CS 1675 Introduction to ML

Lecture 3

Introduction to Machine Learning

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

people.cs.pitt.edu/~milos/courses/cs1675/

Administration

Instructor:

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

TA:

Amin Sobhani
ams543@pitt.edu
6804 Sennott Square

Homework assignment

Homework assignment 1 is out and due on Thursday

Two parts: **Report + Programs**

Submission:

- via Courseweb
- Report (submit in pdf)
- Programs (submit using the zip or tar archive)
- Deadline 4:00pm (prior to the lecture)

Rules:

- Strict deadline
- No collaboration on the programming and the report part

A learning system: basics

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 $\mathbf{x}$ using learned $f(\mathbf{x})$
- Evaluate on the test data

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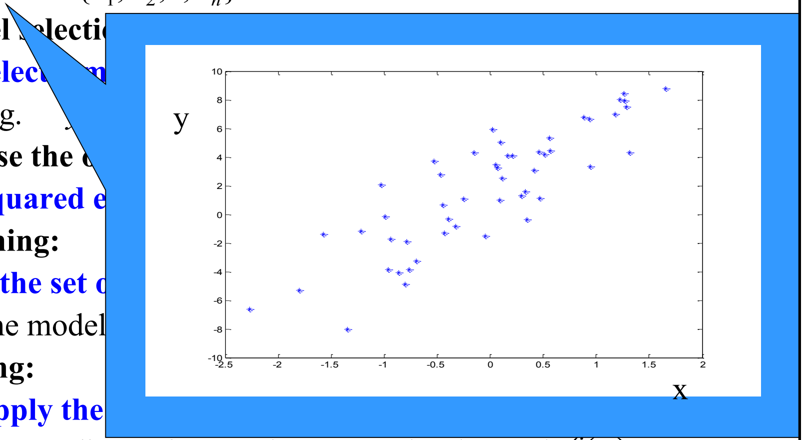

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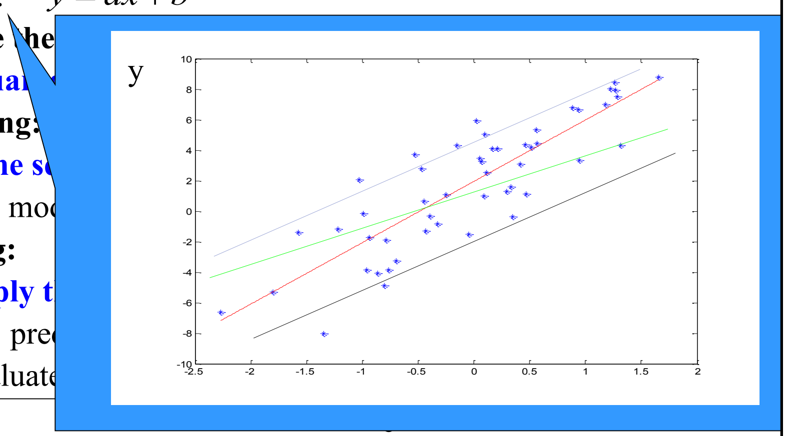

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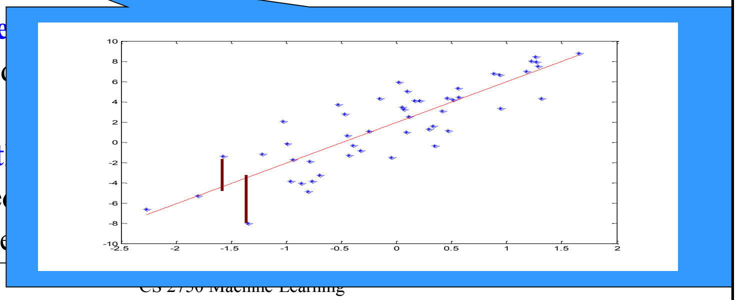
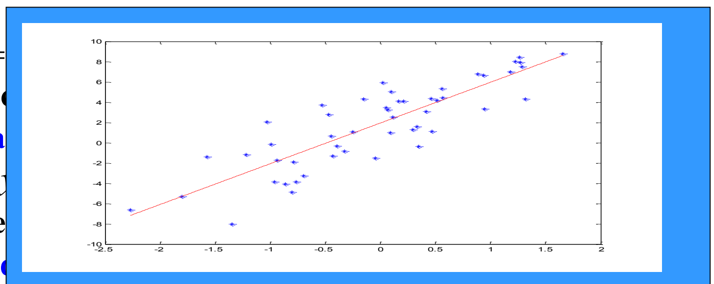


A learning system: basics



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A learning system: basics

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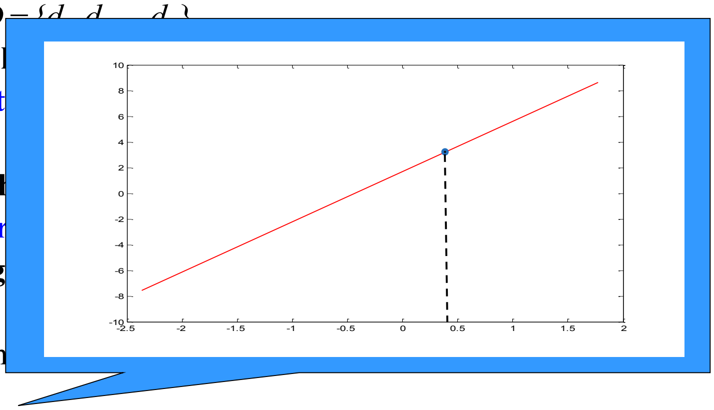
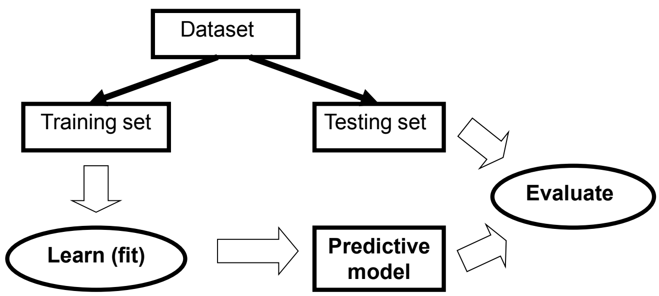


5. **Testing:**
   – **Apply the learned model to new data**
   – E.g. predict ys for new inputs **x** using learned $f(\mathbf{x})$
   – Evaluate on the test data

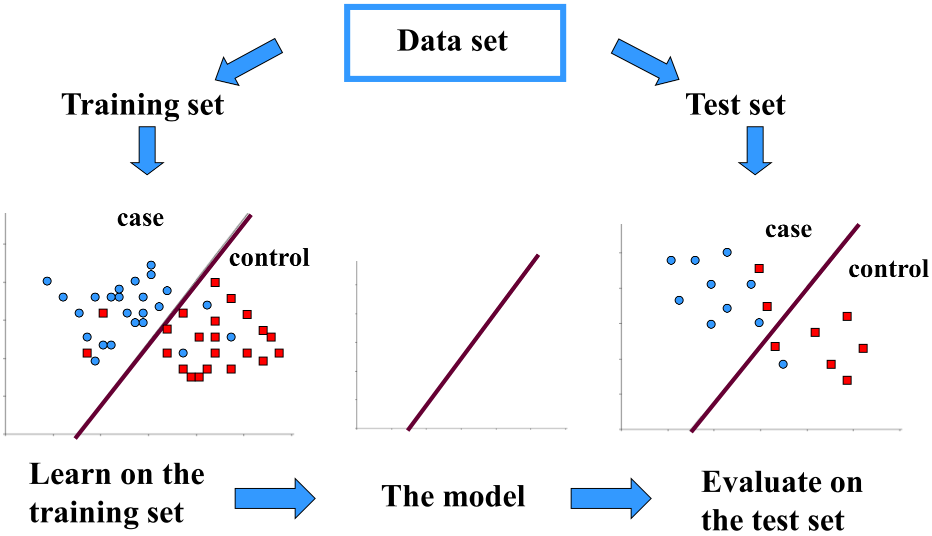
Testing of learning models

• **Simple holdout method**
   – Divide the data to the training and test data



   – Typically 2/3 training and 1/3 testing

Testing of models



Learning process (second look)

1. Data
   – Understand the source of data
   – Real data may need a lot of cleaning/preprocessing
2. Model selection:
   – How to pick the models: manual/automatic methods
3. Choice of the objective (error or loss) function
   – Many functions possible: Squared error, negative log-likelihood, hinge loss
4. Learning:
   – Find the set of parameters optimizing the error function
5. Application/Testing:
   – Evaluate on the test data
   – Apply the learned model to new data

Data source and data biases

- **Understand the data source**
- **Understand the data your models will be applied to**
- **Watch out for data biases:**
  - 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

- **Results (conclusions) derived for a biased dataset do not hold in general !!!**

Data

Example: Assume you want to build an ML program for predicting the stock behavior and for choosing your investment strategy

Data extraction:

- pick companies that are traded on the stock market on January 2017
- Go back 30 years and extract all the data for these companies
- Use the data to build an ML model supporting your future investments

Question:

- **Would you trust the model?**
- **Are there any biases in the data?**

Data cleaning and preprocessing

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

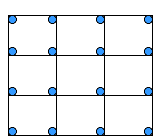
- **Renaming** (relabeling) categorical values to numbers
  - dangerous in conjunction with some learning methods
  - numbers will impose an order that is not warranted

High → 2
Normal → 1
Low → 0

True → 2
False → 1
Unknown → 0

Red → 2
Blue → 1
Green → 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

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)

Feature selection/dimensionality reduction

Feature/dimensionality reduction selection:

- **One way to prevent overfitting for high dimensional data**

  $x_i = (x_i^1, x_i^2, .., x_i^d)$ $\quad d$ - very large

- It reduces the dimensionality of data and expresses them in terms of a smaller sets of inputs/features:
  - Feature filtering
  - Multiple features are combined together

Example: document classification

- **thousands of documents**, >10,000 different words
- **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

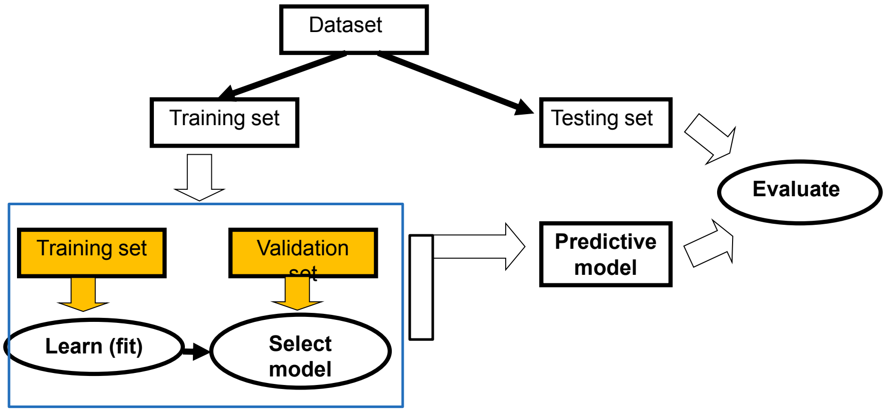
Solutions for overfitting

How to make the learner avoid overfitting?

- **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)

Model selection using validation sets

- Select a model from multiple model choices
- Training set is split to training and validation set
- Validation set is used to decide which model is better



Solutions for overfitting

How to make the learner avoid the overfit?

- **Regularization (Occam's Razor)**
  - Explicit preference towards simple models
  - Penalize for the model complexity (number of parameters) by modifying the objective function

Objective function =

error from the data fit +

regularization penalty for the model complexity

- **Solved through the optimization**

Objective criteria

- **Measure how well the model fits the data**:
  - **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)**

$$\Theta^* = \arg\max_{\Theta} P(\Theta \mid D) \qquad P(\Theta \mid D) = \frac{P(D \mid \Theta)P(\Theta)}{P(D)}$$

Other criteria:

  - **hinge loss (used in the support vector machines)**

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)

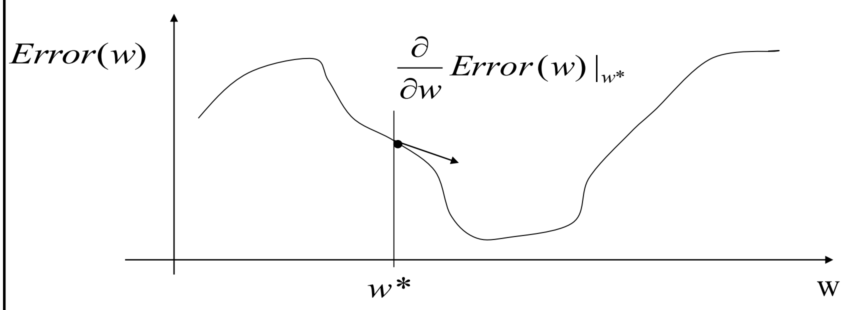
  Goal: $\mathbf{w}^* = \arg\min_{\mathbf{w}} f(\mathbf{w})$

- **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

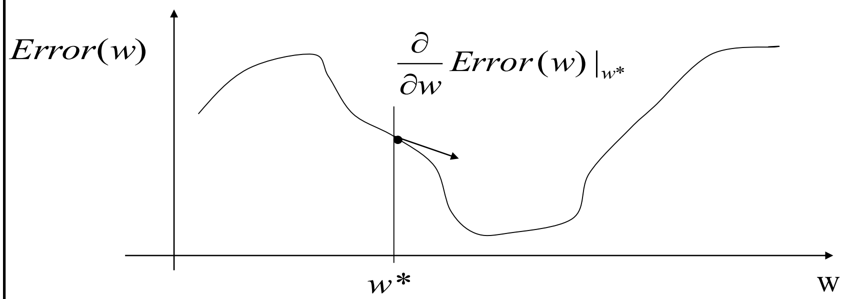


- Change the parameter value of w according to the gradient

  $w \leftarrow w^* + ?$

Gradient descent method

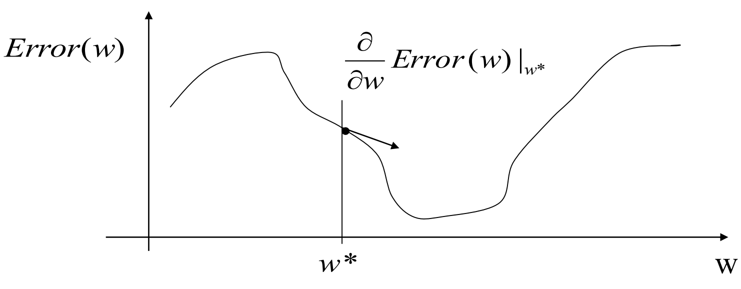
- Descend to the minimum of the function using the gradient information



- Change the parameter value of w according to the gradient

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

Gradient descent method



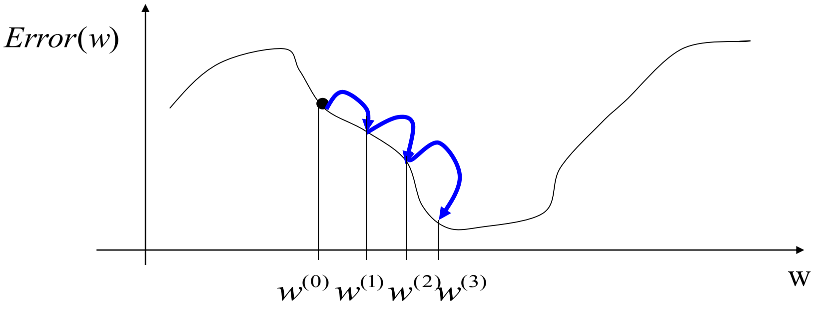
- New value of the parameter

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

$\alpha > 0$ - 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)

Batch vs on-line learning

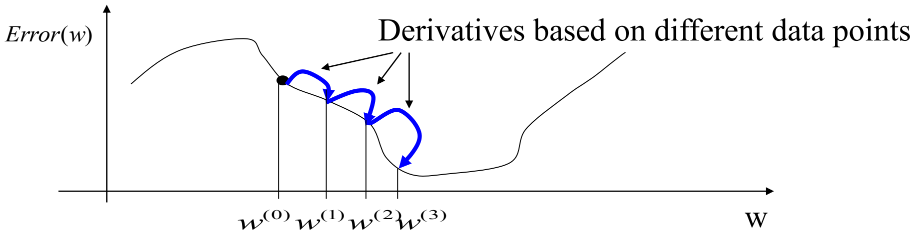
- **Batch learning:** Error function looks at all data points

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

- **On-line learning:** 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)