Feature extraction and selection

Based on slides **Martina Bachlera** martin.bachler@igi.tugraz.at **, Makoto Miwa**

And paper Isabelle Guyon, André Elisseeff: An Introduction to variable and feature selection. *JMLR*, 3 (2003) 1157-1182

Overview

- Introduction/Motivation — WHY ?
- Basic definitions, Terminology — WHAT ?
- Variable Ranking methods — HOW ?
- Feature subset selection

Problem: **Where to focus attention ?**

- **A universal problem of intelligent (learning) agents is where to focus their attentio**n.
- What aspects of the problem at hand are important/necessary to solve it?
- **Discriminate between the relevant and irrelevant parts of experience.**

What is **feature selection ?**

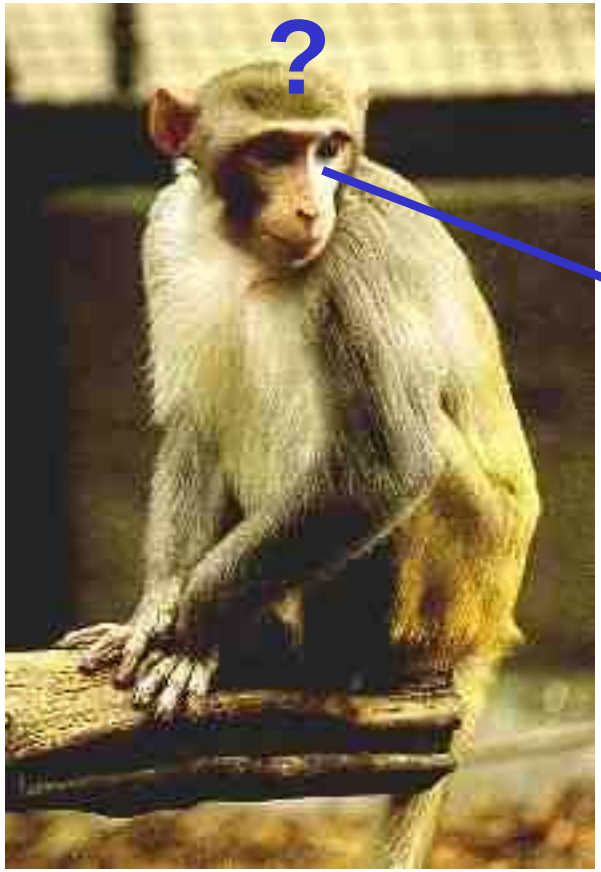
- **Feature selection:**
Problem of selecting some subset of a learning algorithm's input variables upon which it should focus attention, while ignoring the rest (DIMENSIONALITY REDUCTION)

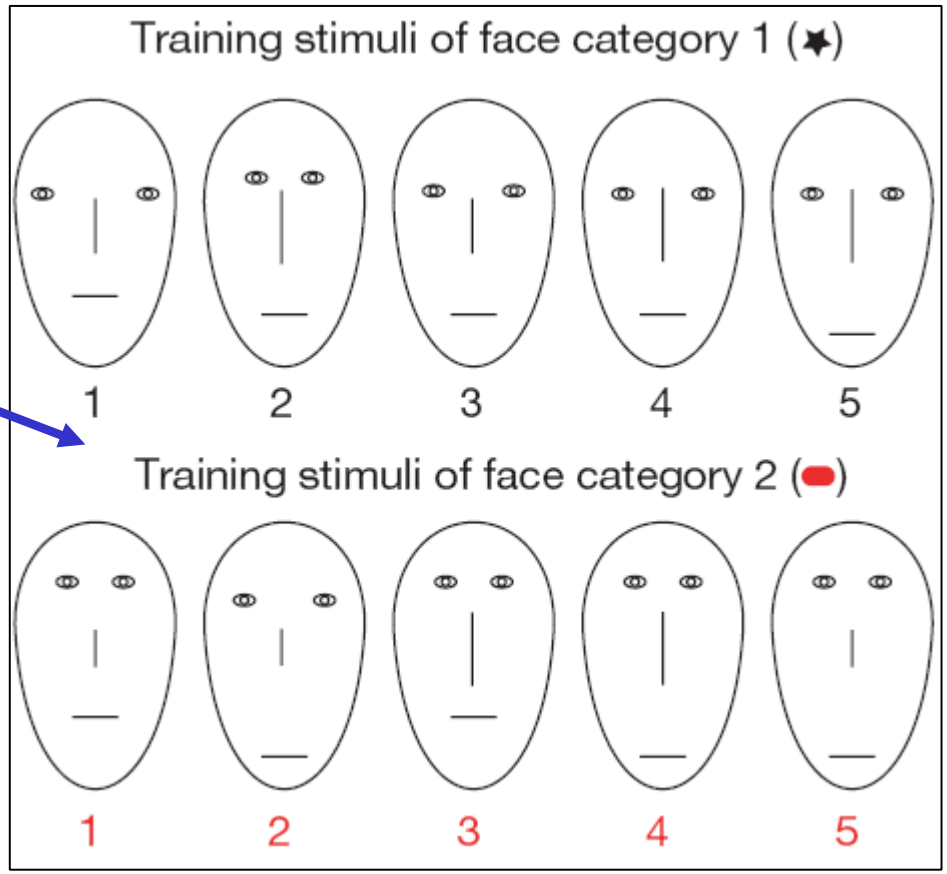
- **Humans/animals do that constantly**!

Motivational example from Biology

[1]

Monkeys performing classification task

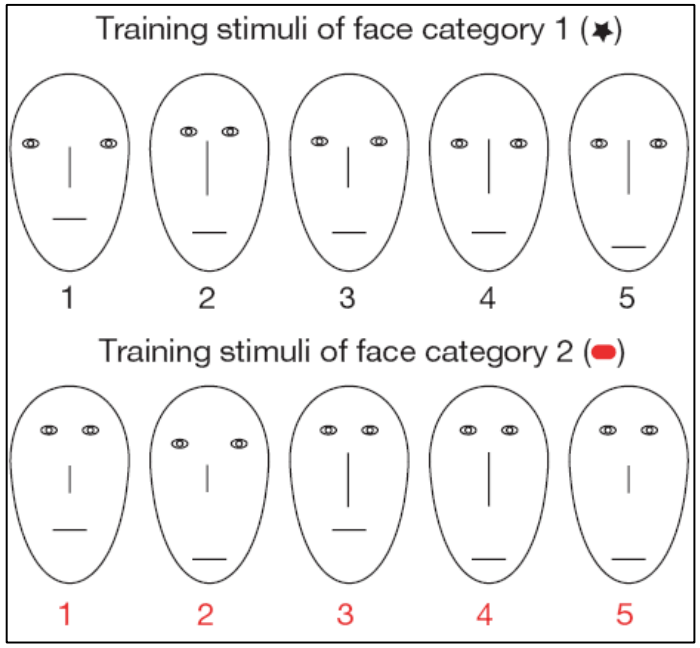


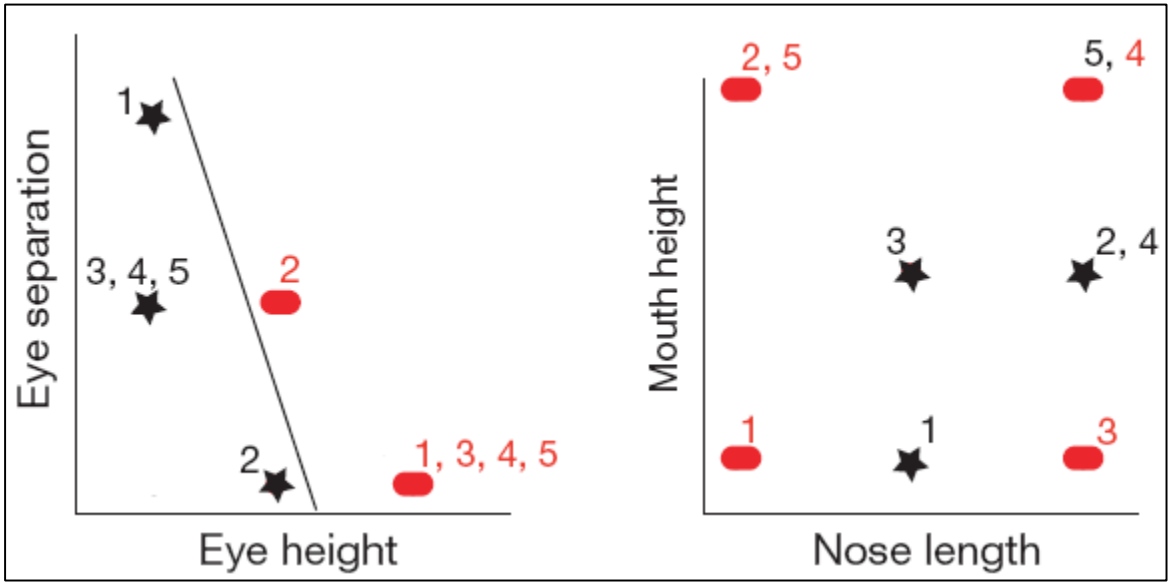


[1] Nathasha Sigala, Nikos Logothetis: Visual categorization shapes feature selectivity in the primate visual cortex. *Nature* Vol. 415(2002)

Motivational example from Biology

Monkeys performing classification task





All considered features:
- Eye height
- Eye separation
- Nose length
- Mouth height

How many pairs of features?

Diagnostic features:
- Eye height
- Eye separation

Non-Diagnostic features:
- Nose length
- Mouth height

Motivational example from Biology

Monkeys performing classification task

Results:

- activity of a population of 150 neurons in the anterior inferior temporal cortex was measured
- 44 neurons responded significantly differently to at least one feature
- After Training: 72% (32/44) were selective to one or both of the diagnostic features (and not for the non-diagnostic features)

Feature Selection in ML ?

Why even think about Feature Selection in ML?

- The information about the target class is **inherent in the variables**!

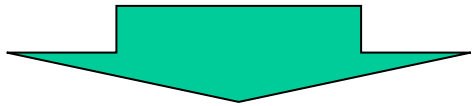
- Naive theoretical view:
  More features
  => More information
  => More discrimination power.

- In practice:
  many reasons why this is not the case!

- Also:
  Optimization is (usually) good, so why not try to optimize the input-coding ?

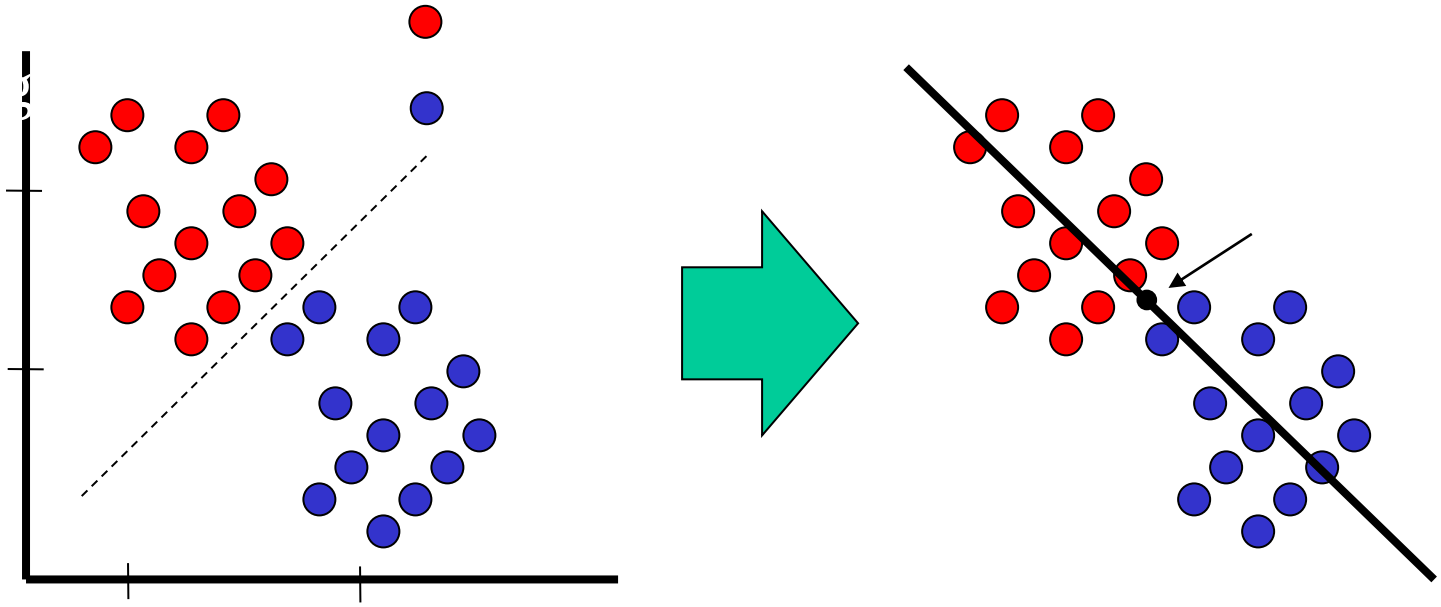
Introduction

- Large and high-dimensional data
  - Web documents, etc…
  - A large amount of resources are needed in
    - Information Retrieval
    - Classification tasks
    - Data Preservation etc…



Dimension Reduction

Dimension Reduction

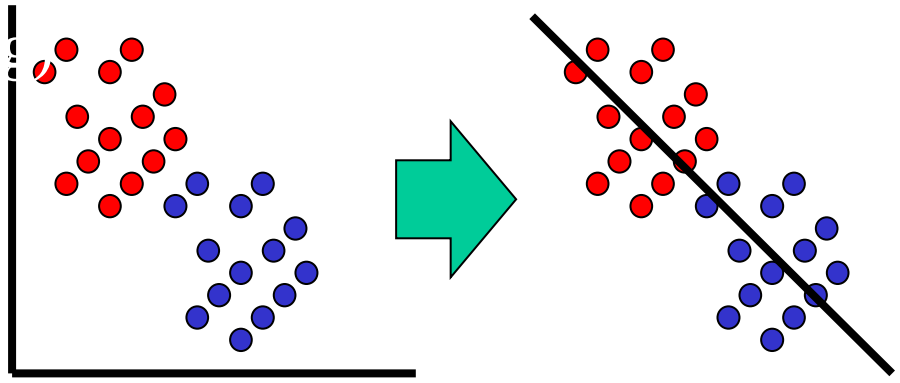


Dimension Reduction

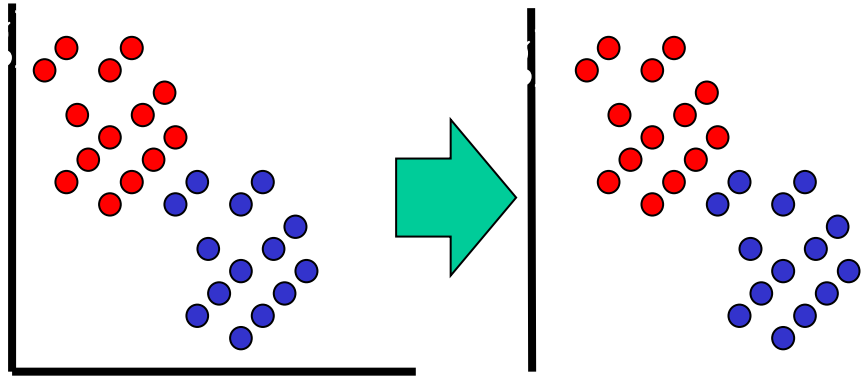
- preserves information on classification of overweight and underweight as much as possible
- makes classification easier
- reduces data size (2 features → 1 feature)

Dimension Reduction

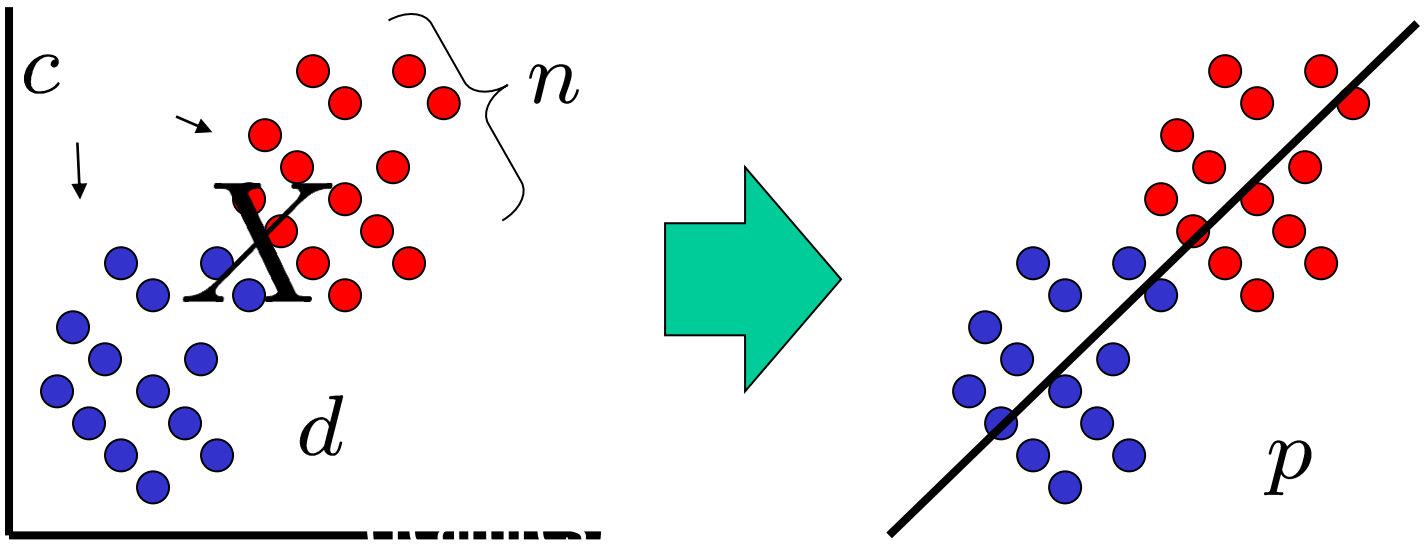
- Feature Extraction (FE)
  - Generates feature
  - ex.
    - Preserves weight / height



- Feature Selection (FS)
  - Selects feature
  - ex.
    - Preserves weight



Problem Setting



- Each of data X (n samples) is represented by d features
- Data belong to c different classes in supervised learning
- Dimension reduction is to generate or select p features preserving original information as much as possible in some criterion

$$1 < p \simeq c \ll d < n$$

Feature Extraction

- Extracts features by projecting data to a lower-dimensional space
  - Unsupervised Method
    - Principal Component Analysis (PCA)
    - Independent Component Analysis (ICA)
  - Supervised Method
    - Linear Discriminant Analysis (LDA)
    - Maximum Margin Criterion (MMC)
    - Orthogonal Centroid algorithm (OC)
- Finds an optimal projection matrix W

W

Principal Component Analysis

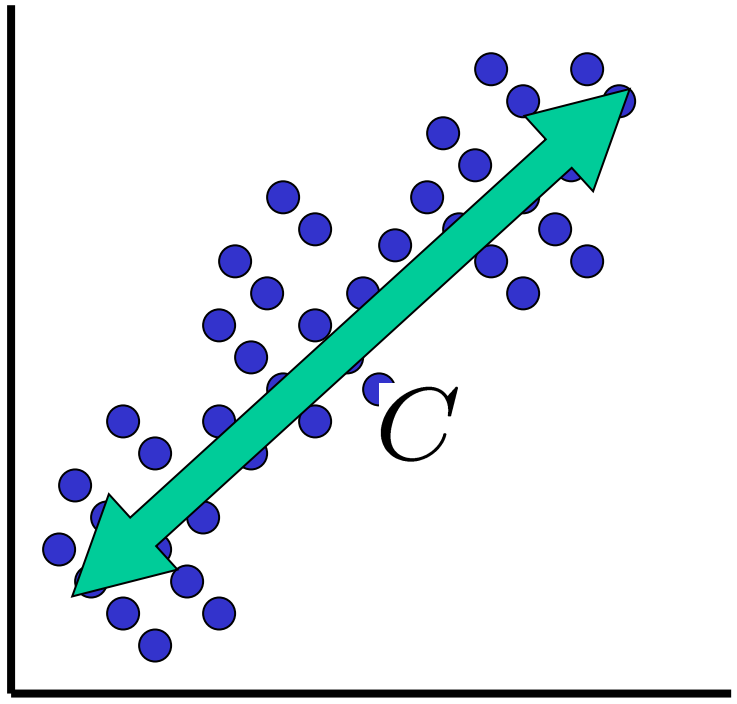
- Unsupervised Method
- PCA tries to maximize

$$J(W) = trace(W^T C W)$$

- PCA needs Singular Value Decomposition calculation (SVD).

  time complexity : $O(n^2 d)$

  space complexity : $O(nd)$



C : covariance matrix

Linear Discriminant Analysis

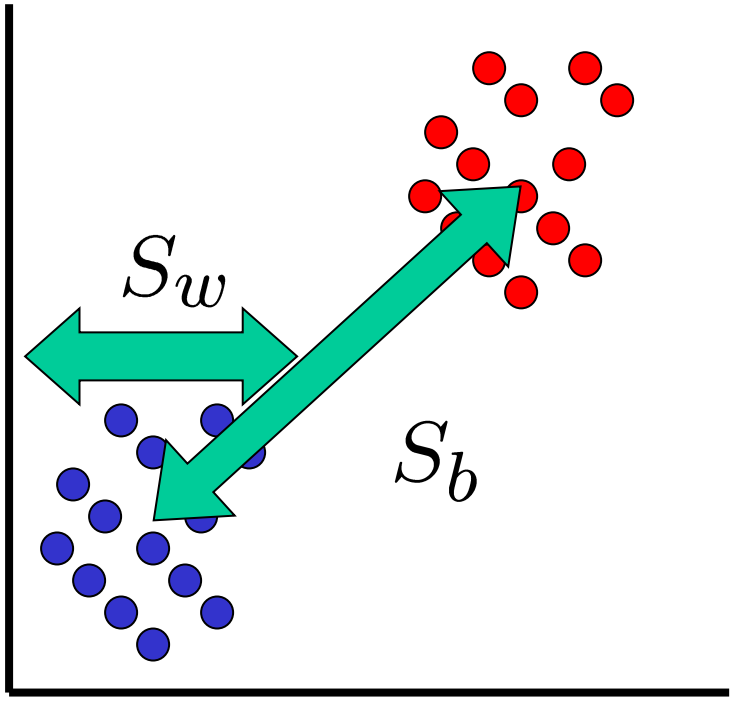
Supervised method

Time complexity

$$O((n+c)^2 d)$$

Space complexity

$$O(nd)$$



S_b Interclass scatter matrix

S_w: Intraclass scatter matrix

Feature Selection in ML ? YES!

- Many explored domains have **hundreds** to **tens of thousands** of variables/features with many irrelevant and redundant ones!

- In domains with many features the underlying probability distribution can be very complex and very hard to estimate (e.g. dependencies between variables) !

- Irrelevant and redundant features can „confuse" learners!

- Limited training data!

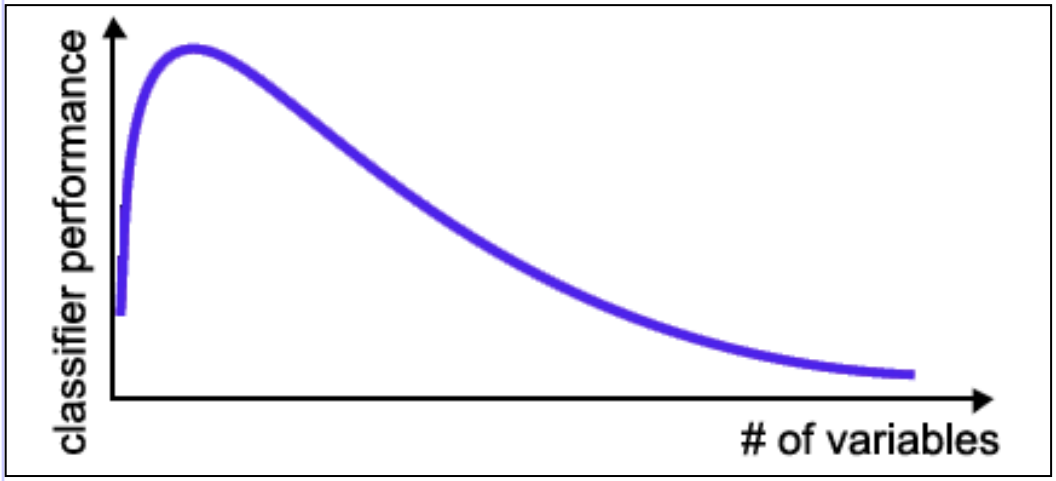
- Limited computational resources!

- **Curse of dimensionality**!

Curse of dimensionality

- The required number ***m*** of samples (to achieve the same accuracy) grows exponentionally with the number of variables! PAC: ***m*** > |Hypothesis_space|
- In practice: number of training examples is fixed!

=> the classifier's performance usually will degrade for a large number of features!



In many cases

- the information that is lost by discarding variables

is made up for by

- a more accurate mapping/sampling in the lower-dimensional space !

Věta o PAC učení rozhodovacího stromu

Nechť objekty jsou charakterizovány pomocí ***n*** binárních atributů a nechť připouštíme jen hypotézy ve tvaru rozhodovacího stromu s maximální délkou větve ***k***. Dále nechť δ, ε jsou malá pevně zvolená kladná čísla blízká 0. Pokud algoritmus strojového učení vygeneruje hypotézu φ, která je konzistentní se všemi **m** příklady trénovací množiny a platí

$$m \geq m_{k\text{-DT}}(n) \geq c\,(\,n^k + \ln(1/\delta))\,/\,\varepsilon$$

pak φ je ε-skoro správná hypotéza s pravděpodobností větší než $(1-\delta)$, t.j. chyba hypotézy φ na celém definičním oboru konceptu je menší než ε s pravděpodobností větší než $(1-\delta)$.

Example for ML-Problem

Gene selection from microarray data

- Variables:
  gene expression coefficients corresponding to the amount of mRNA in a patient's sample (e.g. tissue biopsy)
- Task: Seperate healthy patients from cancer patients
- Usually there are only about 100 examples (patients) available for training and testing (!!!)
- Number of variables in the raw data: 6.000 – 60.000
- Does this work ? ([8])

[8] C. Ambroise, G.J. McLachlan: Selection bias in gene extraction on the basis of microarray gene-expresseion data. *PNAS* Vol. 99 6562-6566(2002)

Example for ML-Problem

Text-Categorization

- Documents are represented by a vector containing word frequency counts (its size ~ number of features is comparable to that of the vocabulary)
- Vocabulary ~ 15.000 words (i.e. each document is represented by a 15.000-dimensional vector)
- Typical tasks:
  - Automatic sorting of documents into web-directories
  - Detection of spam-email

Motivation

- Especially when dealing with a large number of variables there is a need for **dimensionality reduction**!

- Feature Selection can significantly improve a learning algorithm's performance!

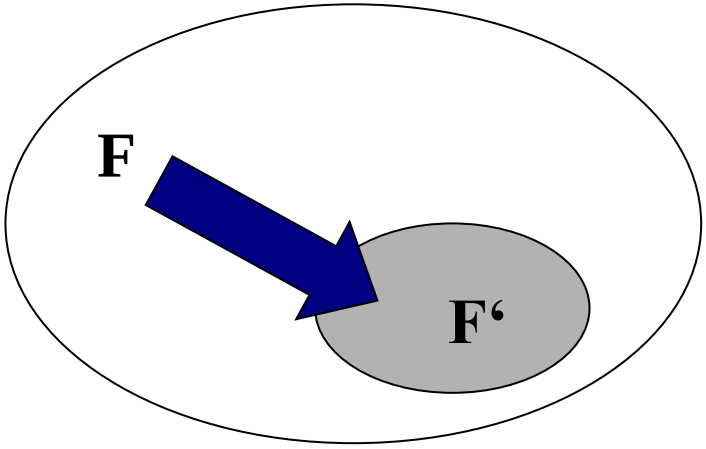
Overview

- Introduction/Motivation
- Basic definitions, Terminology
- Variable Ranking methods
- Feature subset selection

Feature Selection - Definition

- Given a set of features $F=\{f_1,\ldots,f_i,\ldots,f_n\}$

the Feature Selection problem is
to find **a subset** $F'\subseteq F$ that "maximizes the learners ability to classify patterns".



$$\{f_1,\ldots,f_i,\ldots,f_n\} \xrightarrow{f.selection} \{f_{i_1},\ldots,f_{i_j},\ldots,f_{i_m}\}$$

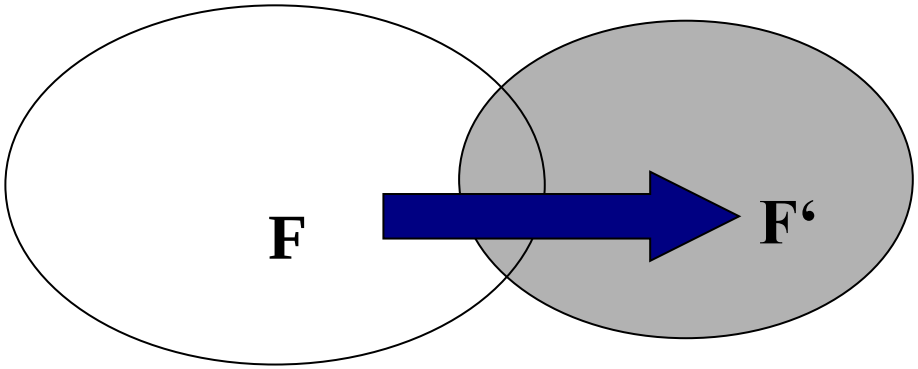
$$i_j \in \{1,\ldots,n\};\ j=1,\ldots,m$$

$$i_a = i_b \Rightarrow a=b;\ \ a,b \in \{1,\ldots,m\}$$

Feature Extraction-Definition

- Given a set of features $F=\{f_1,\ldots,f_i,\ldots,f_n\}$

  the Feature Extraction("Construction") problem is
  is to map F to some feature set F'' that maximizes the learner's ability to classify patterns (design new derived attributes) .



$$\{f_1,\ldots,f_i,\ldots,f_n\} \xrightarrow[f.extraction]{} \{g_1(f_1,\ldots,f_n),\ldots,g_j(f_1,\ldots,f_n),\ldots,g_m(f_1,\ldots,f_n)\}$$

Feature Selection – Optimality ?

- In theory the goal is to find an optimal feature-subset (one that maximizes the scoring function)

- In real world applications this is usually not possible
  - For most problems it is computationally intractable to search the whole space of possible feature subsets
  - One usually has to settle for approximations of the optimal subset
  - Most of the research in this area is devoted to finding efficient search-heuristics

Optimal feature subset

- Often: Definition of optimal feature subset in terms of classifier's performance
- The best one can hope for theoretically is the Bayes error rate
- Given a learner I and training data L with features $F = \{f_1, \ldots f_i, \ldots, f_n\}$ an optimal feature subset F_{opt} is a subset of F such that the accuracy of the learner's hypothesis h is maximal (i.e. its performance is equal to an optimal Bayes classifier)*.
  - F_{opt} (under this definition) depends on I
  - F_{opt} need not be unique
  - Finding F_{opt} is usually computationally intractable

* for this definition a possible scoring function is $1 - true\_error(h)$

Relevance of features

- Relevance of a variable/feature:
  - There are several definitions of relevance in literature:
    - Relevance of 1 variable,
    - Relevance of a variable given other variables,
    - Relevance given a certain learning algorithm,..
  - Most definitions are problematic, because there are problems where all features would be declared to be irrelevant
  - The authors of [2] define two degrees of relevance: **weak** and **strong relevance**.
  - A feature is relevant iff it is weakly or strongly relevant and ”irrelevant”(redundant) otherwise.

[2] Ron Kohavi, George H. John: Wrappers for Feature Subset Selection. *AIJ special issue on relevance* (1996)

Relevance of featurs

- **Strong Relevance** of a variable/feature:

Let $S_i = \{f_1, \ldots, f_{i-1}, f_{i+1}, \ldots f_n\}$ be the set of all features except f_i. Denote by s_i a value-assignment to all features in S_i.

A feature f_i is strongly relevant, iff removal of f_i alone will always result in a performance deterioration of an optimal Bayes classifier.

- **Weak Relevance** of a variable/feature:

A feature f_i is weakly relevant, iff it is not strongly relevant, and there exists a subset of features S_i' of S_i for which there exists a subset of features S_i', such that the performance of an optimal Bayes classifier on S_i' is worse than on $S_i' \cup \{f_i\}$

Relevance of features

- Relevance $\not\Rightarrow$ Optimality of Feature-Set
  - Classifiers induced from training data are likely to be suboptimal (no access to the real distribution of the data)
  - Relevance does not imply that the feature is in the optimal feature subset
  - Even "irrelevant" features can improve a classifier's performance
  - Defining relevance in terms of a given classifier (and therefore a hypothesis space) would be better.

Overview

- Introduction/Motivation
- Basic definitions, Terminology
- Variable Ranking methods
- Feature subset selection

Variable Ranking

- Given a set of features F

Variable Ranking is the process of ordering the features by the value of some scoring function $S: F \rightarrow \Omega$ (which usually measures feature-relevance)

- Resulting set:
a permutation of F: $F' = \{ f_{i_1}, \ldots, f_{i_j}, \ldots f_{i_n} \}$ with

$$S(f_{i_j}) \geq S(f_{i_{j+1}}); \quad j = 1, \ldots, n-1;$$

The score $S(f_i)$ is computed from the training data, measuring some criteria of feature f_i.

- By convention a high score is indicative for a valuable (relevant) feature.

Variable Ranking – Feature Selection

- A simple method for feature selection using variable ranking is to select the k highest ranked features according to S.
- This is usually not optimal
- but often preferable to other, more complicated methods
- computationally efficient(!): only calculation and sorting of n scores

Ranking Criteria – Correlation

Correlation Criteria:

- Pearson correlation coefficient

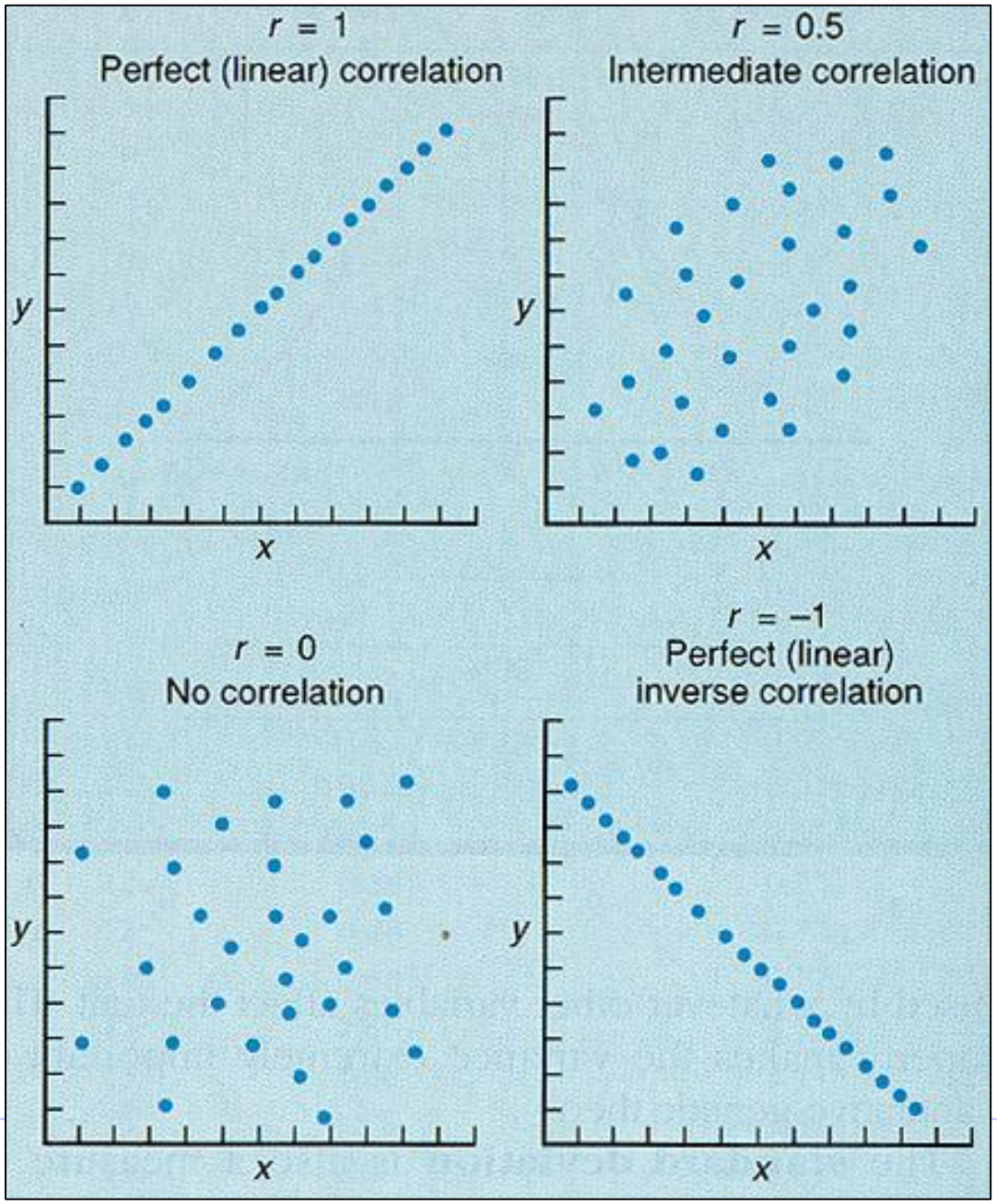
$$R(f_i, y) = \frac{\operatorname{cov}(f_i, y)}{\sqrt{\operatorname{var}(f_i)\operatorname{var}(y)}}$$

- Estimate for m samples:

$$R(f_i, y) = \frac{\sum_{k=1}^{m}\left(f_{k,i} - \overline{f_i}\right)\left(y_k - \overline{y}\right)}{\sqrt{\sum_{k=1}^{m}\left(f_{k,i} - \overline{fi}\right)^2 \sum_{k=1}^{m}\left(y_k - \overline{y}\right)^2}}$$

The higher the correlation between the feature and the target, the higher the score!

Ranking Criteria – Correlation



Ranking Criteria – Correlation

Correlation Criteria:

- $R(X,Y) \in [-1,1]$
- mostly $R(x_i,y)^2$ or $|R(x_i,y)|$ is used
- measure for the goodness of **linear** fit of x_i and y.

  (can only detect linear dependencies between variable and target.)
- what if $y = XOR(x1,x2)$?
- often used for microarray data analysis

Ranking Criteria – Correlation

Questions:

- Can variables with **small score** be automatically discarded ?
- Can a useless variable (i.e. one with a small score) be useful together with others ?
- Can two variables that are useless by themselves can be useful together?)

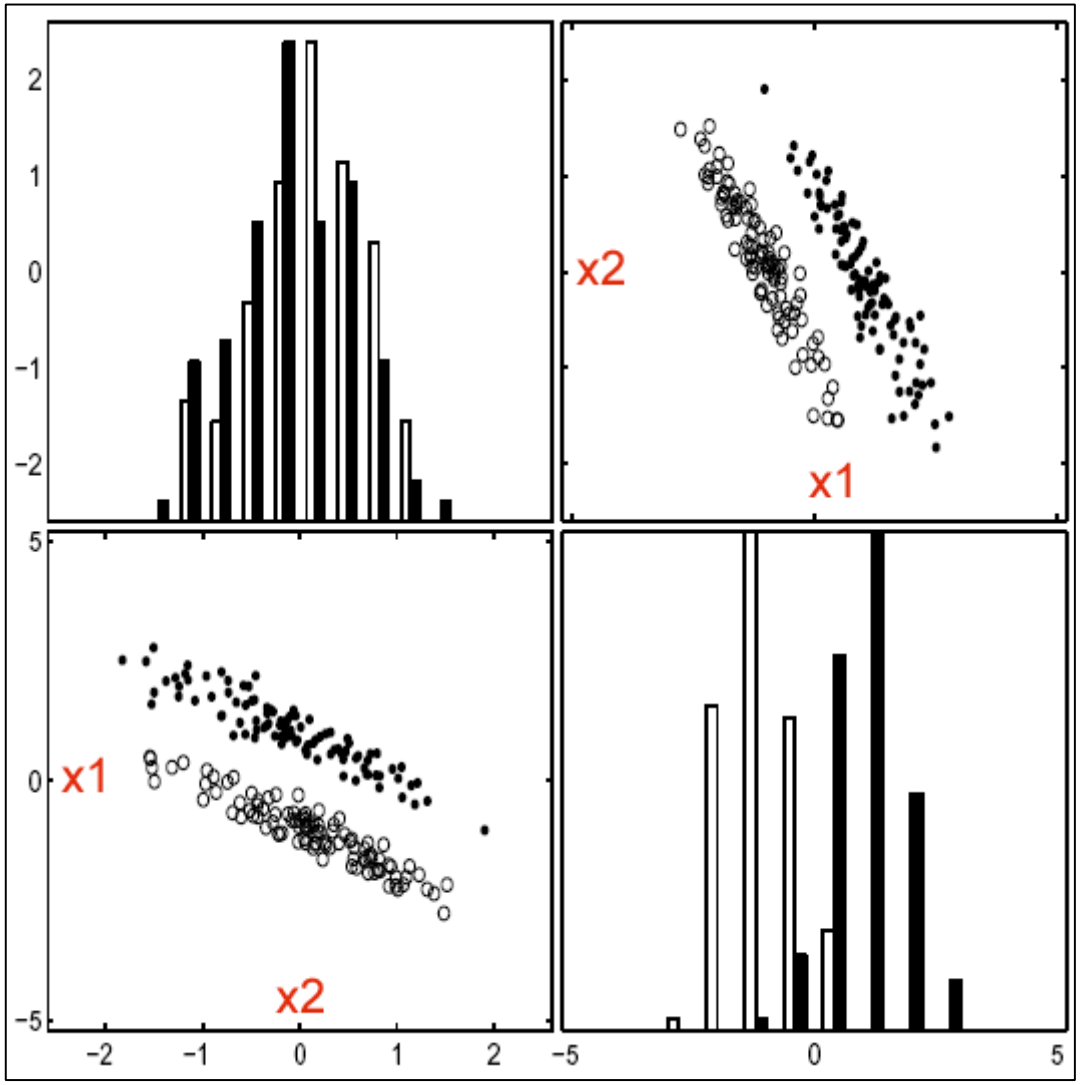
Ranking Criteria – Correlation

- Can variables with small score be discarded without further consideration? **NO!**

- Even variables with small score can improve class seperability!

- Here this depends on the correlation between x_1 and x_2.

(Here the class conditional distributions have a high covariance in the direction orthogonal to the line between the two class centers)

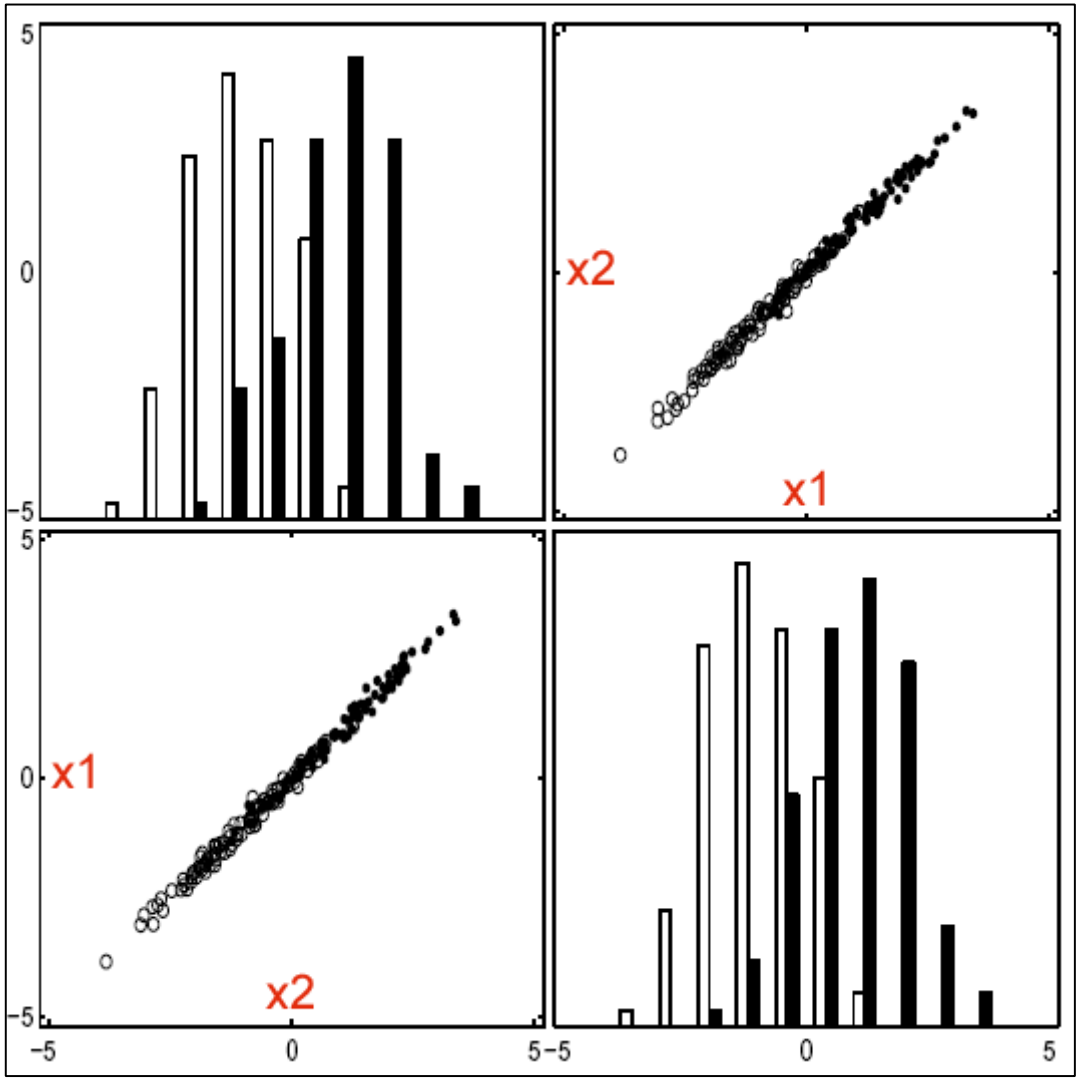


Ranking Criteria – Correlation

- Example with high correlation between x_1 and x_2.

  (Here the class conditional distributions have a high covariance in the direction of the two class centers)

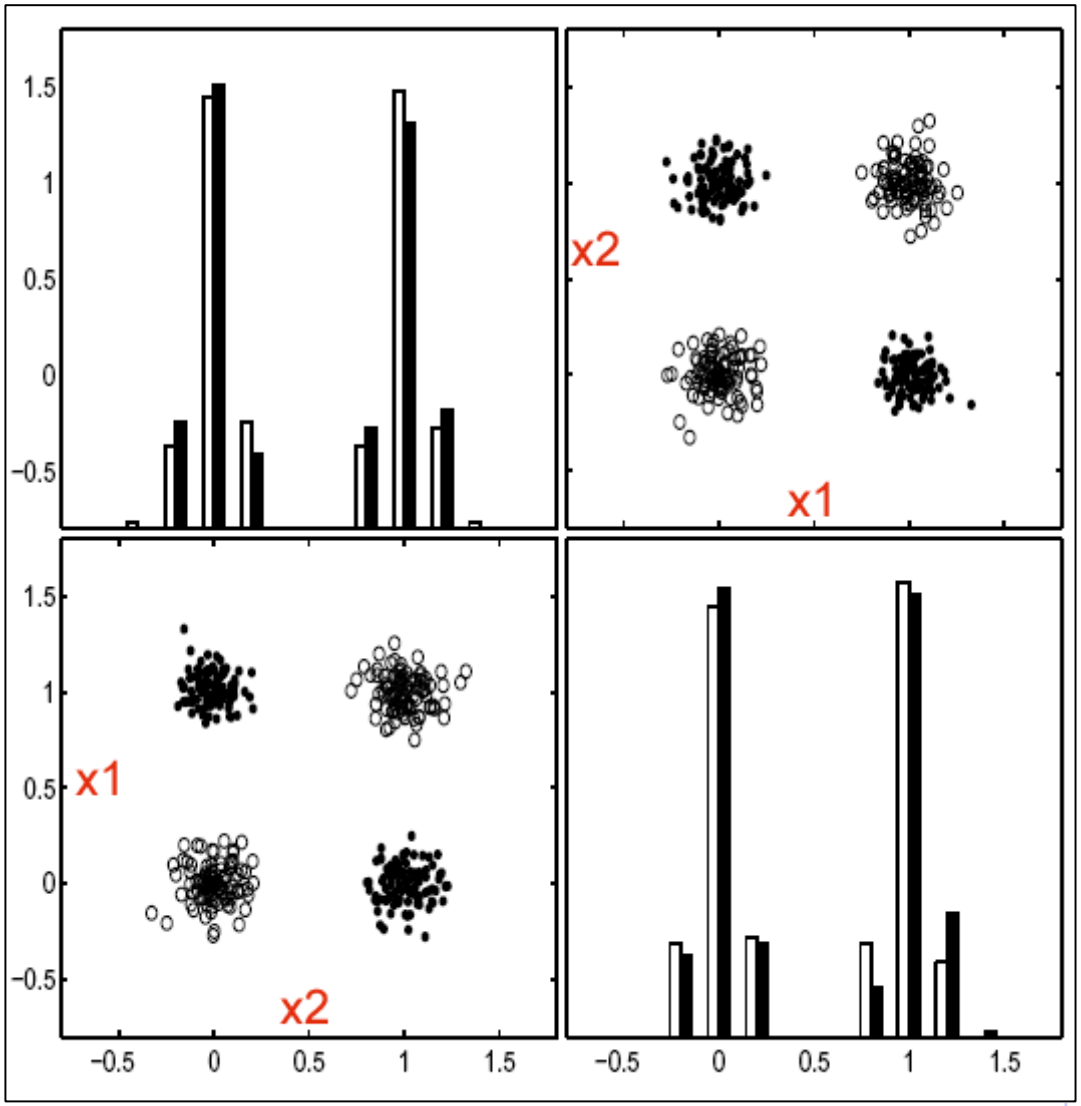
- No gain in seperation ability by using two variables instead of just one!



Ranking Criteria – Correlation

- Can a useless variable be useful together with others ?

YES!



Ranking Criteria – Correlation

- correlation between variables and target are not enough to assess relevance!

- correlation / covariance between pairs of variables has to be considered too!

  (potentially difficult)

- **diversity** of features

Ranking Criteria – Inf. Theory

Information Theoretic Criteria

- Most approaches use (empirical estimates of) mutual information between features and the target:

$$I(x_i, y) = \int_{x_i} \int_{y} p(x_i, y) \log \frac{p(x_i, y)}{p(x_i)\,p(y)}\, dxdy$$

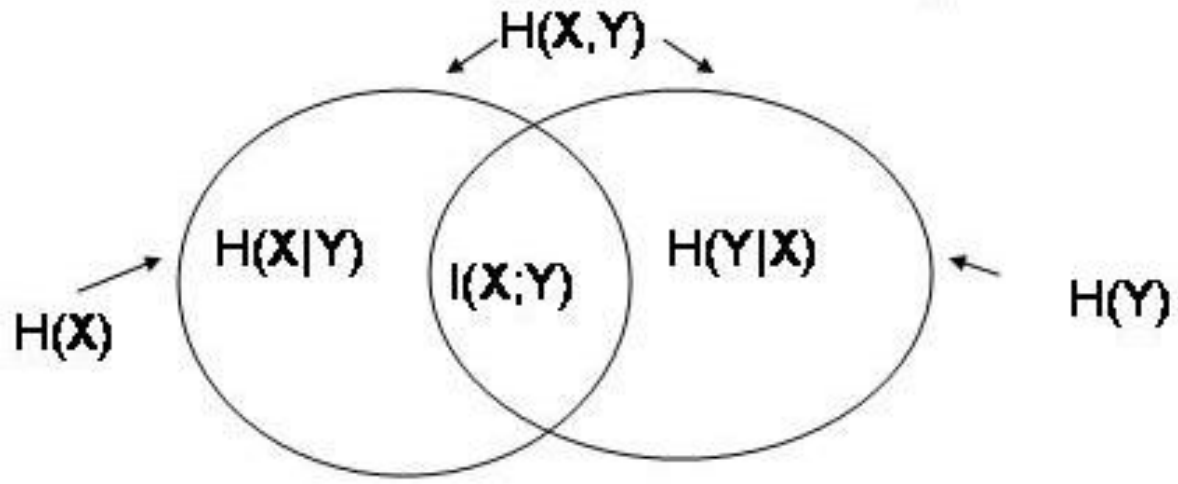
- Case of discrete variables:

$$I(x_i, y) = \sum_{x_i} \sum_{y} P(X = x_i, Y = y) \log \frac{P(X = x_i, Y = y)}{P(X = x_i)P(Y = y)}$$

(probabilities are estimated from frequency counts)

Ranking Criteria – Inf. Theory

- Mutual information can also detect non-linear dependencies among variables!
- But harder to estimate than correlation!
- It is a measure for "how much information (in terms of entropy) two random variables share"



Variable Ranking - SVC

Single **V**ariable **C**lassifiers

- Idea: Select variables according to their **individual predictive power**
- criterion: Performance of a classifier built with 1 variable
- e.g. the value of the variable itself

(set treshold on the value of the variable)

- predictive power is usually measured in terms of error rate (or criteria using fpr, fnr)
- also: combination of SVCs using ensemble methods (boosting,…)

Overview

- Introduction/Motivation
- Basic definitions, Terminology
- Variable Ranking methods
- Feature subset selection

Feature Subset Selection

- Goal:

  - Find the optimal feature subset.

    (or at least a "good one.")

- Classification of methods:
  - Filters
  - Wrappers
  - Embedded Methods

Feature Subset Selection

- You need:
  - a measure for assessing the goodness of a feature subset (scoring function)
  - a strategy to search the space of possible feature subsets
- Finding a minimal optimal feature set for an arbitrary target concept is NP-hard

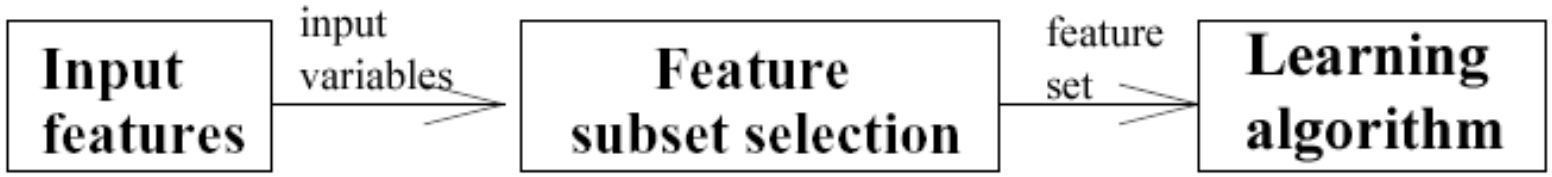
=> Good heuristics are needed!

[9] E. Amaldi, V. Kann: The approximability of minimizing nonzero variables and unsatisfied relations in linear systems. (1997)

Feature Subset Selection

❖ Filter Methods

- Select subsets of variables as a pre-processing step,
  independently of the used classifier!!



- Note that Variable Ranking-FS is a filter method

Feature Subset Selection

- Filter Methods
- usually fast
- provide generic selection of features, not tuned by given learner (universal)
- this is also often criticised (feature set not optimized for used classifier)
- sometimes used as a preprocessing step for other methods

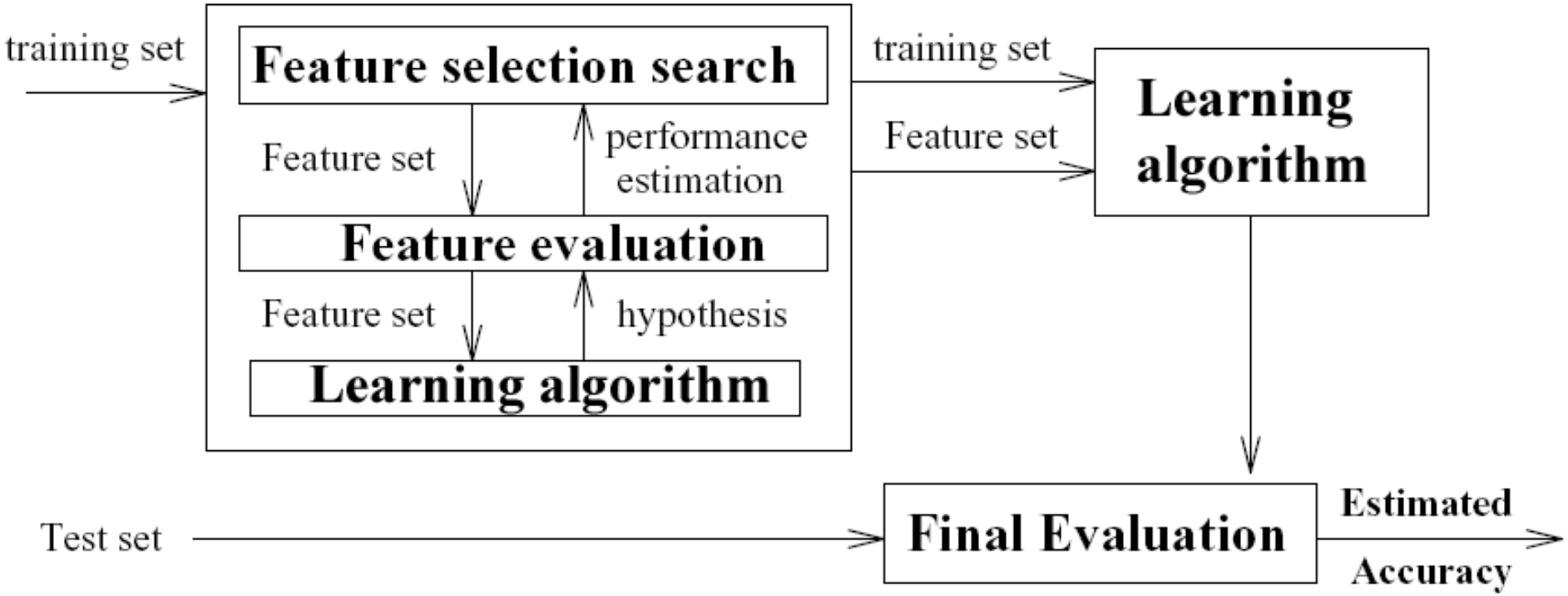
Feature Subset Selection

❖ Wrapper Methods

- Learner is considered a black-box
- Interface of the black-box is used to score subsets of variables according to the predictive power of the learner when using the subsets.
- Results vary for different learners
- One needs to define:
  - how to search the space of all possible variable subsets ?
  - how to assess the prediction performance of a learner ?

Feature Subset Selection

Wrapper Methods



Feature Subset Selection

❖ Wrapper Methods

- The problem of finding the optimal subset is NP-hard!

- A wide range of heuristic search strategies can be used.
  Two different classes:
  - **Forward selection**
    (start with empty feature set and add features at each step)
  - **Backward elimination**
    (start with full feature set and discard features at each step)

- predictive power is usually measured on a validation set or by cross-validation
- By using the learner as a black box wrappers are universal and simple!
- Criticism: a large amount of computation is required.

Feature Subset Selection

- Embedded Methods
- Specific to a given learning machine!
- Performs variable selection (implicitly) in the process of training
- E.g. WINNOW-algorithm
- (linear unit with multiplicative updates)

Important points 1/2

- Feature selection can significantly increase the performance of a learning algorithm (both accuracy and computation time) – but it is not easy!
- One can work on problems with very high-dimensional feature-spaces
- Relevance <-> Optimality
- Correlation and Mutual information between single variables and the target are often used as Ranking-Criteria of variables.

Important points 2/2

- One can not automatically discard variables with small scores – they may still be useful together with other variables.
- Filters – Wrappers - Embedded Methods
- How to search the space of all feature subsets ?
- How to asses performance of a learner that uses a particular feature subset ?

THANK YOU!

Sources

1. Nathasha Sigala, Nikos Logothetis: Visual categorization shapes feature selectivity in the primate visual cortex. *Nature* Vol. 415(2002)
2. Ron Kohavi, George H. John: Wrappers for Feature Subset Selection. *AIJ special issue on relevance* (1996)
3. Isabelle Guyon and Steve Gunn. Nips feature selection challenge. http://www.nipsfsc.ecs.soton.ac.uk/, 2003.
4. Isabelle Guyon, Andre Elisseeff: An Introduction to Variable and Feature Selection. *Journal of Machine Learning Research 3* (2003) 1157-1182
5. Nathasha Sigala, Nikos Logothetis: Visual categorization shapes feature selectivity in the primate visual cortex. *Nature* Vol. 415(2002)
6. Daphne Koller, Mehran Sahami: Toward Optimal Feature Selection. *13. ICML* (1996) p. 248-292
7. Nick Littlestone: Learning Quickly When Irrelevant Attributes Abound: A New Linear-treshold Algorithm. *Machine Learning 2*, p. 285-318 (1987)
8. C. Ambroise, G.J. McLachlan: Selection bias in gene extraction on the basis of microarray gene-expresseion data. *PNAS* Vol. 99 6562-6566(2002)
9. E. Amaldi, V. Kann: The approximability of minimizing nonzero variables and unsatisfied relations in linear systems. (1997)