Machine Learning

0. Overview

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Outline

Outline

Exam and Credit Points

- The course is now a BSc course and can be used as MSc course **only** for those students who are now **not** in their first MSc semester.
- Exceptions might exist, for external MSc students for example if they have to get additional credit points from BSc courses.
- There will be a written exam at end of term (2h, 4 problems).
- The course gives 6 ECTS (2+2 SWS).

Exercises and Tutorials

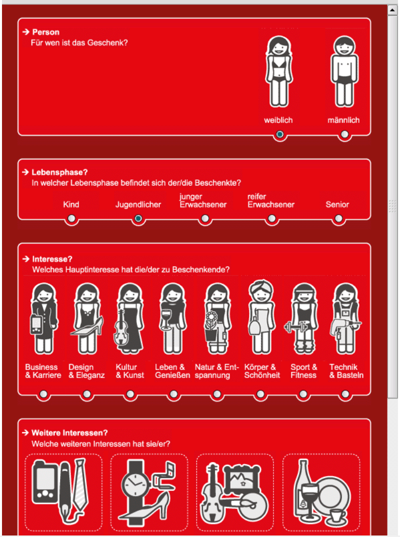
- There will be a weekly sheet with 4 exercises uploaded **every Wednesday** to our webpage. First sheet will be handed out next week.
- Solutions to the exercises can be submitted until **next Tuesday noon** 1st sheet is due Tue. 27.10.
- Exercises will be corrected.
- Tutorials **each Wednesday 2pm–4pm**, 1st tutorial at Wed. 28.10.
- Successful participation in the tutorial gives up to 10% bonus points for the exam.

Outline

What is Machine Learning?

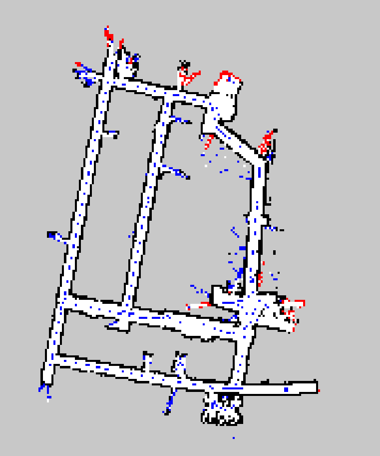
What is Machine Learning?

1. E-Commerce: predict what customers will buy.



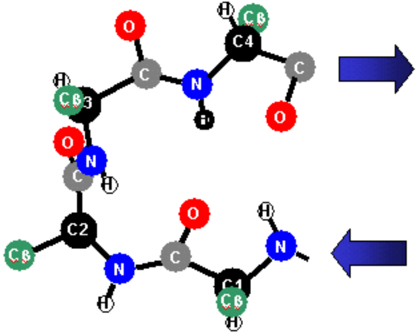
What is Machine Learning?

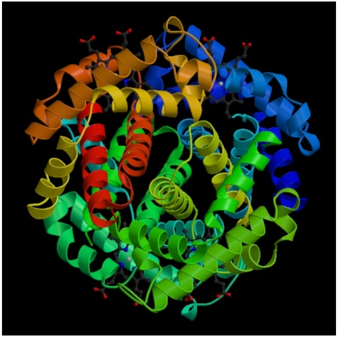
2. Robotics: Build a map of the environment based on sensor signals.



What is Machine Learning?

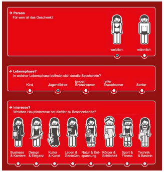
3. Bioinformatics: predict the 3d structure of a molecule based on its sequence.





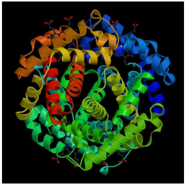
What is Machine Learning?

Information Systems



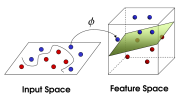
Robotics

Bioinformatics



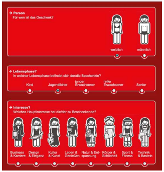
Many Further Applications!

MACHINE LEARNING



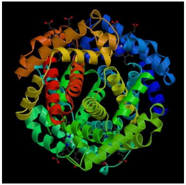
What is Machine Learning?

Information Systems



Robotics

Bioinformatics



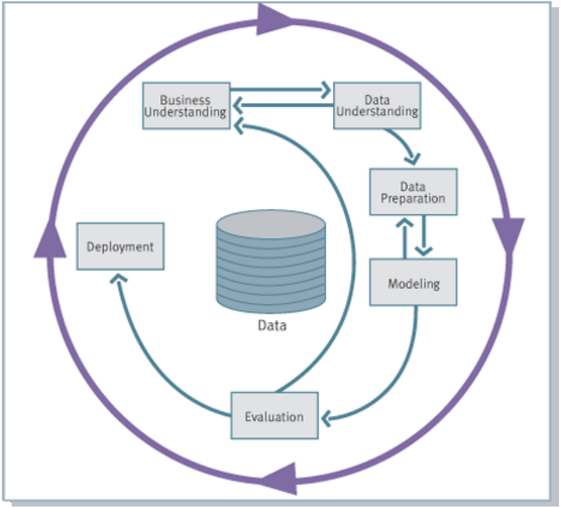
Many Further Applications!

MACHINE LEARNING

OPTIMIZATION

NUMERICS

Process models



Cross Industry Standard Process for Data Mining (CRISP-DM)

One area of research, many names (and aspects)

machine learning
historically, stresses learning logical or rule-based models (vs. probabilistic models).

data mining stresses the aspect of large datasets and complicated tasks.

knowledge discovery in databases (KDD)
stresses the embedding of machine learning tasks in applications, i.e., preprocessing & deployment; data mining is considered the core process step.

data analysis historically, stresses multivariate regression methods and many unsupervised tasks.

pattern recognition
name prefered by engineers, stresses cognitive applications such as image and speech analysis.

applied statistics
stresses underlying statistical models, testing and methodical rigor.

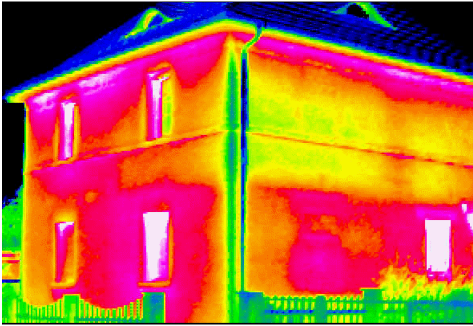
Outline

Example

How does gas consumption depend on external temperature?

Example data (Whiteside, 1960s):
weekly measurements of

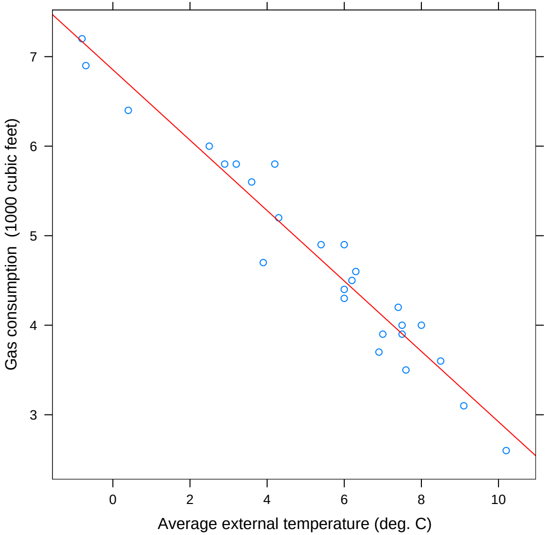
- average external temperature
- total gas consumption
  (in 1000 cubic feets)



How does gas consumption depend on external temperature?

How much gas is needed for a given temperature ?

Example


Gas consumption (1000 cubic feet)
Average external temperature (deg. C)
0
2
4
6
8
10
3
4
5
6
7

The Simple Linear Regression Problem (yet vague)

Given

- a set $\mathcal{D}^{\text{train}} := \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\} \subseteq \mathbb{R} \times \mathbb{R}$ called **training data**,

compute the line that describes the data generating process best.

The Simple Linear Model

For given predictor/input $x \in \mathbb{R}$, the **simple linear model** predicts/outputs

$$\hat{y}(x) := \hat{\beta}_0 + \hat{\beta}_1 x$$

with **parameters** $(\hat{\beta}_0, \hat{\beta}_1)$ called

$\hat{\beta}_0$ **intercept** / **bias** / **offset**

$\hat{\beta}_1$ **slope**

```
procedure PREDICT-SIMPLE-LINREG(x ∈ ℝ, β̂0, β̂1 ∈ ℝ)
    ŷ := β̂0 + β̂1 x
    return ŷ
```

When is a Model Good?

We still need to specify what "describes the data generating process best" means. — What are good predictions $\hat{y}(x)$?

Predictions are considered better the smaller the difference between

- an **observed** y_n (for predictors x_n) and
- a **predicted** $\hat{y}_n := \hat{y}(x_n)$

are, e.g., the smaller the **L2 loss** / **squared error**:

$$\ell(y_n, \hat{y}_n) := (y_n - \hat{y}_n)^2$$

Note: Other error measures such as absolute error $\ell(y_n, \hat{y}_n) = |y_n - \hat{y}_n|$ are also possible, but more difficult to handle.

When is a Model Good?

Pointwise losses are usually averaged over a dataset $\mathcal{D}$

$$\text{err}(\hat{y}; \mathcal{D}) := \frac{1}{N}\text{RSS}(\hat{y}; \mathcal{D}) = \frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}(x_n))^2$$

$$\text{or} \quad \text{err}(\hat{y}; \mathcal{D}) := \text{RSS}(\hat{y}; \mathcal{D}) := \sum_{n=1}^{N}(y_n - \hat{y}(x_n))^2$$

called **residual sum of squares** (RSS) or generally **error**/**risk**.

Equivalently, often **Root Mean Square Error** (RMSE) is used:

$$\text{err}(\hat{y}; \mathcal{D}) := \text{RMSE}(\hat{y}; \mathcal{D}) := \sqrt{\frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}(x_n))^2}$$

Note: RMSE has the same scale level / unit as the original target y, e.g., if y is measured in meters so is RMSE.

Generalization

We can trivially get a model with error zero on training data, e.g., by simply looking up the corresponding y_n for each x_n:

$$\hat{y}^{\text{lookup}}(x) := \begin{cases} y_n, & \text{if } x = x_n \\ 0, & \text{else} \end{cases}$$

$$\text{with } \text{RSS}(\hat{y}^{\text{lookup}}, \mathcal{D}^{\text{train}}) = 0 \text{ optimal}$$

Models should not just reproduce the data, but **generalize**, i.e., predict well on fresh / unseen data (called **test data**).

The Simple Linear Regression Problem

Given

- a set $\mathcal{D}^{\text{train}} := \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\} \subseteq \mathbb{R} \times \mathbb{R}$ called **training data**,

compute the **parameters** $(\hat{\beta}_0, \hat{\beta}_1)$ of a linear **regression function**

$$\hat{y}(x) := \hat{\beta}_0 + \hat{\beta}_1 x$$

s.t. for a set $\mathcal{D}^{\text{test}} \subseteq \mathbb{R} \times \mathbb{R}$ called **test set** the **test error**

$$\text{err}(\hat{y}; \mathcal{D}^{\text{test}}) := \frac{1}{|D^{\text{test}}|} \sum_{(x,y)\in\mathcal{D}^{\text{test}}} (y - \hat{y}(x))^2$$

is minimal.

Note: $\mathcal{D}^{\text{test}}$ has (i) to be from the same data generating process and (ii) not to be available during training.

Least Squares Estimates

As $\mathcal{D}^{\text{test}}$ is not accessible during training, use $\mathcal{D}^{\text{train}}$ as **proxy** for $\mathcal{D}^{\text{test}}$:

- rationale: models predicting well on $\mathcal{D}^{\text{train}}$ should also predict well on $\mathcal{D}^{\text{test}}$ as both come from the same data generating process.

The parameters with minimal L2 loss for a dataset $\mathcal{D}^{\text{train}} := \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$ are called **(ordinary) least squares estimates**:

$$
\begin{aligned}
(\hat{\beta}_0, \hat{\beta}_1) :=& \arg\min_{\hat{\beta}_0, \hat{\beta}_1} \text{RSS}(\hat{y}, \mathcal{D}^{\text{train}}) \\
:=& \arg\min_{\hat{\beta}_0, \hat{\beta}_1} \sum_{n=1}^{N} (y_n - \hat{y}(x_n))^2 \\
=& \arg\min_{\hat{\beta}_0, \hat{\beta}_1} \sum_{n=1}^{N} (y_n - (\hat{\beta}_0 + \hat{\beta}_1 x_n))^2
\end{aligned}
$$

Learning the Least Squares Estimates

The least squares estimates can be written in closed form:

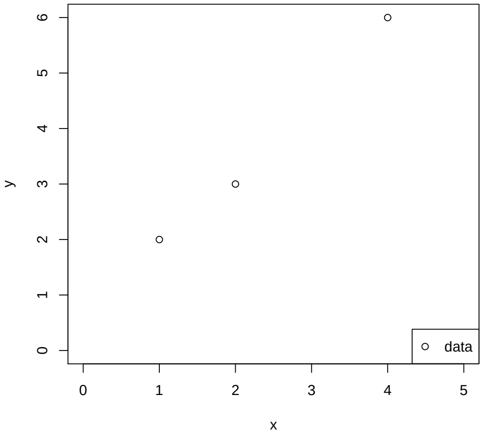
$$\hat{\beta}_1 = \frac{\sum_{n=1}^N (x_n - \bar{x})(y_n - \bar{y})}{\sum_{n=1}^N (x_n - \bar{x})^2}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

1: **procedure** LEARN-SIMPLE-LINREG($\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\} \in \mathbb{R} \times \mathbb{R}$)
2: $\quad \bar{x} := \frac{1}{N} \sum_{n=1}^N x_n$
3: $\quad \bar{y} := \frac{1}{N} \sum_{n=1}^N y_n$
4: $\quad \hat{\beta}_1 := \frac{\sum_{n=1}^N (x_n - \bar{x})(y_n - \bar{y})}{\sum_{n=1}^N (x_n - \bar{x})^2}$
5: $\quad \hat{\beta}_0 := \bar{y} - \hat{\beta}_1 \bar{x}$
6: $\quad$ **return** $(\hat{\beta}_0, \hat{\beta}_1)$

A Toy Example

Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.



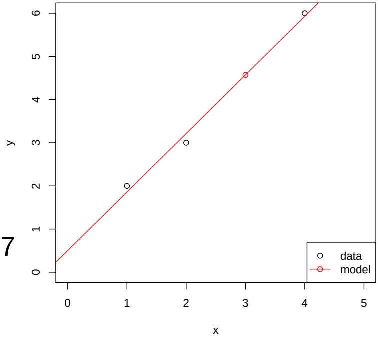
A Toy Example / Least Squares Estimates

Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.
Use a simple linear model.
$\bar{x} = 7/3$, $\bar{y} = 11/3$.

n	$x_n - \bar{x}$	$y_n - \bar{y}$	$(x_n - \bar{x})^2$	$(x_n - \bar{x}) \cdot (y_n - \bar{y})$
1	$-4/3$	$-5/3$	$16/9$	$20/9$
2	$-1/3$	$-2/3$	$1/9$	$2/9$
3	$5/3$	$7/3$	$25/9$	$35/9$
$\sum$			$42/9$	$57/9$

$$\hat{\beta}_1 = \frac{\sum_{n=1}^N (x_n - \bar{x})(y_n - \bar{y})}{\sum_{n=1}^N (x_n - \bar{x})^2} = 57/42 = 1.357$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = \frac{11}{3} - \frac{57}{42} \cdot \frac{7}{3} = \frac{63}{126} = 0.5$$



A Toy Example / Least Squares Estimates

Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.
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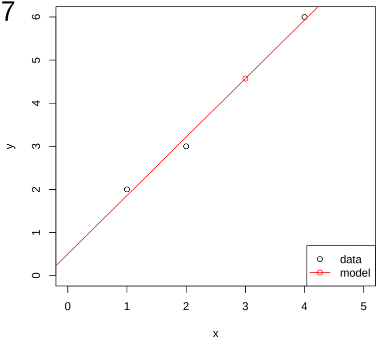
$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1\bar{x} = \frac{11}{3} - \frac{57}{42}\cdot\frac{7}{3} = \frac{63}{126} = 0.5$$

RSS:

n	y_n	$\hat{y}_n$	$(y_n - \hat{y}_n)^2$
1	2	1.857	0.020
2	3	3.214	0.046
3	6	5.929	0.005
$\sum$			0.071

$\hat{y}(3) = 4.571$



Outline

Regression

Real regression problems are more complex than simple linear regression in many aspects:

- There is more than one predictor.
- The target may depend non-linearly on the predictors.

Examples:

- predict sales figures.
- predict rating for a customer review.
- ...

Classification

Example: classifying iris plants (Anderson 1935).

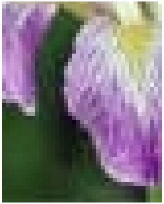
150 iris plants (50 of each species):

- species: setosa, versicolor, virginica
- length and width of sepals (in cm)
- length and width of petals (in cm)

Given the lengths and widths of sepals and petals of an instance, which iris species does it belong to?

iris setosa

iris versicolor

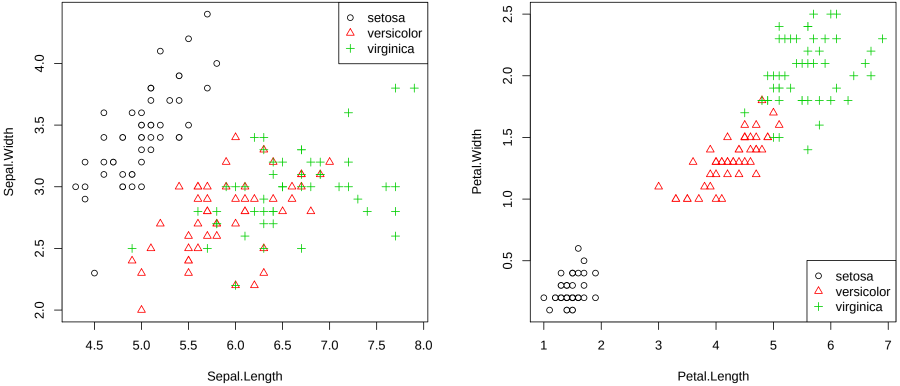


iris virginica

Classification

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.10	3.50	1.40	0.20	setosa
2	4.90	3.00	1.40	0.20	setosa
3	4.70	3.20	1.30	0.20	setosa
4	4.60	3.10	1.50	0.20	setosa
5	5.00	3.60	1.40	0.20	setosa
⋮	⋮	⋮	⋮	⋮	
51	7.00	3.20	4.70	1.40	versicolor
52	6.40	3.20	4.50	1.50	versicolor
53	6.90	3.10	4.90	1.50	versicolor
54	5.50	2.30	4.00	1.30	versicolor
⋮	⋮	⋮	⋮	⋮	
101	6.30	3.30	6.00	2.50	virginica
102	5.80	2.70	5.10	1.90	virginica

Classification



Classification

Example: classifying email (lingspam corpus)

Subject: query: melcuk (melchuk) does anybody know a working email (or other) address for igor melcuk (melchuk) ?	Subject: ' hello ! come see our naughty little city made especially for adults http://208.26.207.98/freeweek/enter.html once you get here, you won't want to leave !
legitimate email ("ham")	spam

How to classify email messages as spam or ham?

Classification

Subject: query: melcuk (melchuk)

does anybody know a working email (or other) address for igor melcuk (melchuk) ?

$\Rightarrow$

$$\begin{pmatrix} \text{a} & 1 \\ \text{address} & 1 \\ \text{anybody} & 1 \\ \text{does} & 1 \\ \text{email} & 1 \\ \text{for} & 1 \\ \text{igor} & 1 \\ \text{know} & 1 \\ \text{melcuk} & 2 \\ \text{melchuk} & 2 \\ \text{or} & 1 \\ \text{other} & 1 \\ \text{query} & 1 \\ \text{working} & 1 \end{pmatrix}$$

Classification

lingspam corpus:

- email messages from a linguistics mailing list.
- 2414 ham messages.
- 481 spam messages.
- 54742 different words.
- an example for an early, but very small spam corpus.

Classification

All words that occur at least in each second spam or ham message on average (counting multiplicities):

	!	your	will	we	all	mail	from	do	our	email
spam	14.18	7.45	4.36	3.42	2.88	2.77	2.69	2.66	2.46	2.24
ham	0.38	0.46	1.93	0.94	0.83	0.79	1.60	0.57	0.30	0.39

	out	report	order	as	free	language	university
spam	2.19	2.14	2.09	2.07	2.04	0.04	0.05
ham	0.34	0.05	0.27	2.38	0.97	2.67	2.61

example rule:

if freq("!") $\geq$ 7 and freq("language")=0 and freq("university")=0 then spam,
else ham

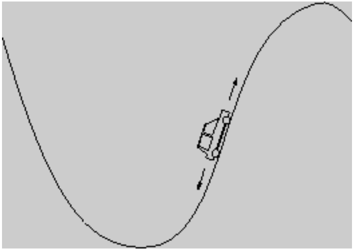
Should we better normalize for message length?

Reinforcement Learning

A class of learning problems where

- the correct / optimal action never is shown,
- but only positive or negative feedback for an action actually taken is given.

Example: steering the mountain car.



Observed are

- x-position of the car,
- velocity of the car

Possible actions are

- accelerate left,
- accelerate right,
- do nothing

The goal is to steer the car on top of the right hill.

Reinforcement Learning / TD-Gammon

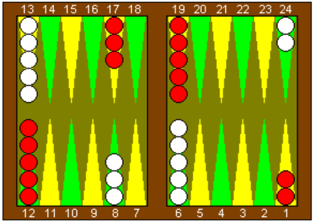


Figure 2. An illustration of the normal opening position in backgammon. TD-Gammon has sparked a near-universal conversion in the way experts play certain opening rolls. For example, with an opening roll of 4-1, most players have now switched from the traditional move of 13-9, 6-5, to TD-Gammon's preference, 13-9, 24-23. TD-Gammon's analysis is given in Table 2.

Program	Hidden Units	Training Games	Opponents	Results
TD-Gam 0.0	40	300,000	Other Programs	Tied for Best
TD-Gam 1.0	80	300,000	Robertie, Magriel, ...	−13 pts / 51 games
TD-Gam 2.0	40	800,000	Var. Grandmasters	−7 pts / 38 games
TD-Gam 2.1	80	1,500,000	Robertie	−1 pts / 40 games
TD-Gam 3.0	80	1,500,000	Kazaros	+6 pts / 20 games

Cluster Analysis

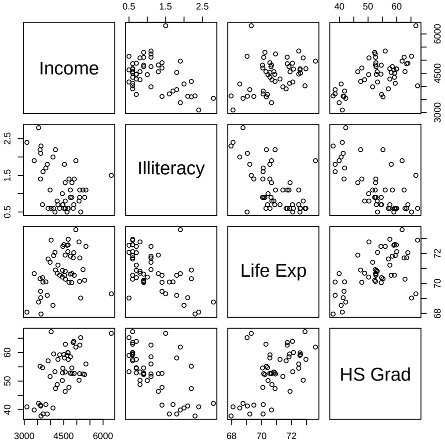
Finding groups of similar objects.

Example: sociographic data of the 50 US states in 1977.

state dataset:

- income (per capita, 1974),
- illiteracy (percent of population, 1970),
- life expectancy (in years, 1969–71),
- percent high-school graduates (1970).

(and some others not used here).



Fundamental Machine Learning Problems

1. Density Estimation	
2. Regression 3. Classification	} Supervised Learning
4. Optimal Control	} Reinforcement Learning
5. Clustering 6. Dimensionality Reduction 7. Association Analysis	} Unsupervised Learning

Supervised learning: correct decision is observed (**ground truth**).
Unsupervised learning: correct decision never is observed.

Outline

Syllabus

Wed. 21.10.	(1)	0. Introduction
		A. Supervised Learning
Wed. 28.10.	(2)	A.1 Linear Regression
Wed. 04.11.	(3)	A.2 Linear Classification
Wed. 11.11.	(4)	A.3 Regularization (Given by Martin)
Wed. 18.11.	(5)	A.4 High-dimensional Data
Wed. 25.11.	(6)	A.5 Nearest-Neighbor Models
Wed. 02.12.	(7)	A.6 Support Vector Machines
Wed. 09.12.	(8)	A.7 Decision Trees
Wed. 06.01.	(9)	A.8 A First Look at Bayesian and Markov Networks
		Extra:
Wed. 16.12.	(E)	Invited Talk: Recommender Systems in work at Volkswagen
		B. Unsupervised Learning
Wed. 13.01.	(10)	B.1 Clustering
Wed. 20.01.	(11)	B.2 Dimensionality Reduction
Wed. 27.01.	(12)	B.3 Frequent Pattern Mining
		C. Reinforcement Learning
Wed. 03.02.	(13)	C.1 State Space Models
Wed. ??.??.	(14)	C.2 Markov Decision Processes

Outline

Some Books

- Gareth James, Daniela Witten, Trevor Hastie, R. Tibshirani (2013): *An Introduction to Statistical Learning with Applications in R*, Springer.
- Kevin P. Murphy (2012): *Machine Learning, A Probabilistic Approach*, MIT Press.
- Trevor Hastie, Robert Tibshirani, Jerome Friedman (^{2}2009): *The Elements of Statistical Learning*, Springer.

  Also available online as PDF at `http://www-stat.stanford.edu/~tibs/ElemStatLearn/`
- Christopher M. Bishop (2007): *Pattern Recognition and Machine Learning*, Springer.
- Richard O. Duda, Peter E. Hart, David G. Stork (^{2}2001): *Pattern Classification*, Springer.

Some First Machine Learning Software

- R (v3.0.0, 3.4.2013; `http://www.r-project.org`).
- Weka (v3.6.9, 22.1.2013; `http://www.cs.waikato.ac.nz/~ml/`).
- SAS Enterprise Miner (commercially).

Public data sets:

- UCI Machine Learning Repository (`http://www.ics.uci.edu/~mlearn/`)
- UCI Knowledge Discovery in Databases Archive (`http://kdd.ics.uci.edu/`)

Further Readings

- For a general introduction: [JWHT13, chapter 1&2], [Mur12, chapter 1], [HTFF05, chapter 1&2].
- For linear regression: [JWHT13, chapter 3], [Mur12, chapter 7], [HTFF05, chapter 3].

References

Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin.
The elements of statistical learning: data mining, inference and prediction, volume 27.
2005.

Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani.
An introduction to statistical learning.
Springer, 2013.

Kevin P. Murphy.
Machine learning: a probabilistic perspective.
The MIT Press, 2012.

Simple Linear Regression / Least Squares Estimates / Proof (p. 20):

$$\text{RSS} = \sum_{i=1}^{n} (y_i - (\hat\beta_0 + \hat\beta_1 x_i))^2$$

$$\frac{\partial\,\text{RSS}}{\partial \hat\beta_0} = \sum_{i=1}^{n} 2(y_i - (\hat\beta_0 + \hat\beta_1 x_i))(-1) \stackrel{!}{=} 0$$

$$\implies \quad n\hat\beta_0 = \sum_{i=1}^{n} (y_i - \hat\beta_1 x_i)$$

Simple Linear Regression / Least Squares Estimates / Proof

Proof (ctd.):

$$
\begin{aligned}
\text{RSS} &= \sum_{i=1}^{n} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2 \\
&= \sum_{i=1}^{n} (y_i - (\bar{y} - \hat{\beta}_1 \bar{x}) - \hat{\beta}_1 x_i)^2 \\
&= \sum_{i=1}^{n} (y_i - \bar{y} - \hat{\beta}_1 (x_i - \bar{x}))^2 \\
\frac{\partial \, \text{RSS}}{\partial \hat{\beta}_1} &= \sum_{i=1}^{n} 2(y_i - \bar{y} - \hat{\beta}_1 (x_i - \bar{x}))(-1)(x_i - \bar{x}) \stackrel{!}{=} 0 \\
\implies \quad \hat{\beta}_1 &= \frac{\sum_{i=1}^{n} (y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}
\end{aligned}
$$