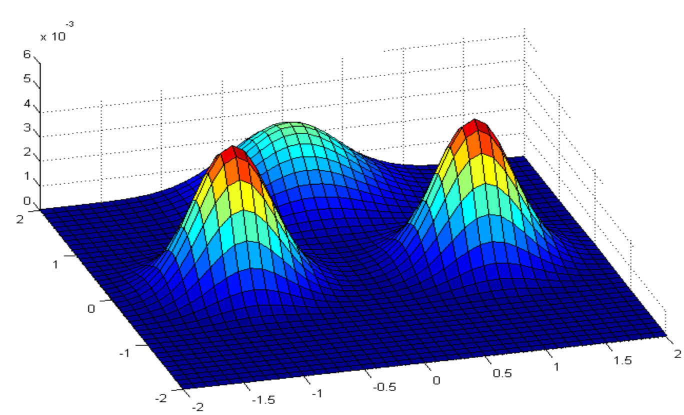
Unsupervised learning example.

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



Unsupervised learning. Density estimation

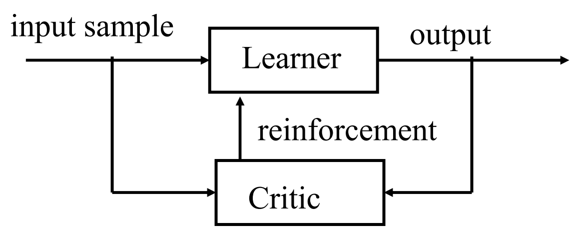
- A probability density of a point in the two dimensional space
  - Model used here: **Mixture of Gaussians**



CS 2750 Machine Learning

Reinforcement learning

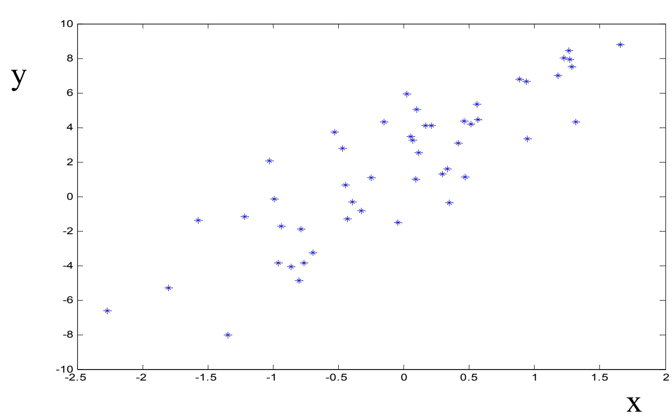
- We want to learn: $f : X \to Y$
- We see samples of **x** but not y
- Instead of y we get a feedback (reinforcement) from a **critic** about how good our output was



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

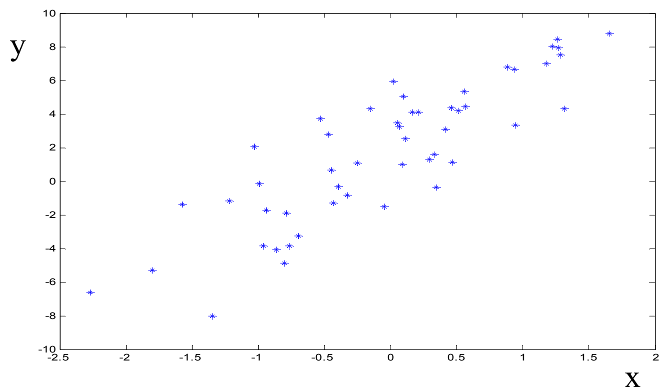
Learning

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



Learning bias

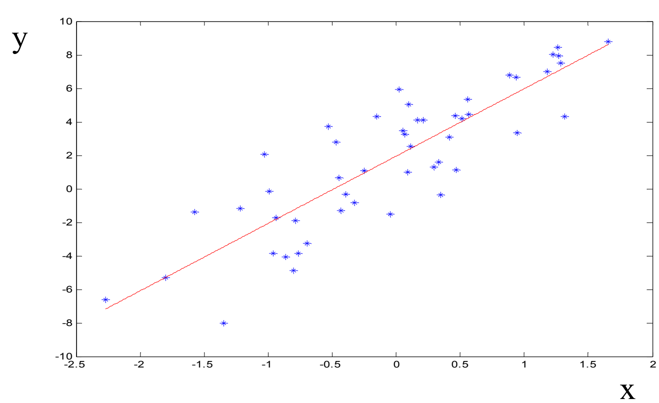
- **Problem:** many possible functions $f : X \to Y$ exists for representing the mapping between **x** and y
- Which one to choose? Many examples still unseen!



Learning bias

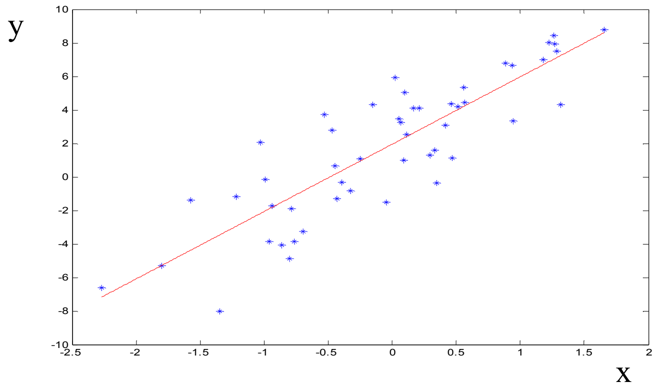
- Problem is easier when we make an assumption about the model, say, $f(x) = ax + b + \varepsilon$

  $\varepsilon = N(0, \sigma)$ - random (normally distributed) noise
- Restriction to a linear model is an example of learning bias



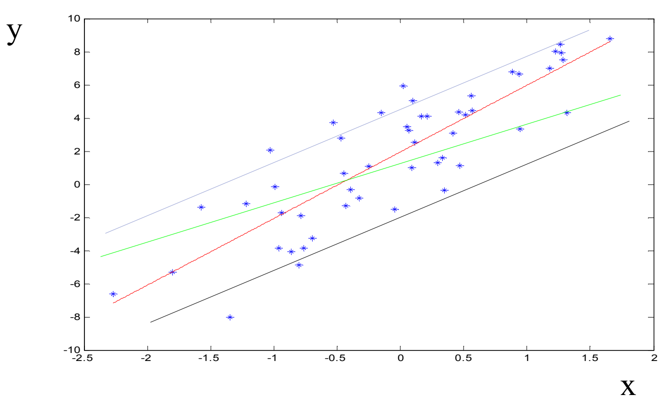
Learning bias

- **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 $f(x) = ax + b + \varepsilon \quad \varepsilon = N(0, \sigma)$
  - 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:

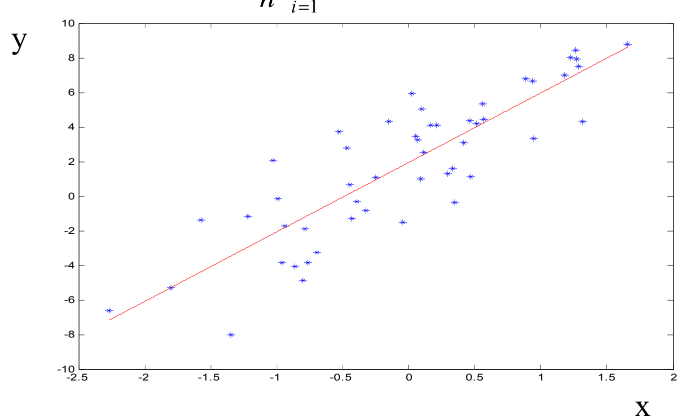
Measure of misfit between the data and the model

- **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**
  – 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. $y = ax + b + \varepsilon \qquad \varepsilon = N(0, \sigma)$

- **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):

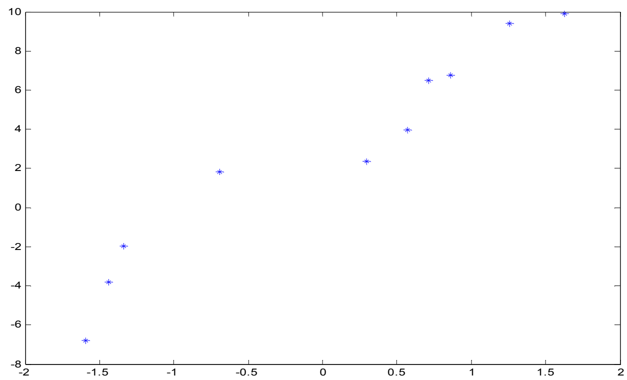
$$E_{(x,y)}[(y - f(x))^2] \qquad \text{Mean squared error}$$

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

Does a good training error imply a good generalization error ?

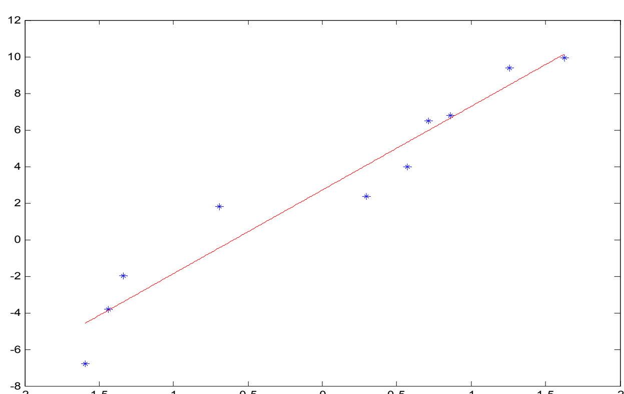
Overfitting

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



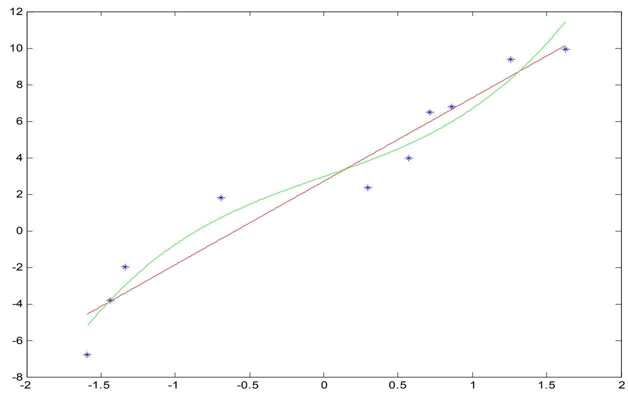
Overfitting

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



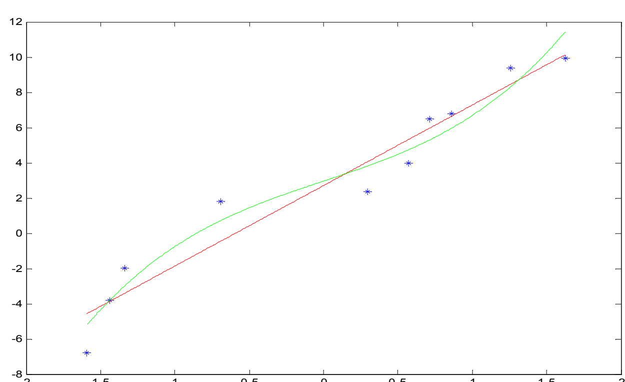
Overfitting

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



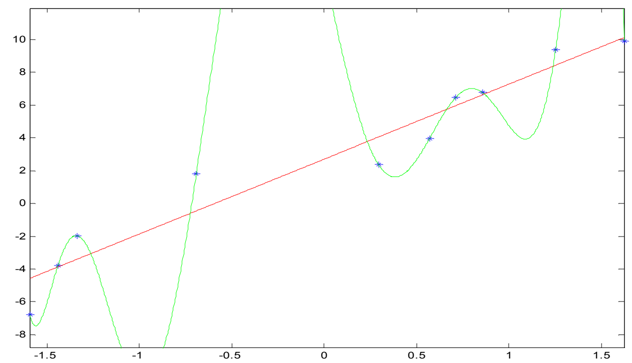
Overfitting

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



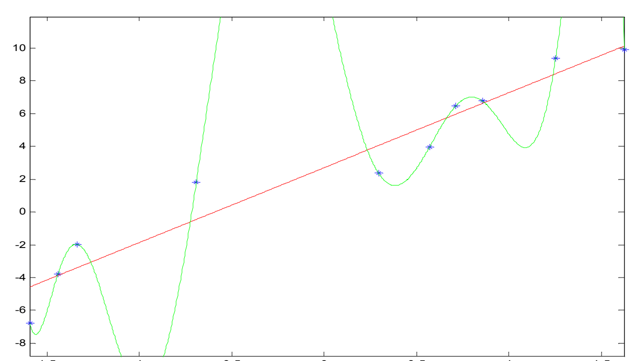
Overfitting

- 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

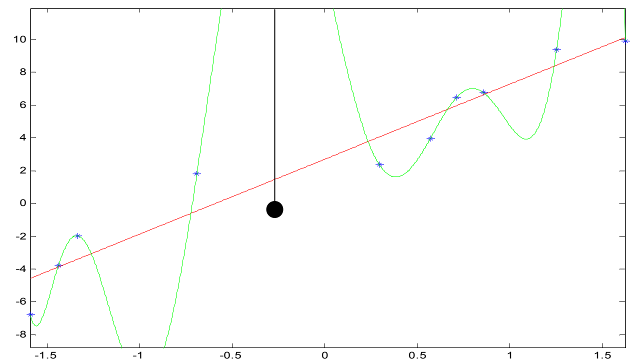
- For 10 data points, degree 9 polynomial gives a perfect fit (Lagrange interpolation). Error is zero.
- Is it always good to minimize the training error? NO !!
- **More important:** How do we perform on the unseen data?



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

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

- **Sample mean only approximates it**
- How to measure the generalization error?
- **Two ways:**
  - **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
    - **(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

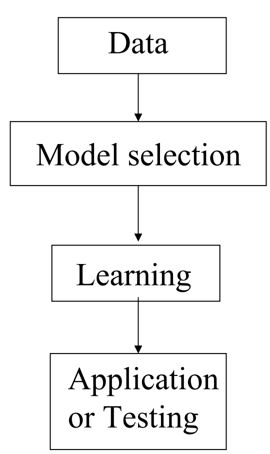
- The results on the testing set can be used to compare different learners powered with different models and learning algorithms

Solutions for overfitting

How to make the learner avoid overfitting?

- **Assure sufficient number of samples** in the training set
  - May not be possible
- **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 (cross-validation techniques)
- **Regularization (Occam's Razor)**
  - Penalize for the model complexity (number of parameters)
  - Explicit preference towards simple models

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. $y = ax + b + \varepsilon \qquad \varepsilon = N(0, \sigma)$

- **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 $f(\mathbf{x})$