CS 1571 Introduction to AI
Lecture 22

Learning

Milos Hauskrecht
milos@cs.pitt.edu
5329 Sennott Square

Administration

- **Problem set 9 is out**
  - **Due November 19, 2002**
  - **No programming part**
- **Final exam**
  - **December 11, 2002 at 2:00-3:50pm**
  - **25 % of the grade**

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 classification, speech recognition, image/text retrieval, commercial software

- Machine learning is not only the deduction but induction of rules from examples that facilitate prediction and decision making

Learning

Learning process:

Learner (a computer program) processes data ***D*** representing past experiences and tries to either to 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 inputs x and desired outputs 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 inputs x and desired outputs 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**

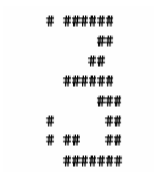
Supervised learning examples

- **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

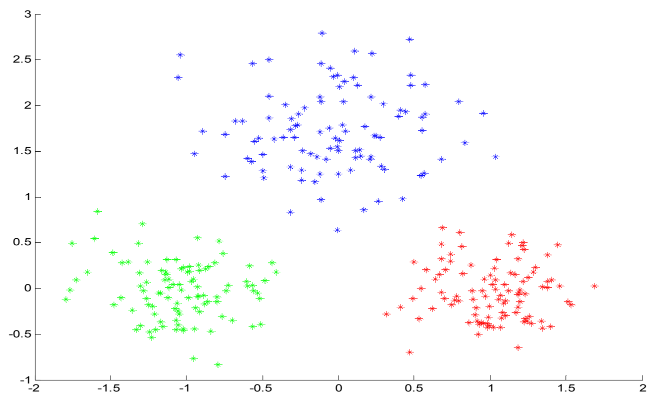
- **Objective:**
  – learn relations between samples, components of samples

Types of problems:

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

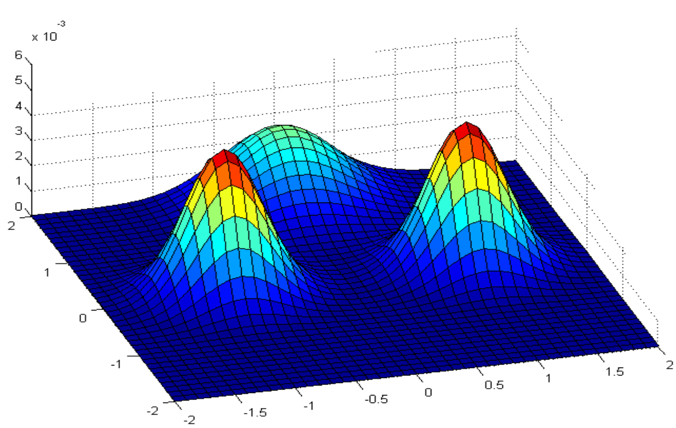
Unsupervised learning example.

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



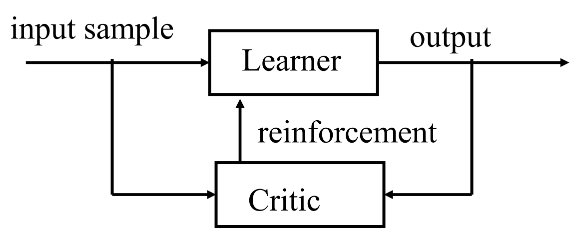
Unsupervised learning. Density estimation

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



Reinforcement learning

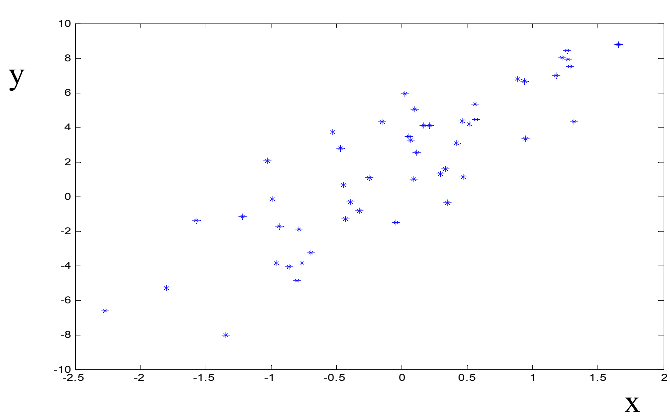
- We want to learn: $f : X \rightarrow Y$
- We see samples of **x** but not y
- Instead of y we get a feedback (reinforcement) from a **critic** about how good our output was



- The goal is to select output that leads to the best reinforcement

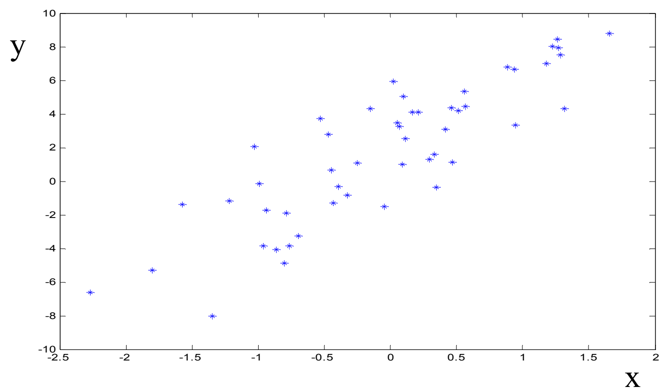
Learning

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



Learning bias

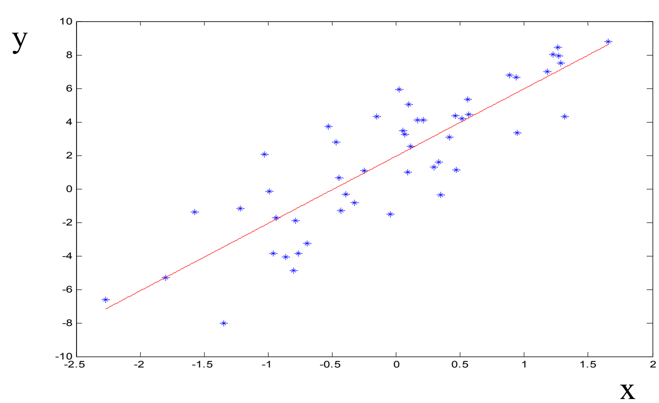
- **Problem:** many possible functions $f : X \rightarrow Y$ exists for representing the mapping between **x** and y
- Which one to choose? Many examples still unseen!



Learning bias

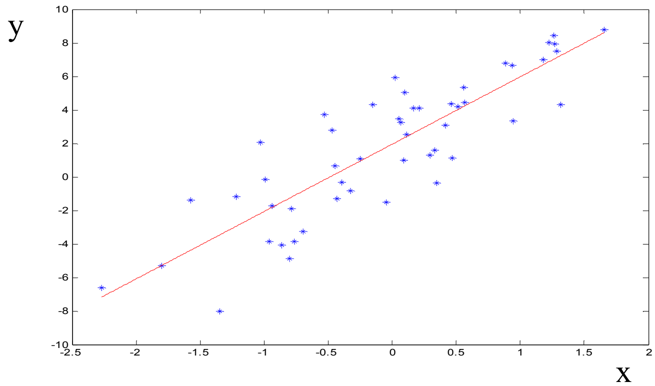
- Problem is easier when we make an assumption about the model, say, $f(x) = ax + b + \varepsilon$

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



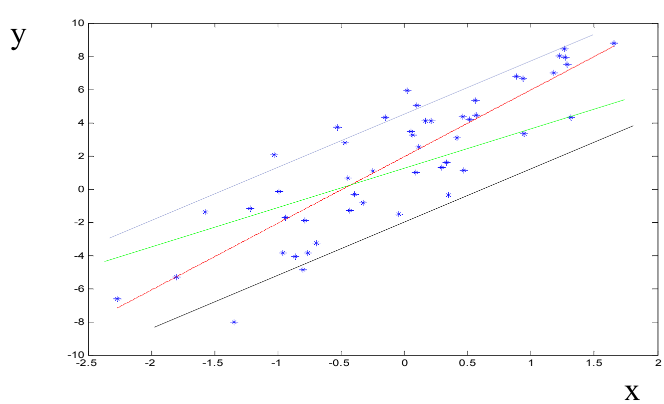
Learning bias

- **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:

- reduce the misfit between what model suggests and what data say
- Or, (in other words) that explain the data the best

Error function:

Measure of misfit between the data and the model

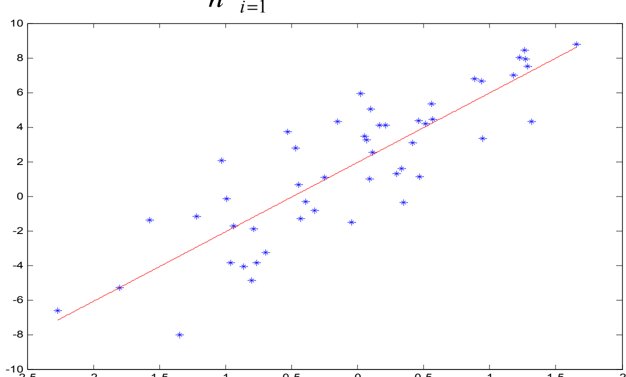
- Examples of error functions:
  – Mean square error $\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$
  – Misclassification error

Average # of misclassified cases $y_i \neq f(x_i)$

Fitting the data to the model

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

y



x

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):

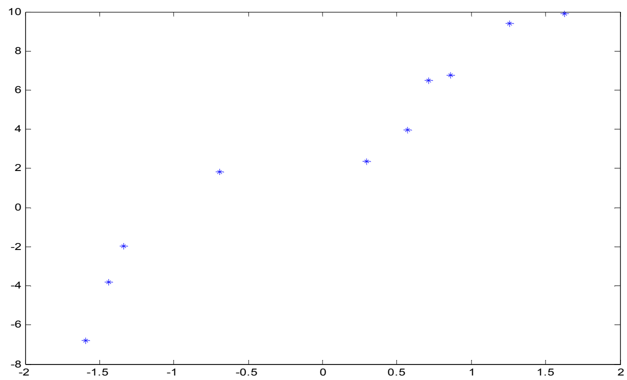
$E_{(x,y)}(y - f(x))^2$ Expected squared error

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

Does a good training error imply a good generalization error ?

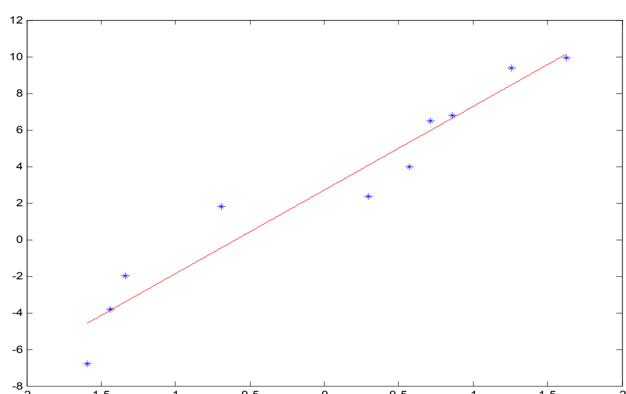
Overfitting

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



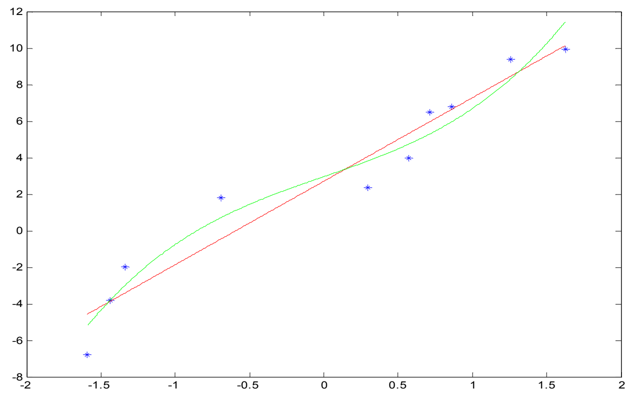
Overfitting

- Fitting a linear function with mean-squares error
- Error is nonzero



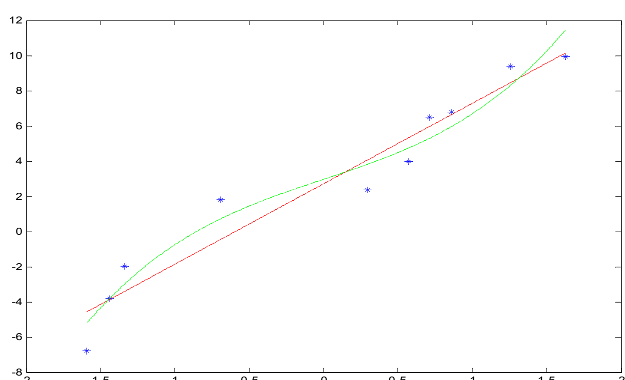
Overfitting

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



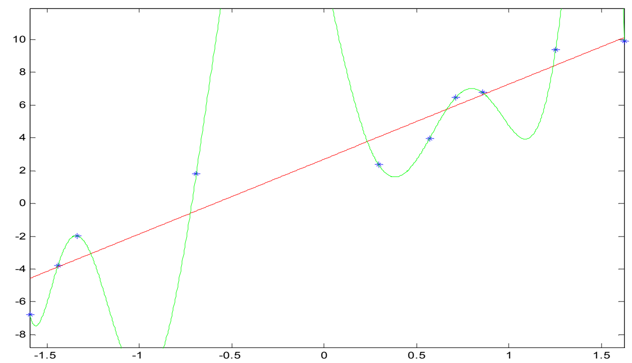
Overfitting

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



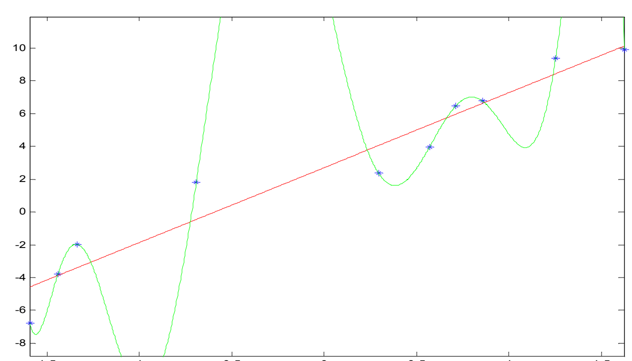
Overfitting

- For 10 data points, degree 9 polynomial gives a perfect fit (Lagrange interpolation). Error is zero.
- Is it always good to minimize the training error?



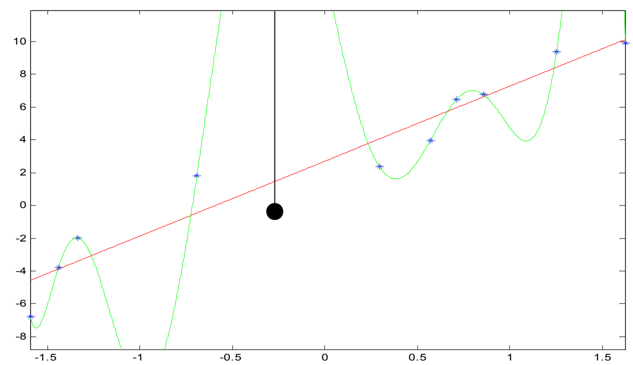
Overfitting

- 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 more degrees of freedom (more parameters)
  - Small data size (as compared to the complexity of 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**
- **Optimizing (mean) training error can lead to 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?

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- How to test the generalization error?
- Use a separate data set with m data samples to test it
- **(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

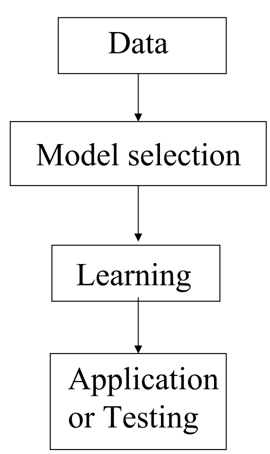
- The results on the testing set can be used to compare different learners powered with different models and learning algorithms

How to deal with 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. $y = ax + b + \varepsilon$ $\varepsilon = N(0, \sigma)$

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