## Machine Learning

Central Problem of Pattern Recognition: Supervised and Unsupervised Learning

Classification<br>Bayesian Decision Theory Perceptrons and SVMs<br>Clustering<br>Dimension Reduction

## The Problem of Pattern Recognition

Machine Learning (as statistics) addresses a number of challenging inference problems in pattern recognition which span the range from statistical modeling to efficient algorithmics. Approximative method which yield good performance on average are particularly important.

- Representation of objects. $\Rightarrow$ Data representation
- What is a pattern? Definition/modeling of structure.
- Optimization: Search for prefered structures
- Validation: are the structures indeed in the data or are they explained by fluctuations?


## Literatur

- Richard O. Duda, Peter E. Hart \& David G. Stork, Pattern Classification. Wiley \& Sons (2001)
- Trevor Hastie, Robert Tibshirani \& Jerome Friedman, The Elements of Statistical Learning: Data Mining, Inference and Prediction. Springer Verlag (2001)
- Luc Devroye, Laslo Györfi \& Gabor Lugosi, A Probabilistic Theory of Pattern Recognition. Springer Verlag (1996)
- Vladimir N. Vapnik, Estimation of Dependences Based on Empirical Data. Springer Verlag (1983); The Nature of Statistical Learning Theory. Springer Verlag (1995)
- Larry Wasserman, All of Statistics. (1st ed. 2004. Corr. 2nd printing, ISBN: 0-387-40272-1) Springer Verlag (2004)


## The Classification Problem





## Classification as a Pattern Recognition Problem

Problem: We look for a partition of the object space $\mathcal{O}$ (fish in the previous example) which corresponds to classification examples.
Distinguish conceptually between "objects" $o \in \mathcal{O}$ and "data" $x \in \mathcal{X}$ !
Data: pairs of feature vectors and class labels

$$
\mathcal{Z}=\left\{\left(x_{i}, y_{i}\right): 1 \leq i \leq n, x_{i} \in \mathbb{R}^{d}, y_{i} \in\{1, \ldots, k\}\right\}
$$

Definitions: feature space $\mathcal{X}$ with $x_{i} \in \mathcal{X} \subset \mathbb{R}^{d}$ class labels $y_{i} \in\{1, \ldots, k\}$

Classifier: mapping $c: \mathcal{X} \rightarrow\{1, \ldots, k\}$
$k$ class problem: What is $y_{n+1} \in\{1, \ldots, k\}$ for $x_{n+1} \in \mathbb{R}^{d}$ ?

## Example of Classification



## Histograms of Length Values



## Histograms of Skin Brightness Values

count


## Linear Classification



## Overfitting



## Optimized Non-Linear Classification

## width



Occam's razor argument: Entia non sunt multiplicanda praeter necessitatem!

## Regression

## (see Introduction to Machine Learning)

Question: Given a feature (vector) $x_{i}$ and a corresponding noisy measurement of a function value $\left(f\left(x_{i}\right)+\right.$ noise $)$ what is the unknown function $f(.) \in$ hypothesis class?

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Data: $\mathcal{Z}=\left\{\left(x_{i}, y_{i}\right) \in \mathbb{R}^{d} \times \mathbb{R}: 1 \leq i \leq n\right\}$
Modeling choice: What is an adequate hypothesis class?
Fitting with linear or nonlinear functions?

## Nonlinear Regression



50 noisy data from a sinc function $\operatorname{sinc}(x):=\sin (x) / x$ (gray) with a regression fit (black).

## The Regression Function

Question: What is the optimal estimate of a function $f: \mathbb{R}^{d} \rightarrow$ $\mathbb{R}$ based on noisy data?

$$
y_{i}=f\left(x_{i}\right)+\eta_{i} \quad \leftarrow \text { noise ? }
$$

Solution: the regression function

$$
y(x)=\mathrm{E}\{y \mid X=x\}=\int_{\Omega} y p(y \mid X=x) d y
$$

Model selection: How many data are required to estimate a model or a regression function?

## Examples of linear and nonlinear regression


linear regression

nonlinear regression

How should we measure the deviations?


## Core Questions of Pattern Recognition: Unsupervised Learning

1. data clustering, vector quantization
2. hierarchical data analysis; search for tree structures in data
3. visualisation, dimension reduction
(a) PCA or principal component analysis
(b) $I C A$, independent component analysis
(c) overcomplete basis
(d) projection pursuit
(e) multidimensional scaling, representation of proximity data as Euclidean distances in $\mathbb{R}^{d}$

## Modes of Learning

Reinforcement Learning: weakly supervised learning Action chains are evaluated at the end.
Backgammon; the neural network TD-Gammon gained the world championship! Quite popular in Robotics

Active Learning: Data are selected according to their expected information gain. Information Filtering

Inductive Learning: the learning algorithm extracts logical rules from the data.
Inductive Logic Programming is a popular sub area of Artificial Intelligence

## Taxonomy of Data with some Examples

Data are representations of measurements / observations!
a) monadic data: $\mathcal{O}=\mathcal{O}^{(1)}$ water depth, temperature, pressure, intensity, ...
b) dyadic data: $\mathcal{O}=\mathcal{O}^{(1)} \times \mathcal{O}^{(2)}$
\{users $\} \times\{$ websites $\}$
\{gene expression levels $\} \times$ \{diseases $\}$ \{word counts\} $\times$ \{documents $\}$ pairwise data: $\mathcal{O}=\mathcal{O}^{(1)} \times \mathcal{O}^{(2)}$ with $\mathcal{O}^{(1)}=\mathcal{O}^{(2)}$ \{proteins $\} \times\{$ proteins $\}$ \{image patches $\} \times\{$ image patches $\}$
c) polyadic data: $R \geq 3$
\{test persons $\} \times$ \{behaviors $\} \times\{$ traits $\}$

## Example for Vectorial Data



## Example of Relational Data

Pairwise dissimilarity of 145 globins which have been selected from 4 classes of $\alpha$-globine, $\beta$-globine, myoglobins and globins of insects and plants.


## Scales for Data

Nominal or categorial scale: qualitative, but without quantitative measurements,
e.g. binary scale $\mathcal{F}=\{0,1\}$ (presence or absence of properties) or
taste categories "sweet, sour, salty and bitter.
Ordinal scale : measurement values are meaningful only with respect to other measurements, i.e., the rank order of measurements carries the information, not the numerical differences (e.g. information on the ranking of different marathon races!?)

## Quantitative scale:

- interval scale: the relation of numerical differences carries the information. Invariance w.r.t. translation and scaling (Fahrenheit scale of temperature).
- ratio scale: zero value of the scale carries information but not the measurement unit. (Kelvin scale).
- Absolute scale: Absolute values are meaningful. (grades of final exams)

