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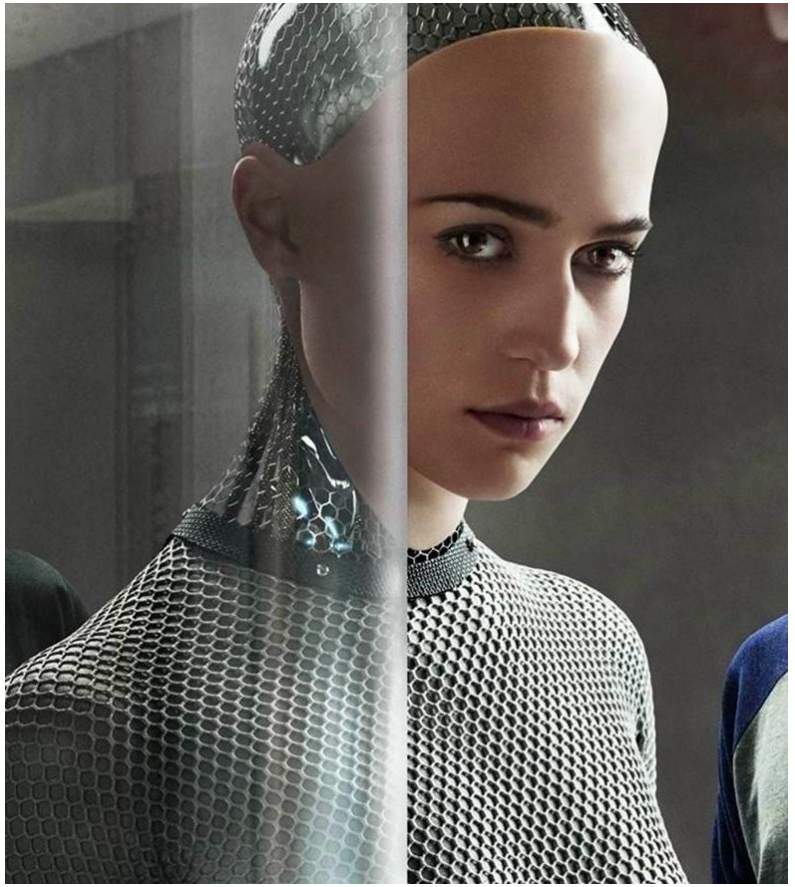
STROJOVÉ UČENÍ

Předměty a návaznost

- SU1/USU ZS, 2+1
  Základní kurz. Existuje i jako ROZP2/ROZRF2
- SU2 ZS, 2+2
- DIZO LS
- SFTO LS

Umělá inteligence (AI)

- Systém (zařízení, stroj, bytost, …), který umí vnímat vnější prostředí, vyhodnocovat ho, rozhodovat se a vykonat akci ke splnění cíle, stanoveného uživatelem.

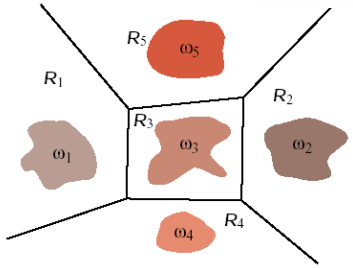


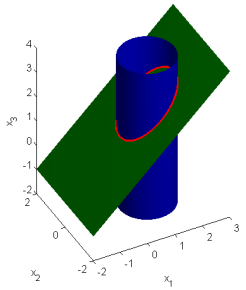
Umělá inteligence dnes

- Jazykové modely (ChatGPT)
- Call centra, vyřizování žádostí
- Generování fotografií a videa
- Autonomní vozidla, drony, roboti
- Specializovaná jednoúčelová zařízení

Umělá inteligence – obecné scéma

- Vnímání: přijímání a zpracování dat
  - senzory, úložiště, software
- Vyhodnocení situace
  - klasifikační problém
- Rozhodnutí
  - optimalizační problém
- Provedení
  - hardware





[Boston Dynamics]

Terminologie

- AI jako vědní obor
- Robotika
- Strojové učení (ML)
- Klasifikátory, rozpoznávání, analýza dat
- Kybernetika

Umělá inteligence

- **OBECNÁ**
- **SPECIÁLNÍ**

Základní odlišnost je v obecnosti zadání
a ve velikosti oblasti přípustných rozhodnutí

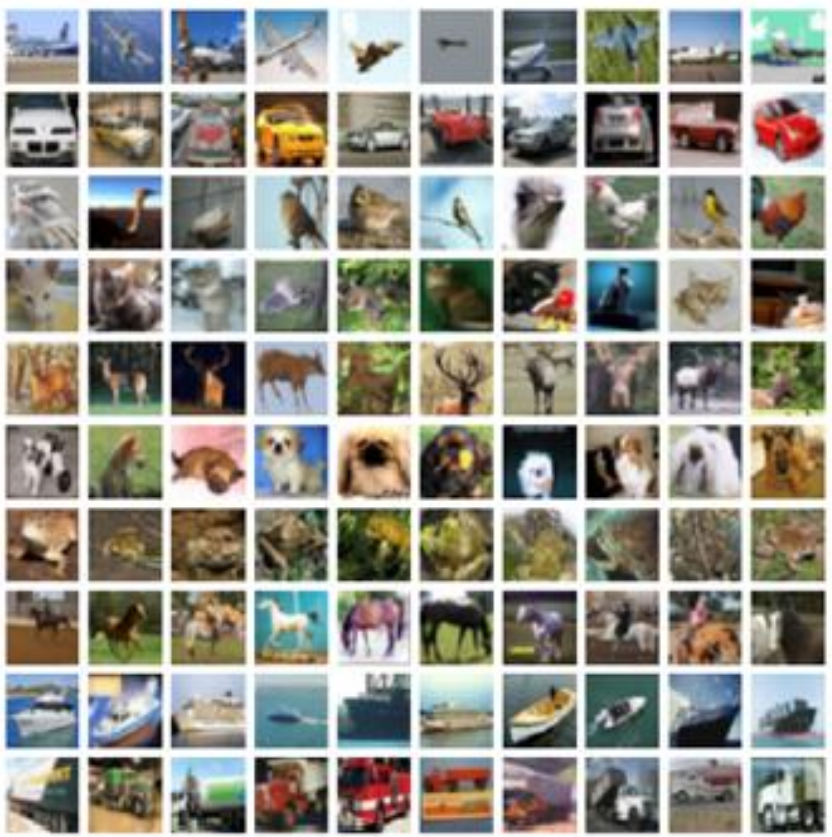
Strojové učení

Volba proměnných, typu a parametrů účelové funkce

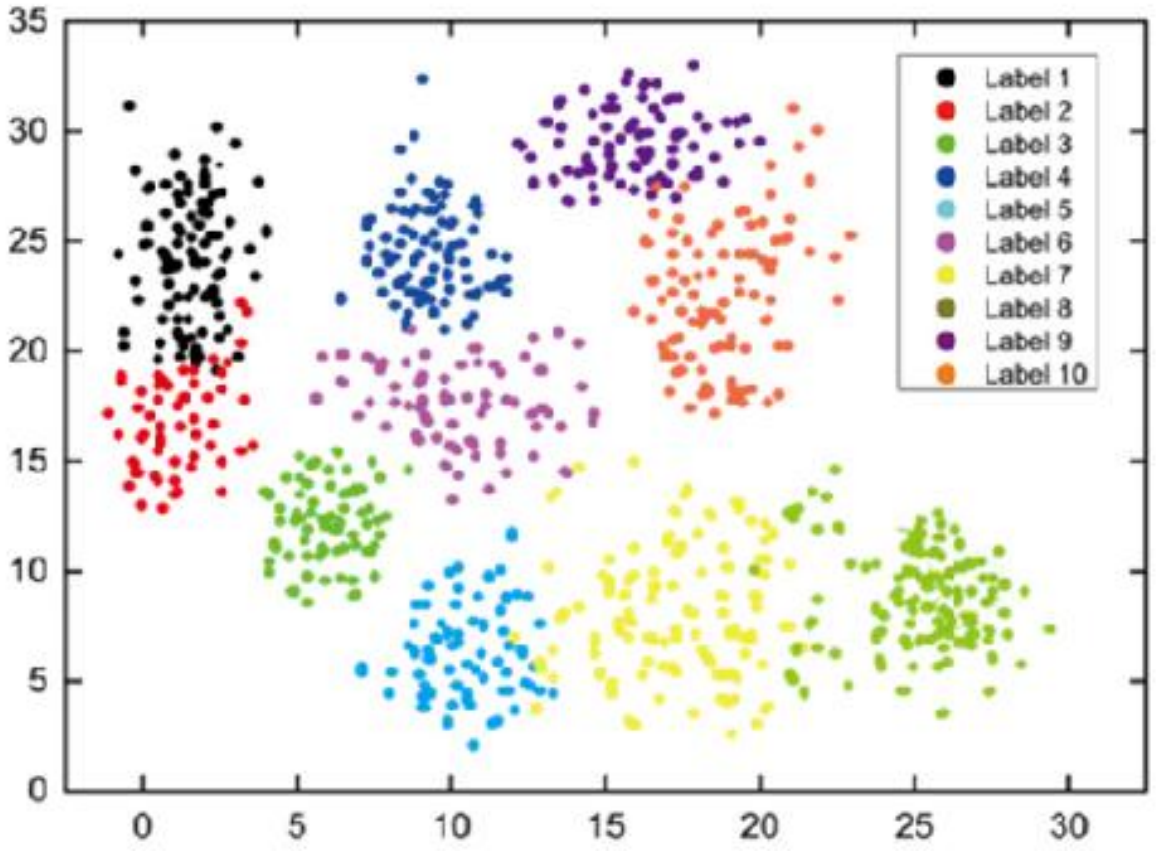
- **Klasické metody**: proměnné definuje uživatel (handcrafted features), parametry (někdy i typ) se trénují na datech

- **Hluboké sítě a podobné metody**: proměnné se určují trénováním (learned features)

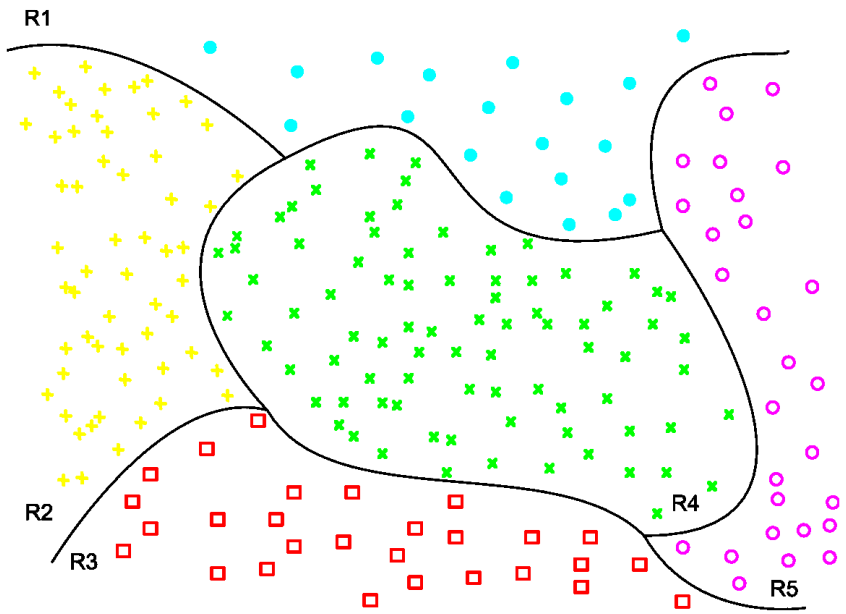
Object space and feature space

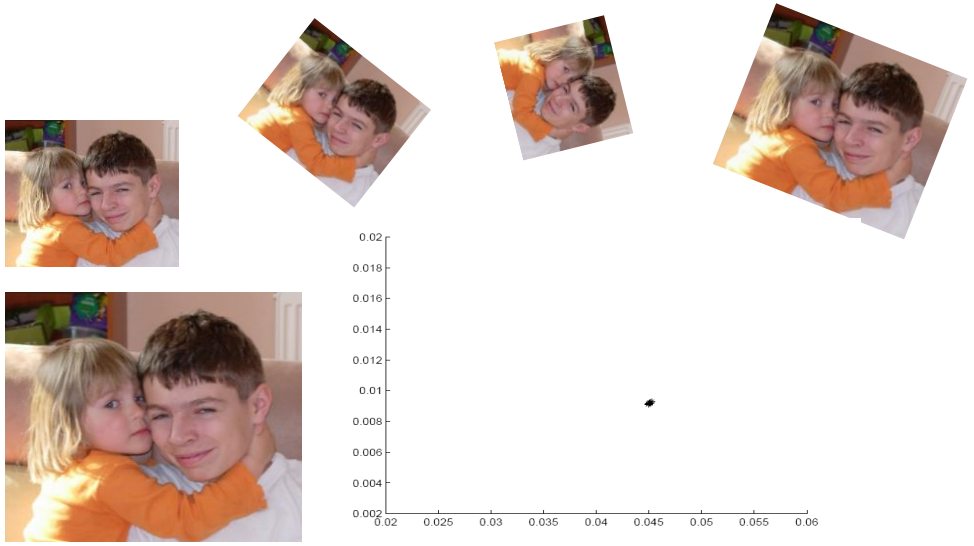


mapping

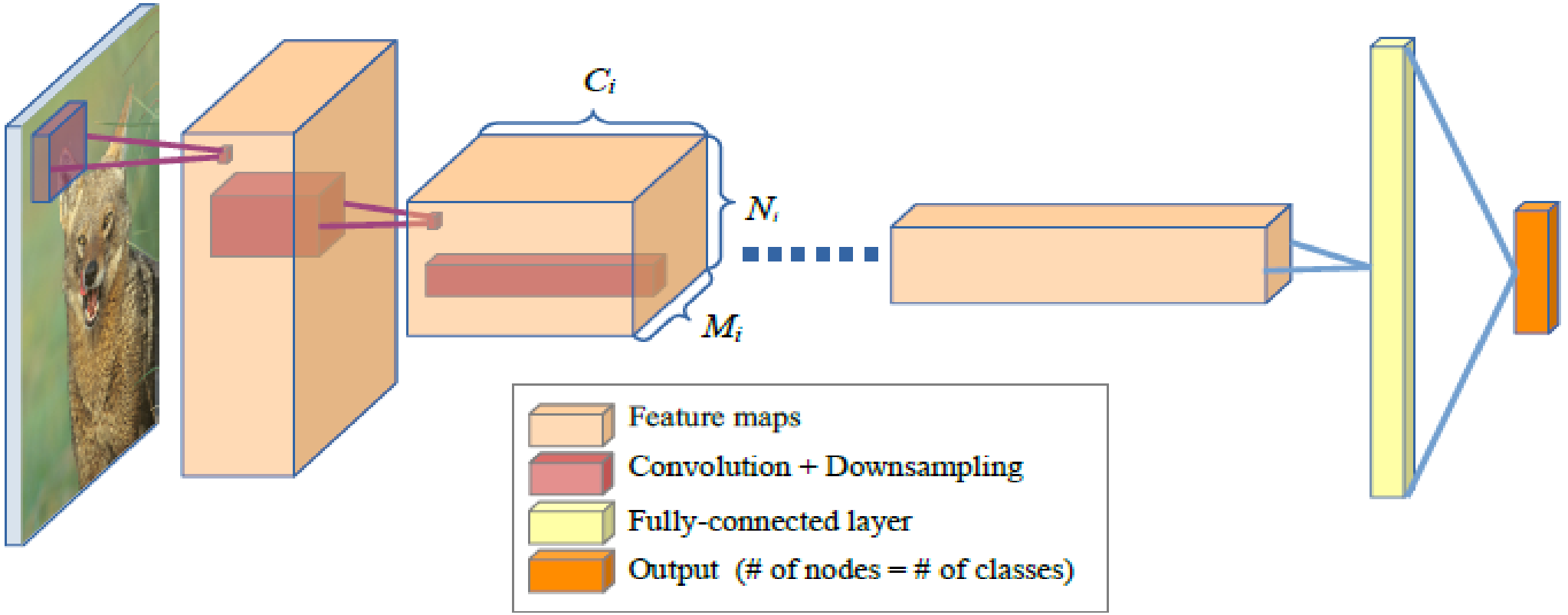


Handcrafted vs. Learned features



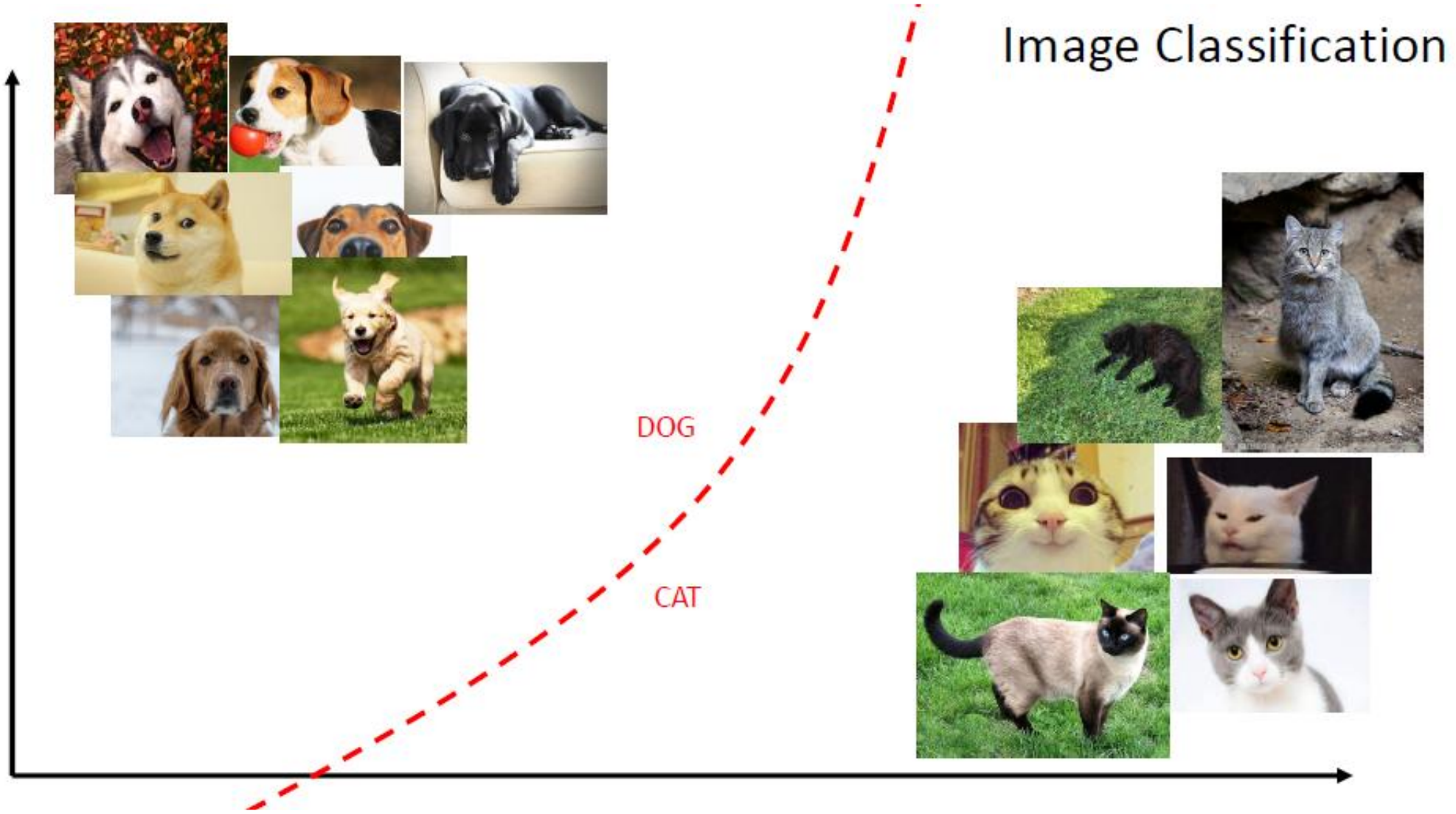


Convolution networks



Teaching by showing many examples without saying what the features are

Properly trained CNN can do this



Handcrafted vs. Learned features

- Teoretický vhled
- Interpretovatelnost
- Závislost na datech
- Hledání příčin chyb
- Trénovací množiny
- Konkurenční nebo komplementární přístupy?

Netechnické aspekty AI

- Právní
- Sociální
- Etické
- Psychologické
- Politické

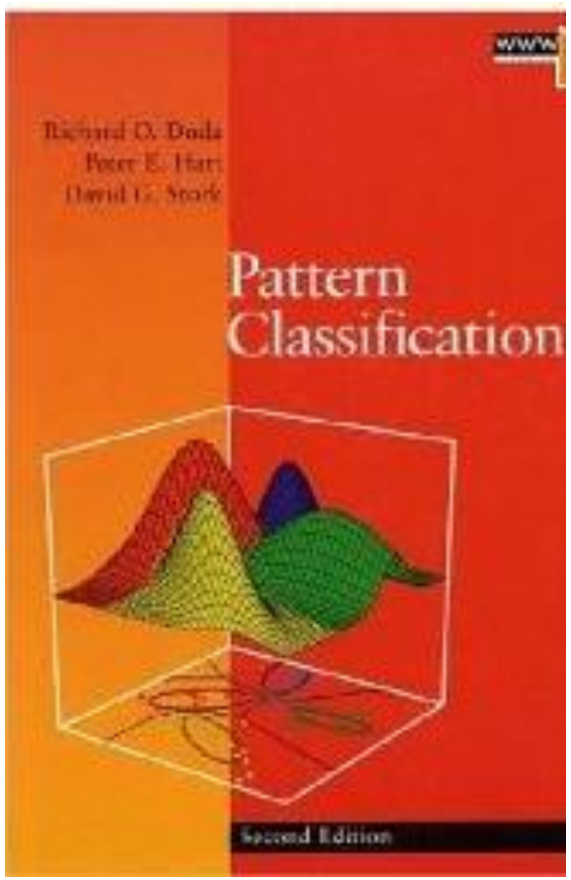
- Máme se příchodu AI bát?

Literatura

Duda, Hart, Stork:

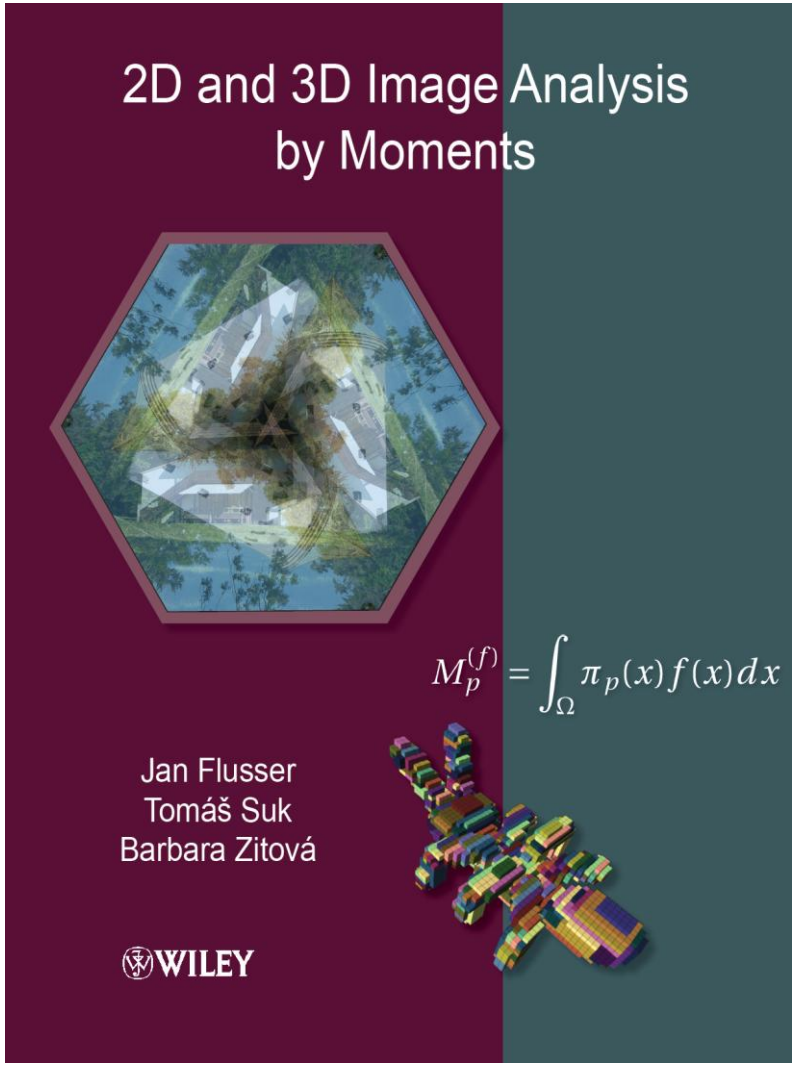
Pattern Classification,

2nd ed., Wiley, 2001



Literatura

Kapitoly 1 a 2 – stručný přehled



Pattern Recognition

- Recognition (classification) = assigning a pattern/object to one of pre-defined classes
- Statistical (feature-based) PR - the pattern is described by features (n-D vector in a metric space)

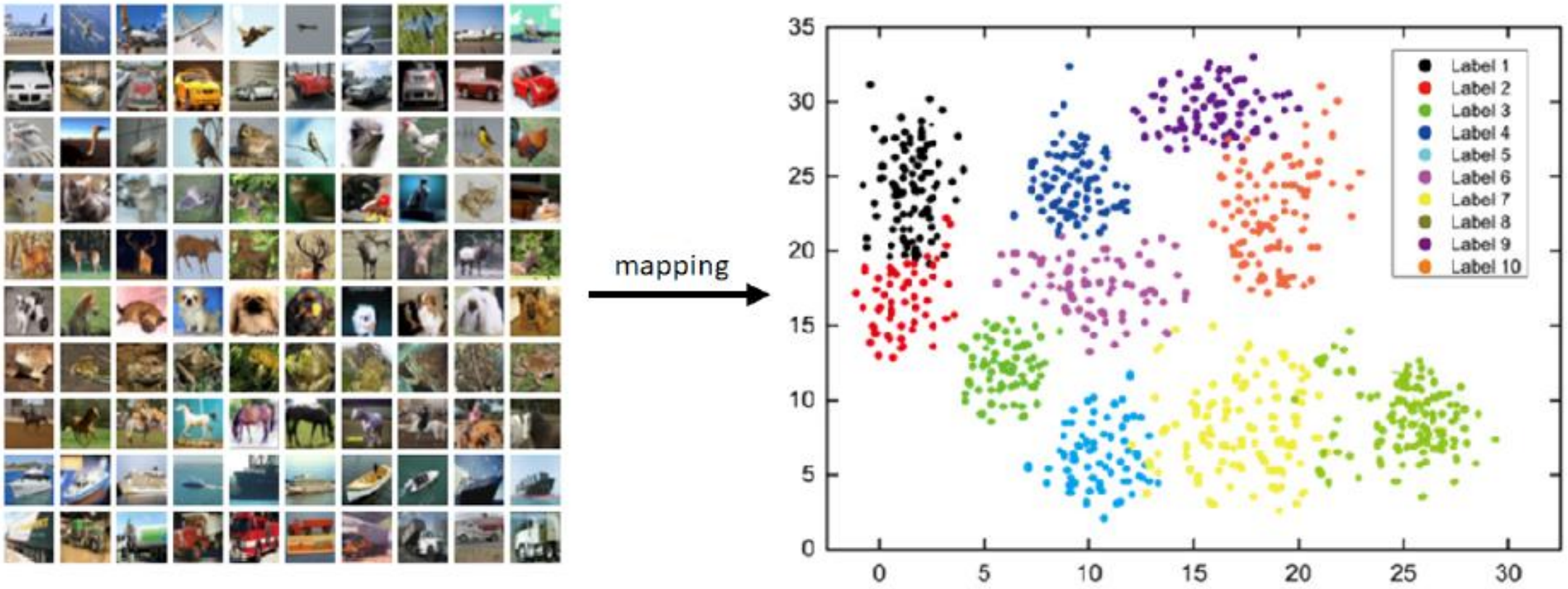
Pattern Recognition

- Supervised PR
  - training set available for each class
- Unsupervised PR (clustering)
  - training set not available, No. of classes may not be known

Desirable properties of the training set

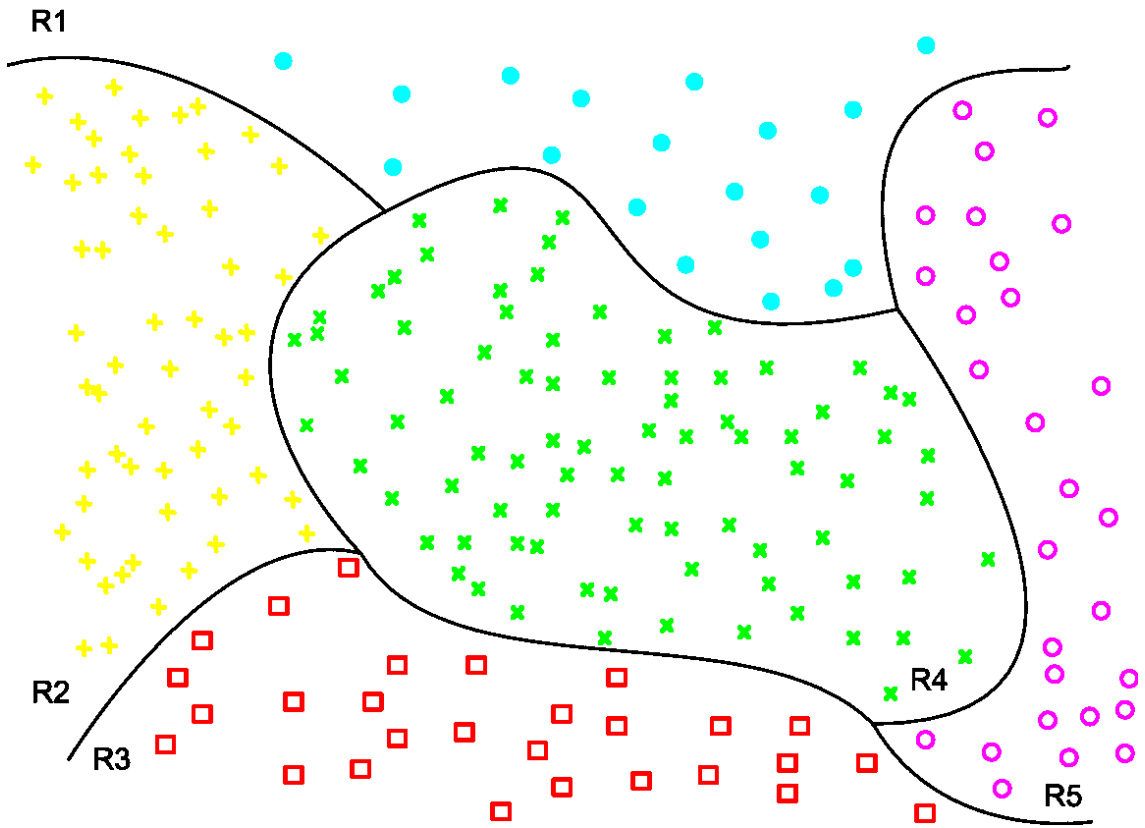
- It should contain typical representatives of each class including intra-class variations
- Reliable and large enough
- Should be selected by the domain experts

Image and feature space



Classification rule setup

Equivalent to a partitioning of the feature space



Independent of the particular application

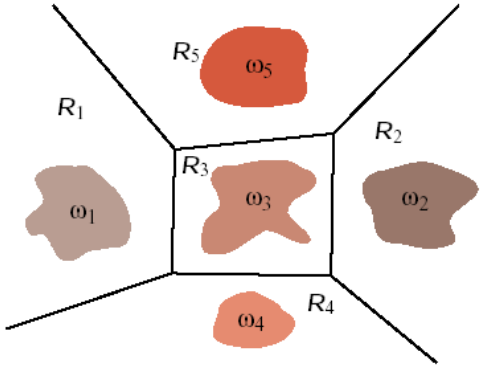
Object Recognition System

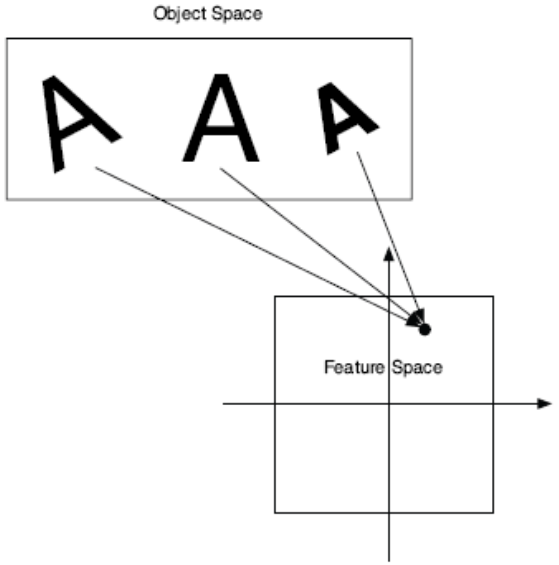
Image acquisition

Preprocessing

Object detection

Computing of the features





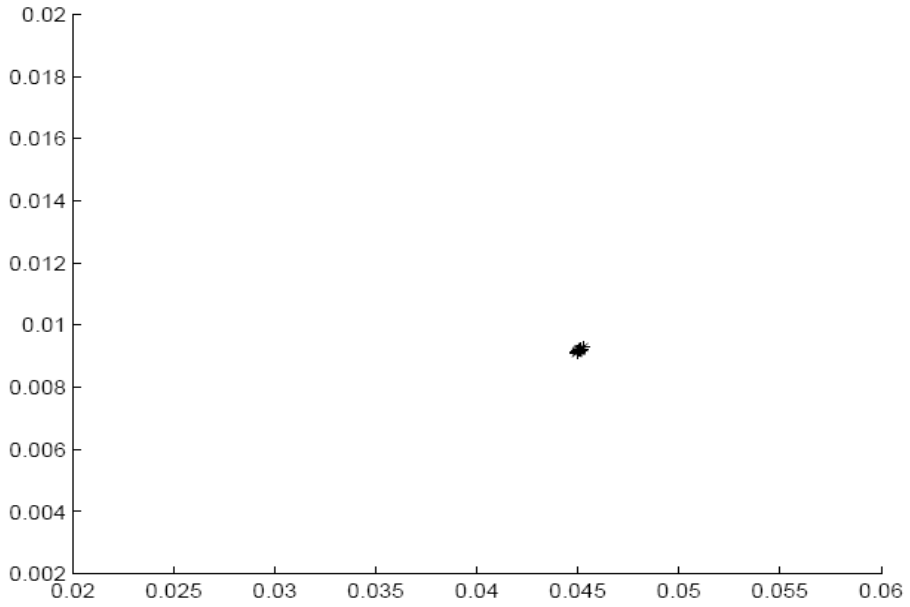
Classification

Class label

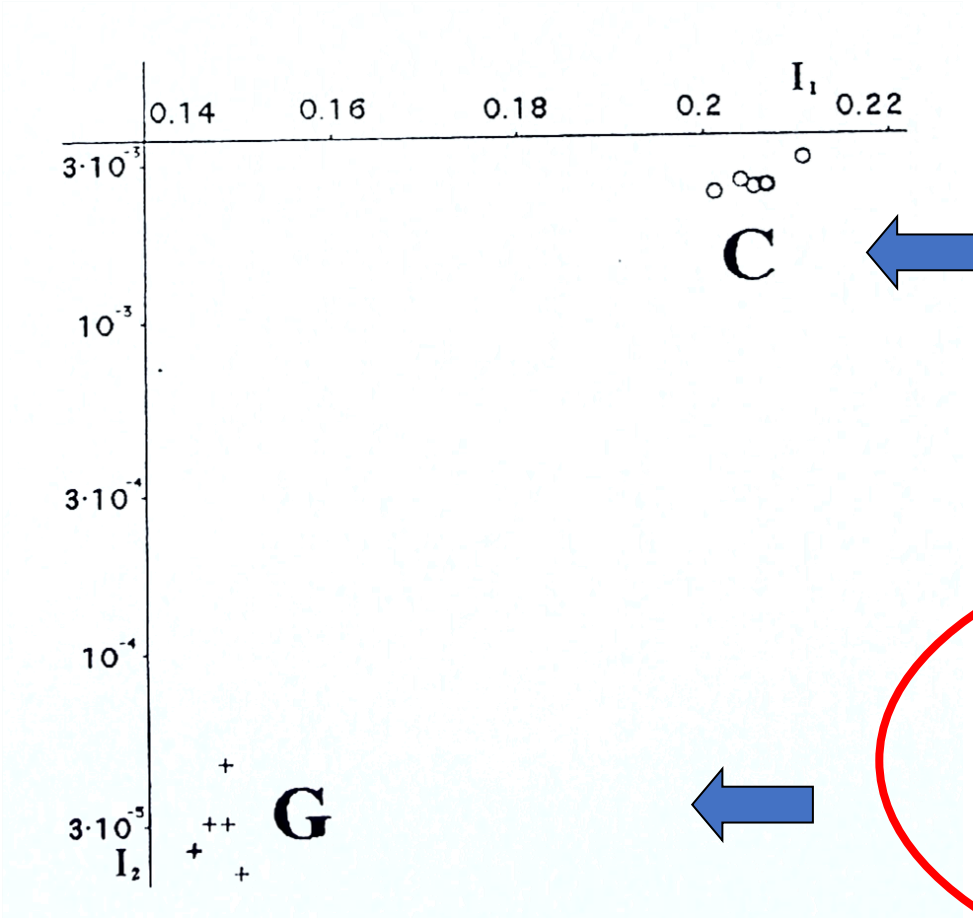
Desirable properties of the features

- **Invariance**
- **Discriminability**
- **Robustness**
- **Efficiency, independence, completeness**

Example: TRS


0.02
0.018
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0.02
0.025
0.03
0.035
0.04
0.045
0.05
0.055
0.06

Discrimination power



What are invariants?

Invariants are **functionals** defined on the image space such that

$$I(D(f)) = I(f) \quad \text{for all admissible } D$$

$$I(D(f)) = D'(I(f)) \text{ - } \textit{equivariance}$$

Groups actions, orbits, equivalence

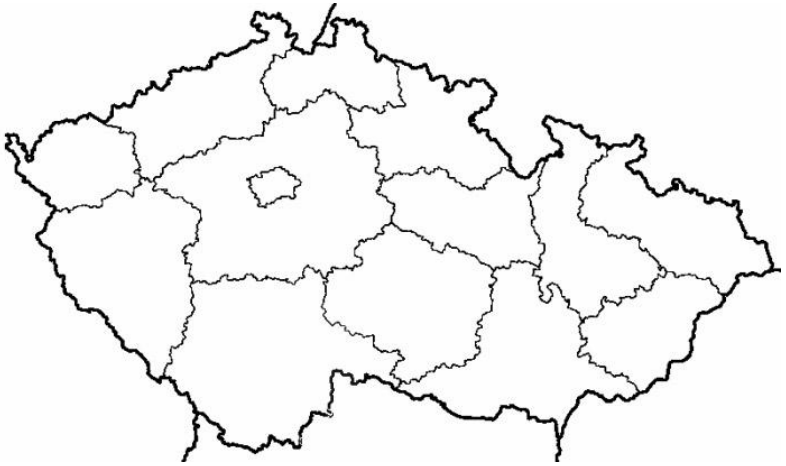
- Let *D* form a group D
- Group action D x I → I
- Orbit *D(f)*
- Orbits are *equivalence classes of I/D*

Orbits are “**classes**” of our classification problem

Invariants and orbits

Orbit space

Invariant forms another factor space (set of equivalence classes) as $I(f) = I(g)$



Complete invariants

Both factor spaces are equal iff

$I(f_1) \neq I(f_2)$ for any $f_1 \neq D(f_2)$

Classification and decision making

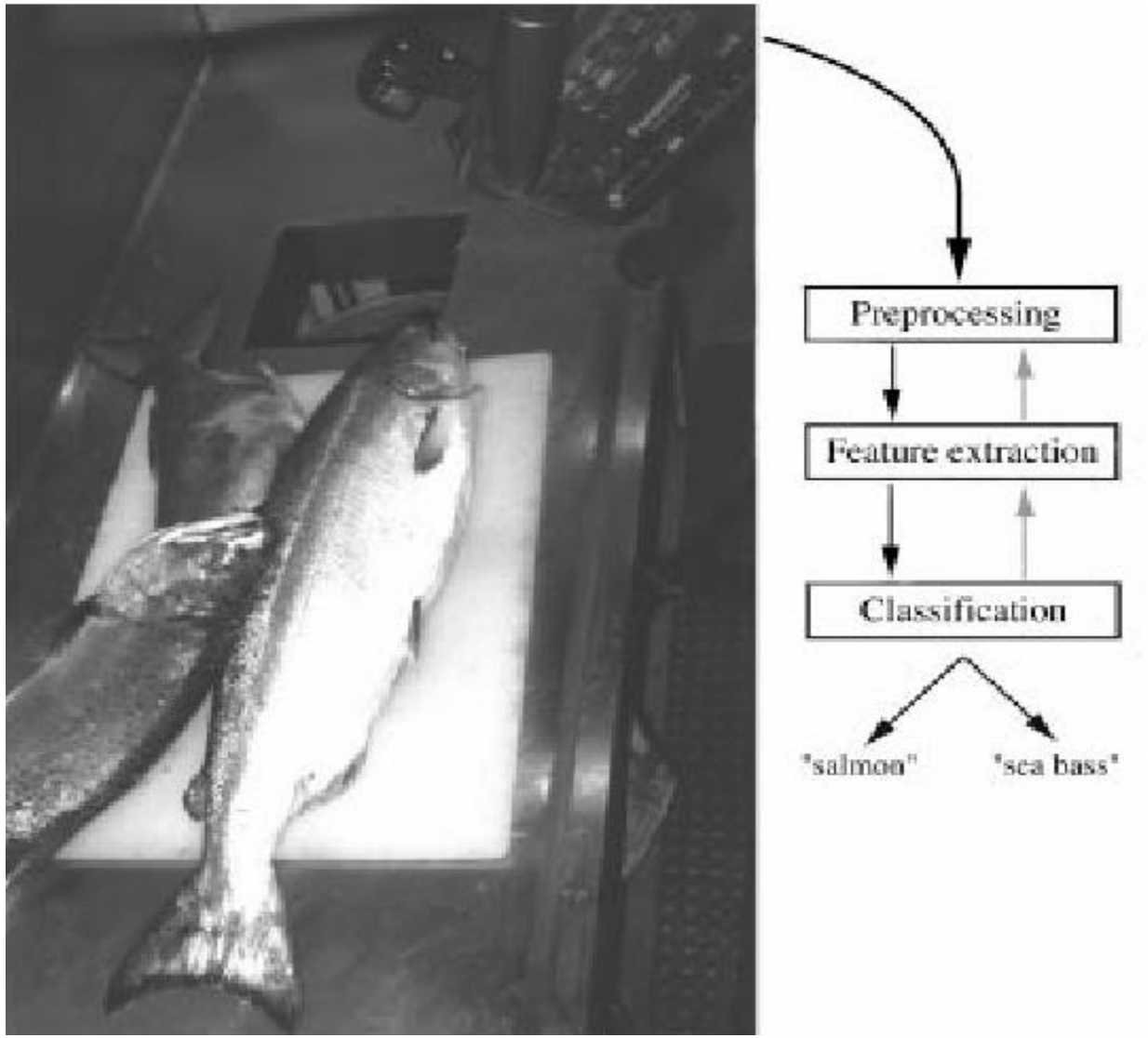
- Sensing, measuring the features

- Classification - Minimization of error probability

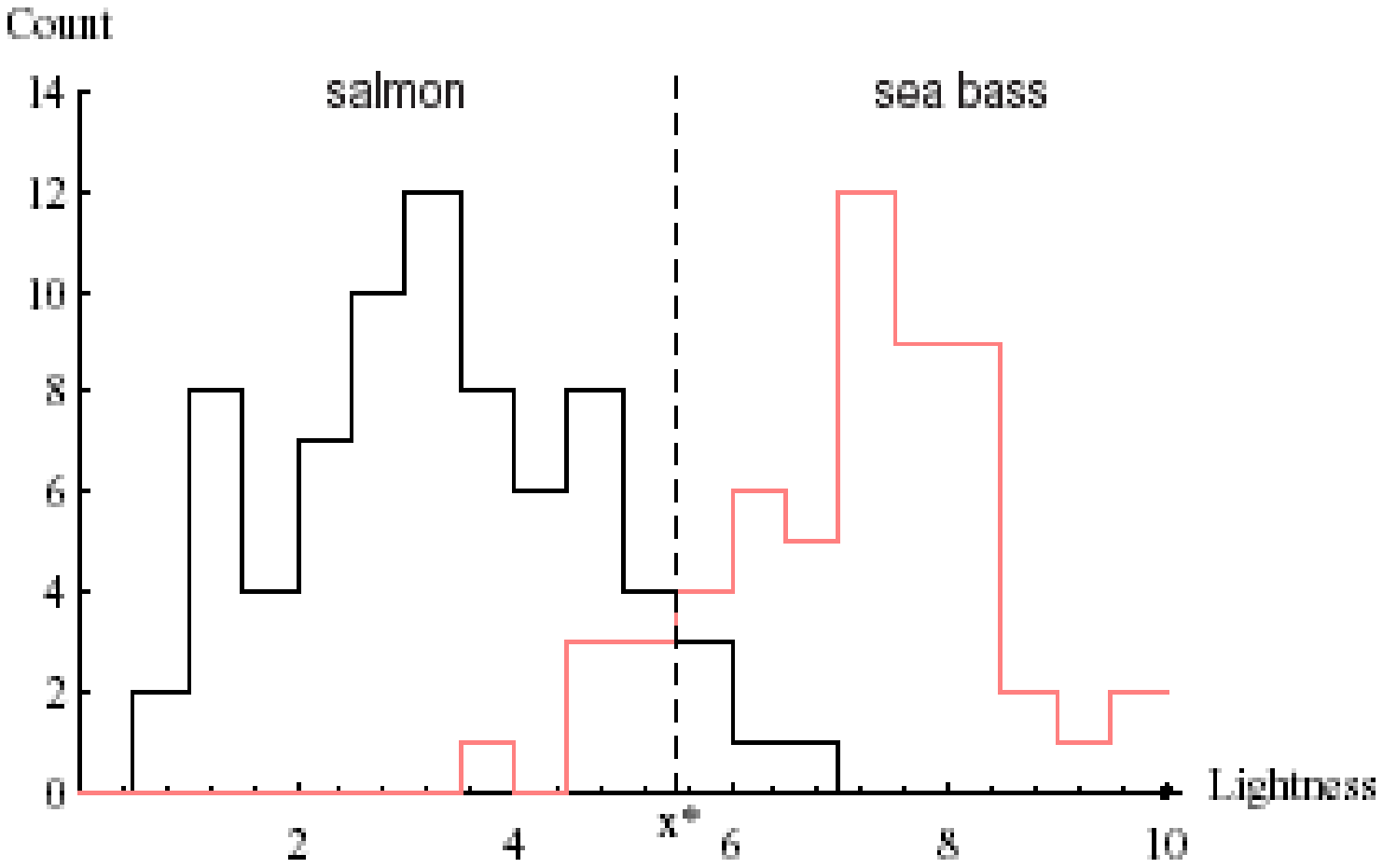
- Decision – Minimization of a loss function

- Action - Hardware

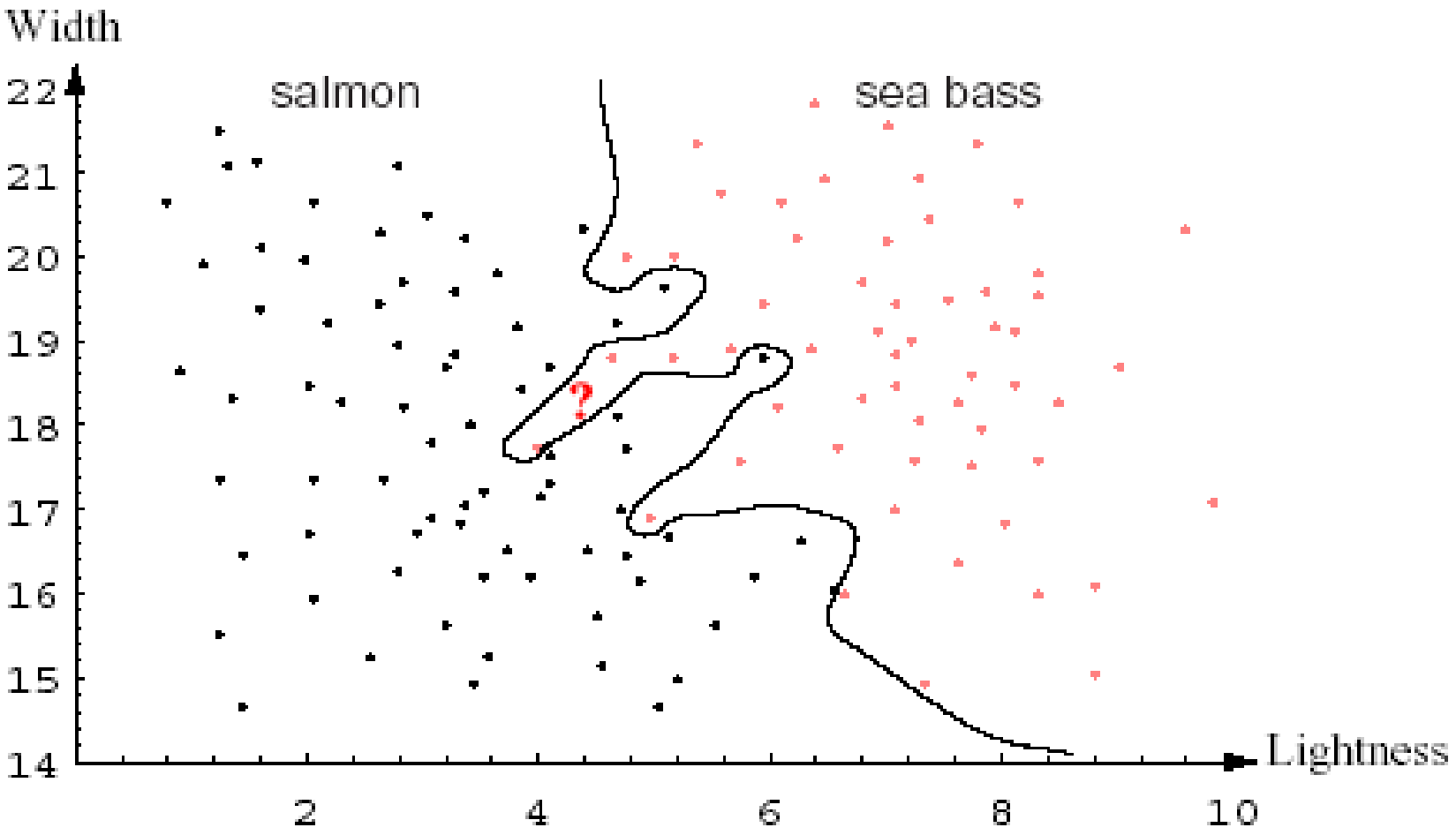
Example – Fish classification



The features: Length, width, brightness



2-D feature space



Empirical observation

- For a given training set, we can have several classifiers (several partitioning of the feature space)
- The training samples are not always classified correctly
- We should avoid overtraining of the classifier

Formal definition of the classifier

- Each class is characterized by its discriminant function *g(x)*
- Classification = maximization of *g(x)*

  Assign *x* to class *i* iff

$$g_i(\mathbf{x}) > g_j(\mathbf{x}) \qquad \forall j \neq i$$

- Discriminant functions define decision boundaries in the feature space

Minimum distance (NN) classifier

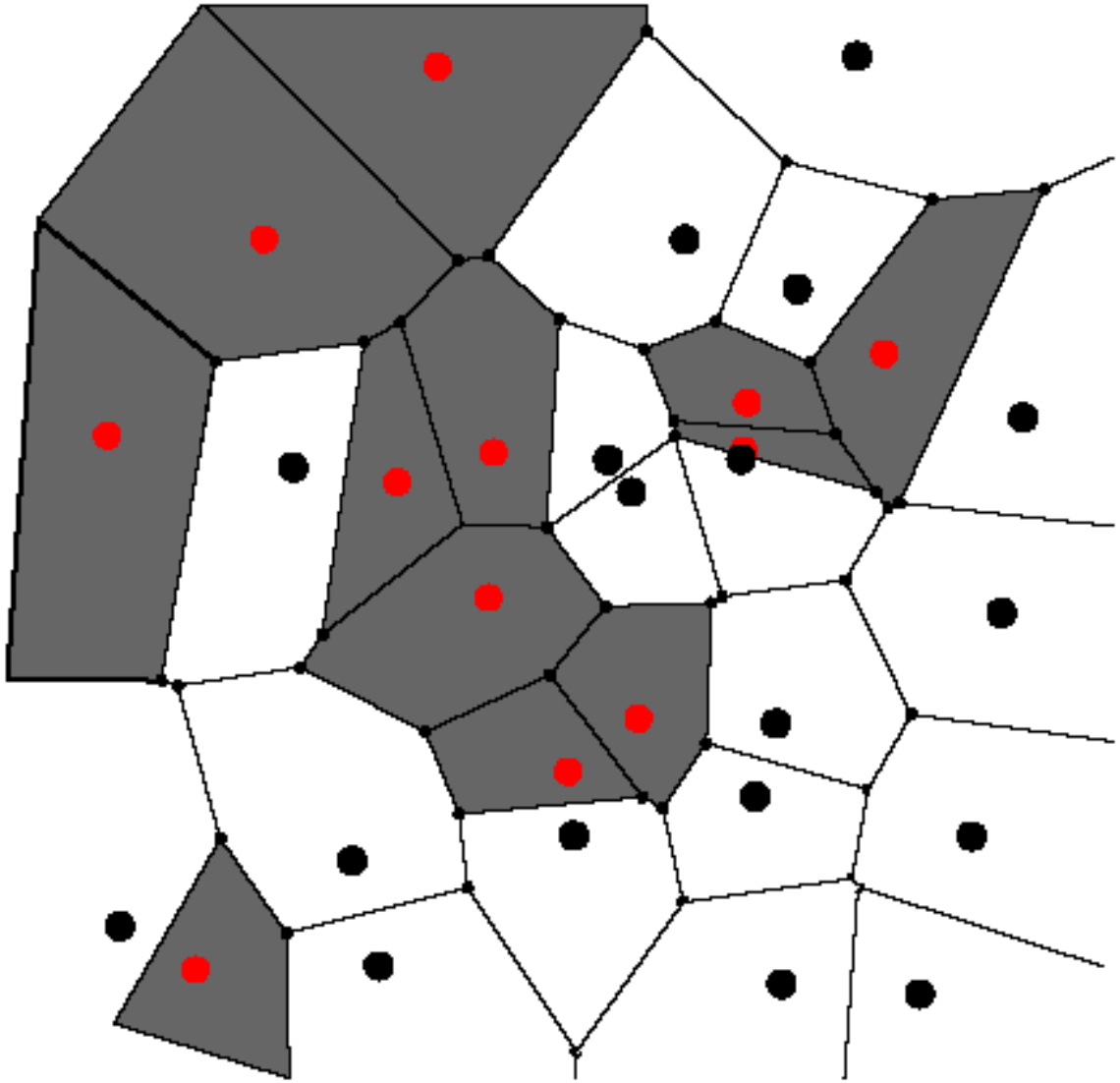
- Discriminant function

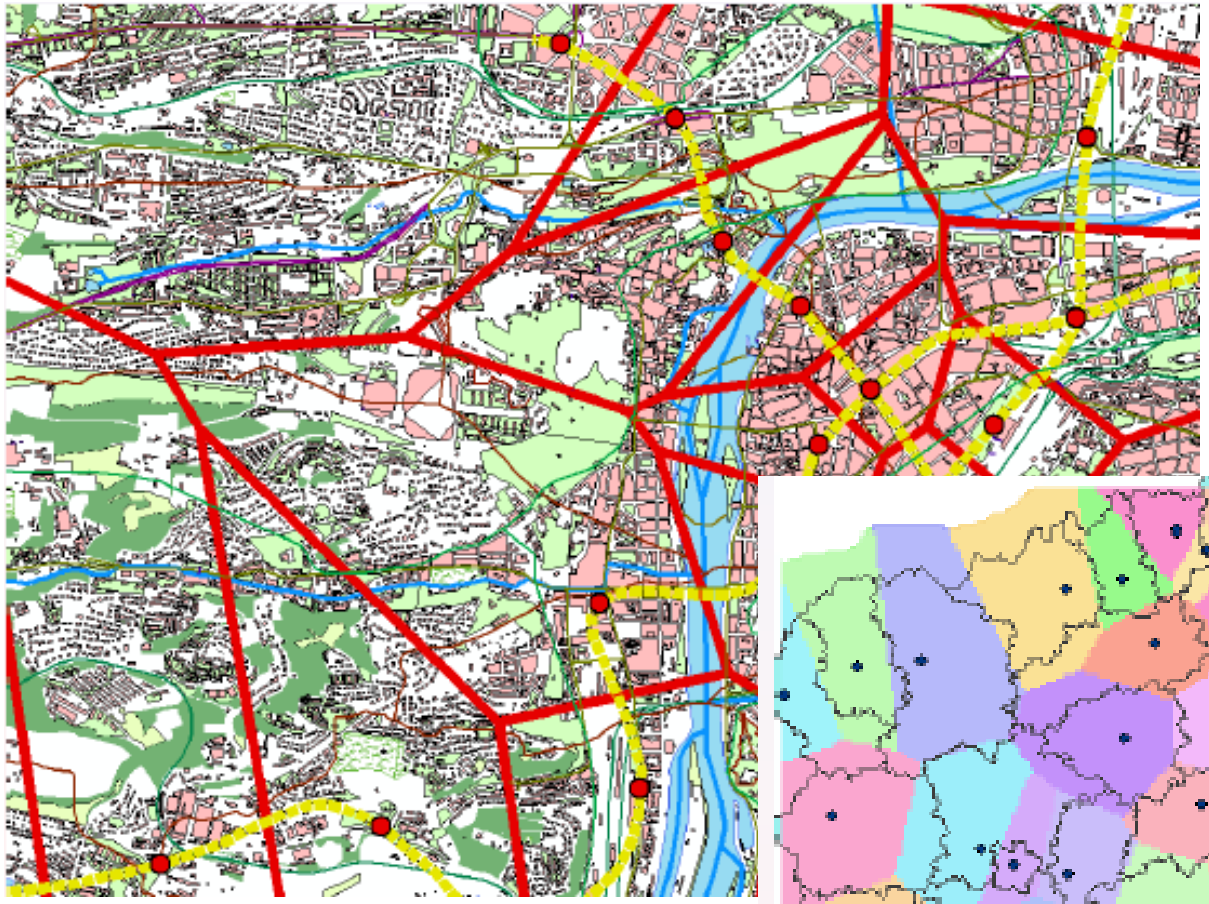
$$g_i(\mathbf{x}) = -d(\mathbf{x}, \omega_i)$$

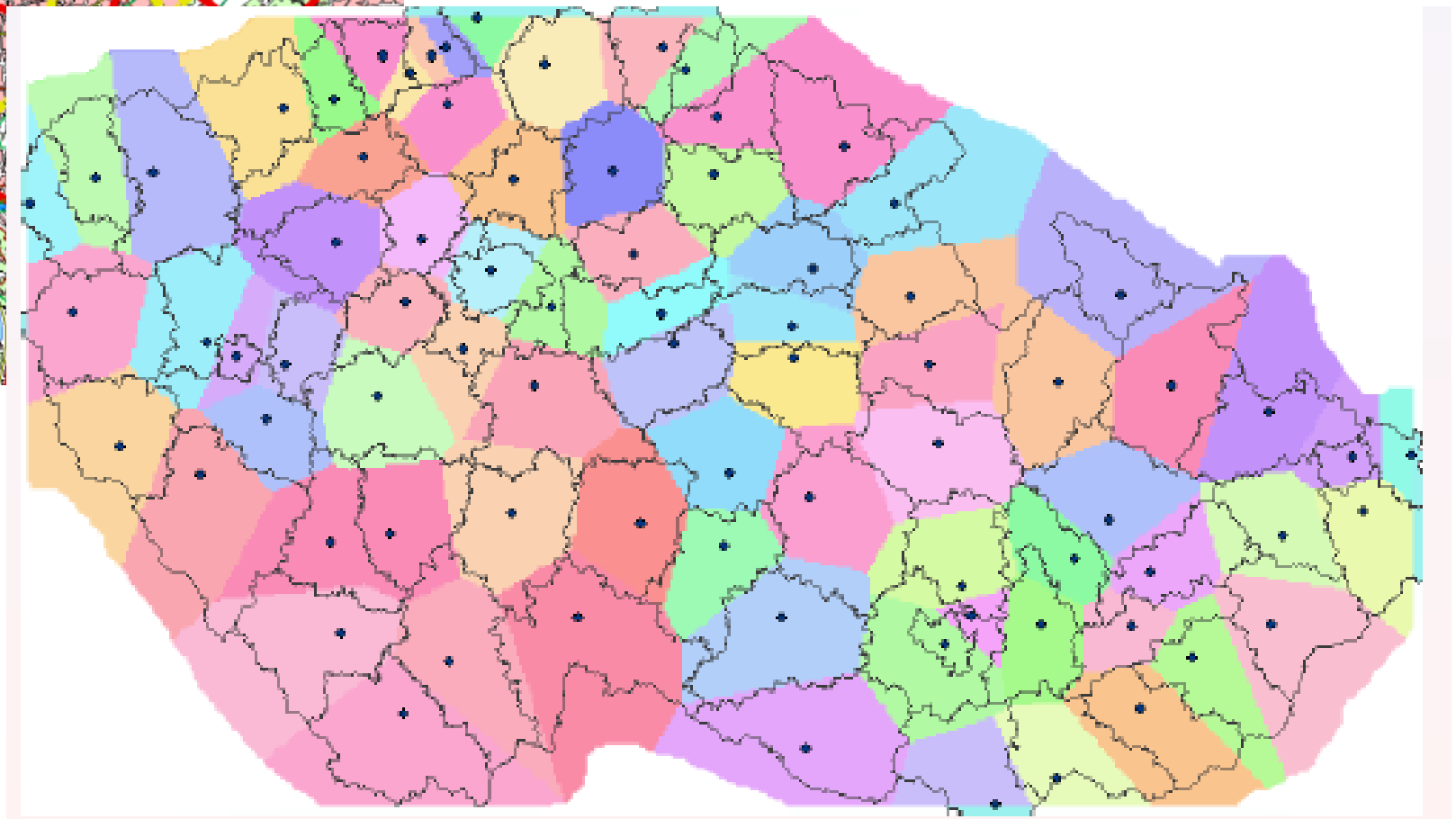
- Various definitions of $d(\mathbf{x}, \omega_i)$

- One-element training set →

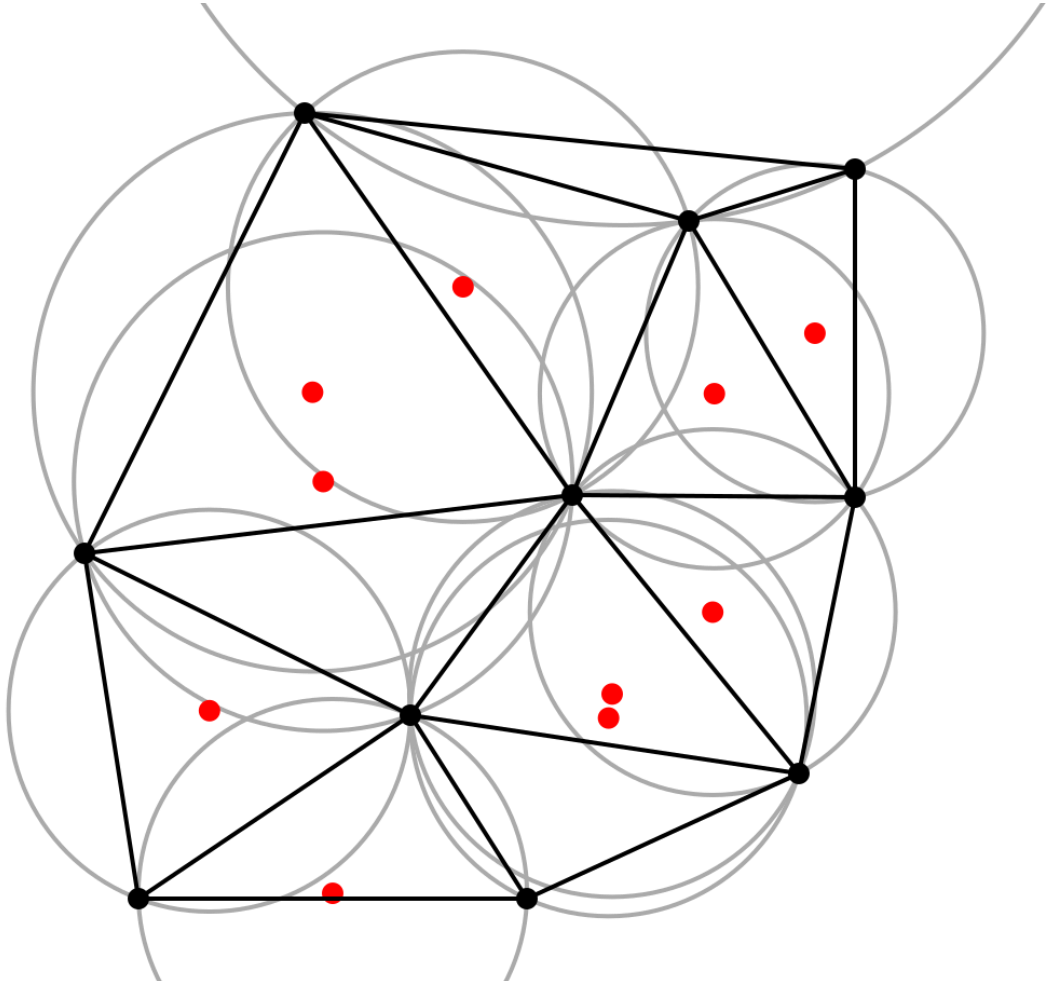
Voronoi polygons

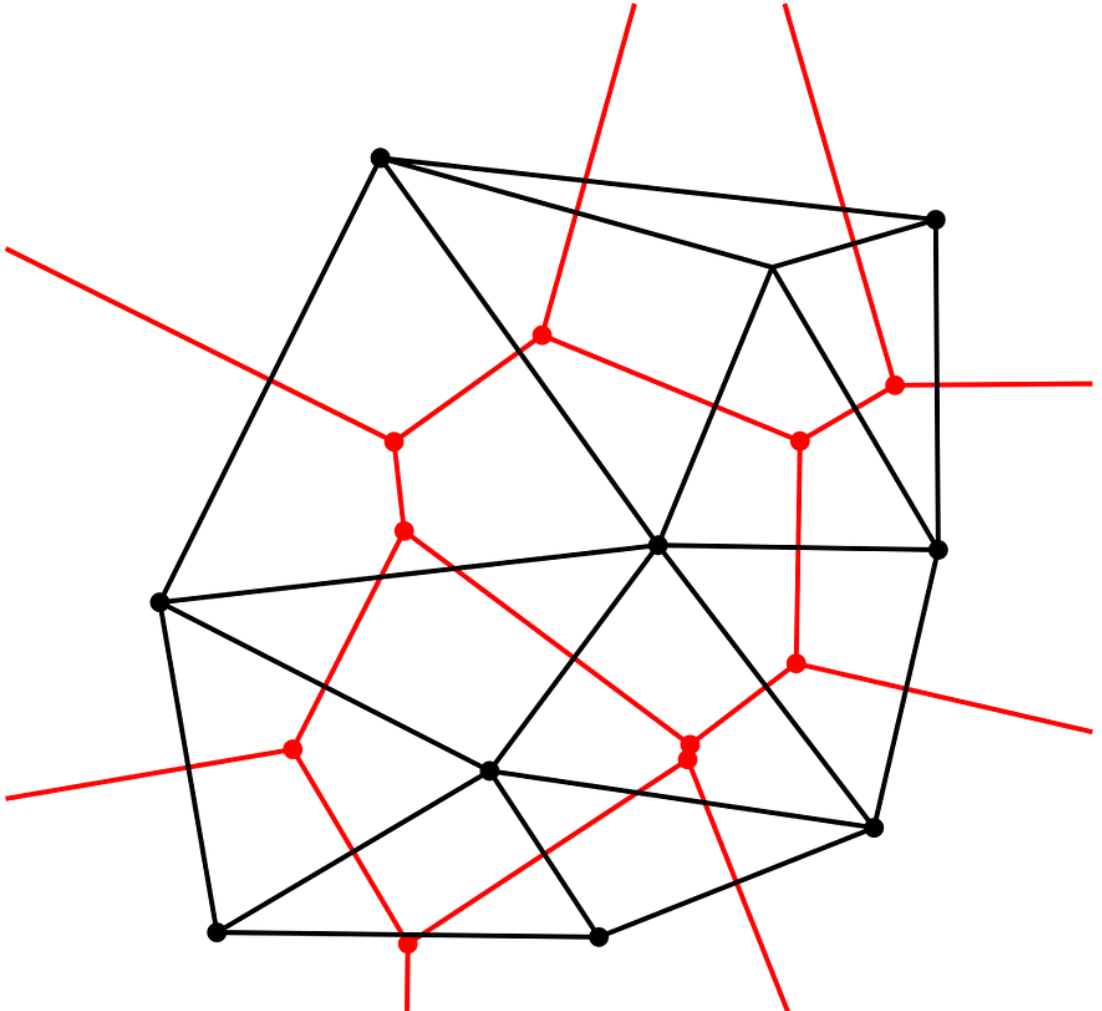






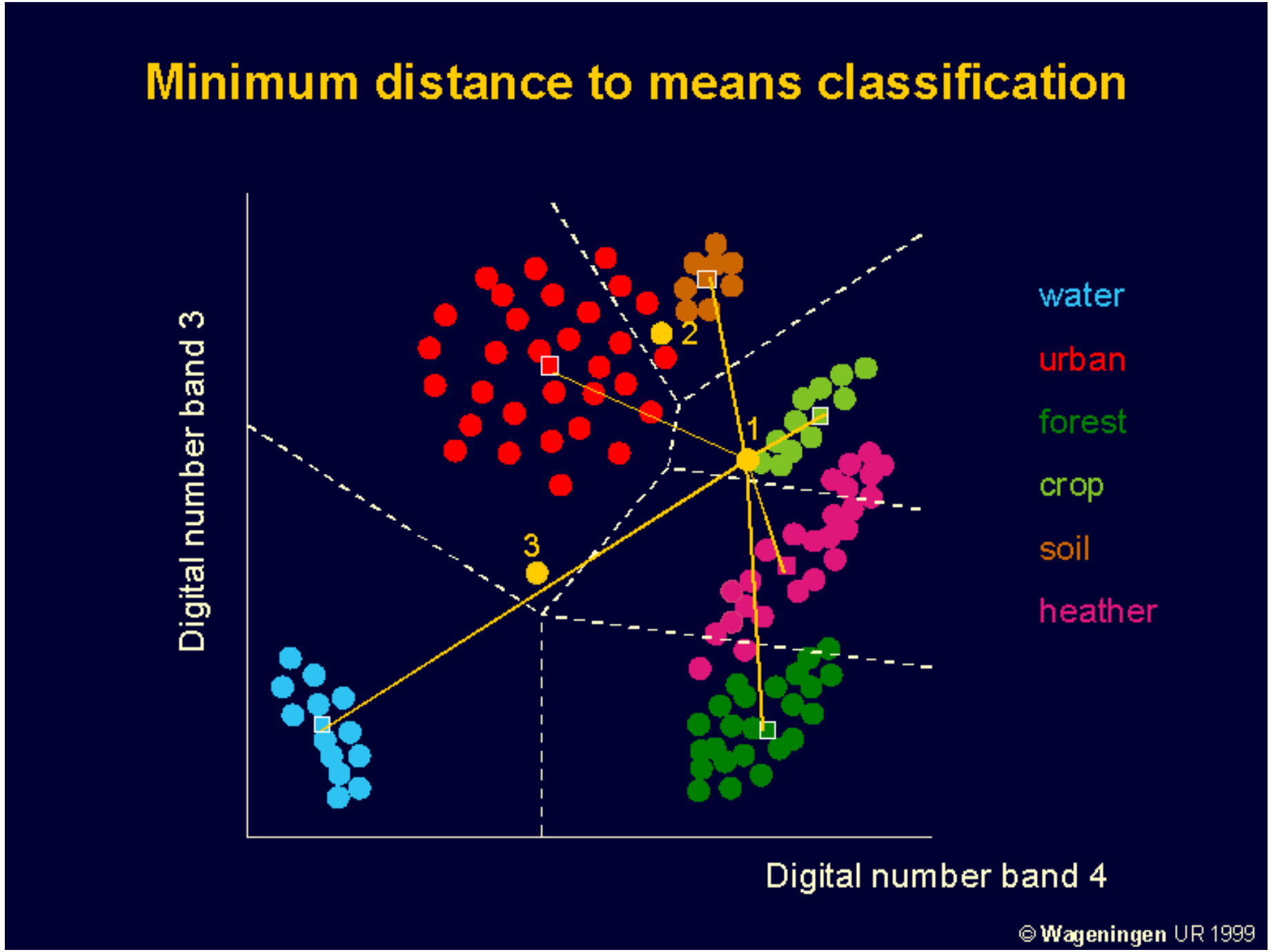
Off-topic: Delaunay triangulation

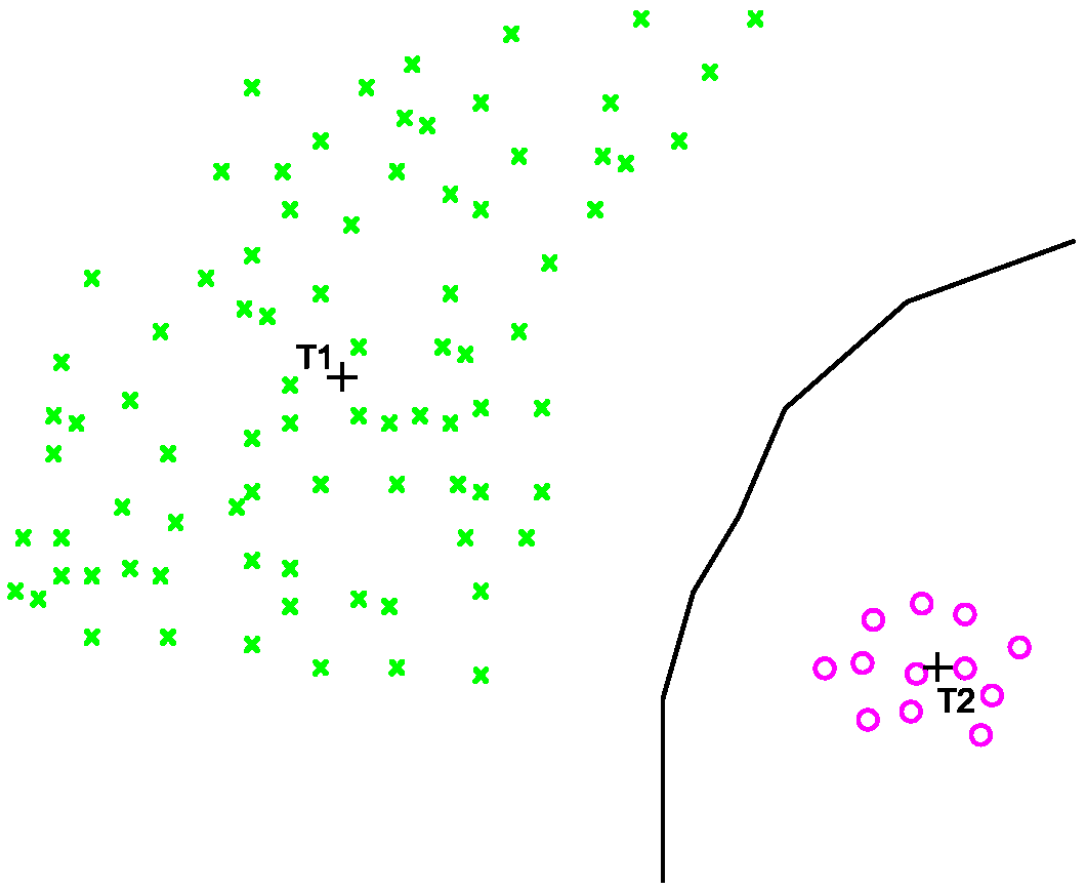


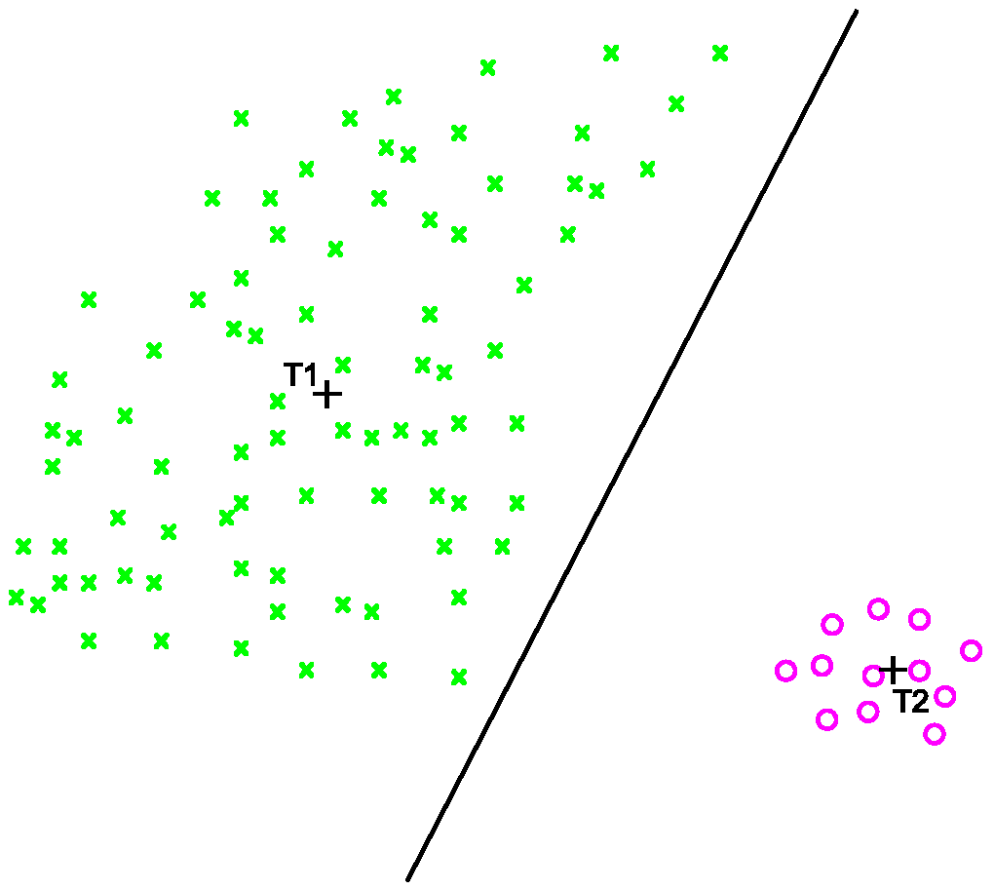


Minimum distance (NN) classifier

- Depending on $d(\mathbf{x}, \omega_i)$, NN classifier may not be linear
- NN classifier is sensitive to outliers → k-NN classifier


Minimum distance to means classification
Digital number band 3
Digital number band 4
1
2
3
water
urban
forest
crop
soil
heather
© Wageningen UR 1999

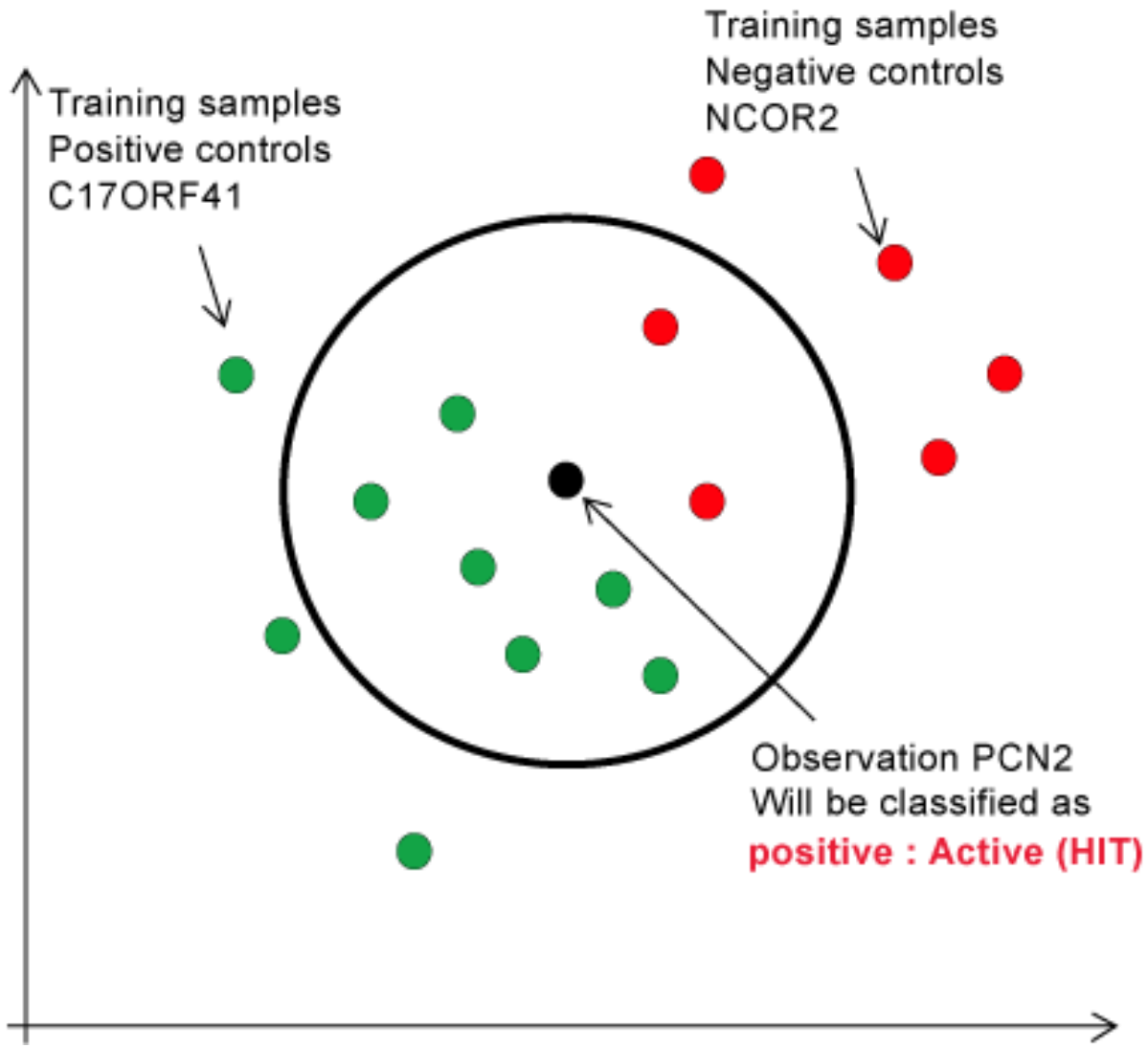

T1
T2


T1
T2

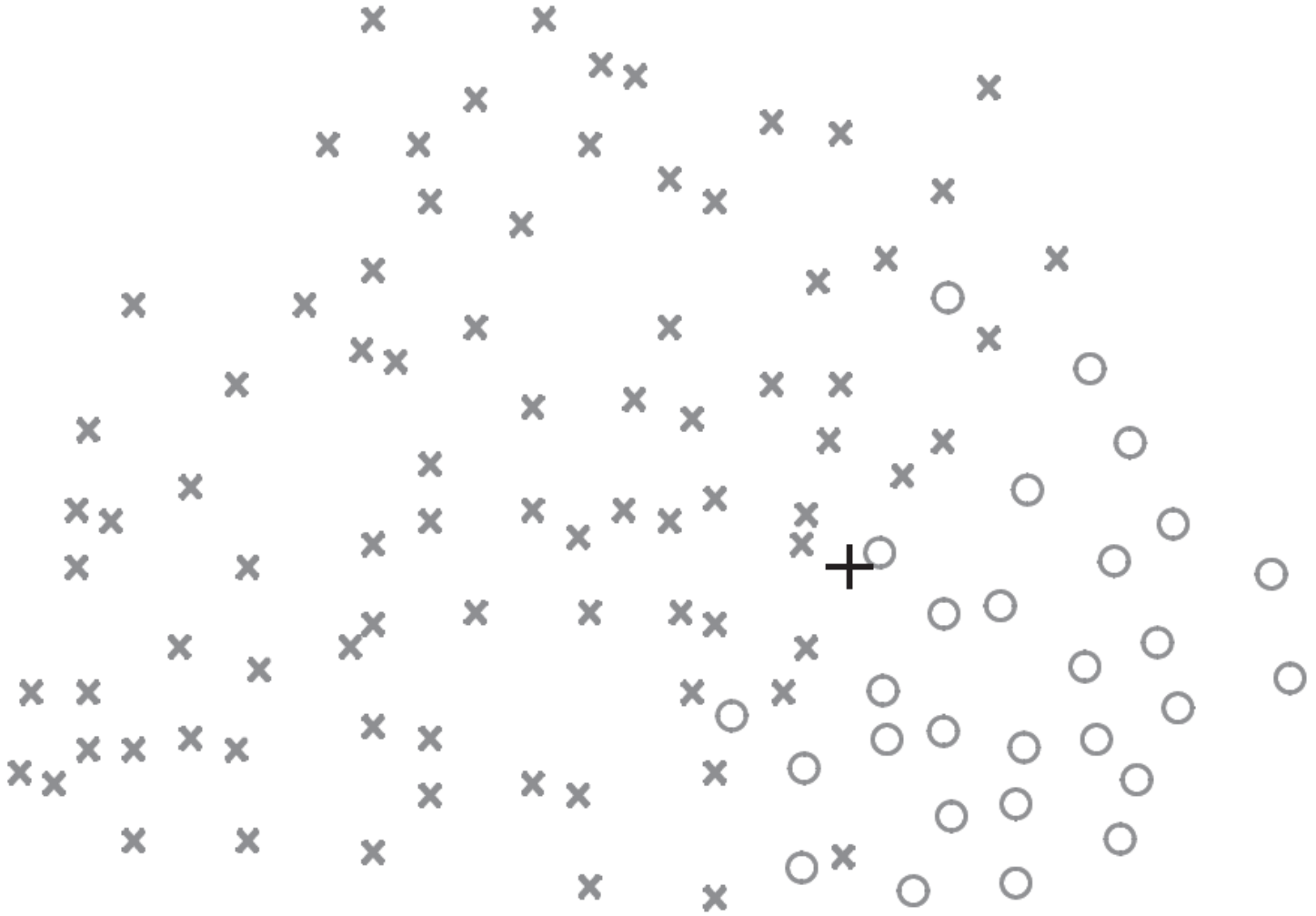
k-NN classifier

- NN classifier is sensitive to outliers → k-NN classifier
- It finds the nearest training points unless *k* samples belonging to one class has been reached

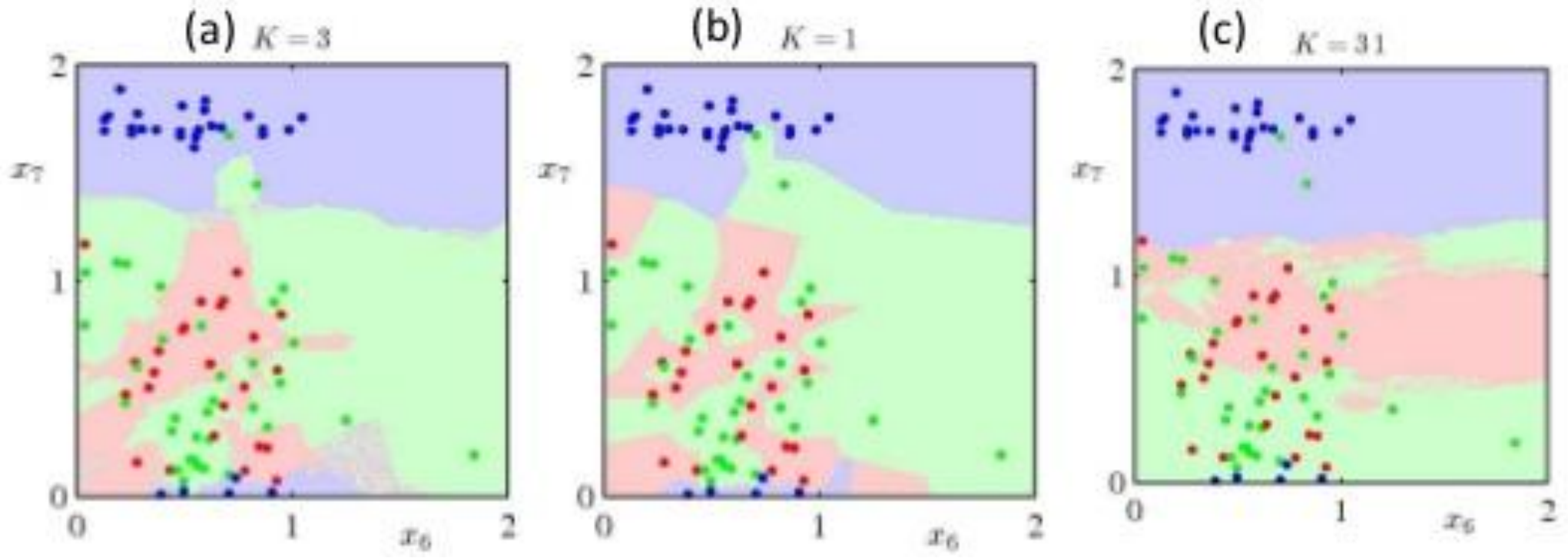
k-NN classifier



k-NN classifier

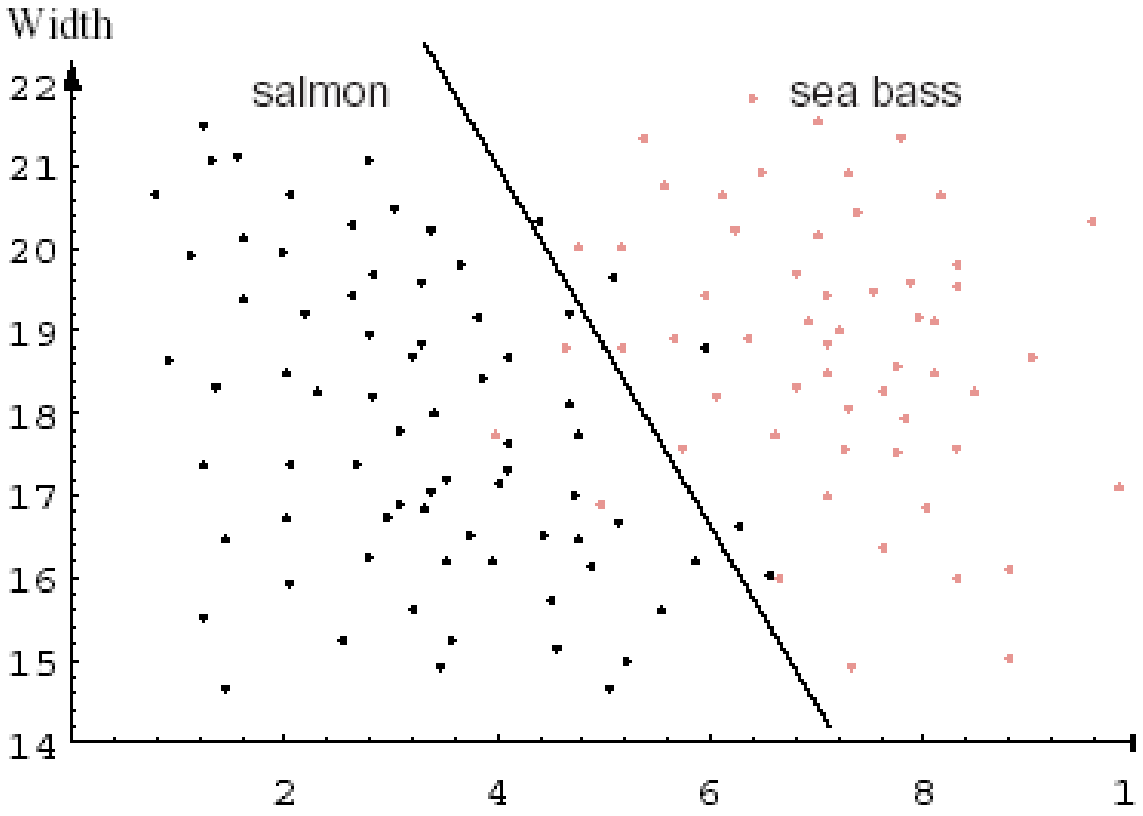


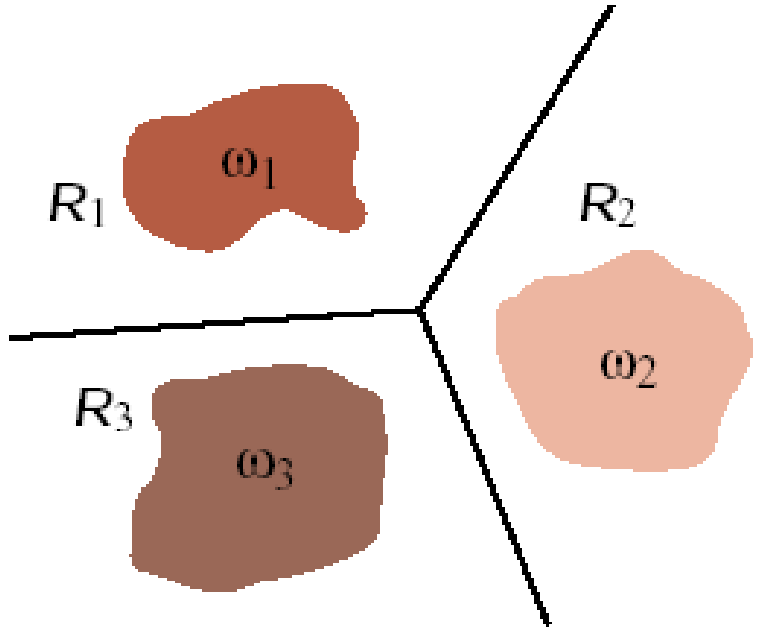
k-NN classifier



Linear classifier

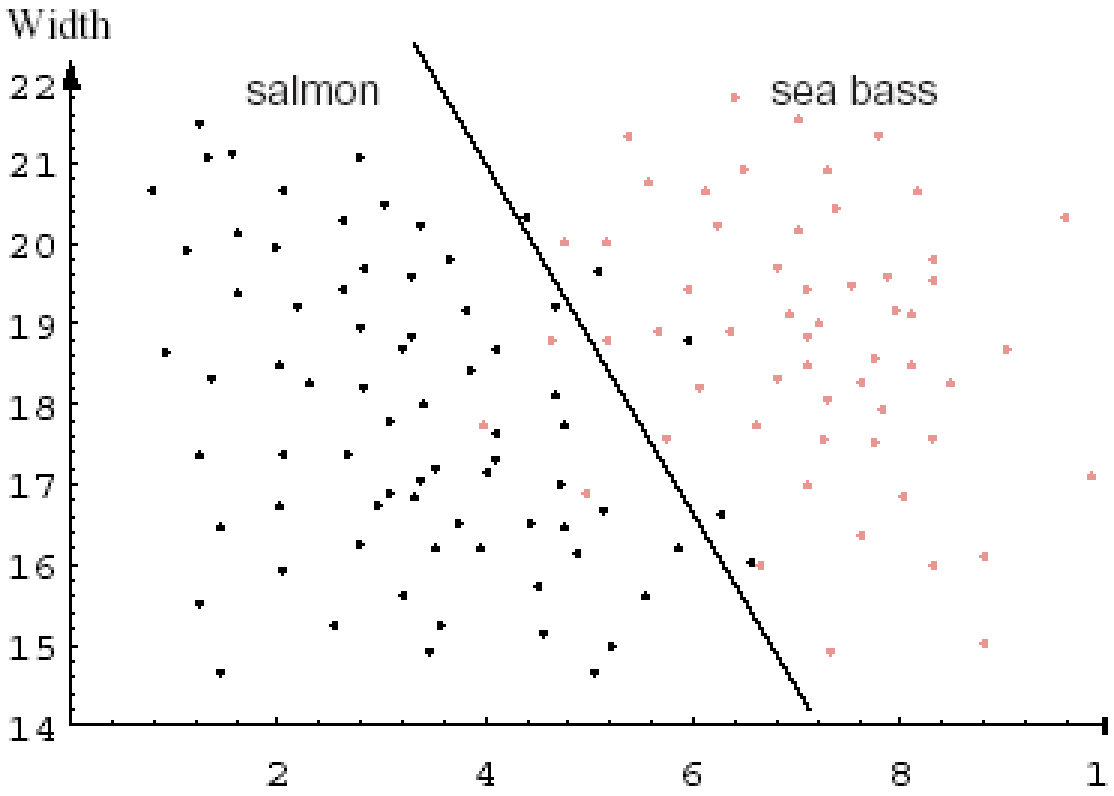
Discriminant functions g(x) are hyperplanes





Simple training algorithms

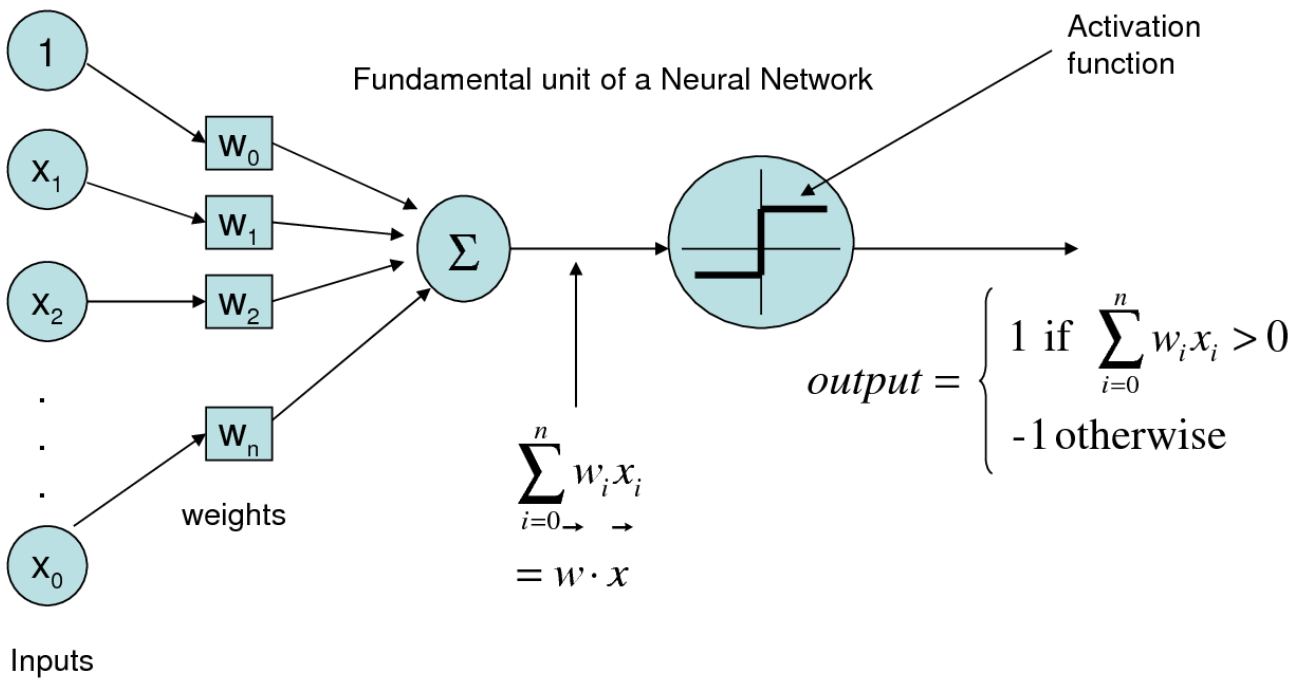
- Many possible hyperplanes
- Perceptron



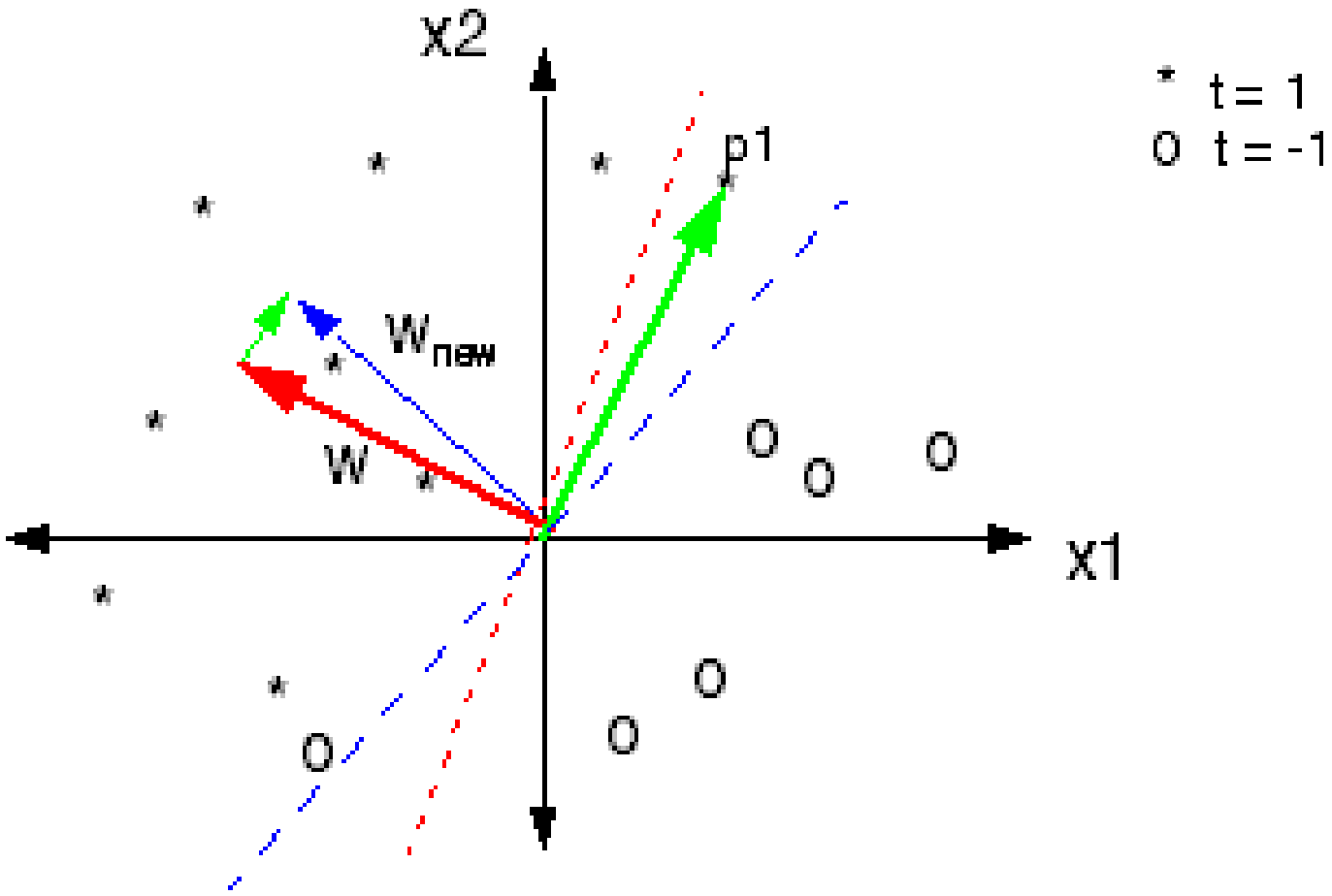
Perceptron

Artificial Neural Networks

The Perceptron

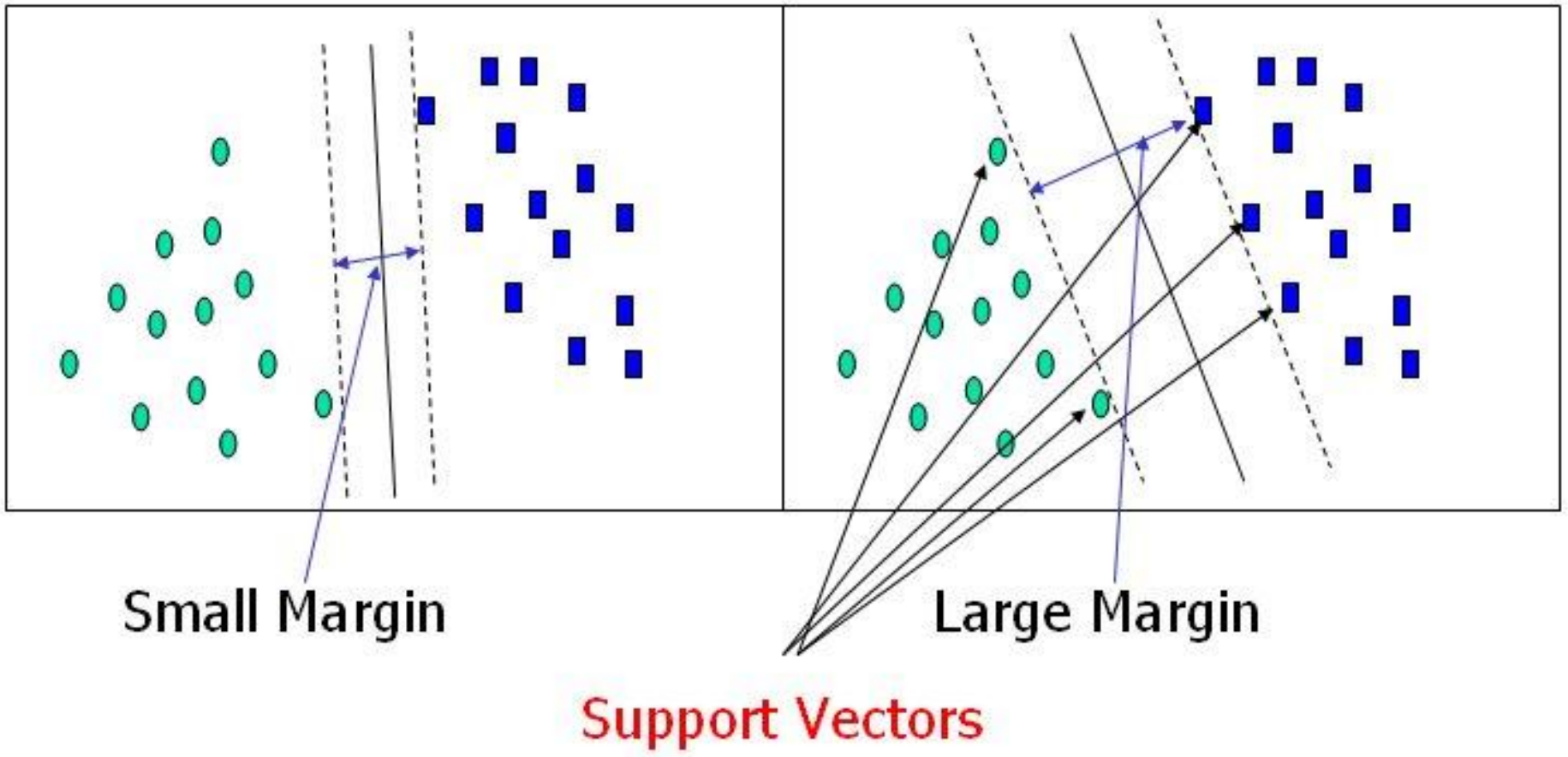


Perceptron – an iterative trainig



Support vector machine (SVM)

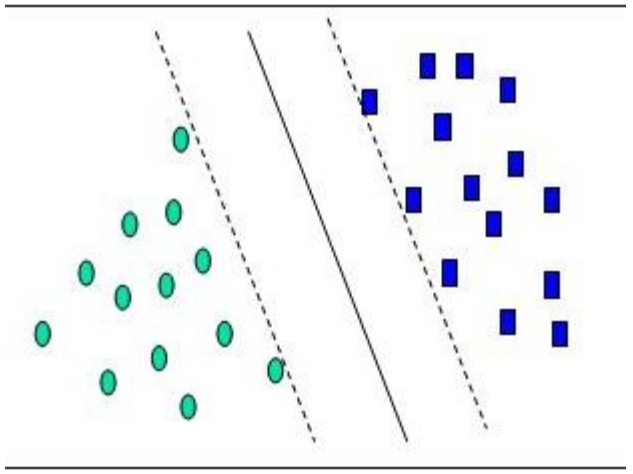
Maximizing the margin



Support vector machine (SVM)

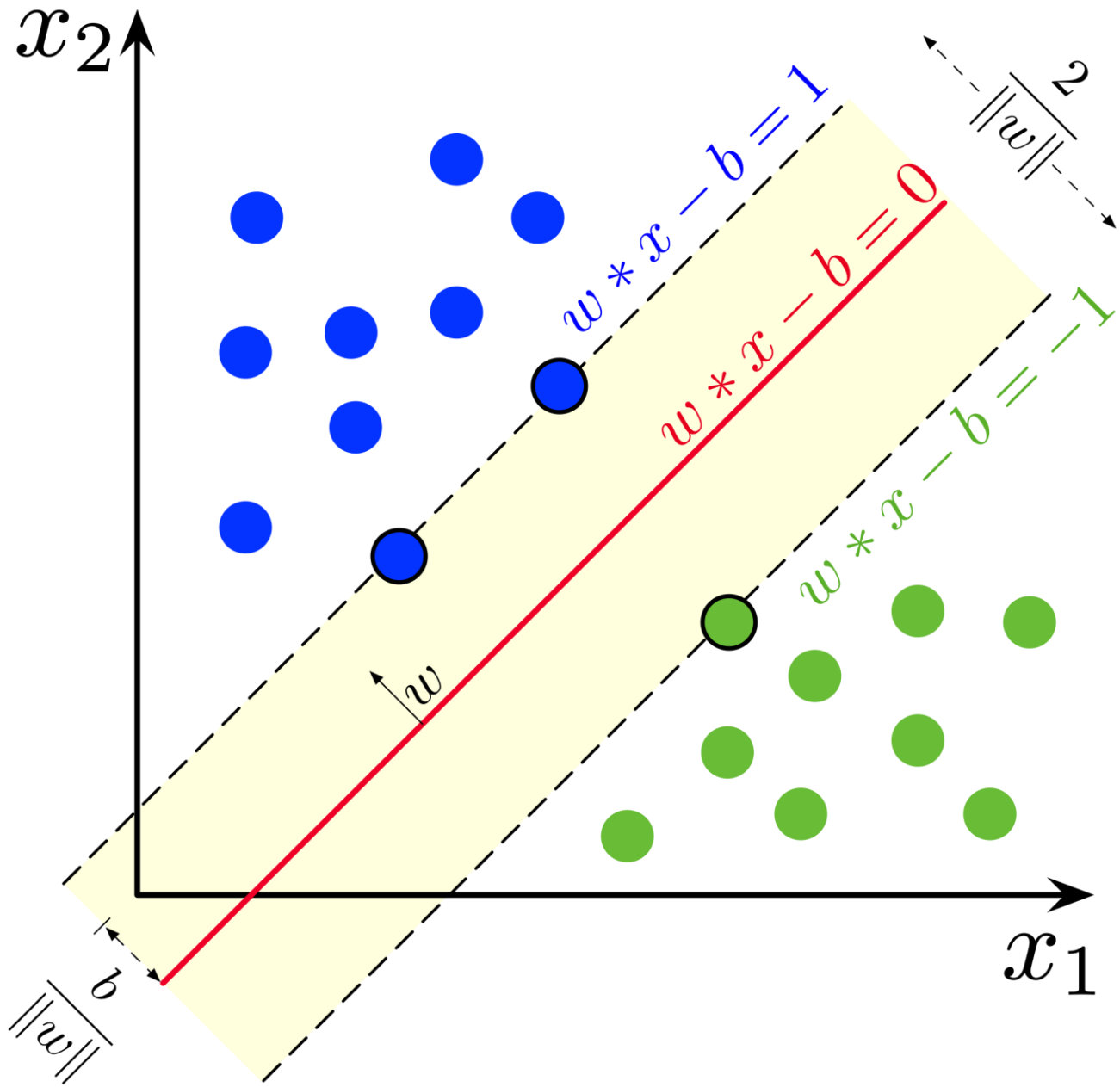
Training algorithm: Discrete optimization

- many versions

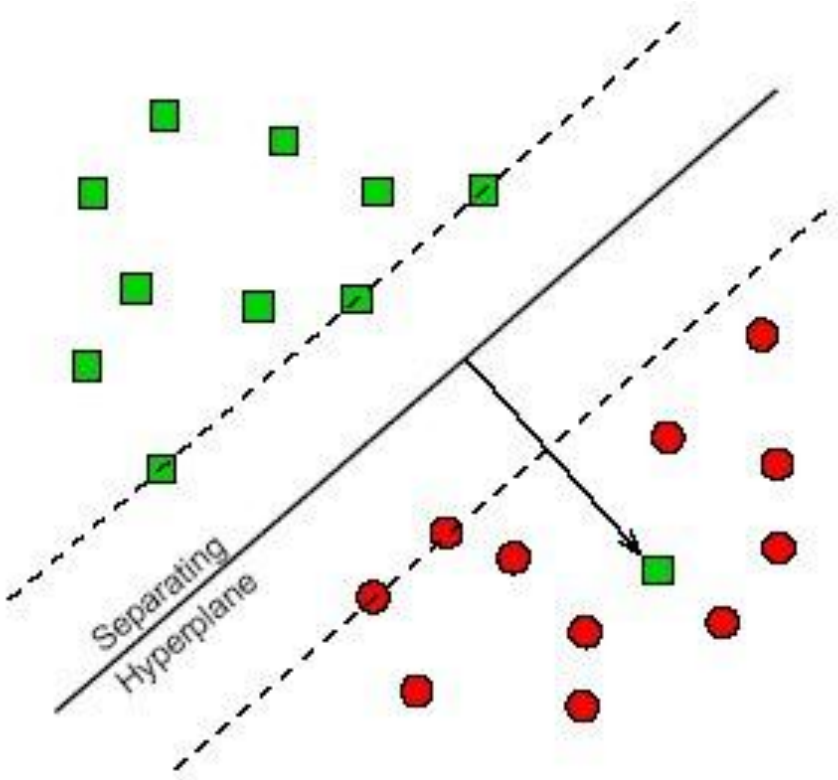


Drawbacks:

- very sensitive to outliers and noise
- does not consider the shape and the size of the training set


x_2
x_1
$w * x - b = 1$
$w * x - b = 0$
$w * x - b = -1$
w
$\frac{2}{\|w\|}$
$\frac{b}{\|w\|}$

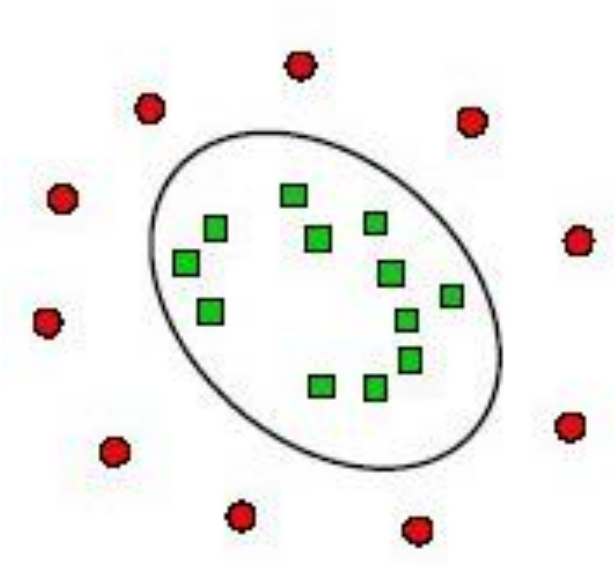
Soft margin SVM



Cost function penalizes the errors

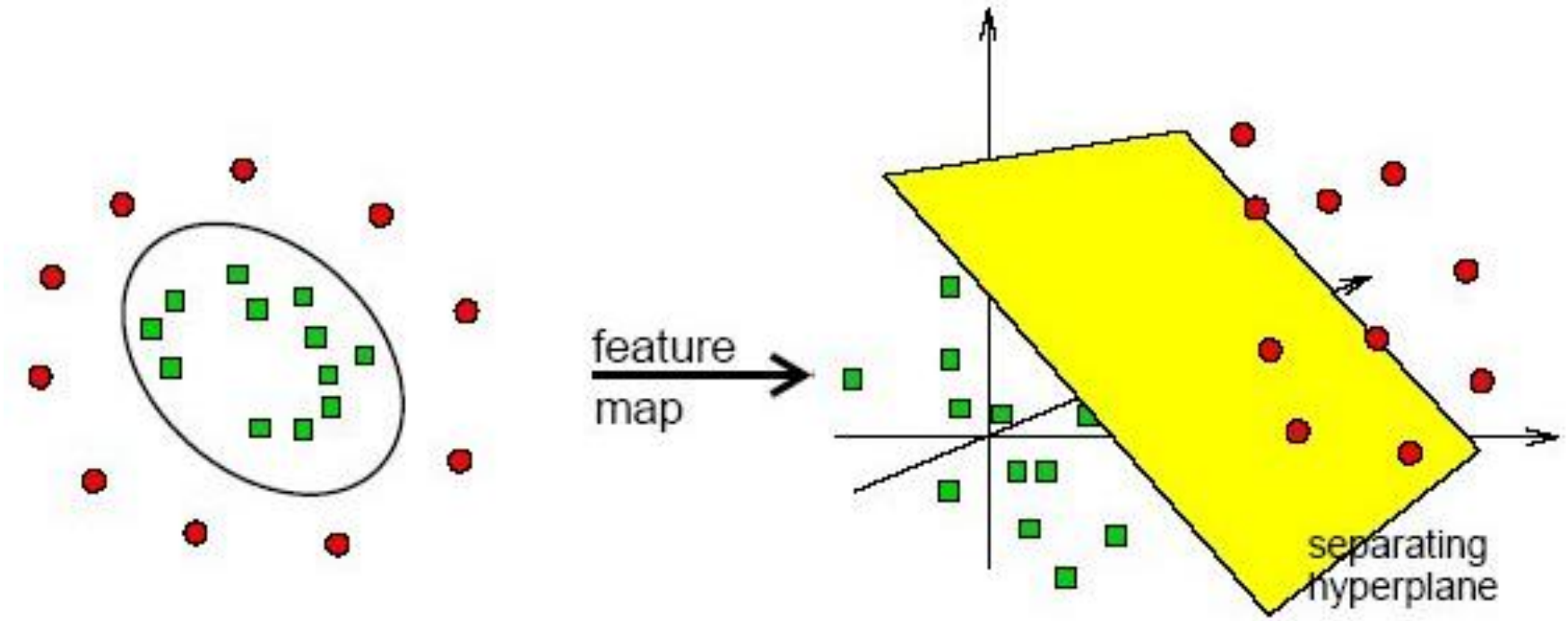
Regularization

SVM for linearly non-separable classes



How to make them linearly separable?

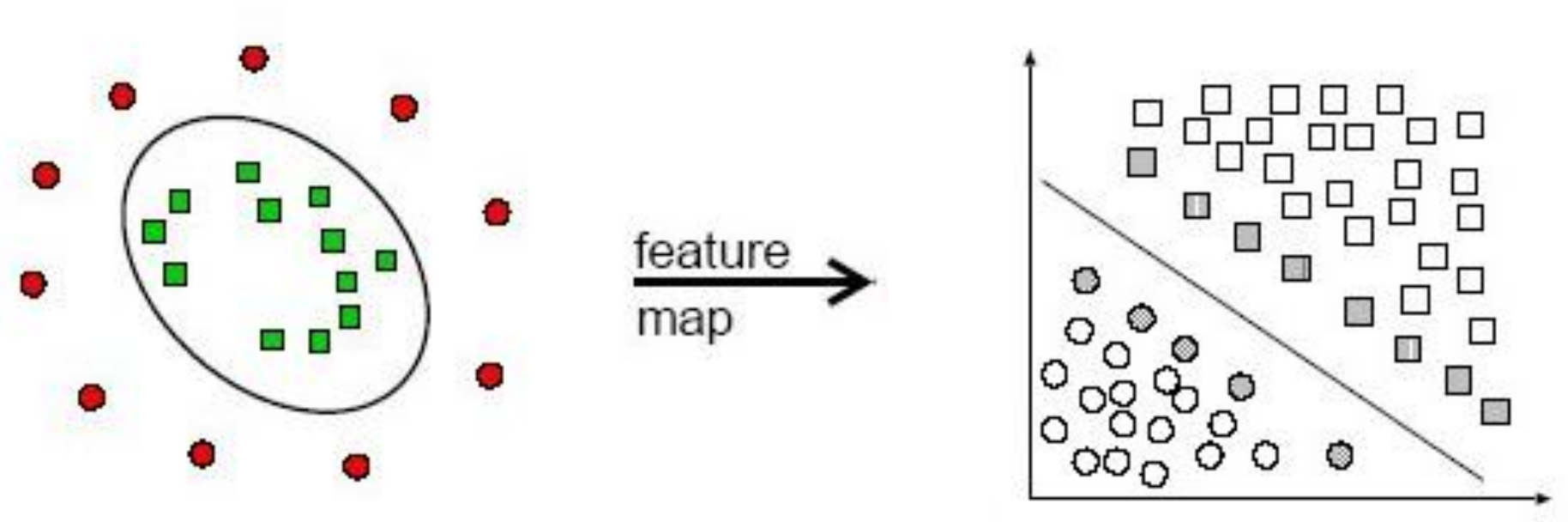
Increasing the number of features



“Curse of dimensionality”

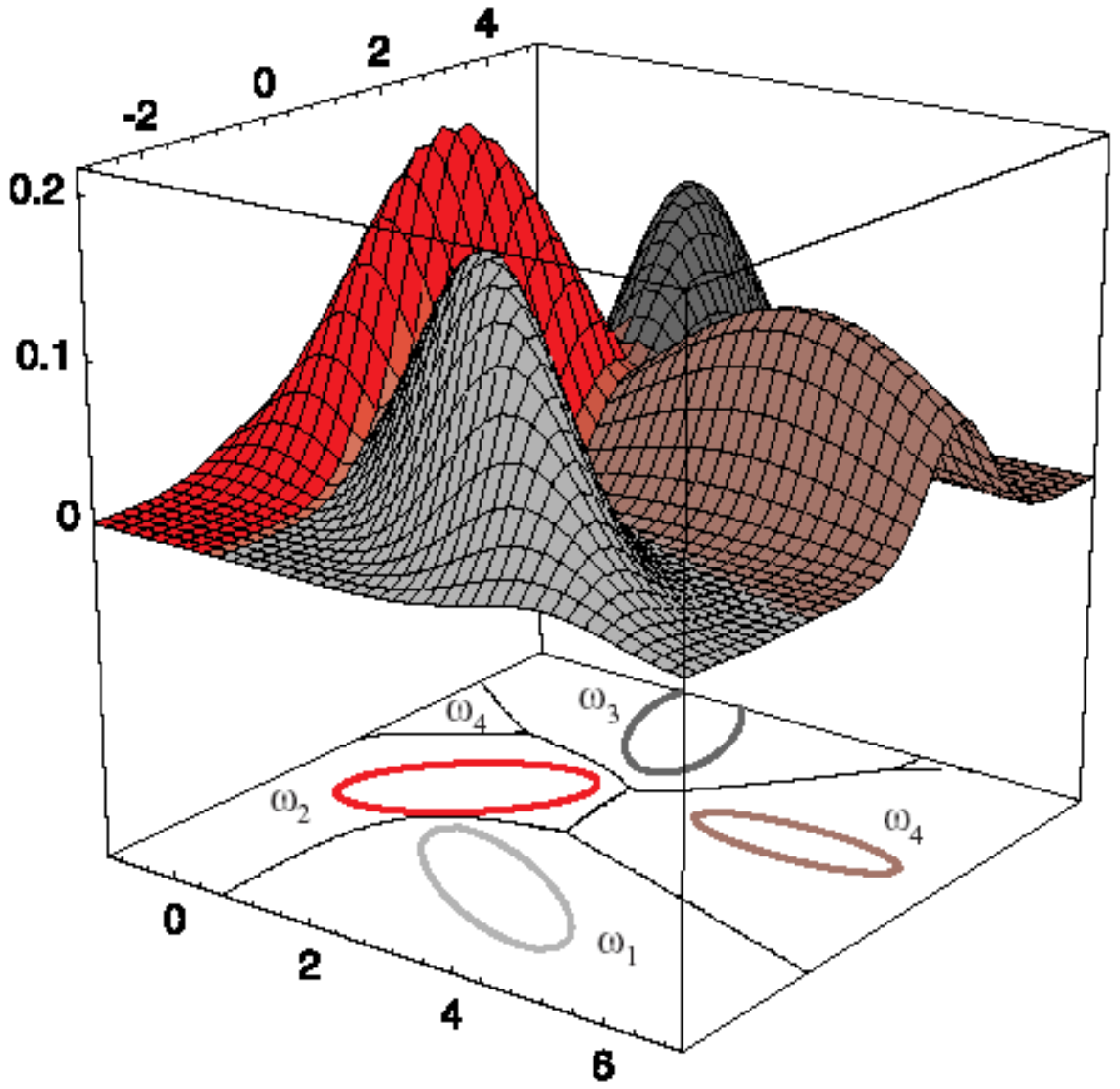
Mapping the features into another space

“The kernel trick”



“Overtraining/undertraining”

Bayesian classifier



Bayesian classifier

Assumption: feature values are random variables

Statistic classifier, the decision is probabilistic

It is based on the **Bayes rule**

The Bayes rule

Class-conditional probability

A posteriori probability

$$P(\omega_j|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_j)P(\omega_j)}{p(\mathbf{x})},$$

A priori probability

Total probability

$$p(\mathbf{x}) = \sum_{j=1}^{c} p(\mathbf{x}|\omega_j)P(\omega_j).$$

Bayesian classifier

Main idea: maximize posterior probability

$$P(\omega_j|\mathbf{x})$$

Since it is hard to do directly, we rather maximize

$$p(\mathbf{x}|\omega_j)P(\omega_j)$$

In case of equal priors, we maximize only

$$p(\mathbf{x}|\omega_j)$$

Equivalent formulation

…in terms of discriminat functions

$$g_i(\mathbf{x}) = P(\omega_i|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x}|\omega_j)P(\omega_j)}$$

$$g_i(\mathbf{x}) = p(\mathbf{x}|\omega_i)P(\omega_i)$$

$$g_i(\mathbf{x}) = \ln\, p(\mathbf{x}|\omega_i) + \ln\, P(\omega_i),$$

How to estimate $p(\mathbf{x}|\omega_j)P(\omega_j)$?

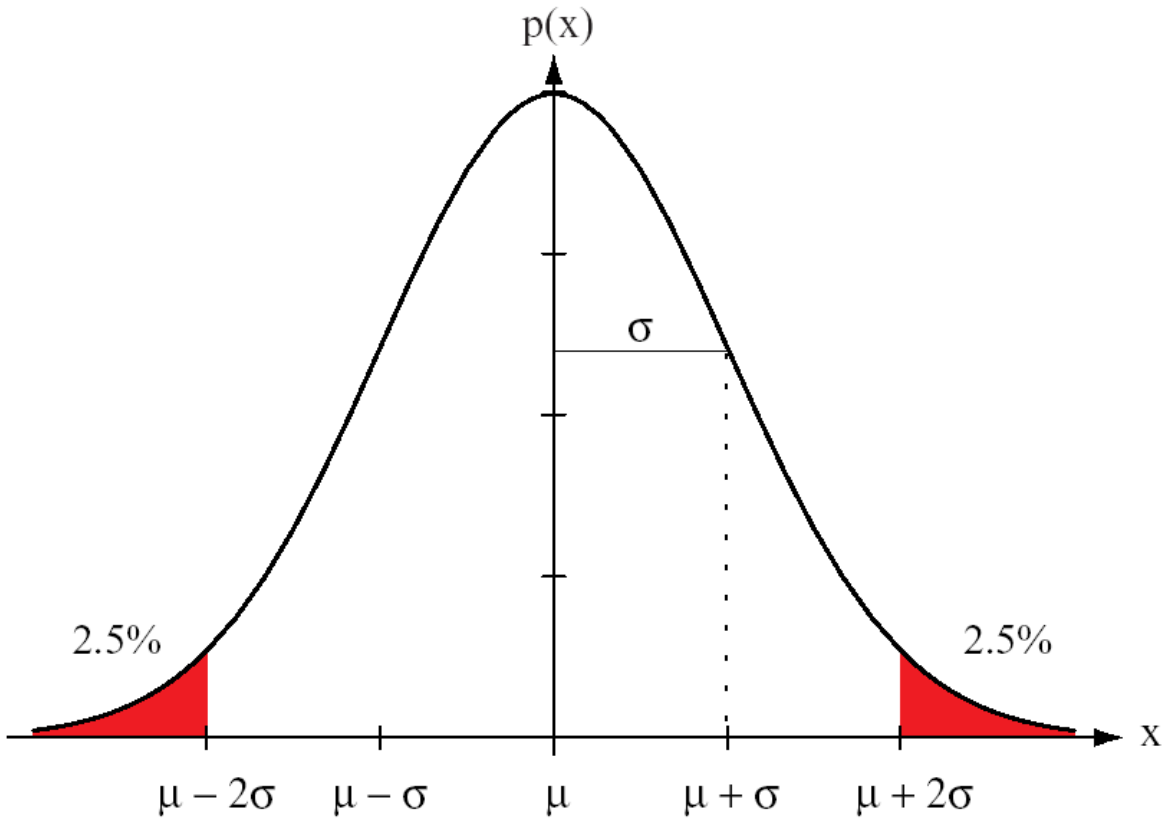
$P(\omega_j)$

- From the case studies performed before (OCR, speech recognition)
- From the occurence in the training set
- Assumption of equal priors

$p(\mathbf{x}|\omega_j)$

- Parametric estimate (assuming pdf is of a known form, e.g. Gaussian)
- Non-parametric estimate (pdf is unknown or too complex)

Parametric estimate of Gaussian $p(\mathbf{x}|\omega_j)$

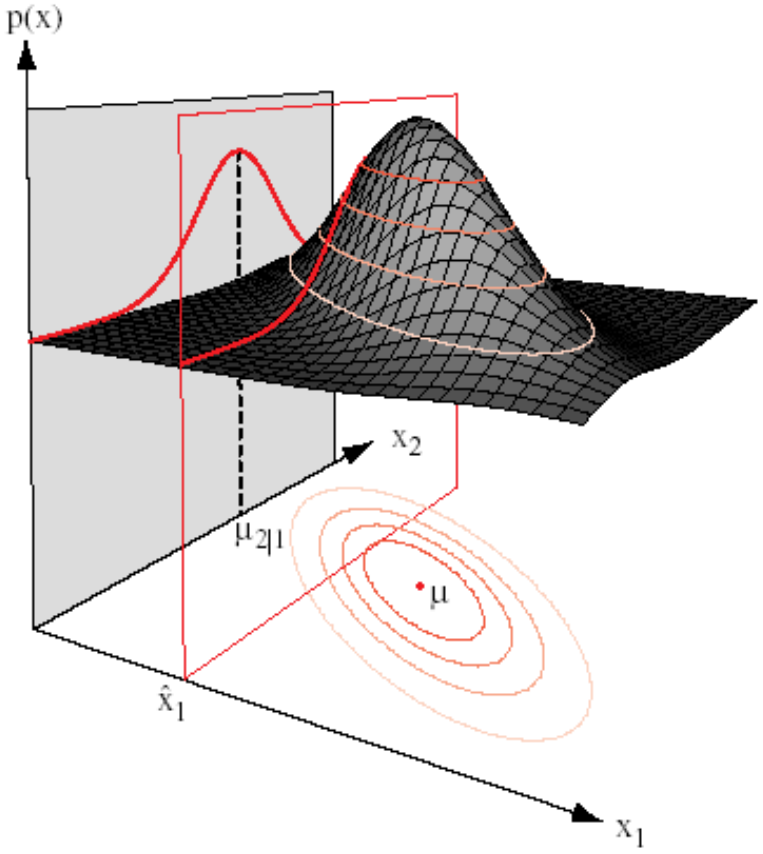


$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} x_k$$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu})^2$$

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

d-dimensional Gaussian pdf

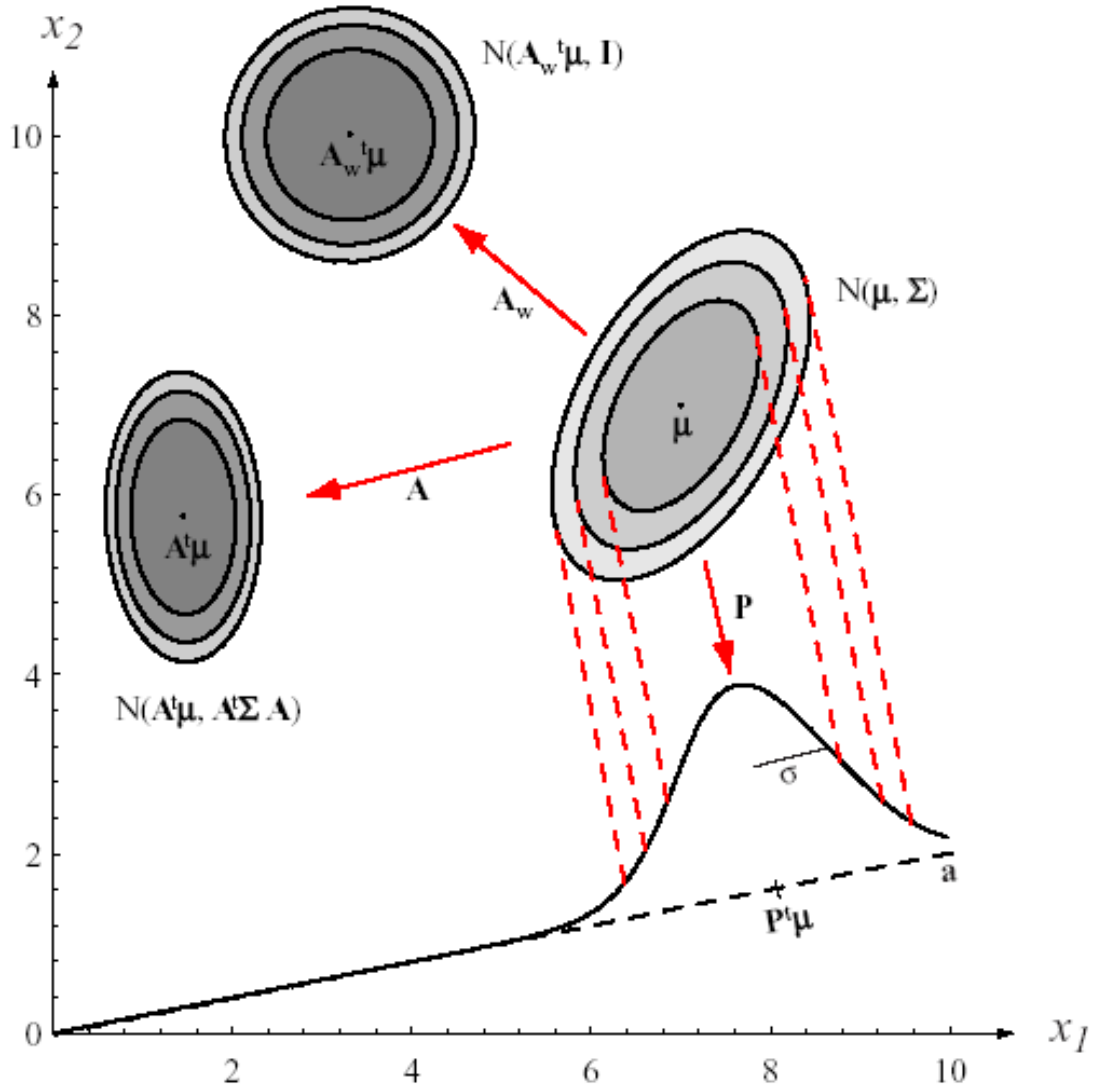


$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_k$$

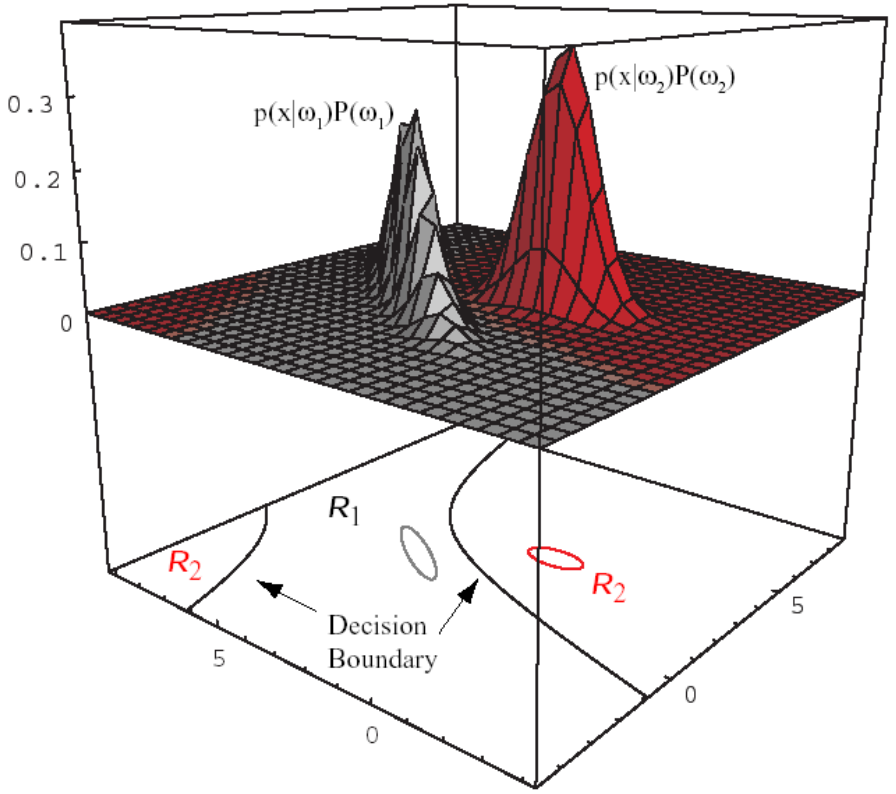
$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n}\sum_{k=1}^{n}(\mathbf{x}_k - \hat{\boldsymbol{\mu}})(\mathbf{x}_k - \hat{\boldsymbol{\mu}})^t.$$

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^t\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

The role of covariance matrix



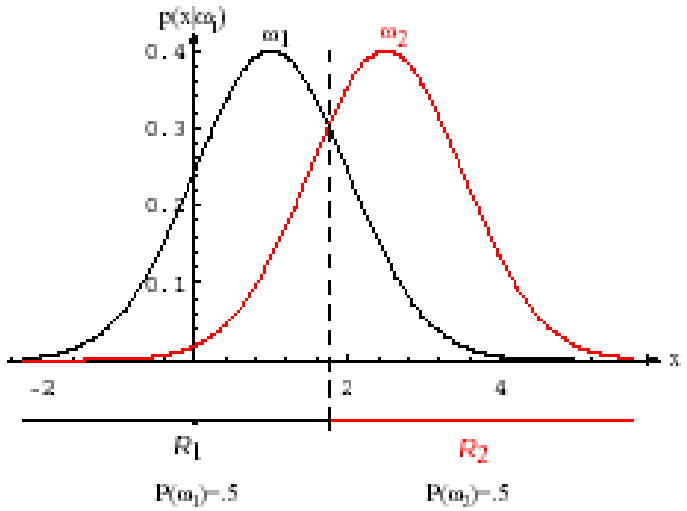
Two-class Gaussian case in 2D

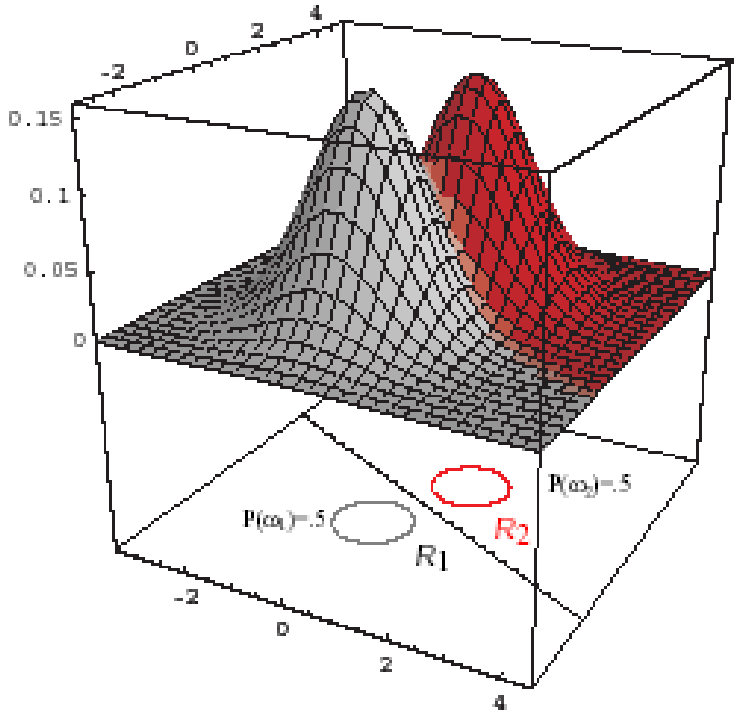


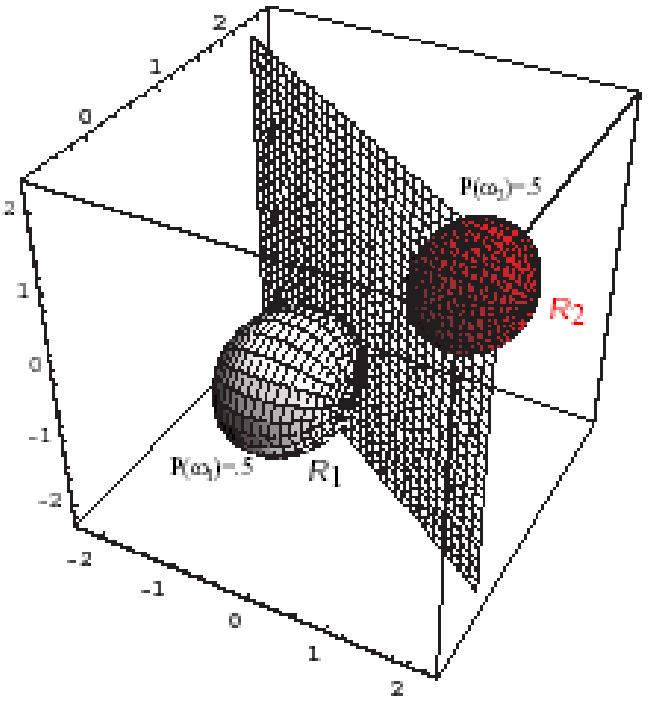
$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}_i^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) - \frac{d}{2}\ln 2\pi - \frac{1}{2}\ln|\boldsymbol{\Sigma}_i| + \ln P(\omega_i).$$

Classification = comparison of two Gaussians

Two-class Gaussian case – Equal cov. mat.







$$g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_i) + \ln P(\omega_i)$$

Linear decision boundary

Equal priors $P(\omega_j)$

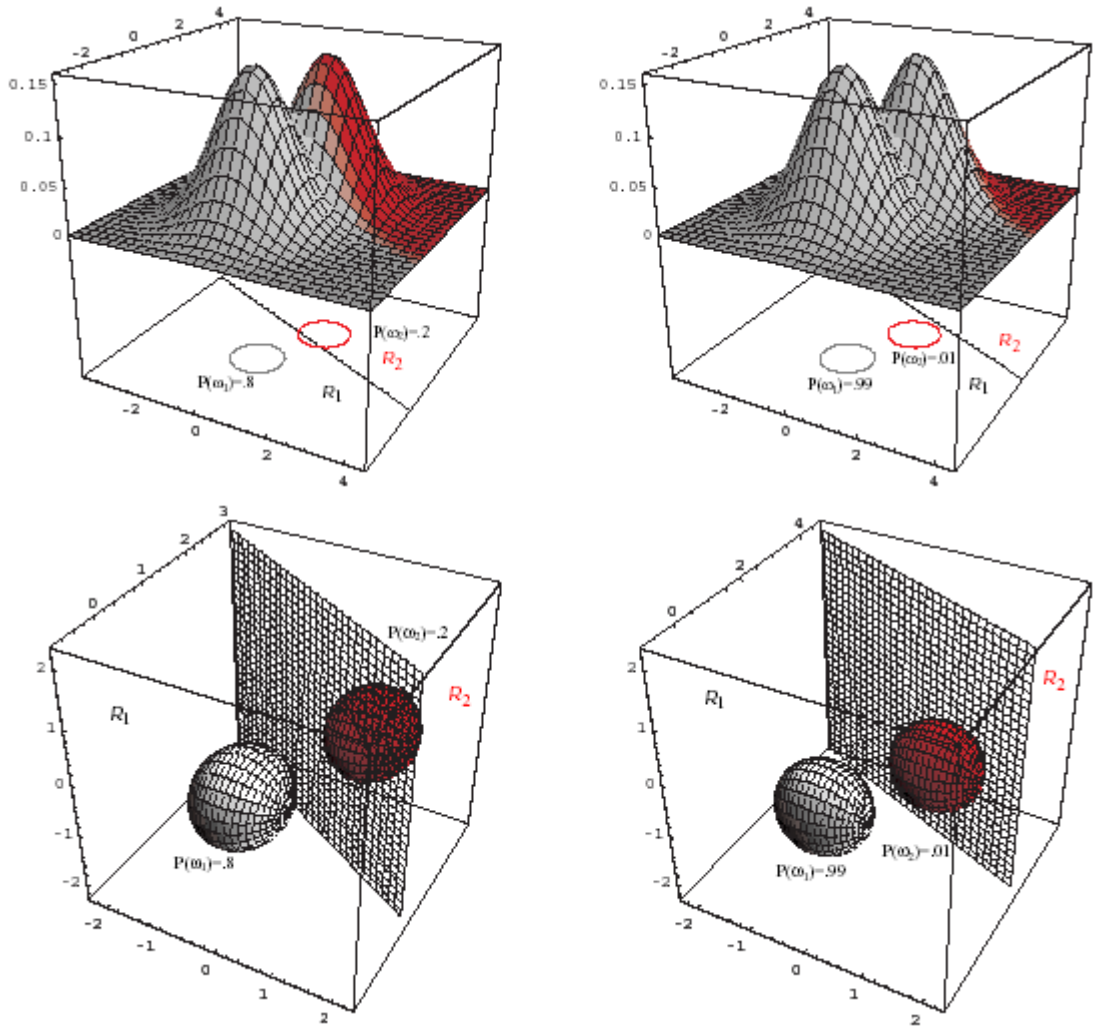
max $g_i(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_i)$.

min $(\mathbf{x}-\boldsymbol{\mu}_i)^t\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_i)$.

Classification by minimum **Mahalanobis distance**

If the cov. mat. is diagonal with equal variances then we get **“standard”** minimum distance rule

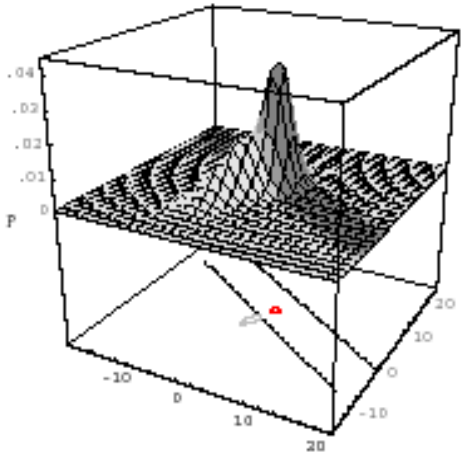
Non-equal priors

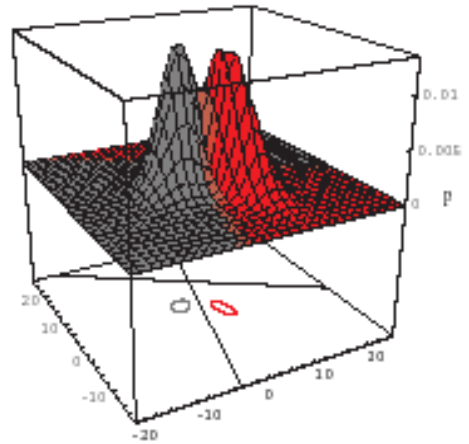


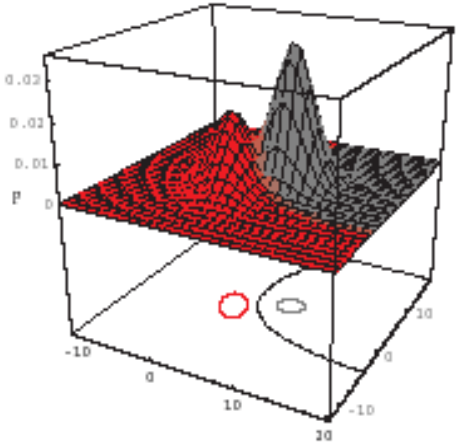
Linear decision boundary still preserved

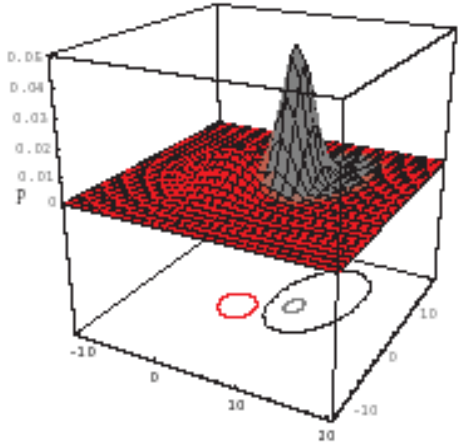
General G case in 2D

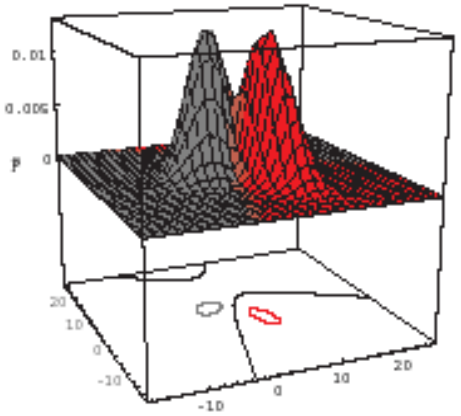
Decision boundary is a hyperquadric

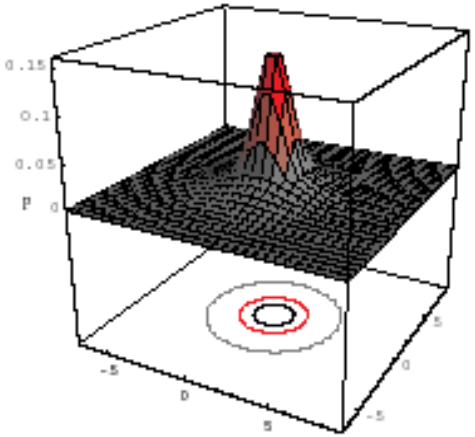






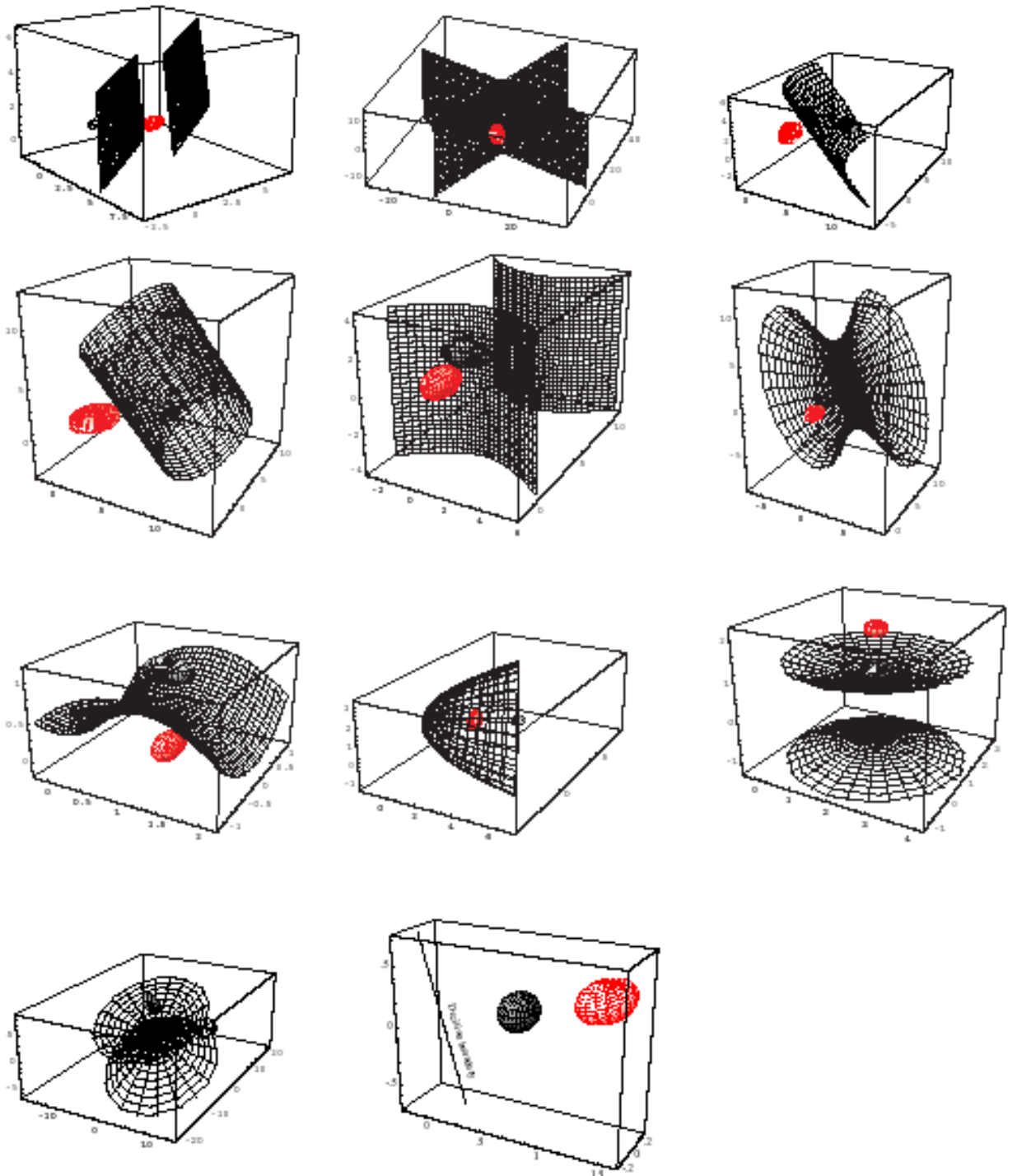




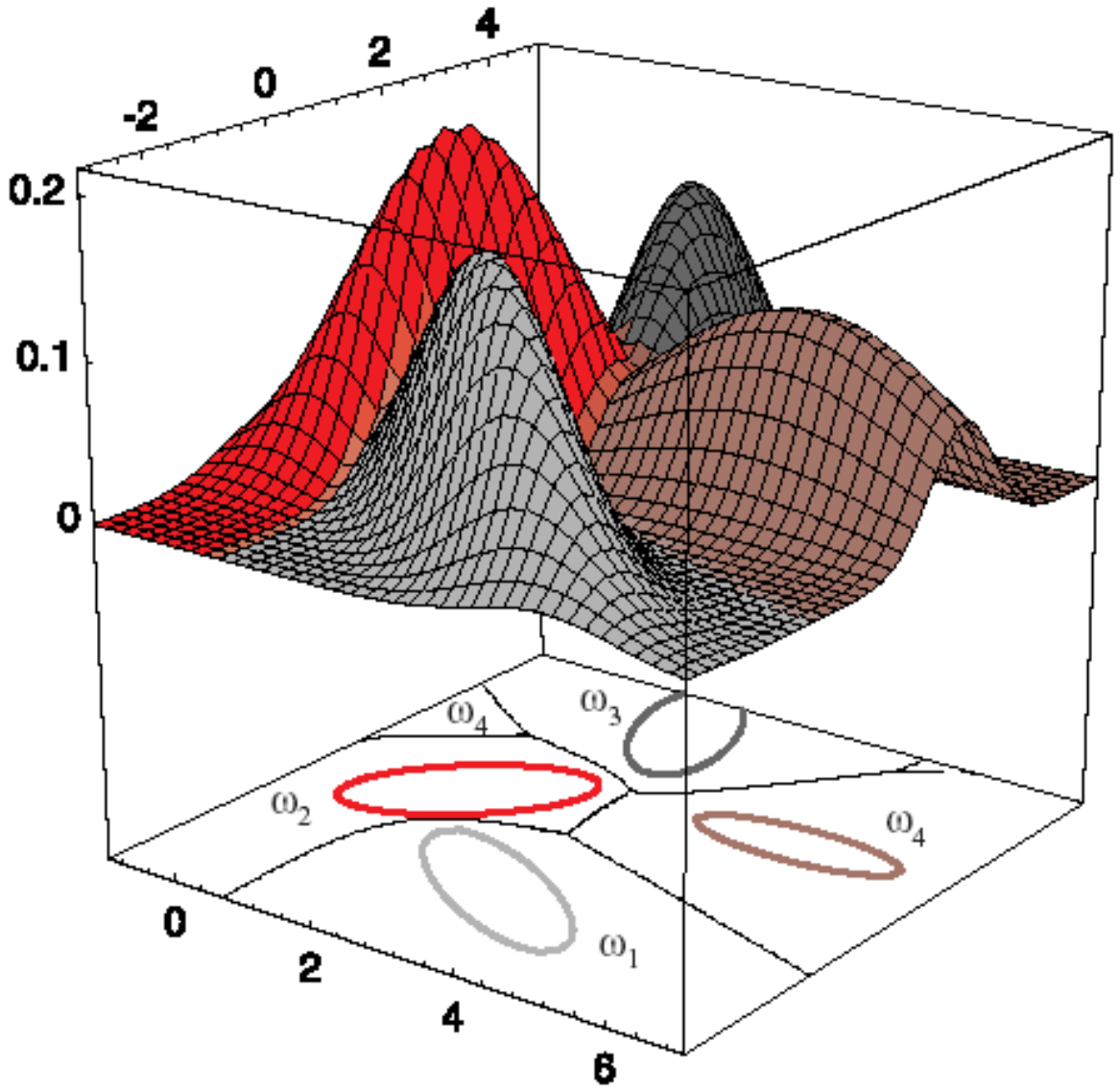


General G case in 3D

Decision boundary is a hyperquadric



More classes, Gaussian case in 2D



How to test the normality

…of the class-conditional distributions?

- Pearson's chi-square test (goodness-of-fit test)

$$X^2 = \sum \frac{(\text{observed} - \text{expected})^2}{\text{expected}}$$

- Moment-based tests
- Visual assessment

What to do

…if the classes are not normally distributed?

- **Gaussian mixtures**
- **Parametric estimation of some other pdf**
- **Non-parametric estimation**

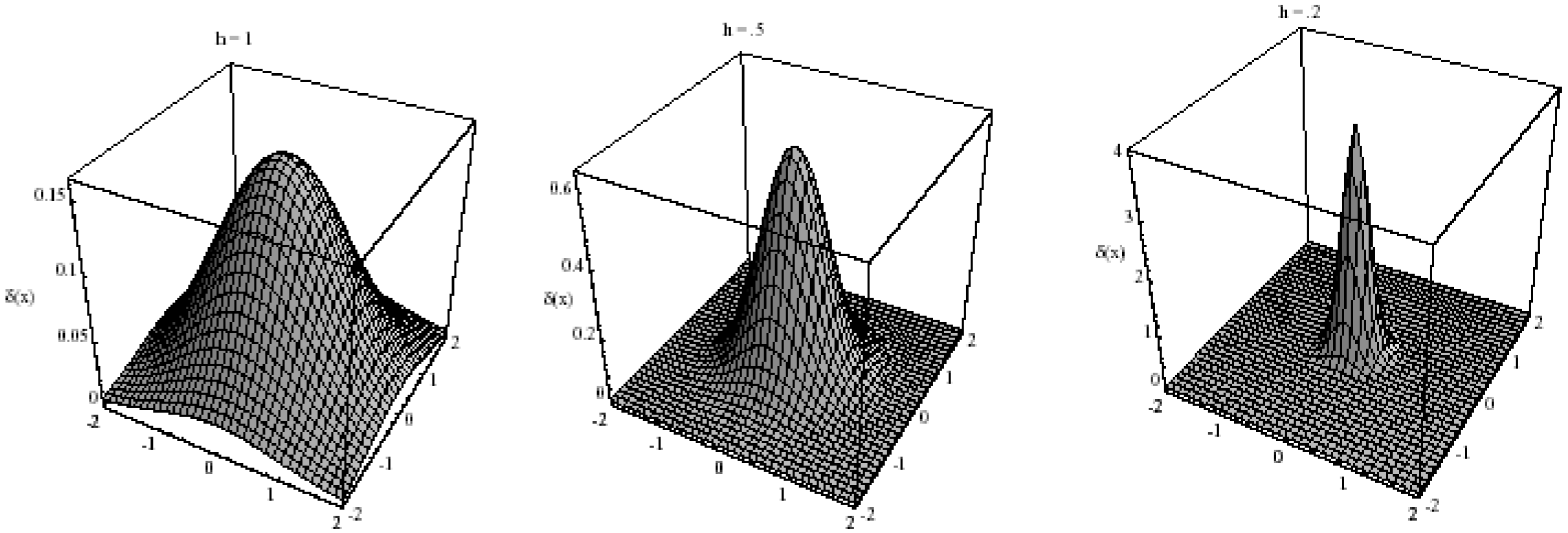
Non-parametric estimation

Estimation of *p(x|w)* by relative frequency in volume *V*

$$p(\mathbf{x}|\omega_j) \simeq \frac{k/n}{V}$$

Non-parametric estimation – Parzen window

Volume *V* is weighted by parametric Parzen window function



The role of the window size

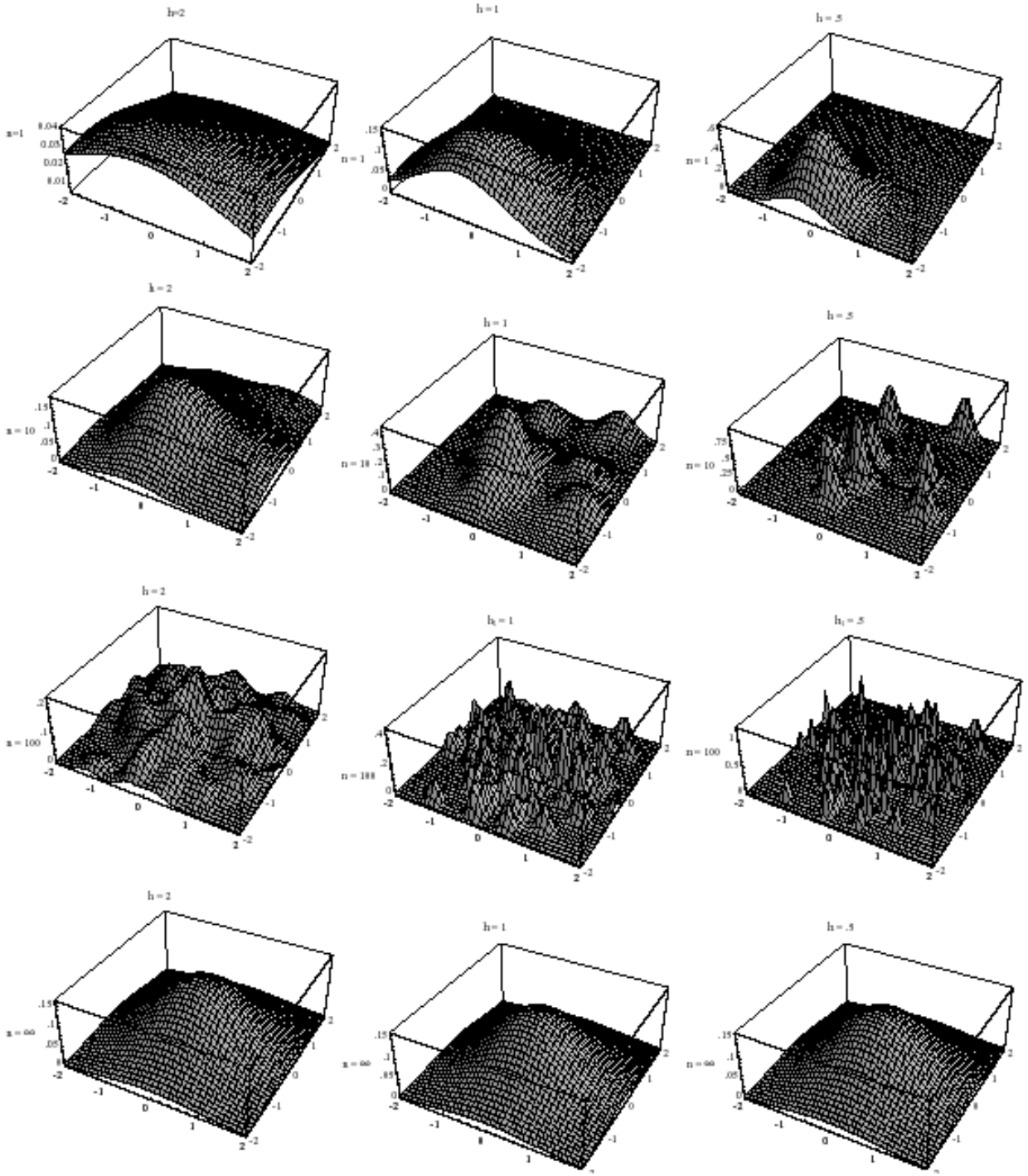
- Small window → overtaining
- Large window → data smoothing
- Continuous data → the size does not matter

n = 1

n = 10

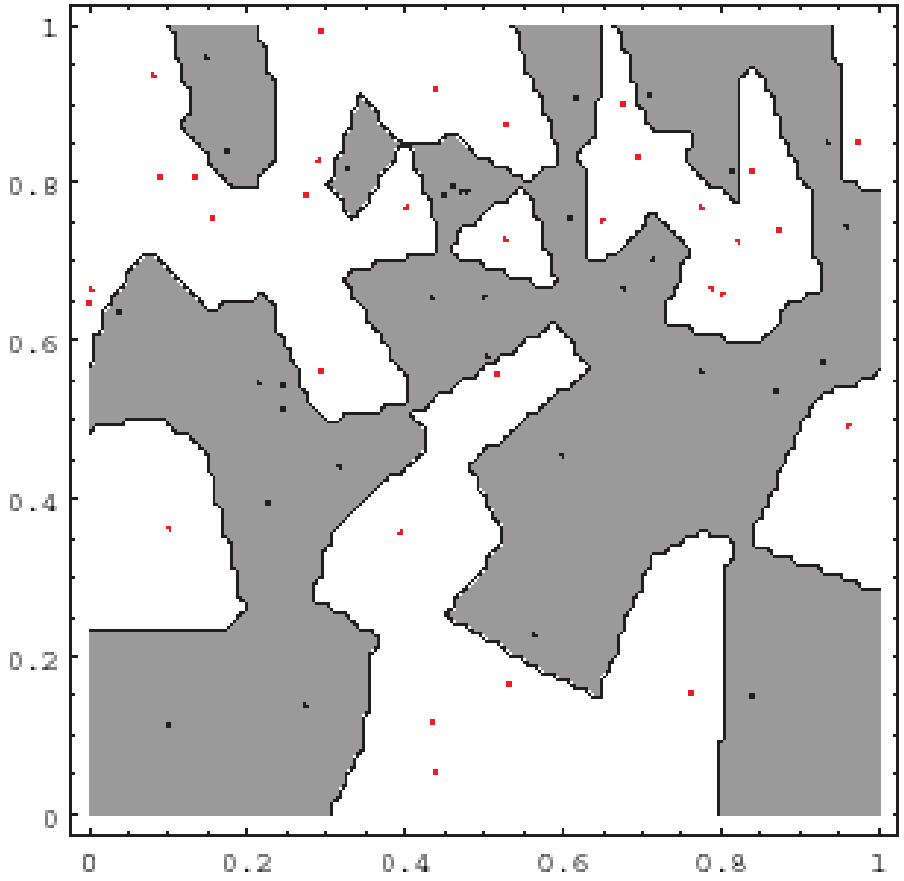
n = 100

n = ∞

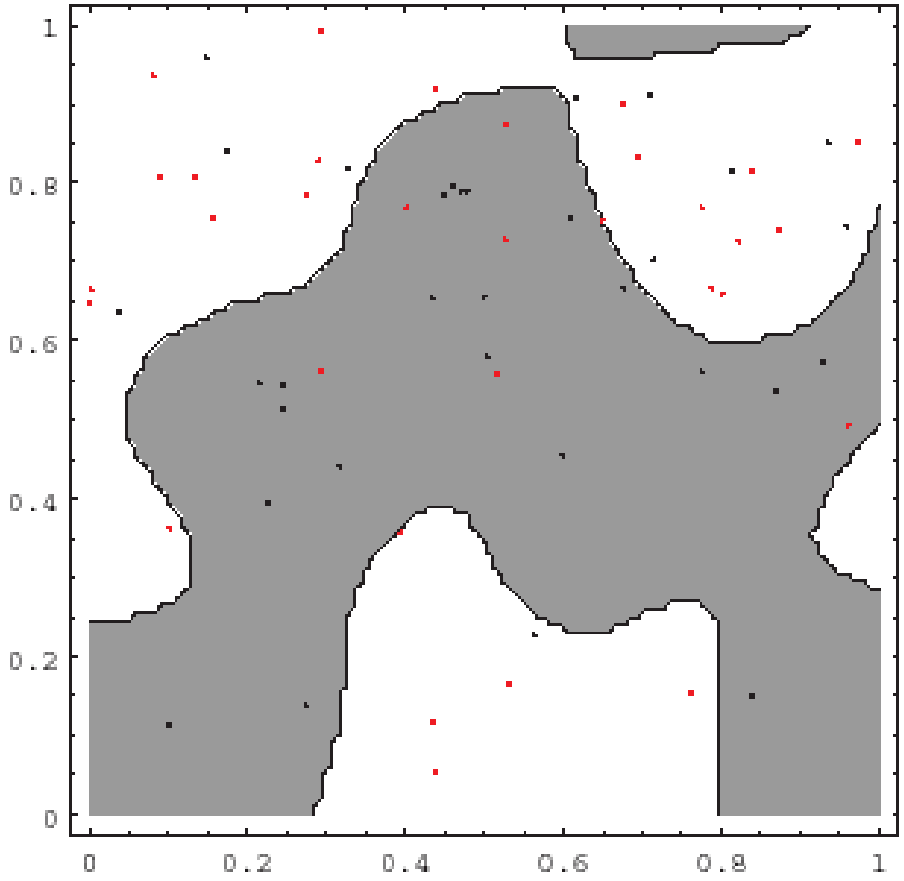


The role of the window size

Small window



Large window



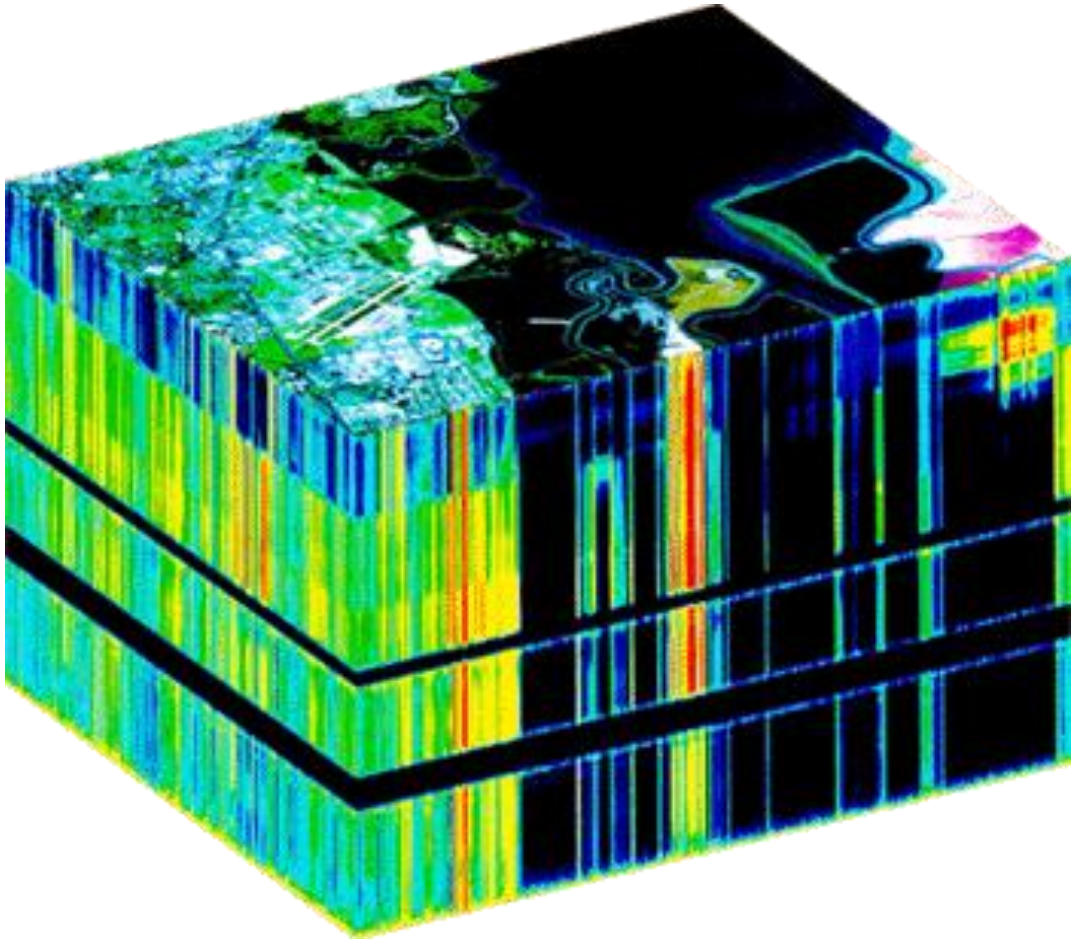
Applications of Bayesian classifier

…in multispectral remote sensing

- Objects = pixels
- Features = pixel values in the spectral bands (from 4 to several hundreds)
- Training set – selected manually by means of thematic maps (GIS), and on-site observation
- Number of classes – typically from 2 to 16

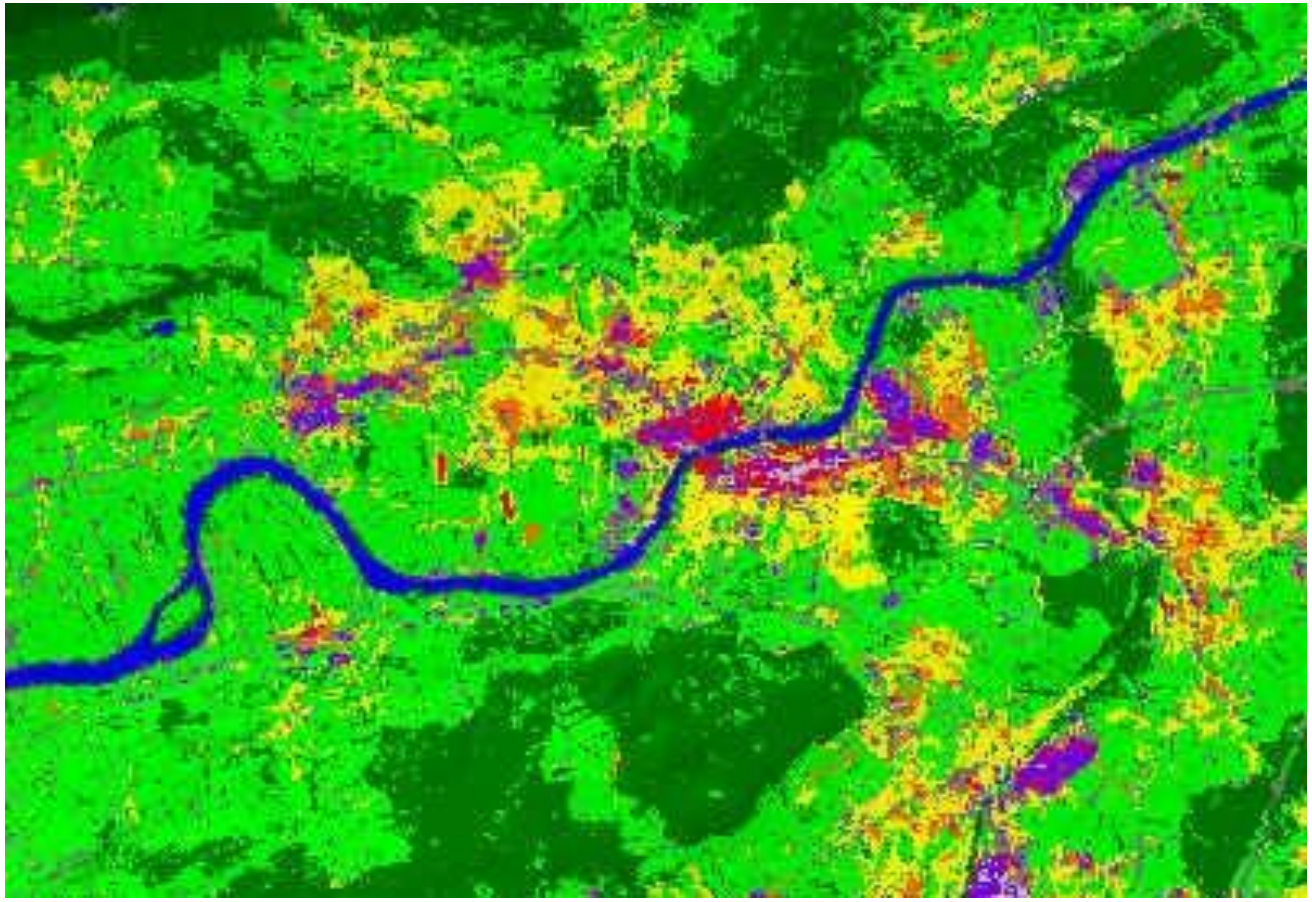
Applications of Bayesian classifier

…in multispectral remote sensing



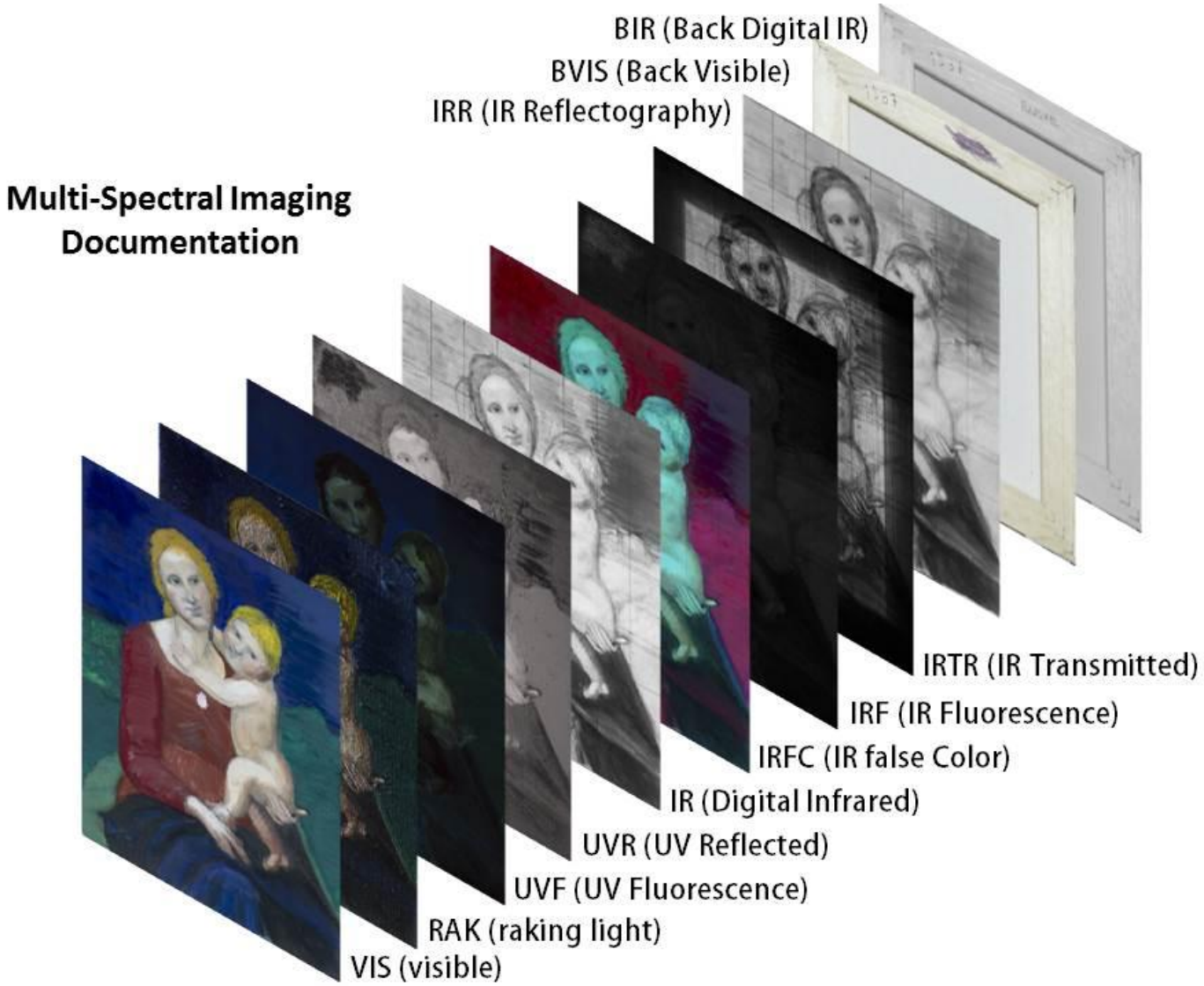
Applications of Bayesian classifier

…in multispectral remote sensing



Applications of Bayesian classifier

…in art



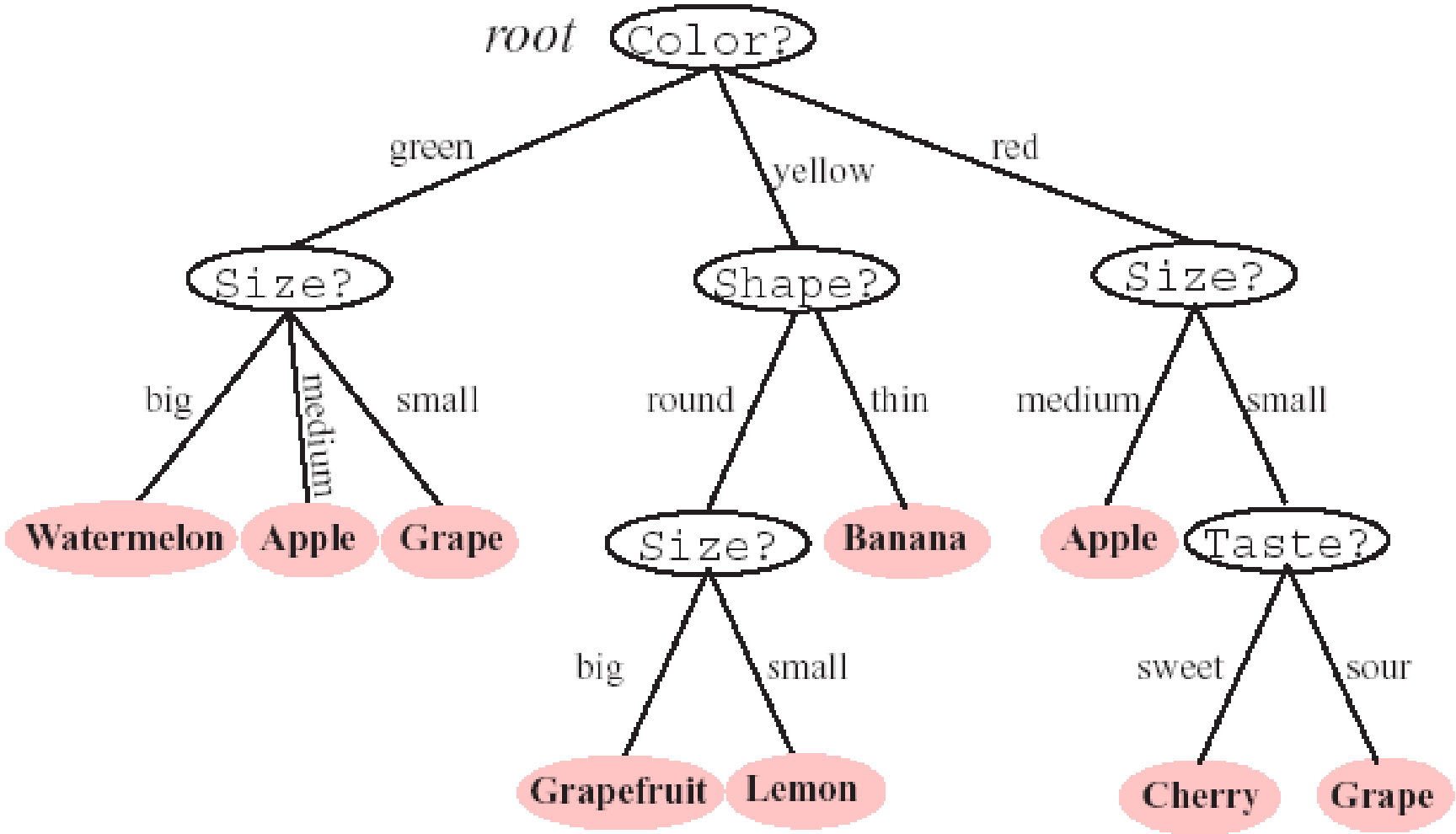
Non-metric classifiers

Typically for “YES – NO” features

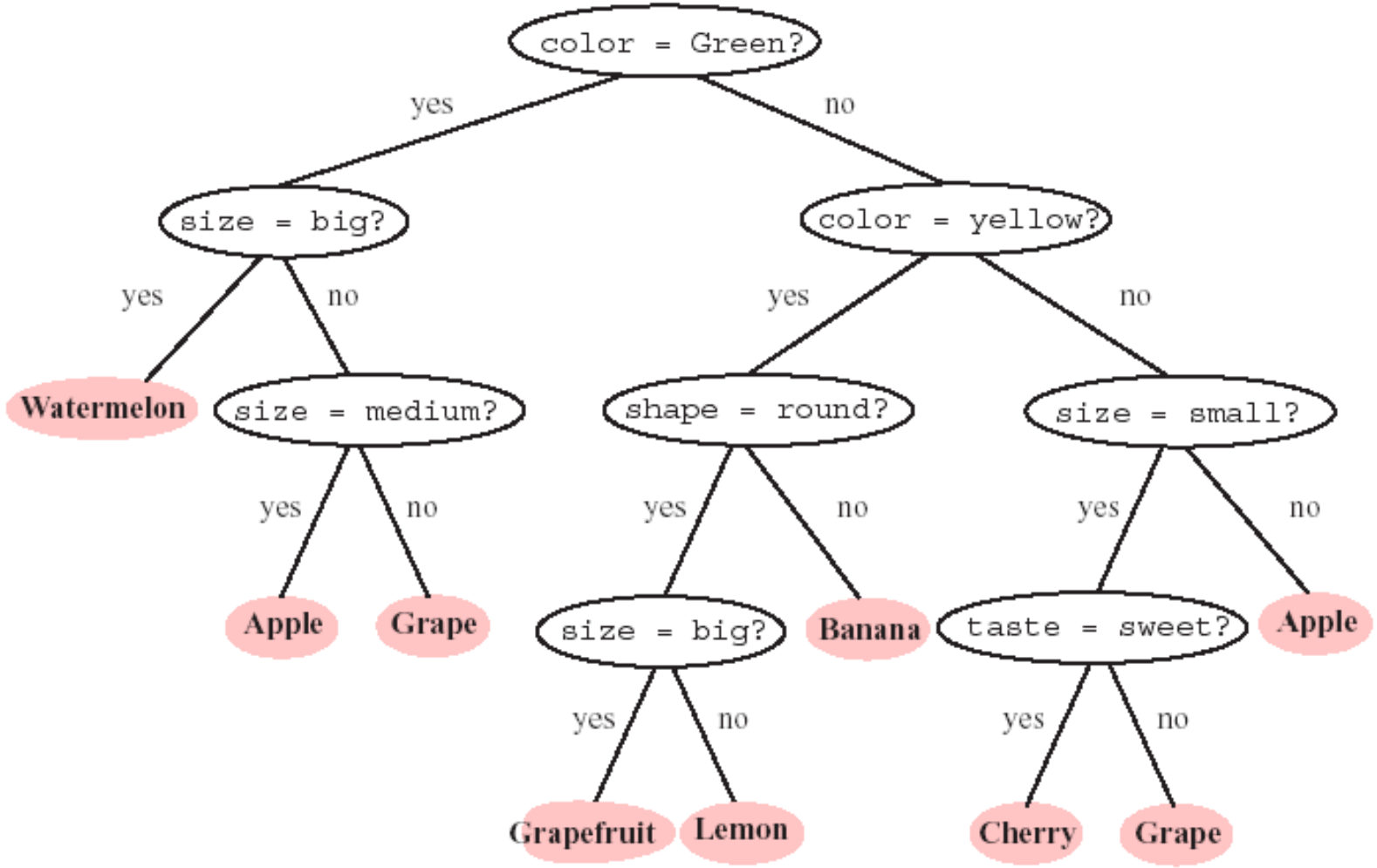
Feature metric is not explicitly defined

Decision trees

General decision tree



Binary decision tree

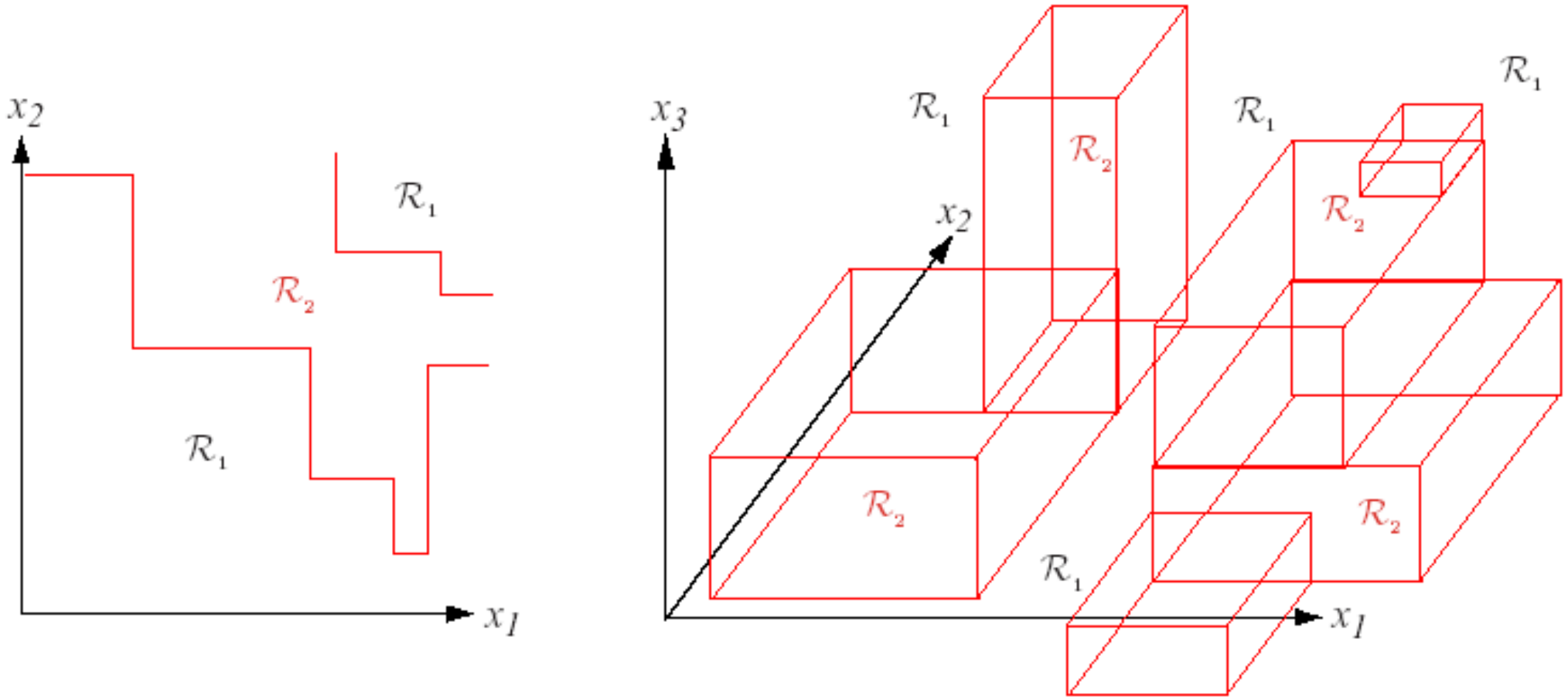


Any decision tree can be replaced by a binary tree

Real-valued features

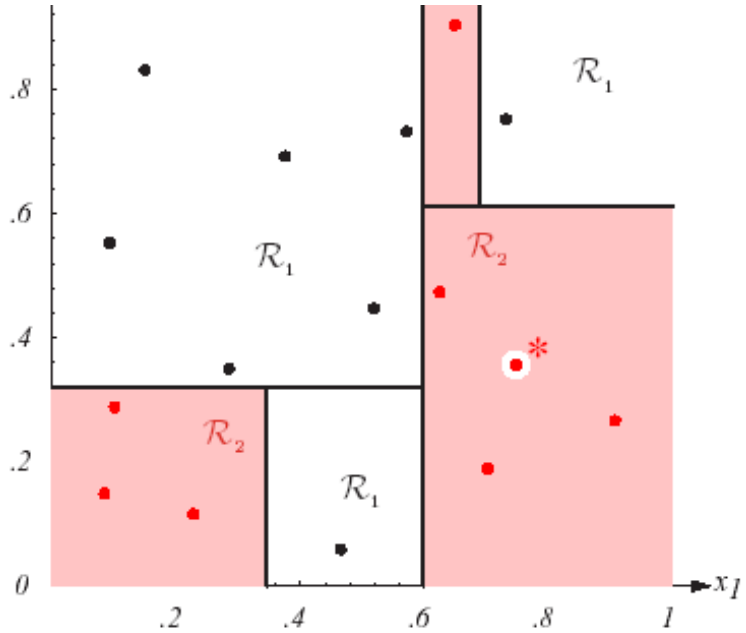
- Node decisions are in form of inequalities
- Training = setting their parameters
- Simple inequalities → stepwise decision boundary

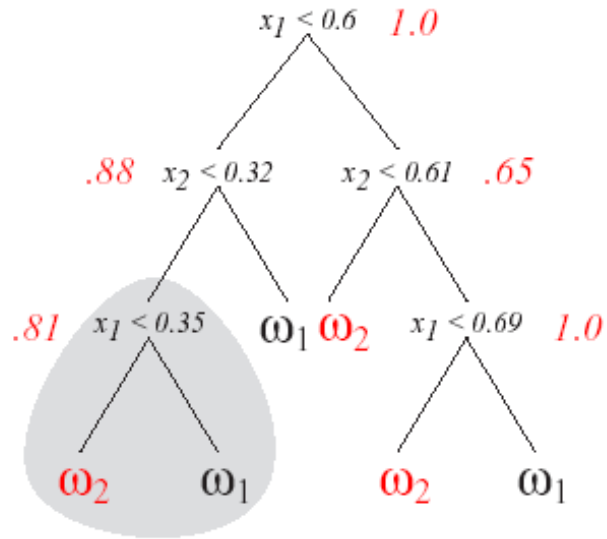
Stepwise decision boundary

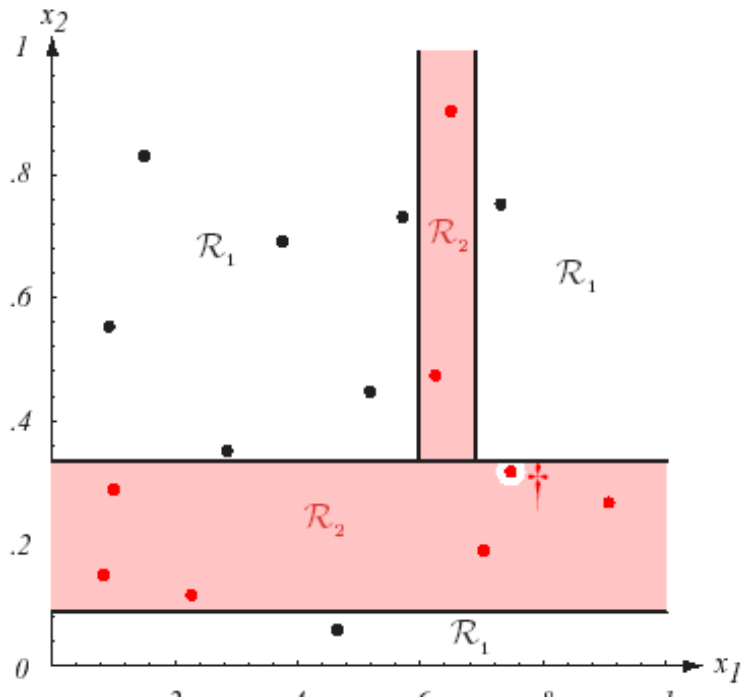


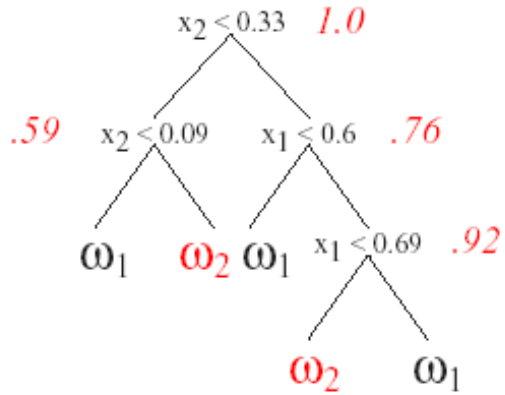
Real-valued features

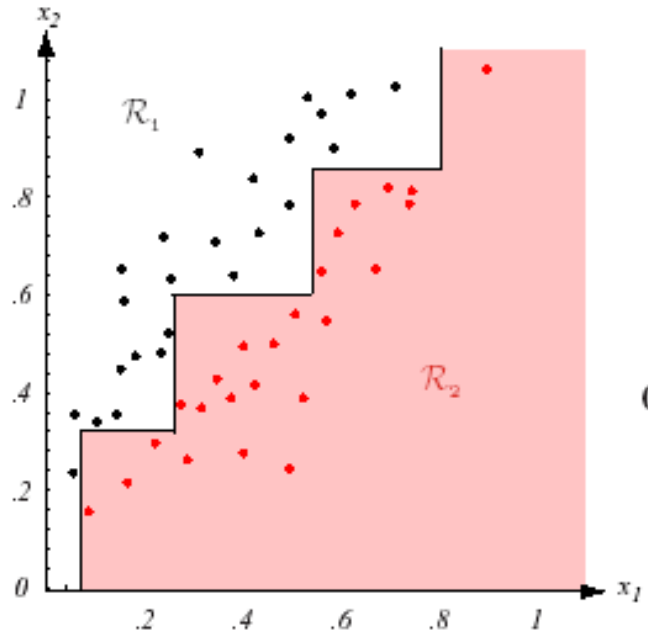
The tree structure and the form of inequalities influence both performance and speed.

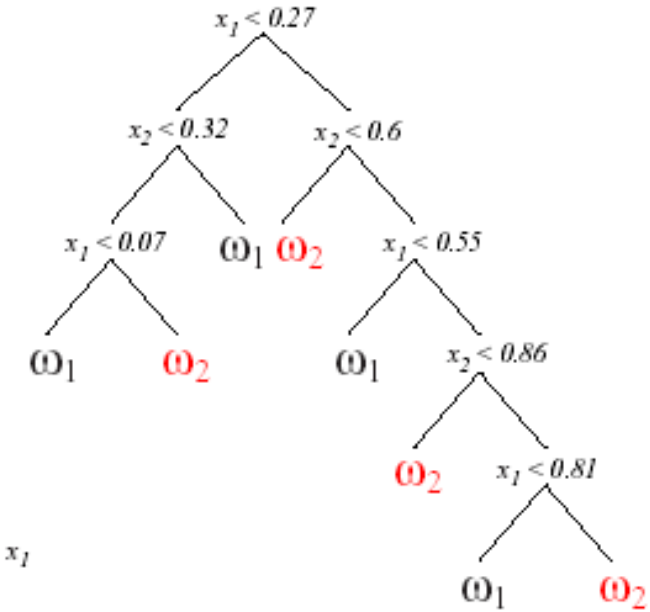

$\mathcal{R}_1$
$\mathcal{R}_2$
$\mathcal{R}_1$
$\mathcal{R}_2$
$\mathcal{R}_1$
0
.2
.4
.6
.8
1
x_1

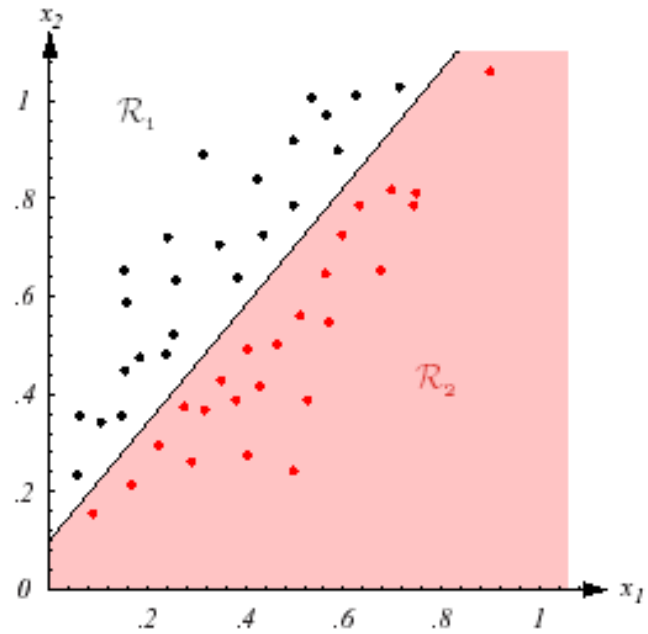

$x_1 < 0.6$ 1.0
.88
$x_2 < 0.32$
$x_2 < 0.61$
.65
.81
$x_1 < 0.35$
ω_1
ω_2
$x_1 < 0.69$
1.0
ω_2
ω_1
ω_2
ω_1

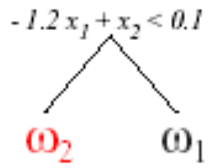

x_2
$\mathcal{R}_1$
$\mathcal{R}_2$
$\mathcal{R}_1$
$\mathcal{R}_2$
$\mathcal{R}_1$
0
.2
.4
.6
.8
1
x_1


$x_2 < 0.33$ 1.0
.59
$x_2 < 0.09$
$x_1 < 0.6$
.76
ω_1
ω_2
ω_1
$x_1 < 0.69$
.92
ω_2
ω_1


x_2
1
.8
.6
.4
.2
0
$\mathcal{R}_1$
$\mathcal{R}_2$
.2
.4
.6
.8
1
x_1


$x_1 < 0.27$
$x_2 < 0.32$
$x_2 < 0.6$
$x_1 < 0.07$
ω_1
ω_2
$x_1 < 0.55$
ω_1
ω_2
ω_1
$x_2 < 0.86$
ω_2
$x_1 < 0.81$
ω_1
ω_2


x_2
1
.8
.6
.4
.2
0
$\mathcal{R}_1$
$\mathcal{R}_2$
.2
.4
.6
.8
1
x_1


$-1.2\,x_1 + x_2 < 0.1$
ω_2
ω_1

Classification performance

How to evaluate the performance of the classifiers?

- Evaluation on the training set (optimistic error estimate).
- Evaluation on the test set (pessimistic error estimate). Intuitive evaluation is misleading, different errors may have different significance

Confusion matrix

		Predicted		
		Greyhound	Mastiff	Samoyed
Actual	Greyhound	250	25	18
	Mastiff	21	320	24
	Samoyed	22	12	180

Confusion matrix 2 x 2

Machine learing \ Manual counting	True	False
True	True Positive (TP)	False Positive (FP)
False	False Negative (FN)	True Negative (TN)

Equations:

$$\text{False positive rate (FPR)} = \frac{FP}{FP+TN}$$

$$\text{False negative rate (FNR)} = \frac{FN}{FN+TP}$$

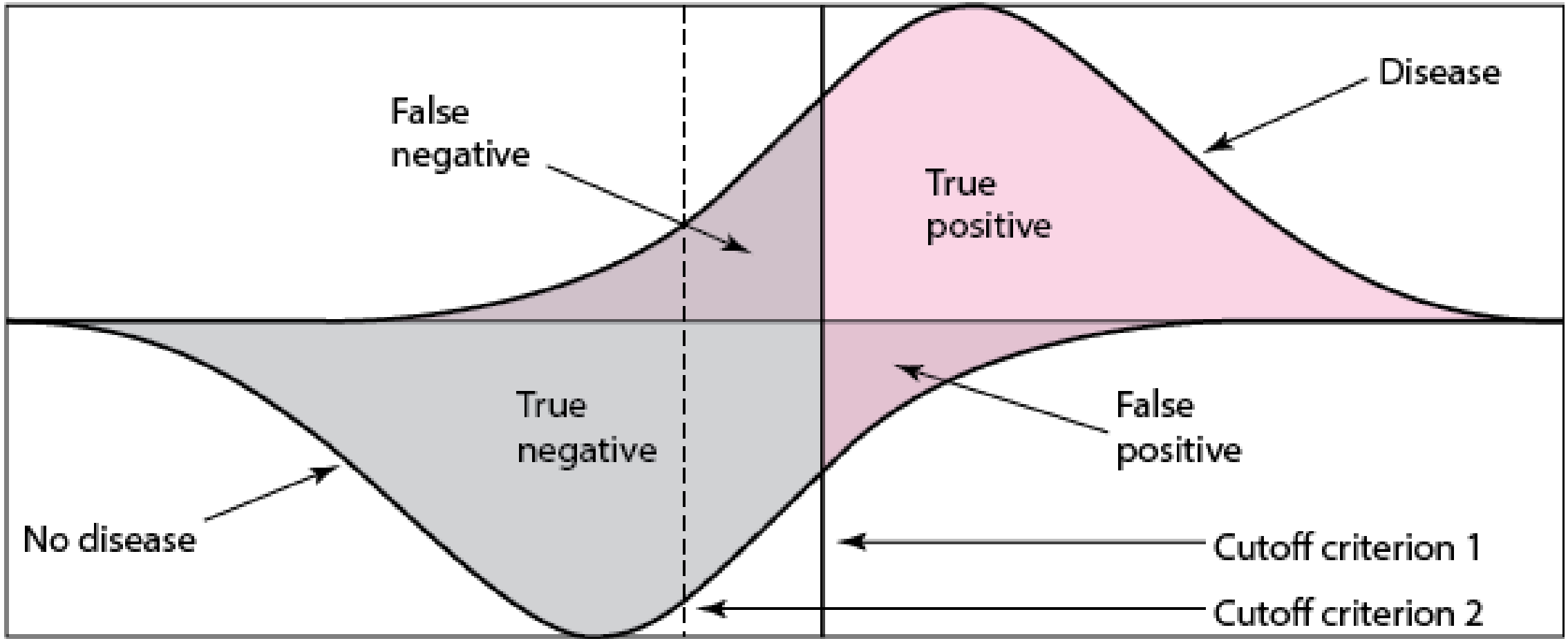
$$\text{Sensitivity} = \frac{TP}{TP+FN}$$

$$\text{Specificity} = \frac{TN}{TN+FP}$$

$$\text{Youden index} = \text{Sensitivity} + \text{Specificity} - 1$$

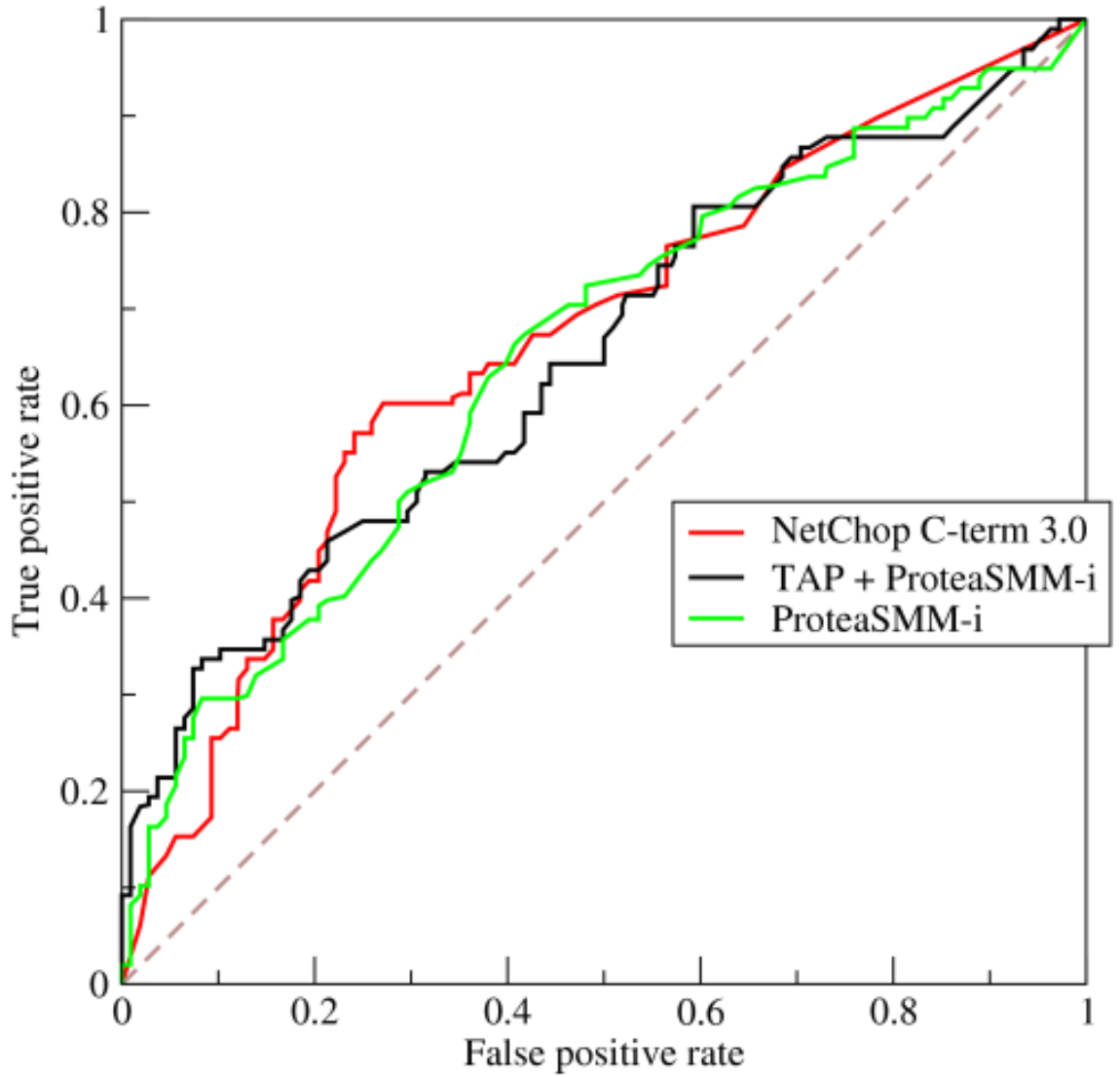
$$\text{Accuracy} = \frac{TP+TN}{TP+TN+FP+FN}$$

Tuning the classifier

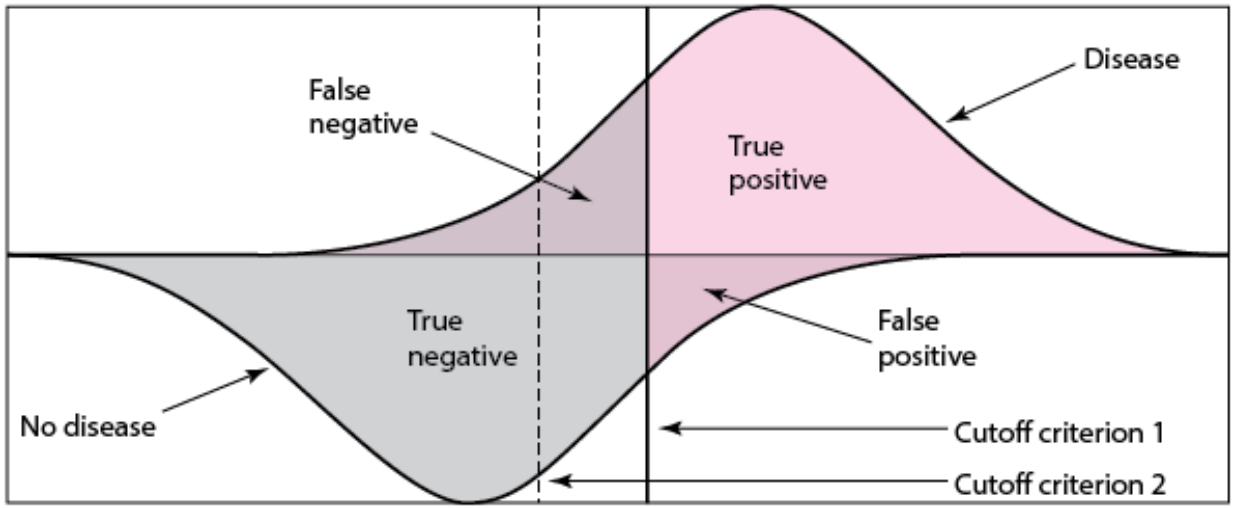


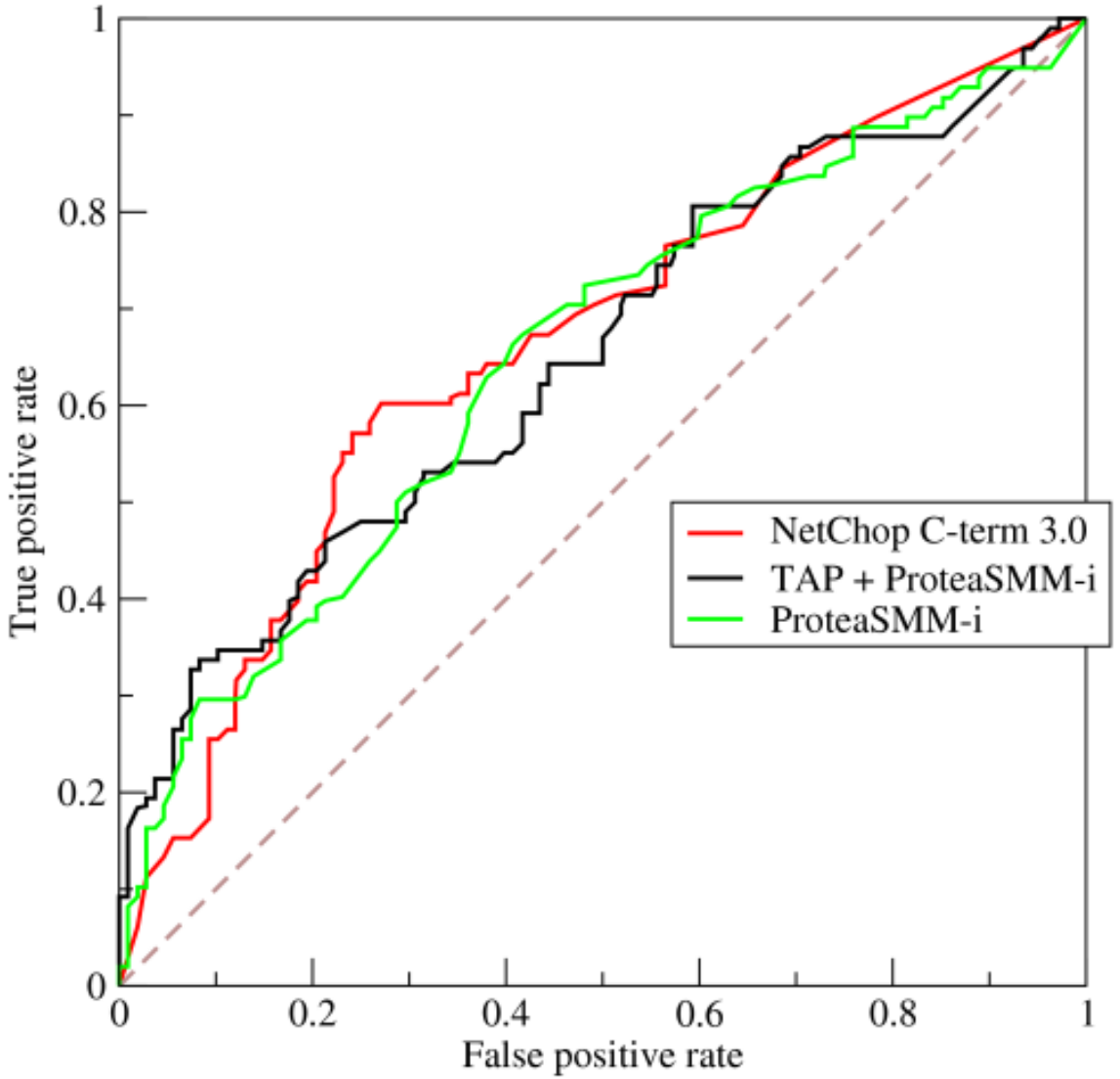
ROC curve

Receiver Operating Characteristic



ROC construction





Classification performance

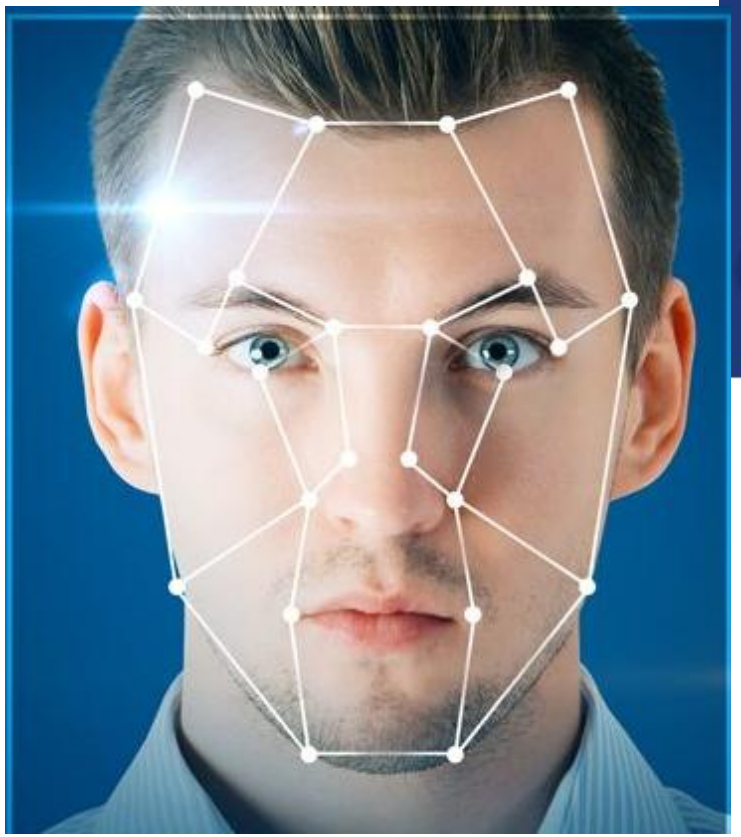
How to increase the performance?

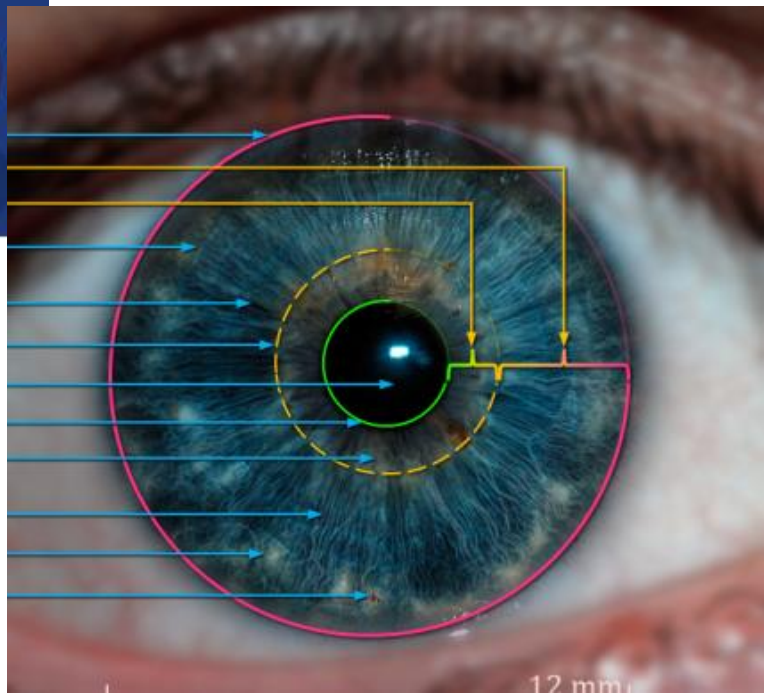
- other features
- more features (dangerous – curse of dimensionality!)
- other (larger, better) training sets
- other parametric models
- other classifiers
- **combining different classifiers**

Combining classifiers

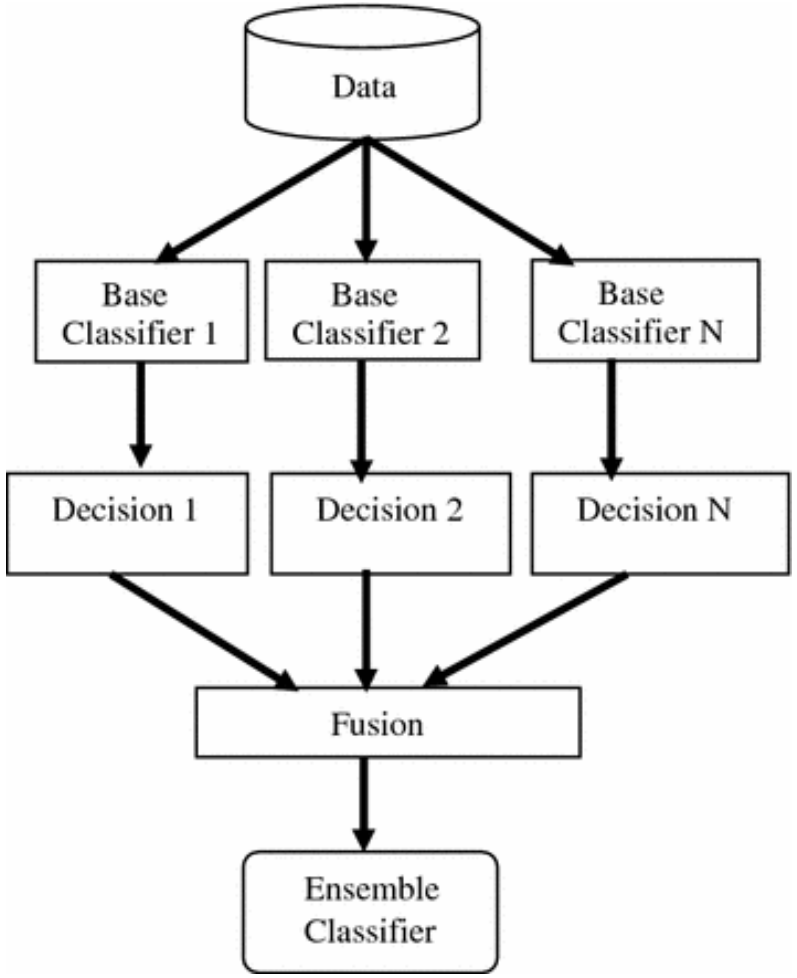
- Several *independent* classifiers
- Averaging of noisy results
- Suppression of extremes
- No guarantee of improvement over the best classifier

Combining classifiers in biometrics





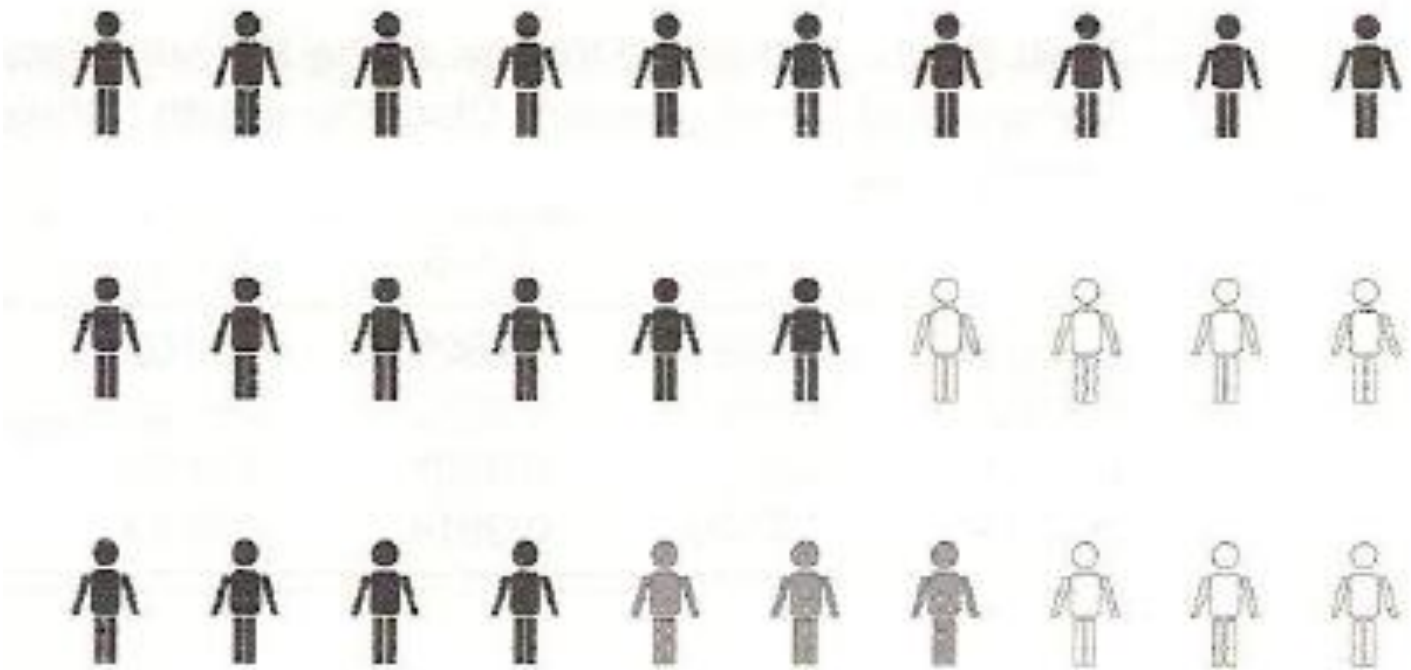
Combining deterministic decisions: voting



$$P_{maj} = \sum_{m=\lfloor L/2 \rfloor + 1}^{L} \binom{L}{m} p^m (1-p)^{L-m}$$

$P > p$ iff $p > 0.5$

Combining deterministic classifiers: voting



Weighted voting: incorporating the expert knowledge

Majority vote – probability of success

Většinové hlasování :

$$P_{maj} = \sum_{m=\lfloor L/2 \rfloor+1}^{L} \binom{L}{m} p^m (1-p)^{L-m}$$

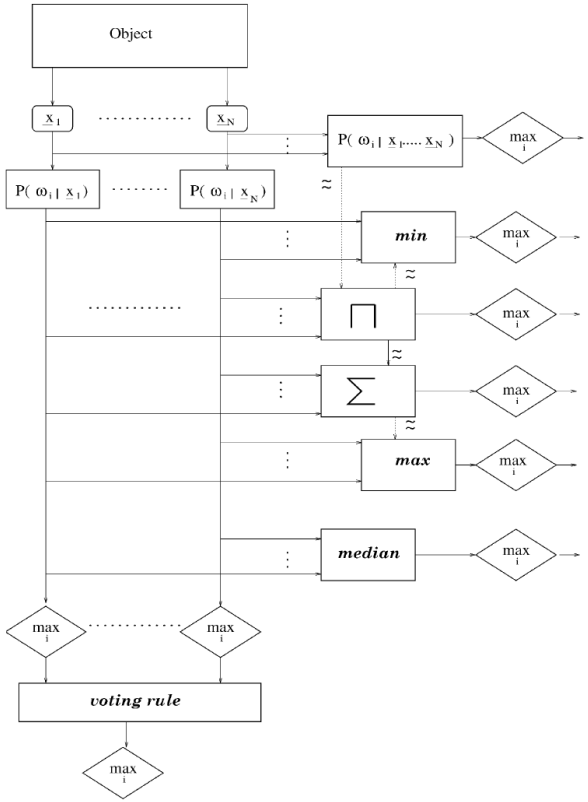
kde L je počet **nezávislých** klasifikátorů a p je jejich úspěšnost.

	$L=3$	$L=5$	$L=7$	$L=9$
$p=0.6$	0.6480	0.6826	0.7102	0.7334
$p=0.7$	0.7840	0.8369	0.8740	0.9012
$p=0.8$	0.8960	0.9421	0.9667	0.9804
$p=0.9$	0.9720	0.9914	0.9973	0.9991

Combining probabilistic classifiers

max $p(\omega_i|x_1, \cdots, x_C)$

$$p(\omega_i) \cdot p(x_1, \cdots, x_C|\omega_i) \quad p(x_1, \cdots, x_C|\omega_i) = \prod_{j=1}^{C} p(x_j|\omega_i)$$



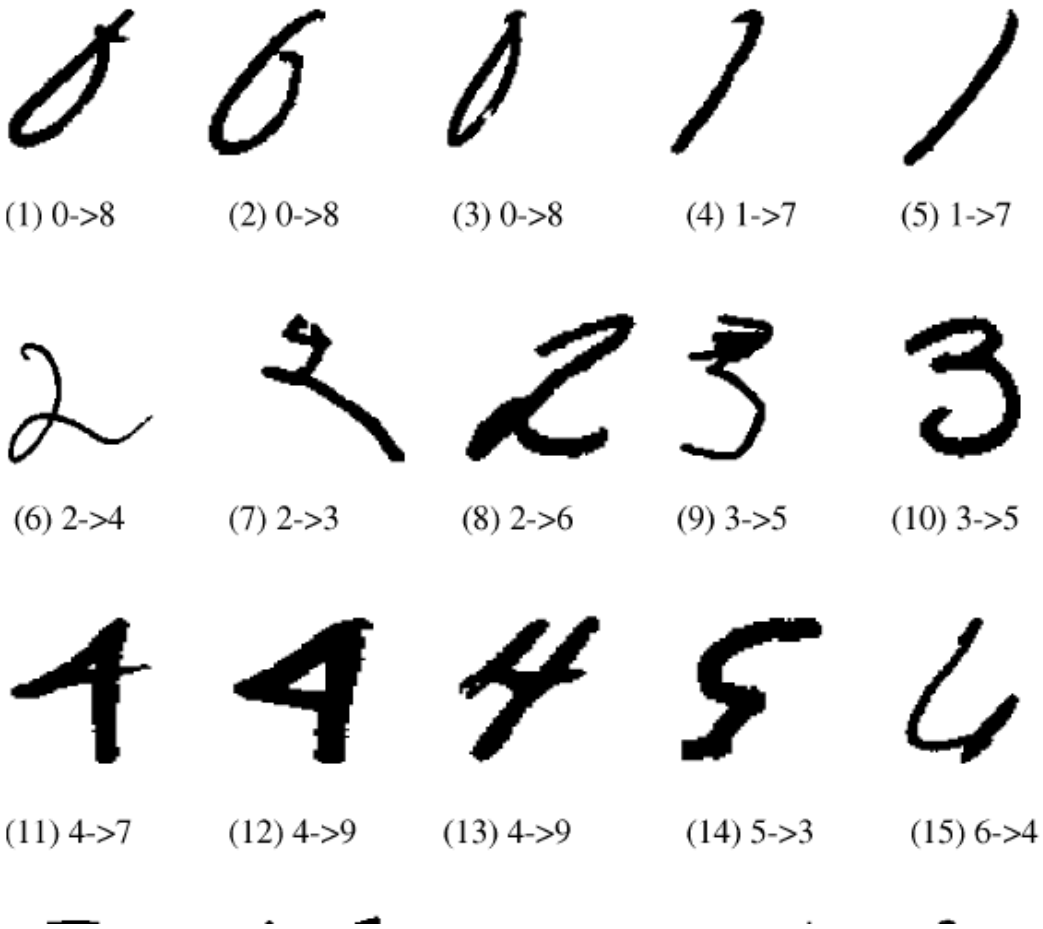
Handwritten digit recognition

TABLE 2
THE CLASSIFICATION RATE FOR EACH CLASSIFIER

Individual classifier	Classification rate %
Structural:	90.85
Gaussian:	93.93
Neural Net:	93.2
HMM:	94.77

TABLE 3
THE CLASSIFICATION RATE USING DIFFERENT COMBINING SCHEMES

Combining rule	Classification rate %
Majority Vote:	97.96
Sum rule:	98.05
Max rule:	93.93
Min rule:	86.00
Product rule:	84.69
Median rule:	98.19



Reprinted from J. Kittler et al., PAMI, 1998

Unsupervised Classification

Cluster analysis

Training set is not available, No. of classes may not be *a priori* known

What are clusters?

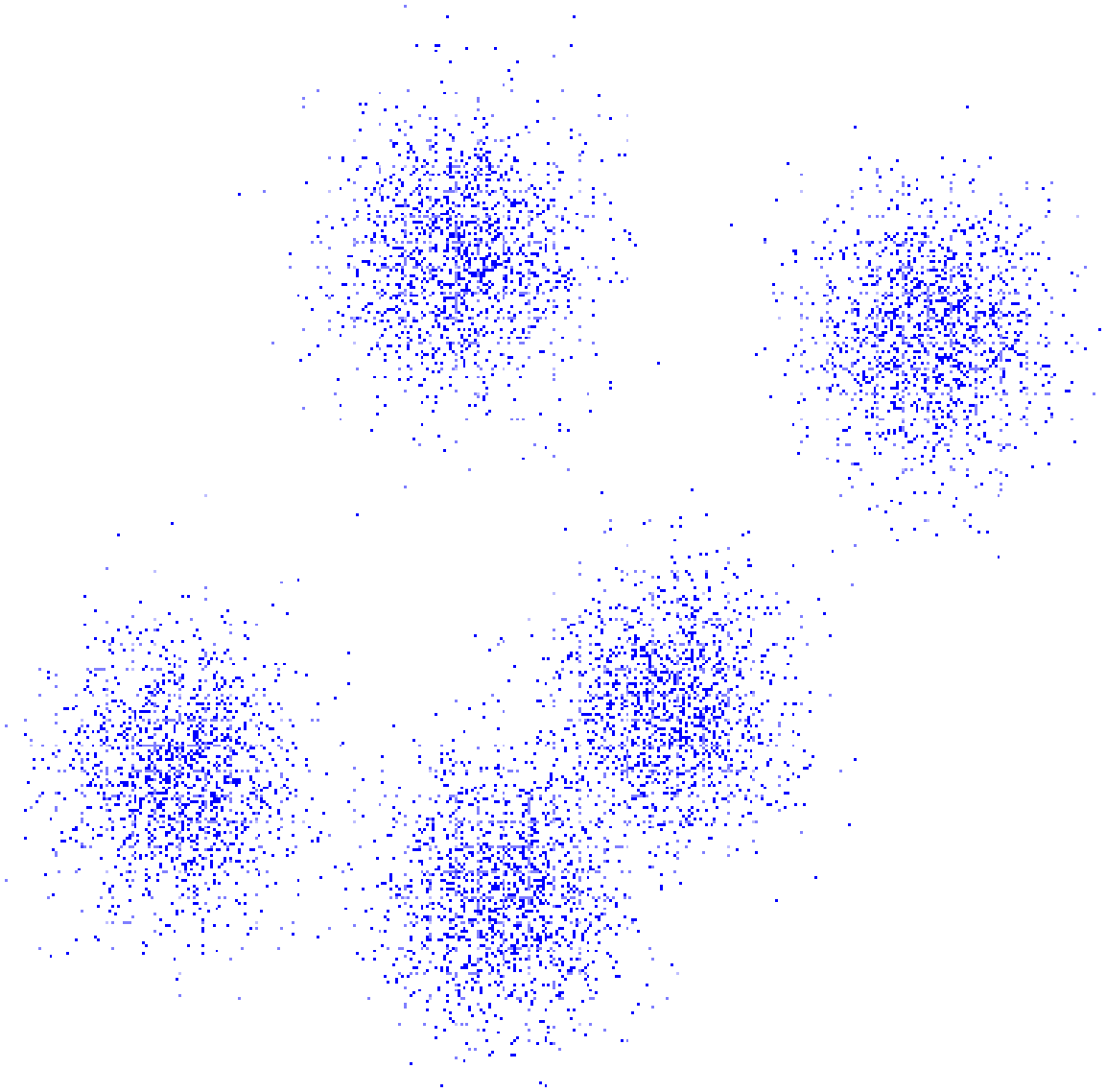
Intuitive meaning

- compact, well-separated subsets

Formal definition

- many attempts, mostly unsatisfactory
  (*t*-connectivity, diameter constraint, ...)
- any partition of the data into disjoint subsets

What are clusters?



How to compare different clusterings?

Ward criterion

Variance measure *J* should be minimized

$$J = \sum_{i=1}^{N} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{m}_i\|^2$$

Drawback – only clusterings with the same *N* can be compared.
Global minimum

J = 0 is reached in the degenerated case.

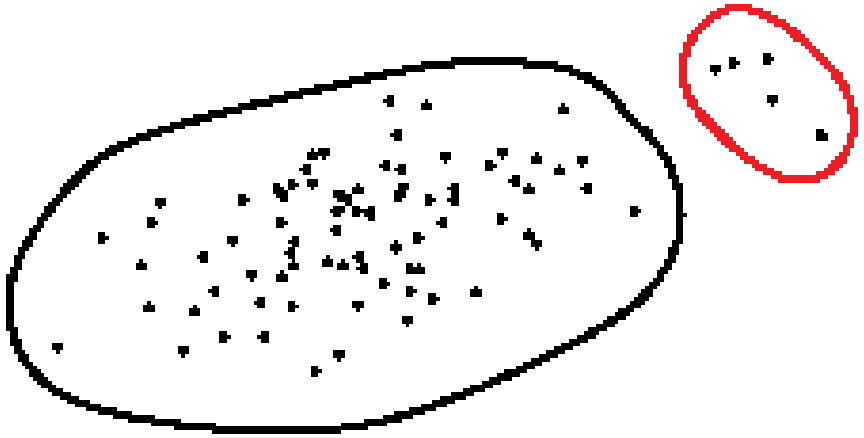
Minimization of *J*

Drawbacks

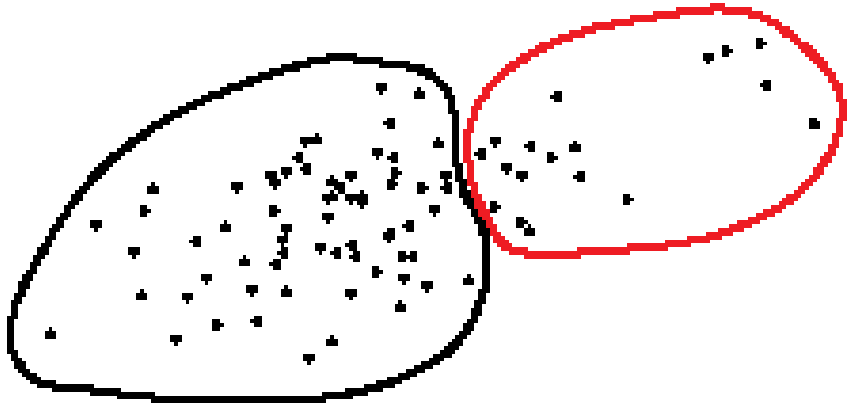
The results are sometimes “intuitively wrong”

because *J* prefers clusters with approx the same size

An example of a „wrong“ result

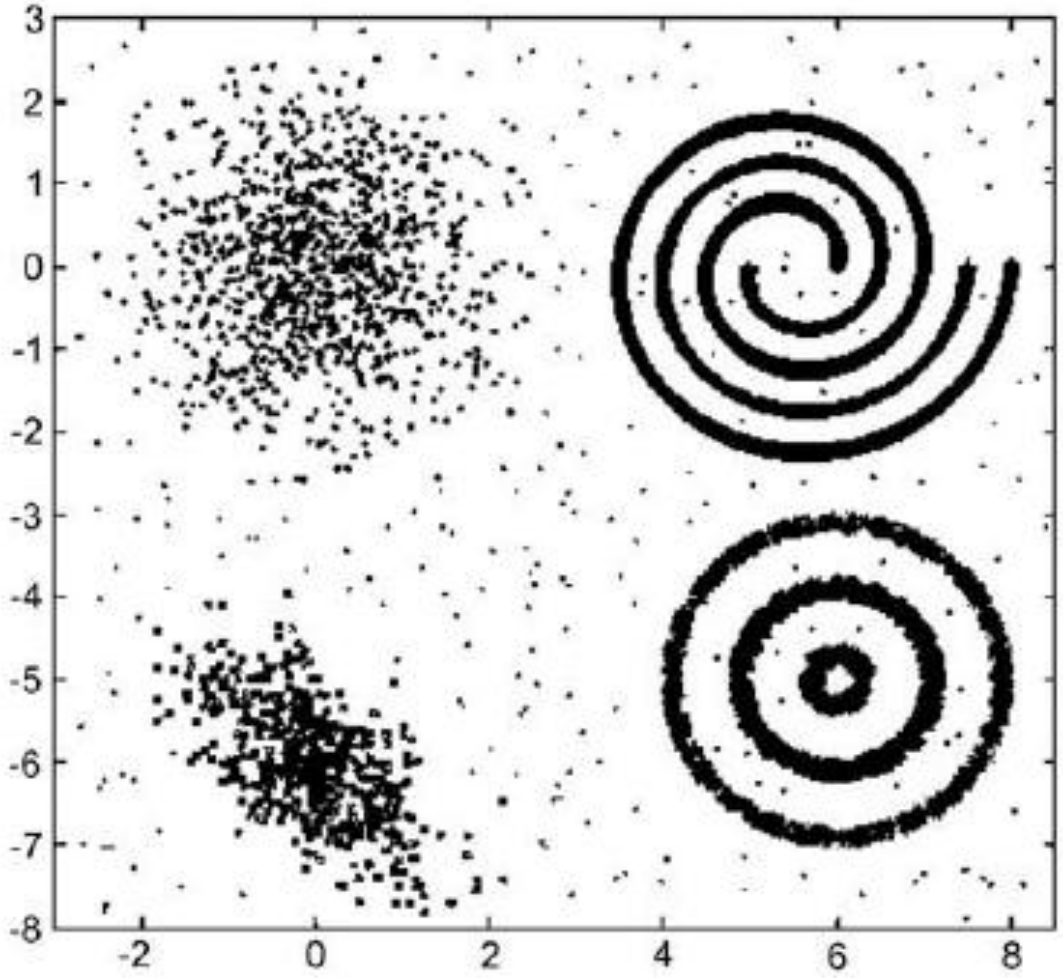


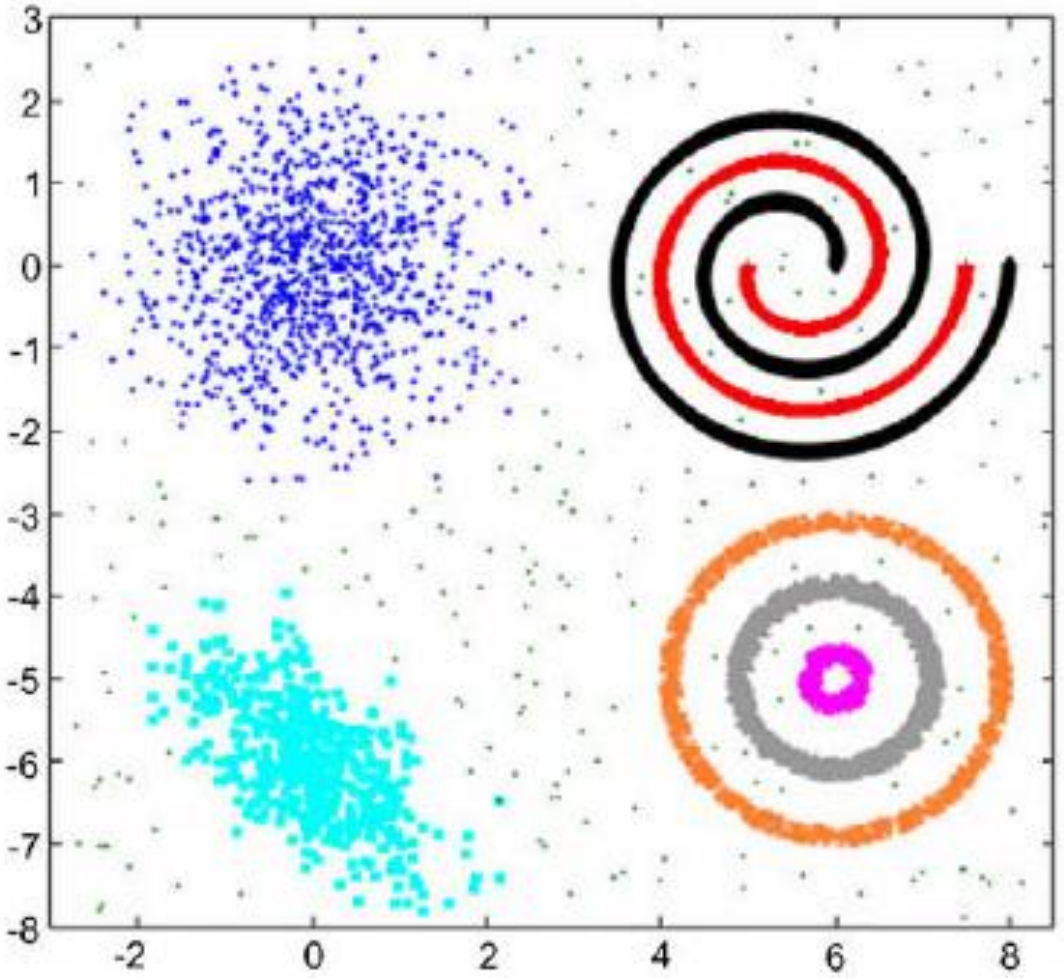
$J_e = large$



$J_e = small$

Drawback – assumes uncorrelated features and “convex” clusters





Clustering techniques

Iterative methods

- typically if *N* is given

Hierarchical methods

- typically if *N* is unknown

Other methods

- sequential, graph-based, branch & bound, fuzzy, genetic, model-based, etc.

Sequential clustering

- *N* may be unknown
- Very fast but not very good
- Each point is considered only once

Idea:

A new point is either added to an existing cluster or it forms a new cluster. The decision is based on the user-defined distance threshold.

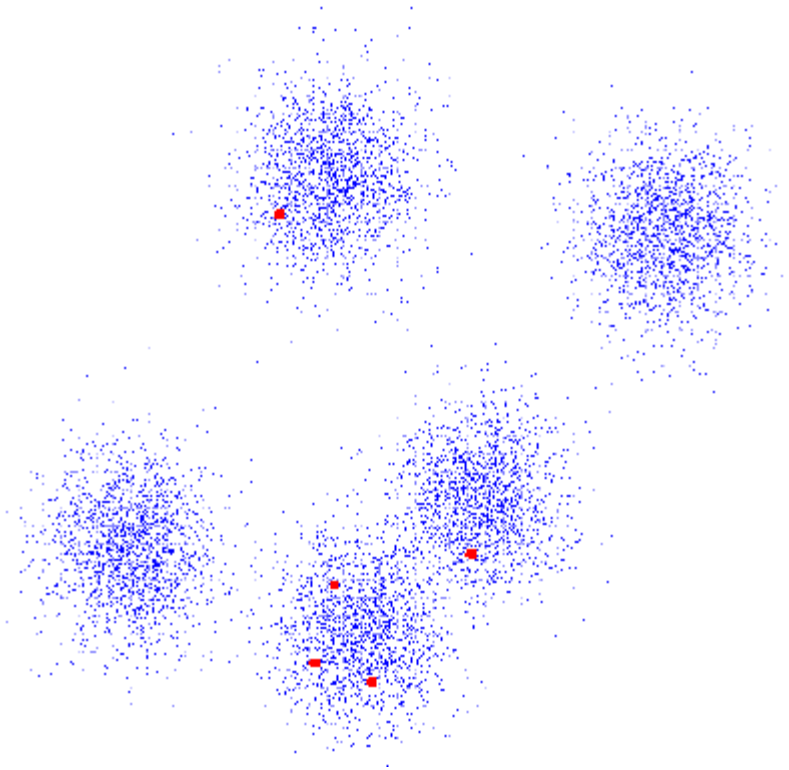
Sequential clustering

Drawbacks:

- Dependence on the distance threshold
- Dependence on the order of data points

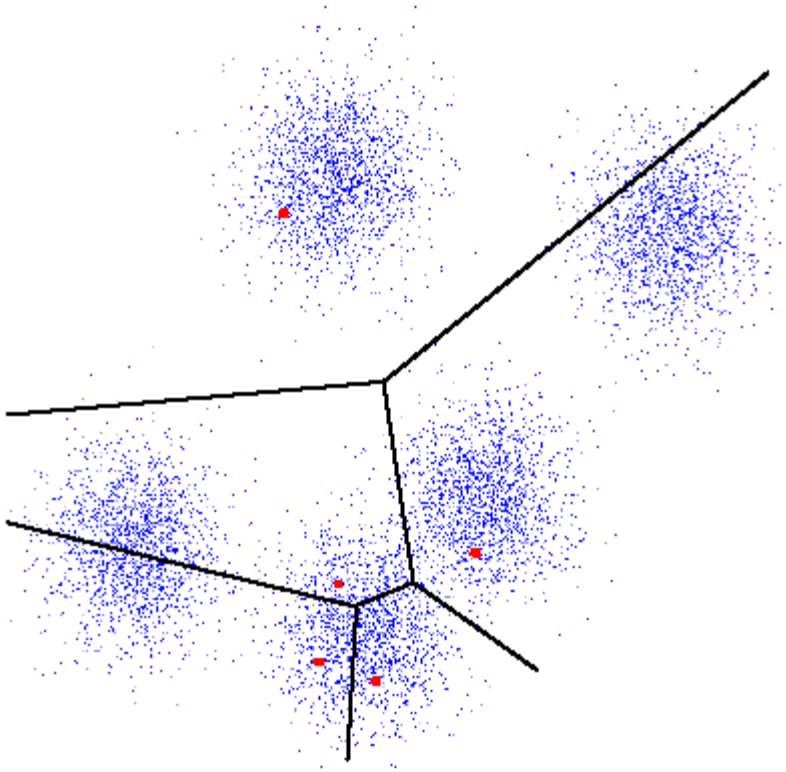
N-means clustering

1. Select *N* initial cluster centroids.



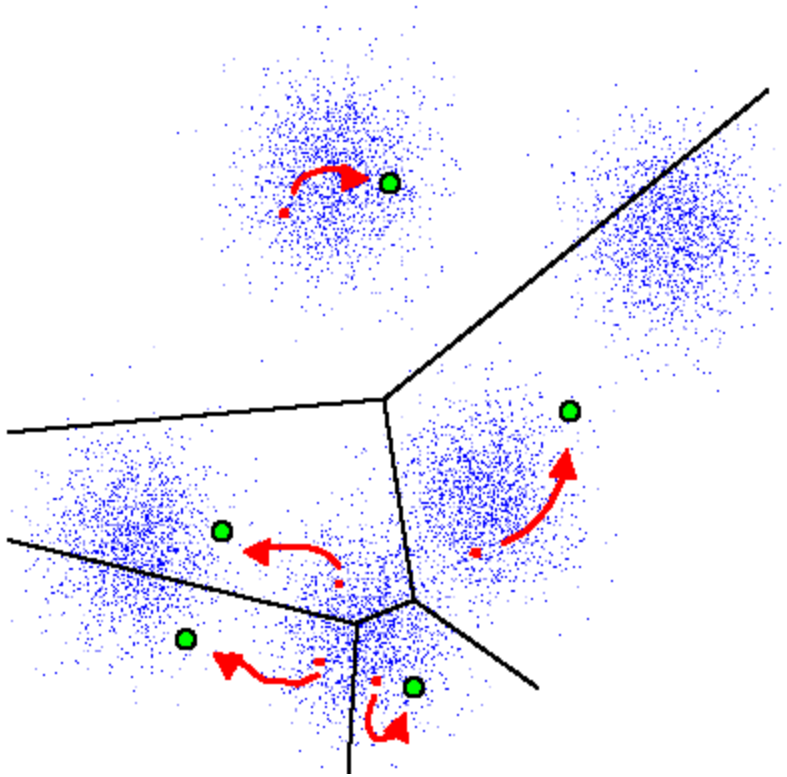
N-means clustering

2. Classify every point *x* according to minimum distance.



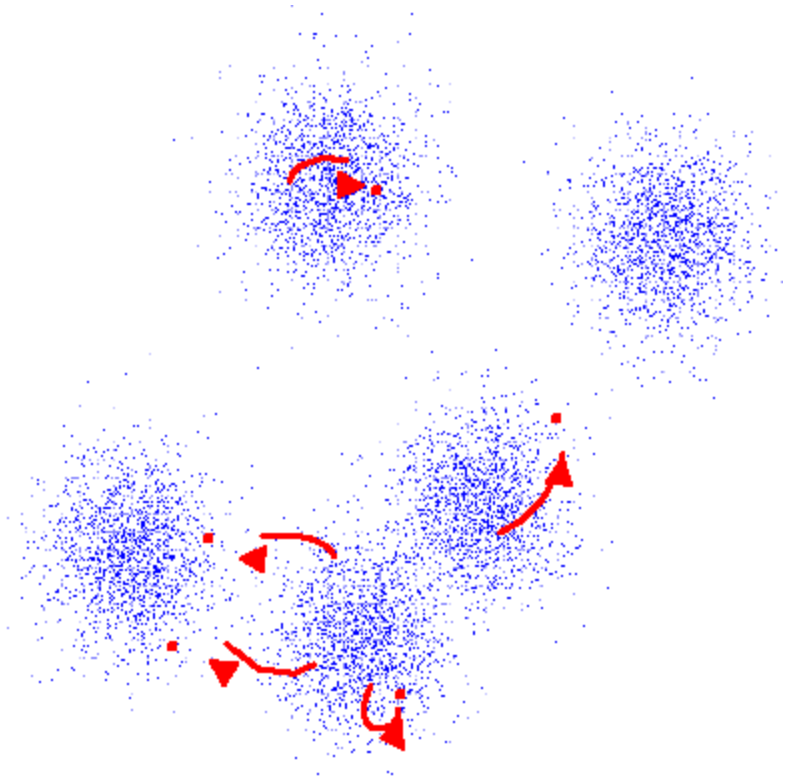
N-means clustering

3. Recalculate the cluster centroids.



N-means clustering

4. If the centroids did not change then STOP else GOTO 2.



N-means clustering

Drawbacks

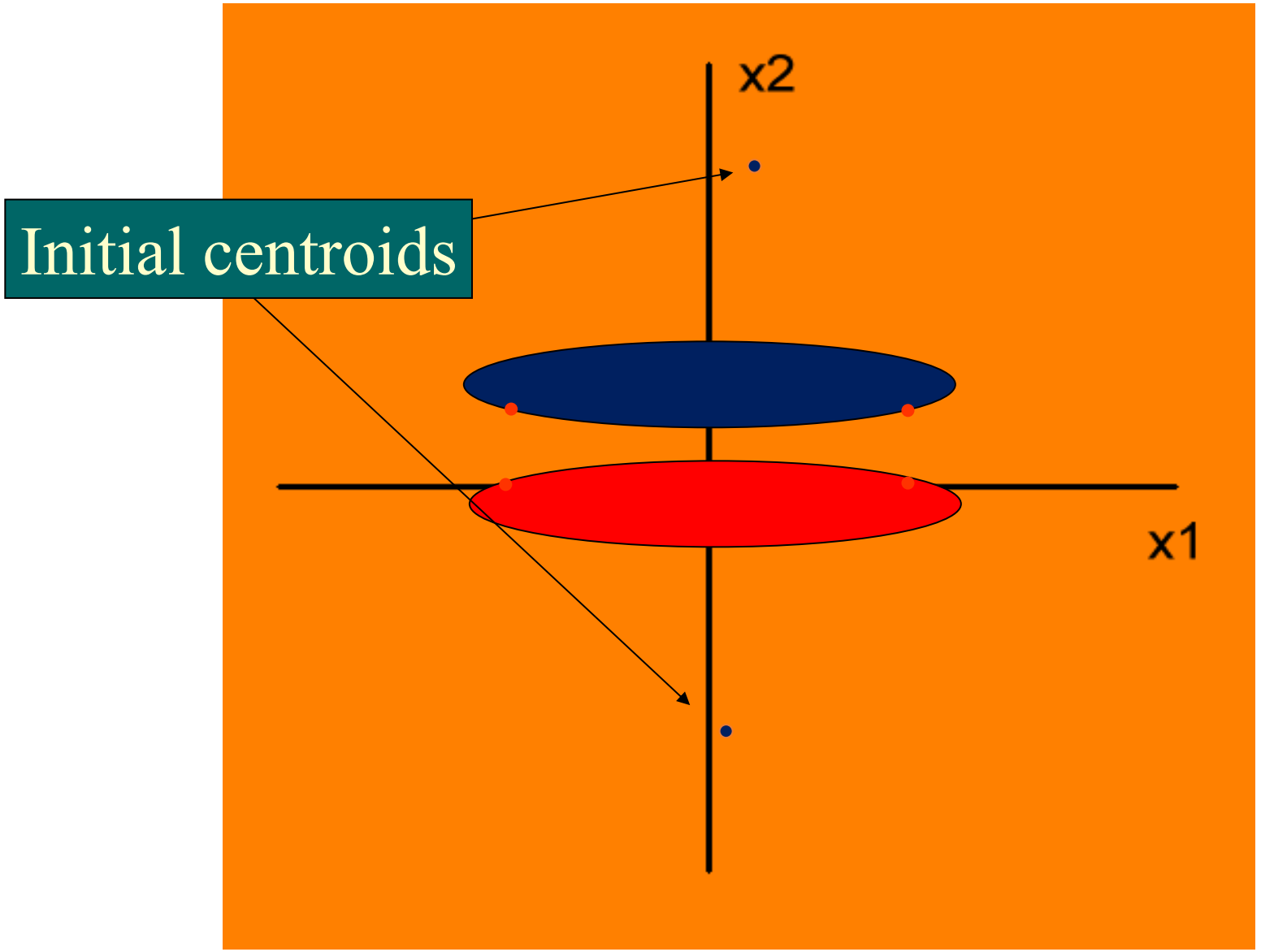
- The result depends on the initialization
- *J* is not minimized
- The results are sometimes “intuitively wrong”

N-means clustering – an example

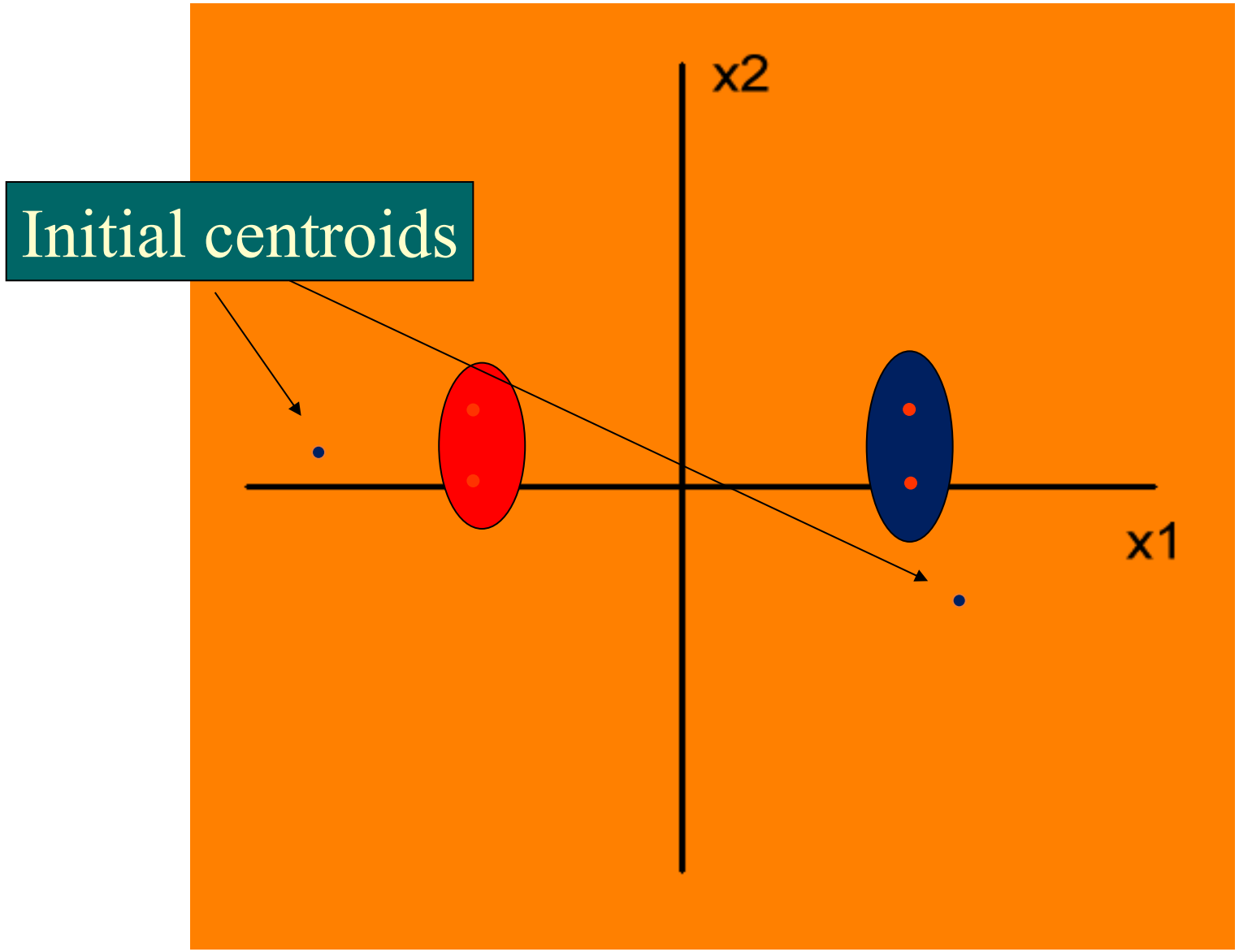
Two features, four points, two clusters ($N = 2$)

Different initializations → different clusterings

N-means clustering – an example



N-means clustering – an example



Iterative minimization of *J*

1. Let's have an initial clustering (by *N*-means)
2. For every point *x* do the following:

   Move *x* from its current cluster to another cluster, such that the decrease of *J* is maximized.
3. If all data points do not move, then STOP

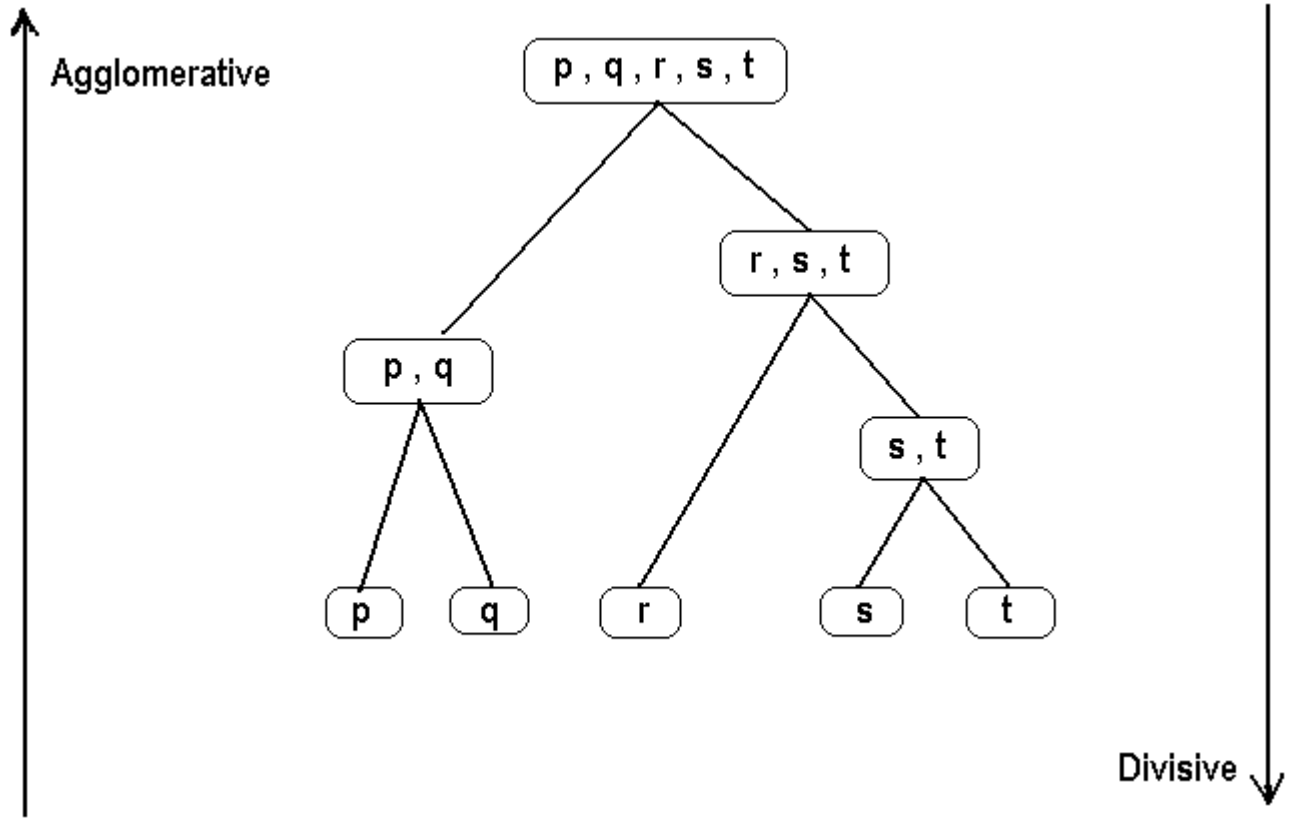
Iterative minimization of J

Drawbacks

The algorithm is optimal in each step but
in general global minimum of J is not reached.

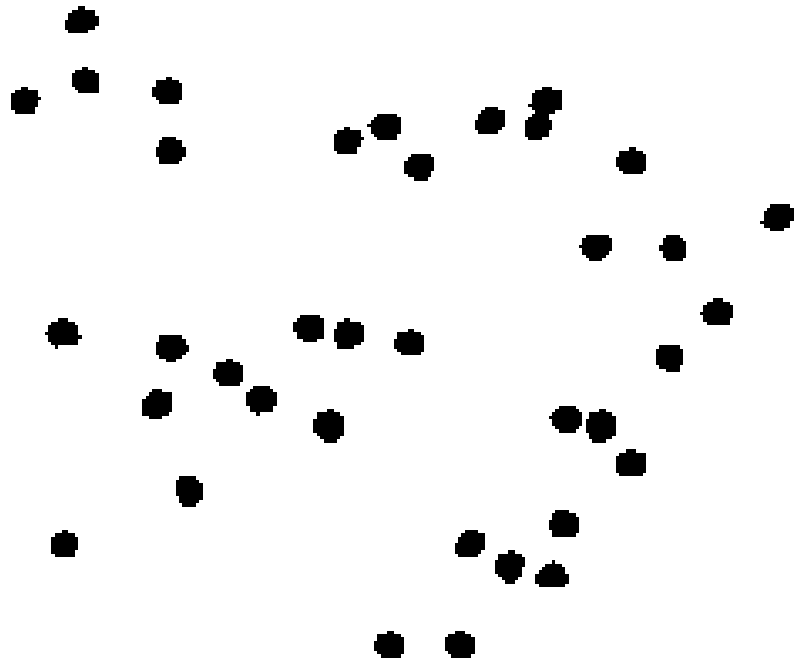
Hierarchical clustering

- Agglomerative clustering
- Divisive clustering



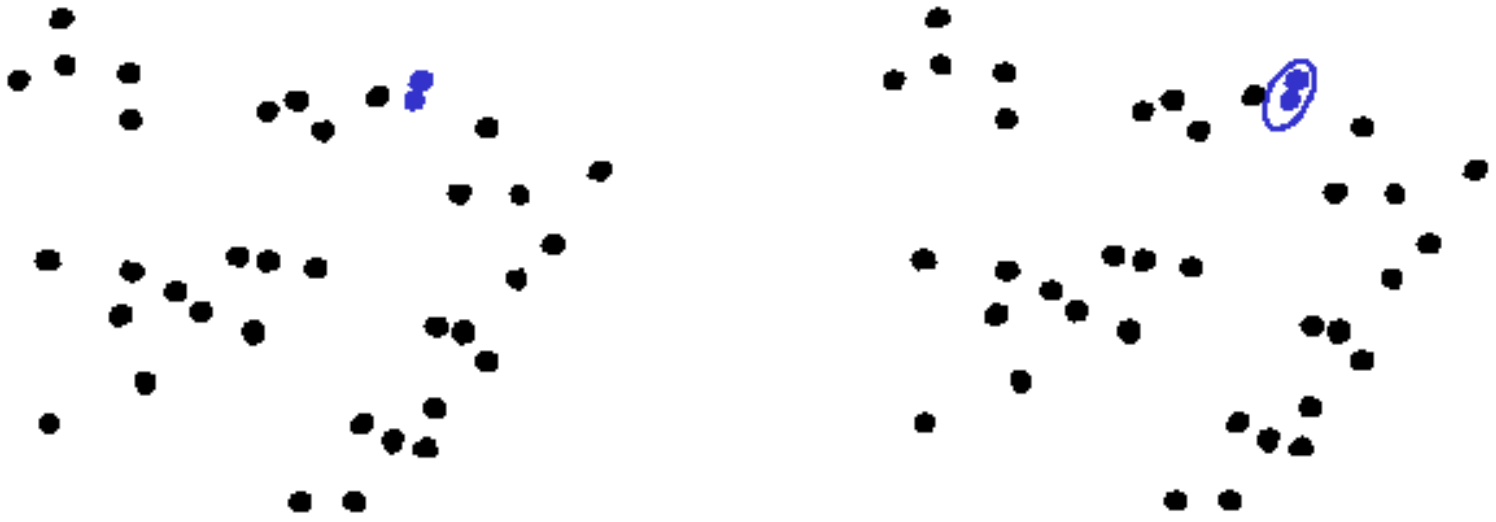
Basic agglomerative clustering

1. Each point = one cluster



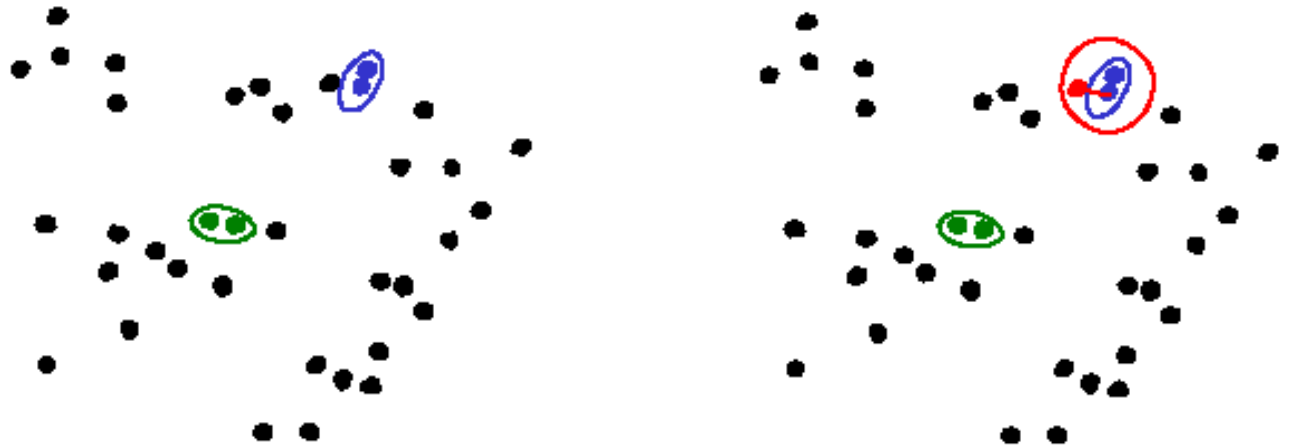
Basic agglomerative clustering

1. Each point = one cluster
2. Find two “nearest” or “most similar” clusters and merge them together



Basic agglomerative clustering

1. Each point = one cluster
2. Find two “nearest” or “most similar” clusters and merge them together
3. Repeat 2 until the stop constraint is reached



Basic agglomerative clustering

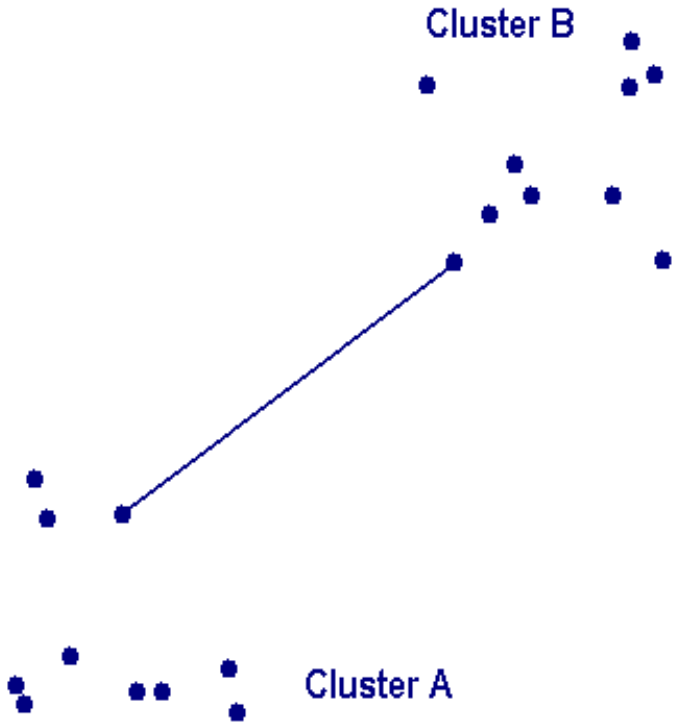
Particular implementations of this method differ from each other by:

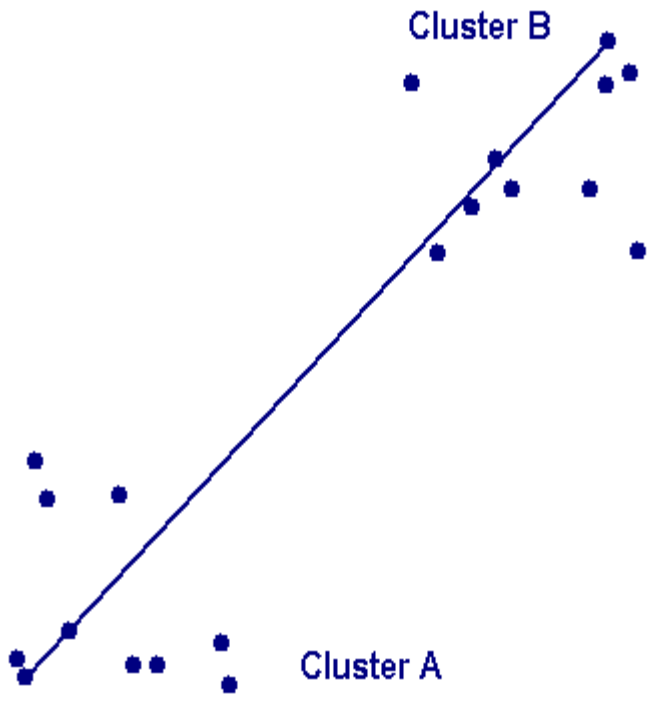
- The STOP constraints
- The distance/similarity measures used

Simple between-cluster distance measures

$$d(A,B) = d(m_1,m_2)$$

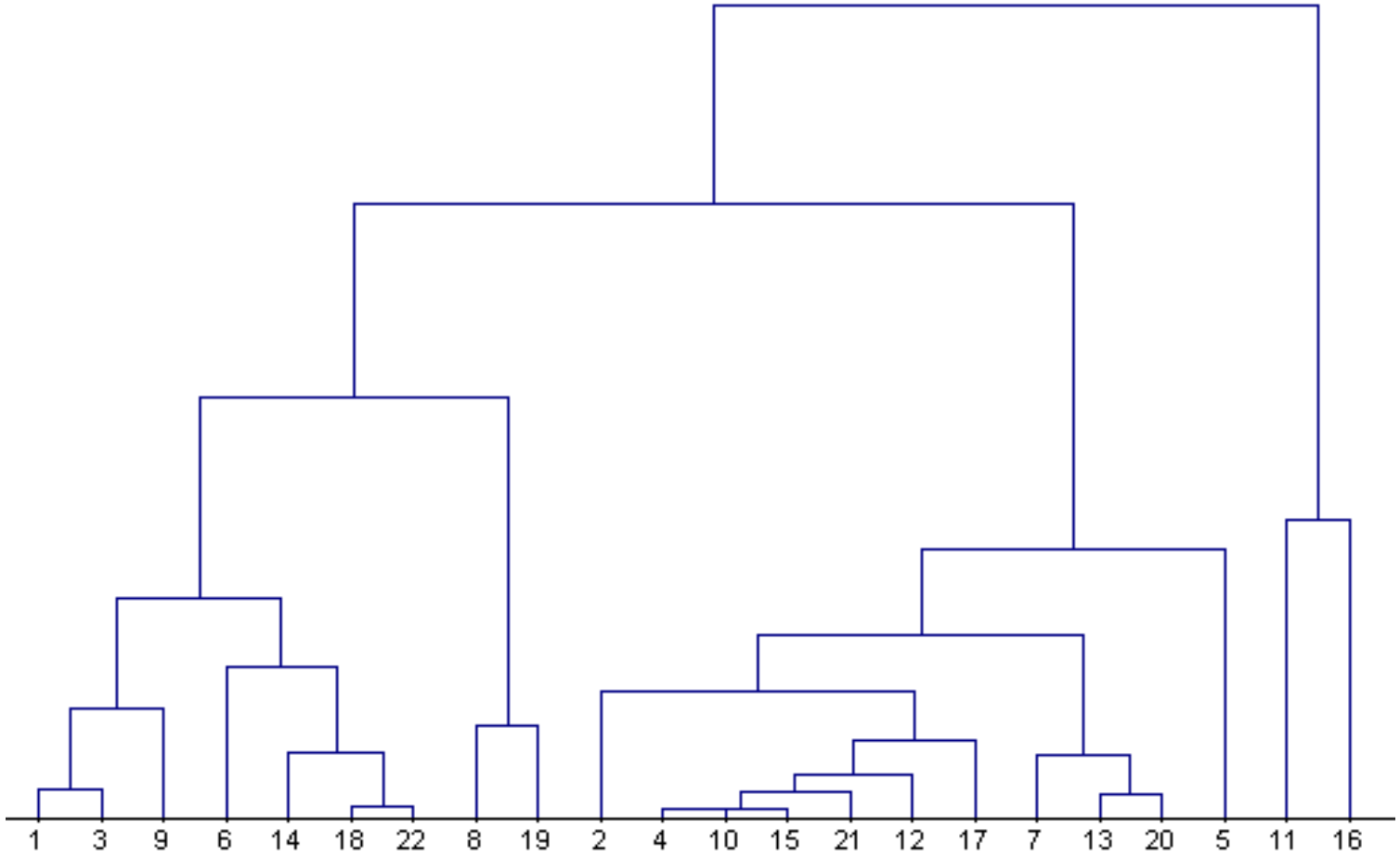
$d(A,B) = \min d(a,b)$ $\quad$ $d(A,B) = \max d(a,b)$





Agglomerative clustering

Representation by a clustering tree (dendrogram)



Definite agglomerative clustering

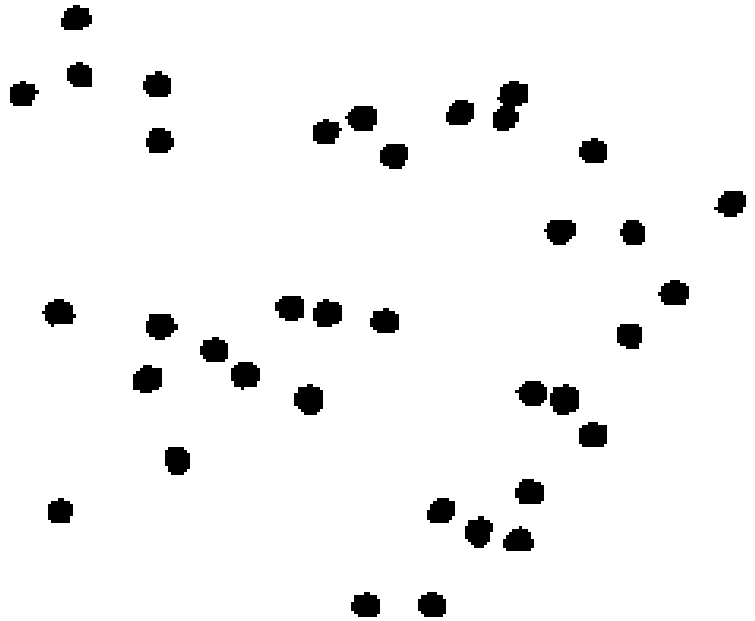
Basic algorithm – at a certain level, there may be multiple candidates of merging.

Random selection leads to ambiguities.

Definite algorithm – **all** such candidates are merged at that level → the number of new clusters emerging at one level may be greater than 1.

Basic divisive clustering

1. All points = one cluster



Basic divisive clustering

1. All points = one cluster
2. Divide the cluster into two parts A,B such that *d(A,B)* is maximized
3. Select a new cluster to split
4. Apply 2 to the selected cluster
5. Repeat 3-4 until the stop constraint is reached

Full search in STEP 2 is very expensive – O(2^n)

Suboptimal STEP 2 of divisive clustering

1. Find point *p* such that the mean of *d(p,x)* is maximized
2. Divide C into A U B, where B={*p*} (*p* is a seed point of a new cluster B)
3. For *x* from A calculate the mean dist *d(x,A)* and *d(x,B).* If *d(x,A)* > *d(x,B)* move *x* into B.
4. Repeat 3 for each *x* from A.

Suboptimal STEP 2 of divisive clustering

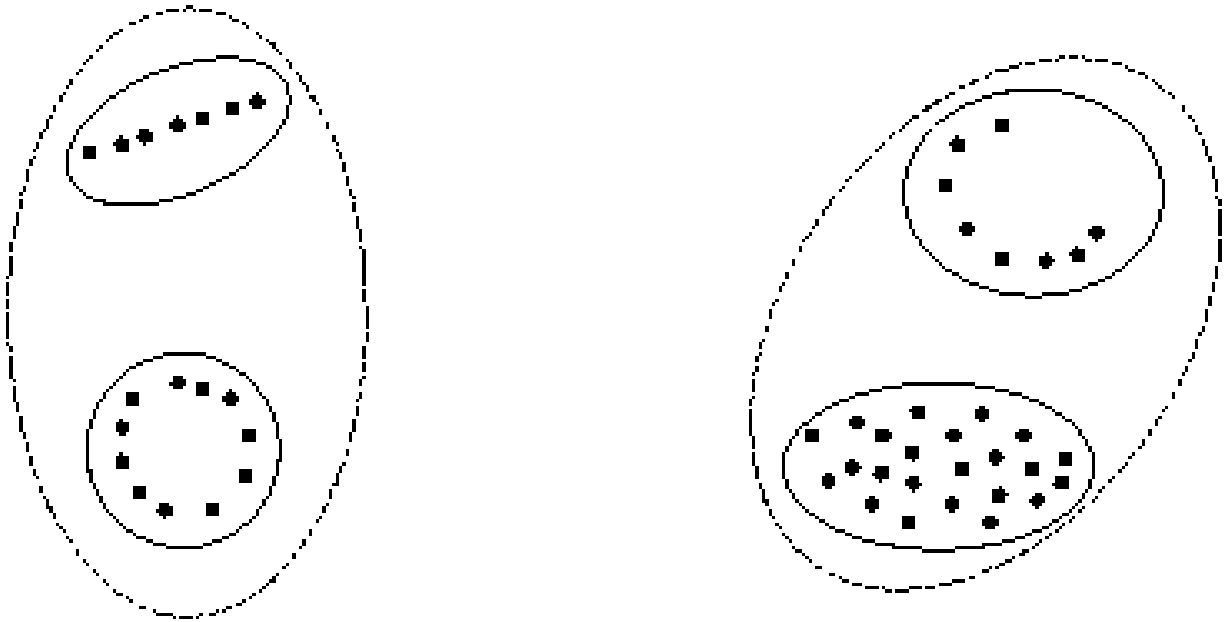
Alternatively, any iterative algorithm for N=2 can be used (N-means, J - minimization, ...)

STEP 3 of divisive clustering

Selecting the next cluster to split

- randomly (when performing complete decomposition)
- by maximum diameter
- by maximum variance
- by maximum *J*

How many clusters are there?



2 or 4?

Clustering is a very subjective task

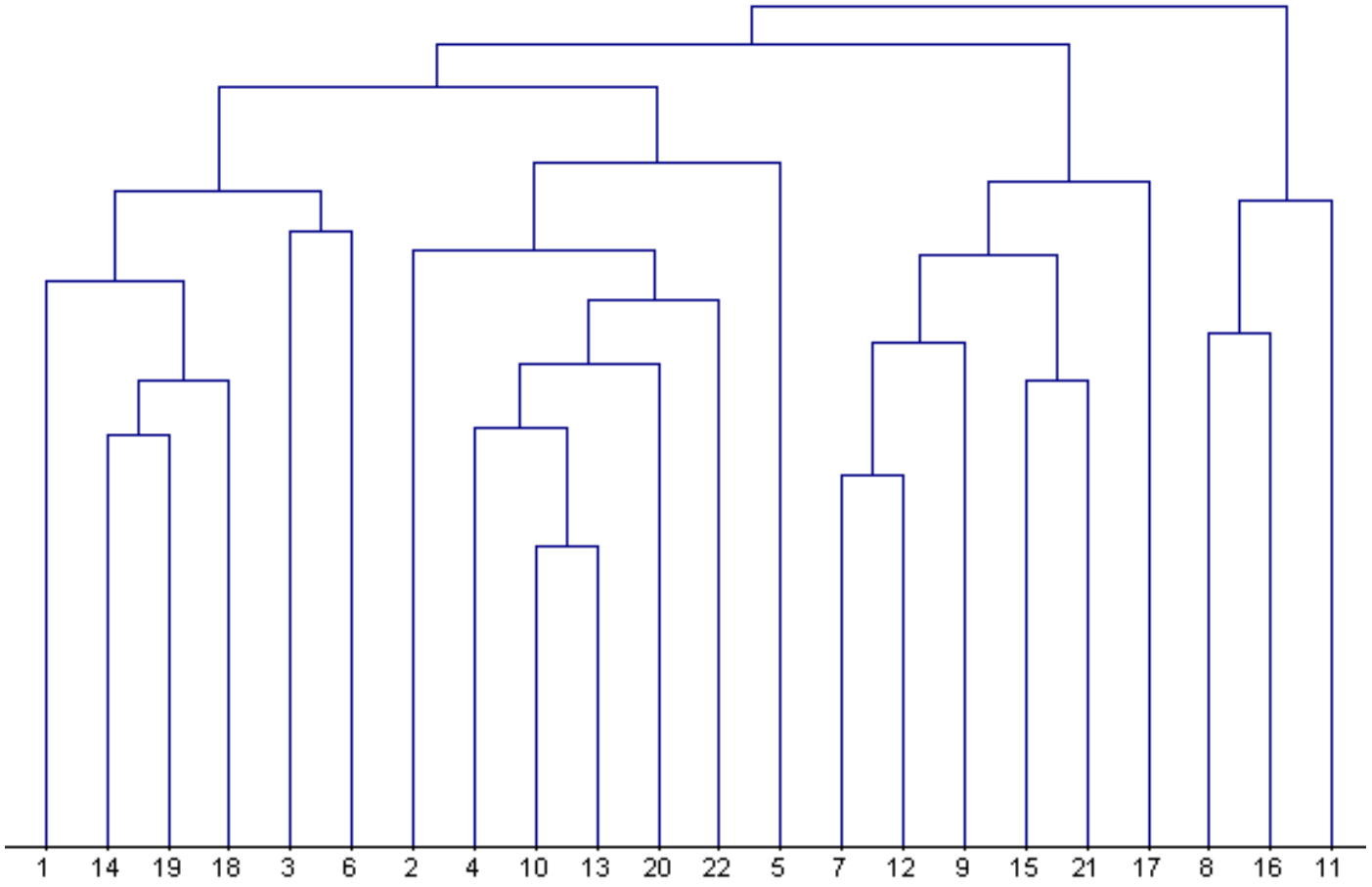
How many clusters are there?

- Difficult to answer even for humans
- “Clustering tendency”, “cluster validity”
- Hierarchical methods:

  N can be estimated from the complete dendrogram
- The methods minimizing a cost function

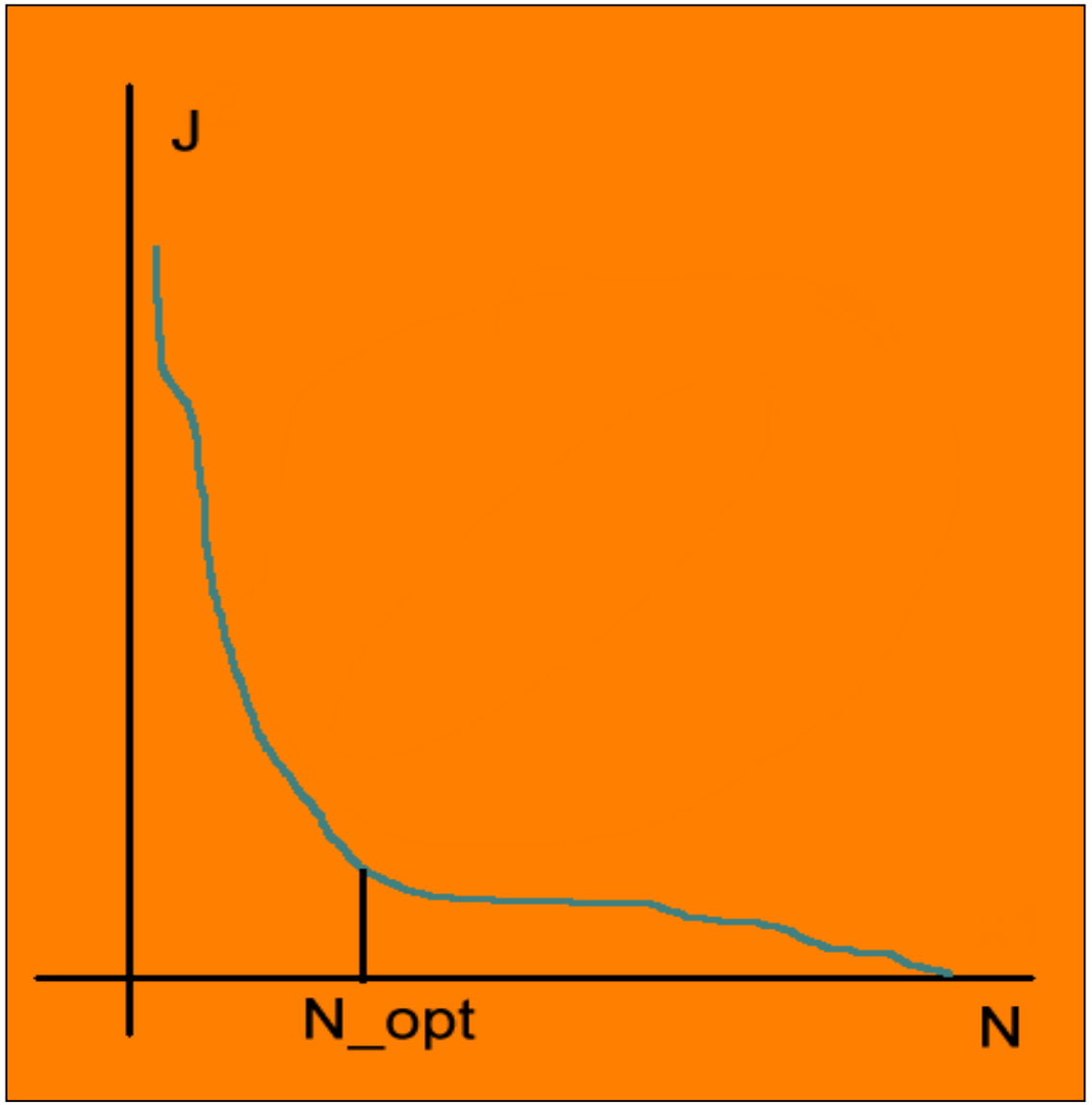
  N can be estimated from the “knees” in *J*-*N* graph

Life time of the clusters



Optimal number of clusters = 4

Optimal number of clusters



Other clustering criteria

Scatter matrices

- between cluster matrix

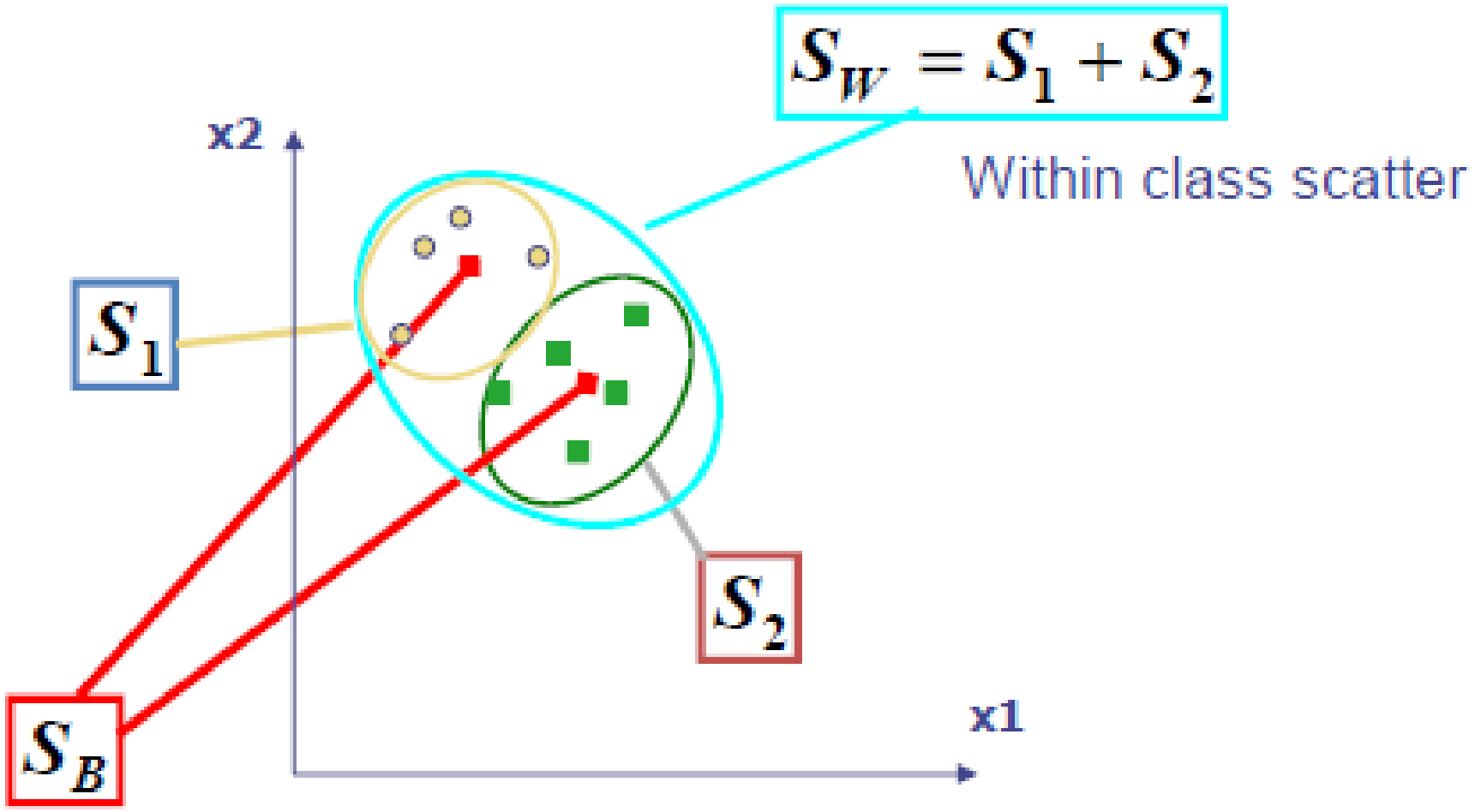
$$B = \sum_{i=1}^{N} n_i(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t$$

- within cluster matrix

$$W = \sum_{i=1}^{N} W_i \qquad W_i = \sum_{\mathbf{x} \in C_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t$$

- total scatter matrix

$$T = \sum_{\mathbf{x}} (\mathbf{x} - \mathbf{m})(\mathbf{x} - \mathbf{m})^t$$


$S_W = S_1 + S_2$
Within class scatter
x2
S_1
S_2
S_B
x1
Between class scatter

Other clustering criteria

min $\operatorname{tr}(W) = \sum_{i=1}^{N} \operatorname{tr}(W_i) = \sum_{i=1}^{N} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{m}_i\|^2 = J$

min $\det(W)$

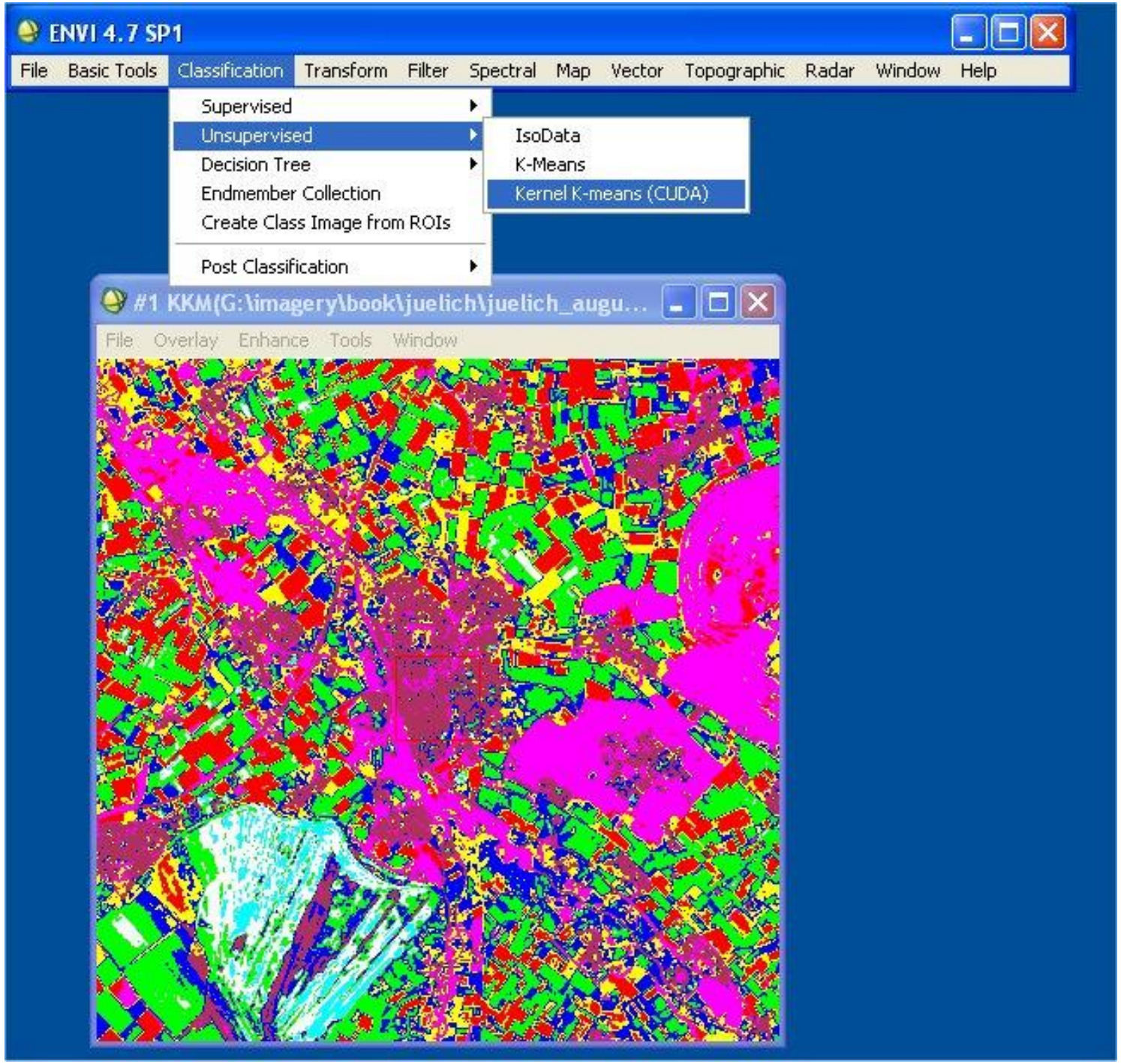
$T = W + B$

max $\operatorname{tr}(W^{-1}B)$

Applications of clustering in image proc.

- **Segmentation – clustering in color space**
- **Preliminary classification of multispectral images**
- **Clustering in parametric space – RANSAC, image registration and matching**

Numerous applications are outside image processing area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Basic Tools
Classification
Transform
Filter
Spectral
Map
Vector
Topographic
Radar
Window
Help
Supervised
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Endmember Collection
Create Class Image from ROIs
Post Classification
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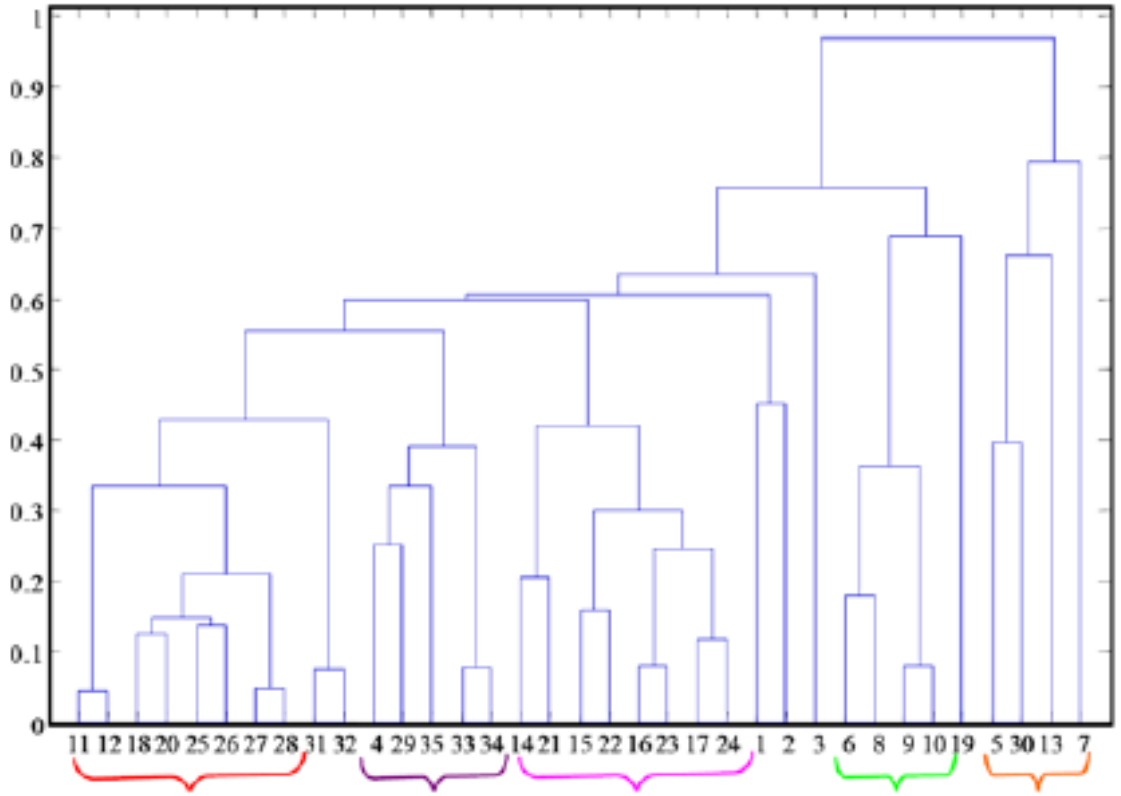
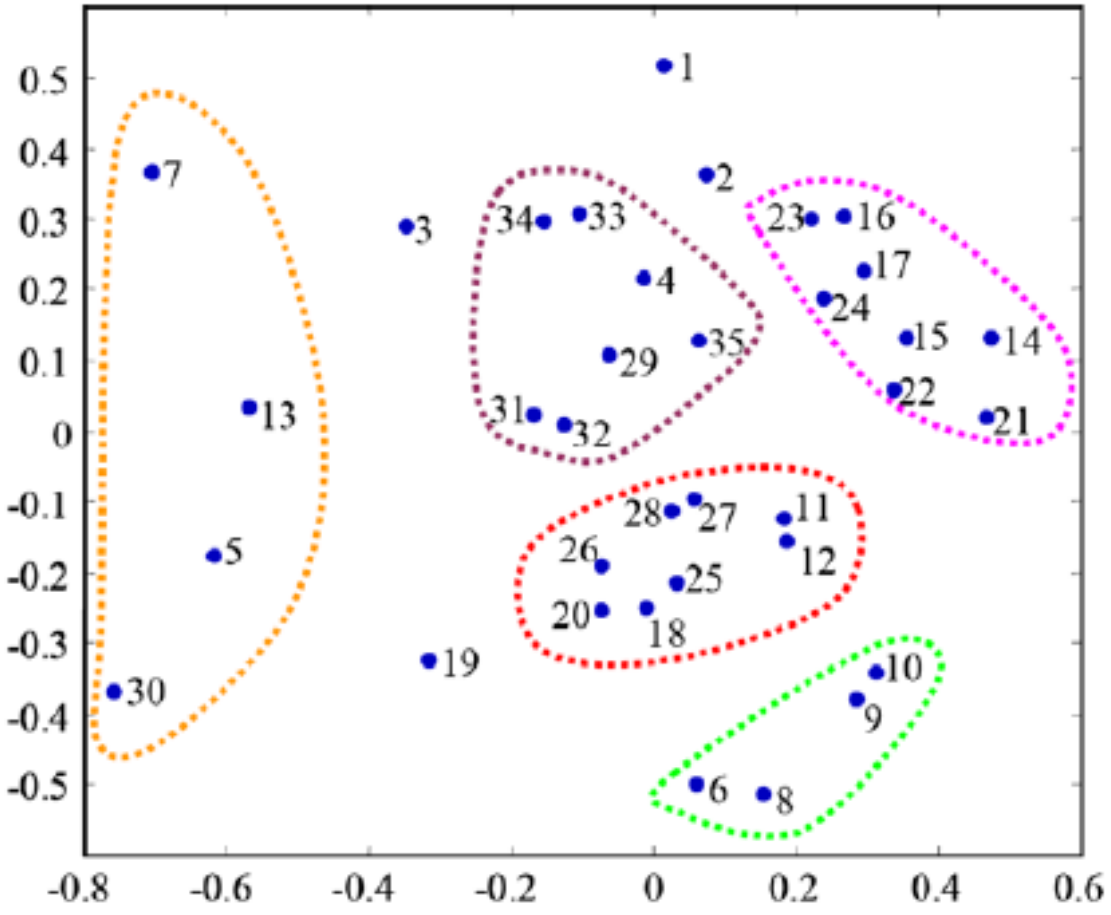
Clustering of clustering methods





Reduction of the Feature Space Dimensionality

Problem formulation

Having *D* features, we want to reduce their number to *n*, where $n \ll D$

$$(x_1, x_2, \cdots, x_D) \longrightarrow (y_1, y_2, \cdots, y_n)$$

Why to reduce the number of the features

- **Pros:** Lower computing complexity
  Improvement of the classification performance
- **Cons:** Possible loss of information

Basic approaches to DR

- **Feature extraction**

  Transform $T: \quad R^D \rightarrow R^n$

  Creation of a new feature space. The features lose their original meaning.

Example: $n = 1$

$$y_1 = \sum_{i=1}^{D} x_i$$

Basic approaches to DR

- **Feature extraction**

  Transform $T: \quad R^D \rightarrow R^n$

  Creation of a new feature space. The features lose their original meaning.

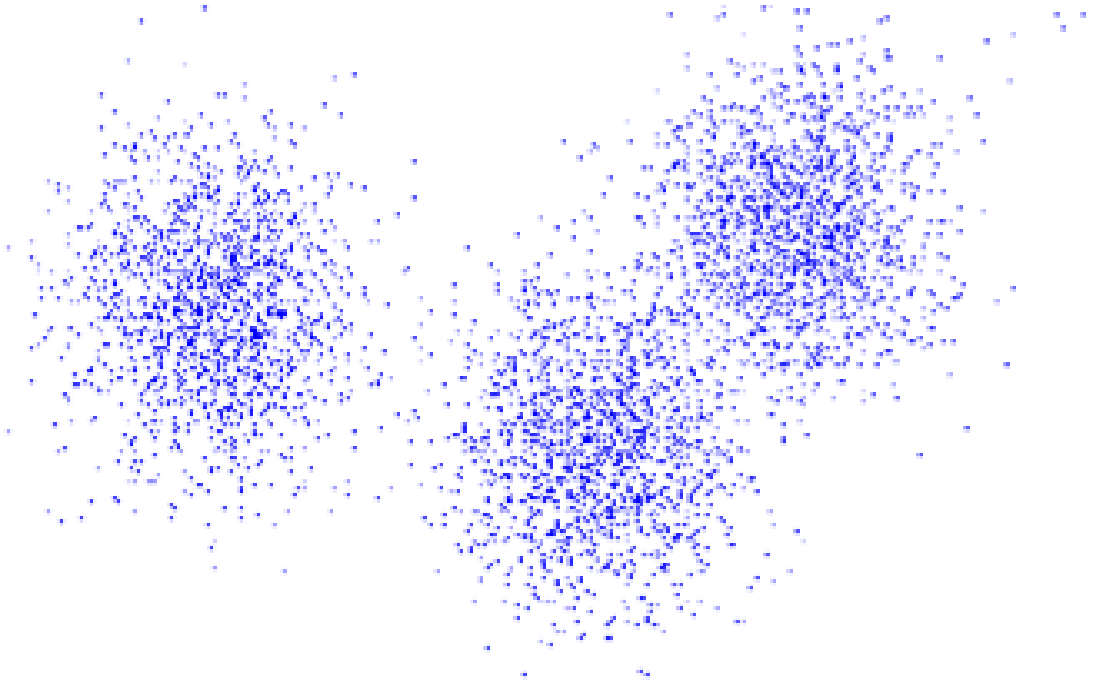
- **Feature selection**

  Selection of a subset of the original features.

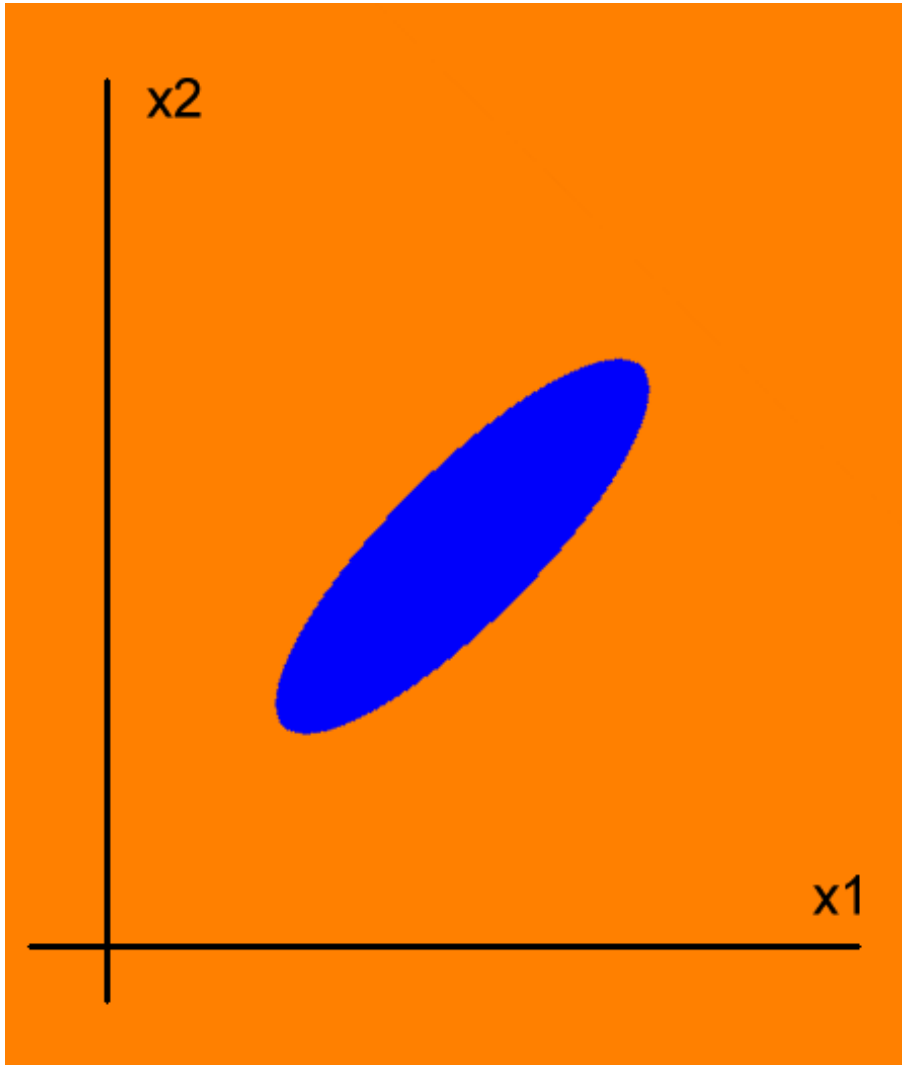
Principal Component Transform

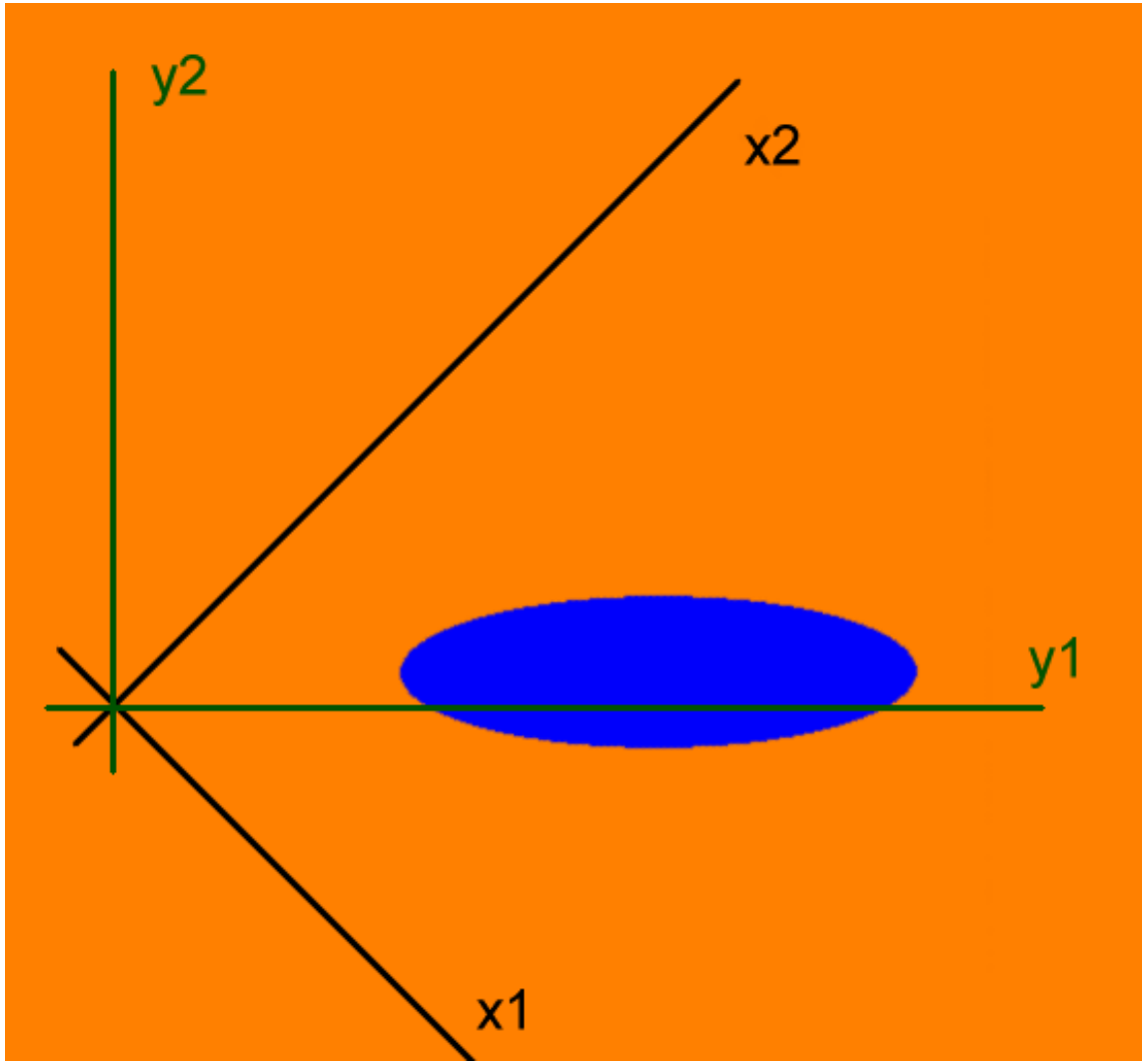
Karhunen-Loeve Transform

PCT is a method for “one-class” problem, i.e. for non-structured data (no class representatives, no training sets, just a cloud of data points in the feature space)



Principal Component Transform





Principal Component Transform

- PCT is a rotation of the feature space

$$y = T'x,$$

  such that the new features y are **uncorrelated**, i.e. covariance matrix C_y is diagonal.

- This is always possible since the original covariance matrix C_x is symmetric and can be diagonalized in the orthonormal basis of its eigenvectors

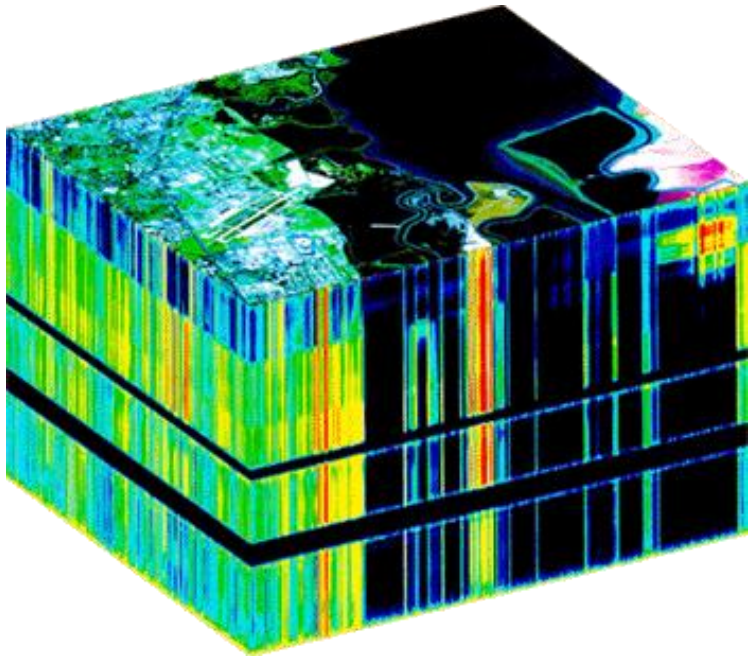
$$C_y = T'C_x T$$

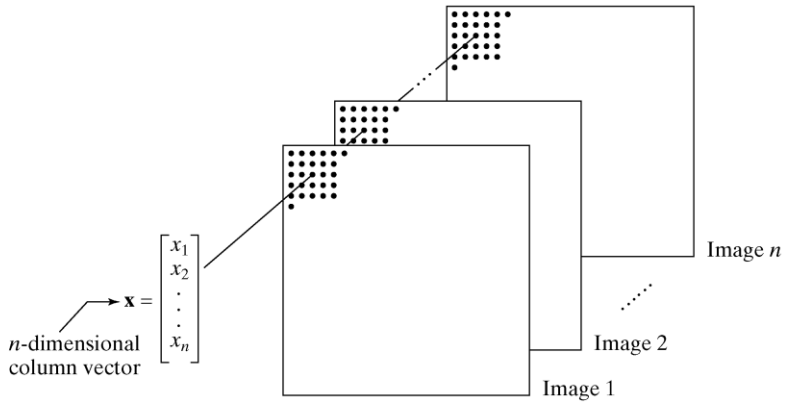
- Features with the highest variances are called **principal components**. First n PC's are kept.

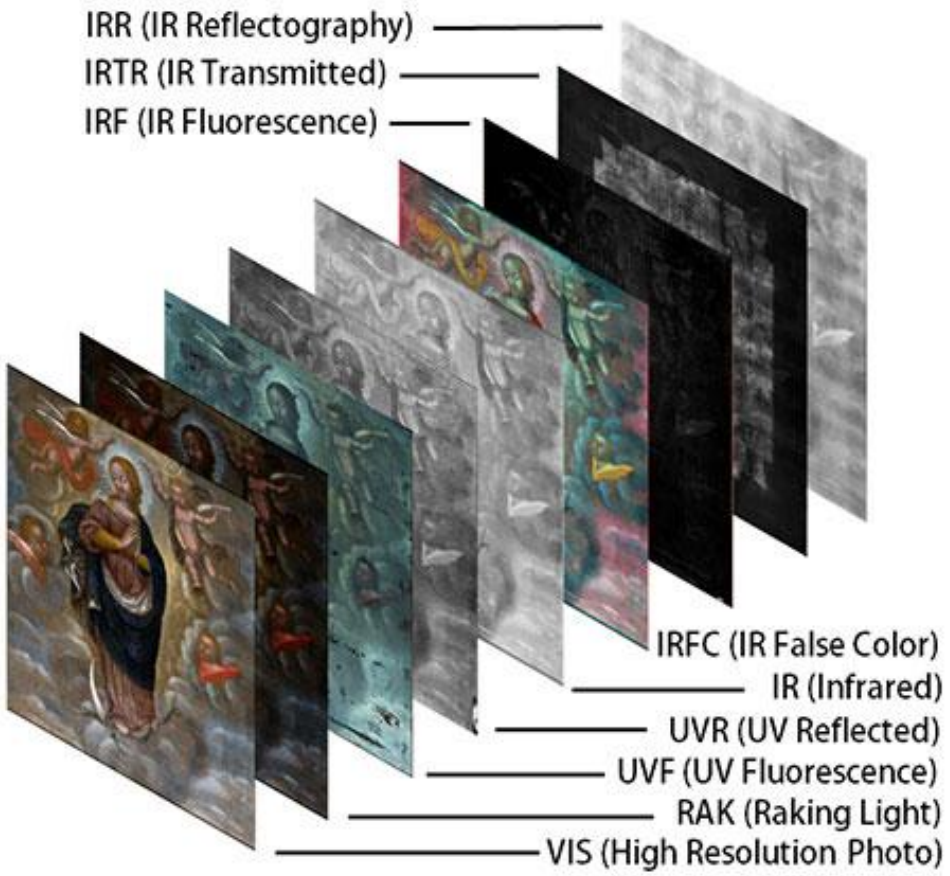
Applications of the PCT

- “Optimal” data representation
- Visualization and compression of multimodal images

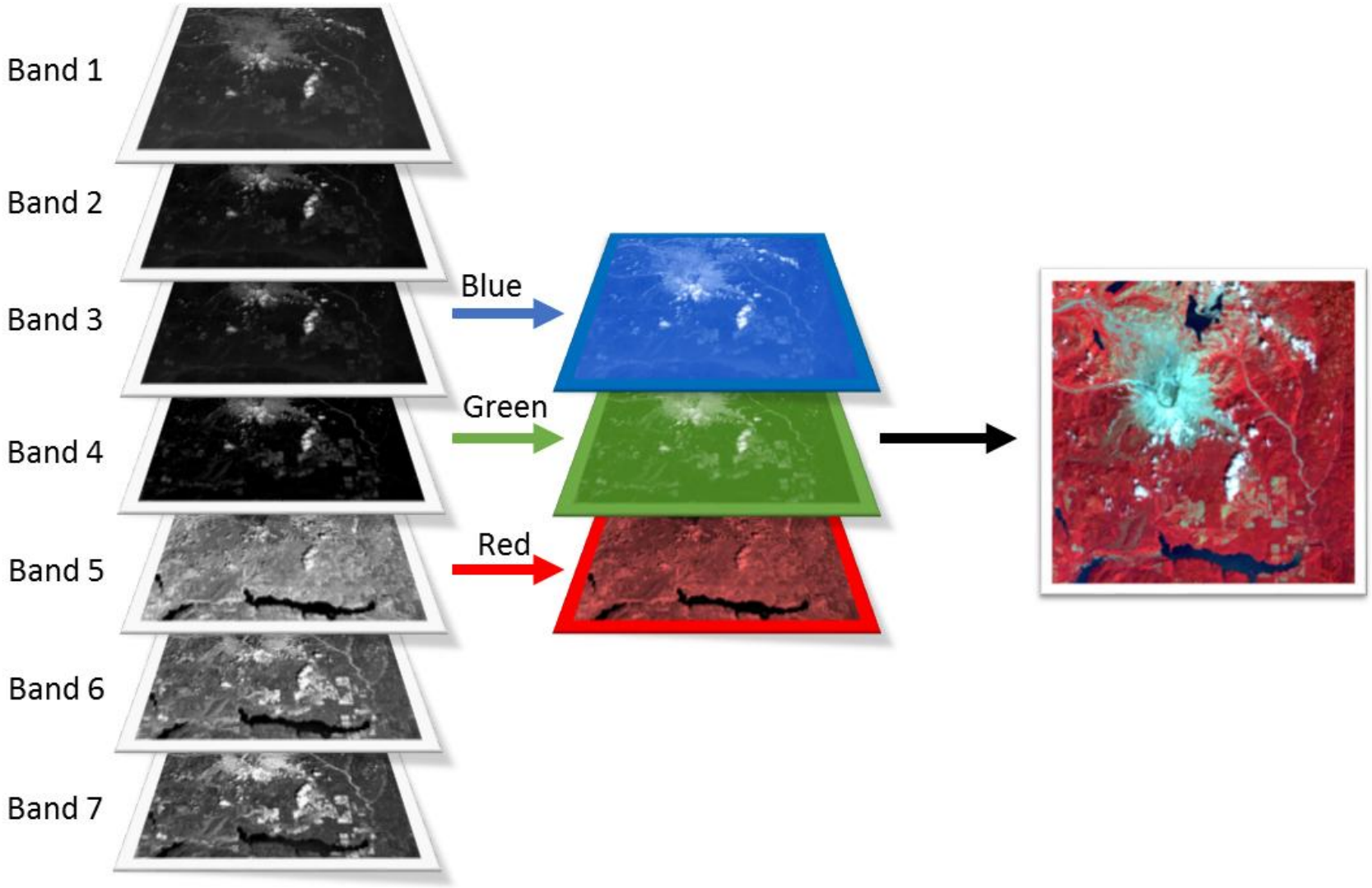
PCT of multispectral images



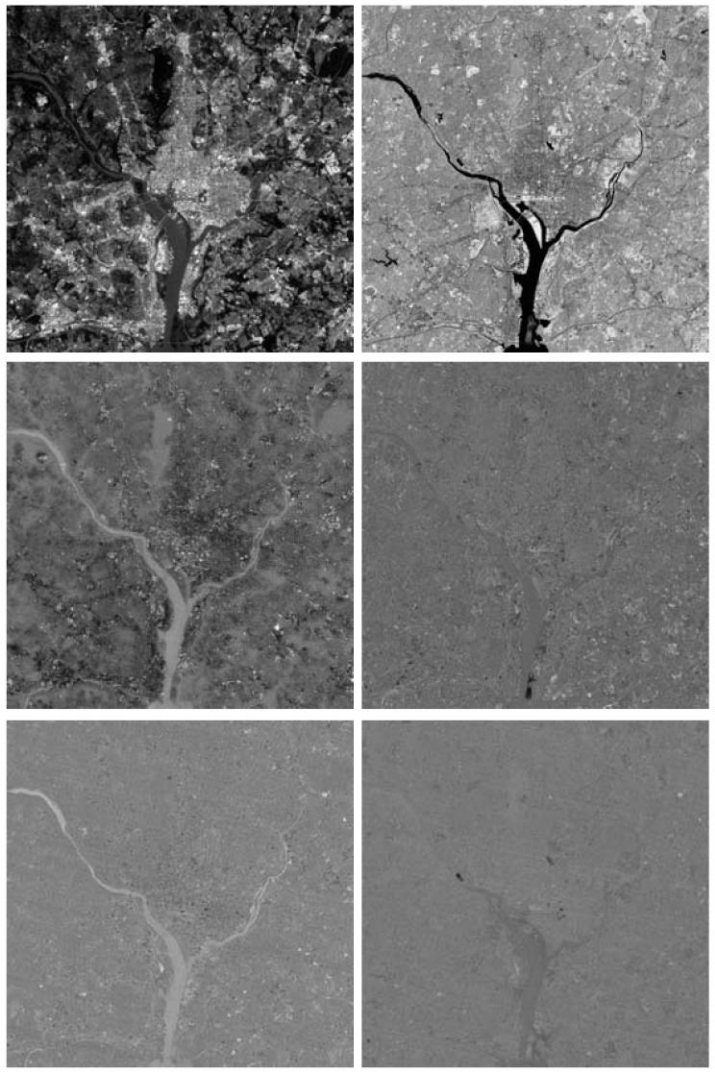




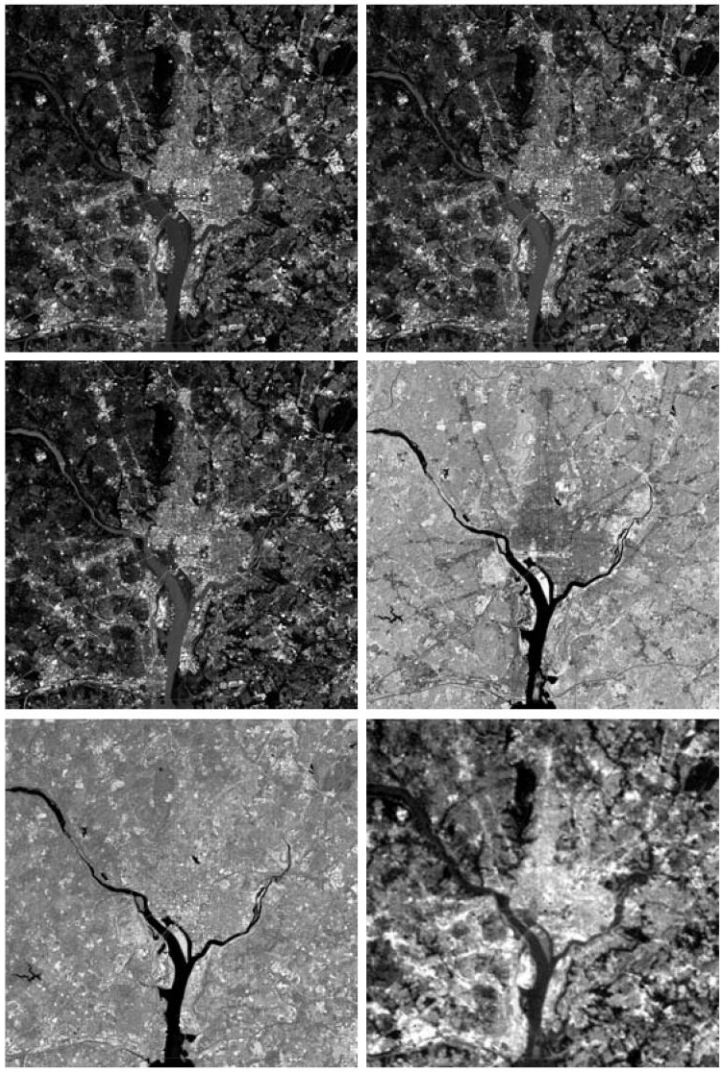
PCT for visualization



PCT



Reconstruction from two PC's



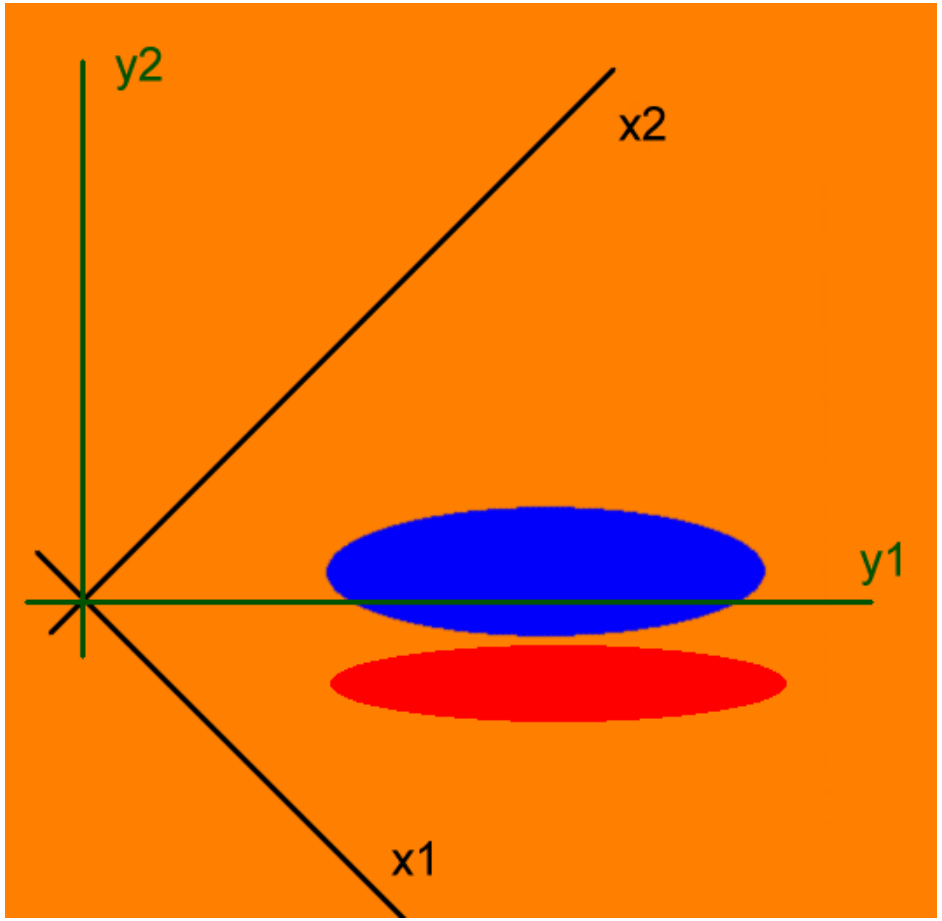
Original

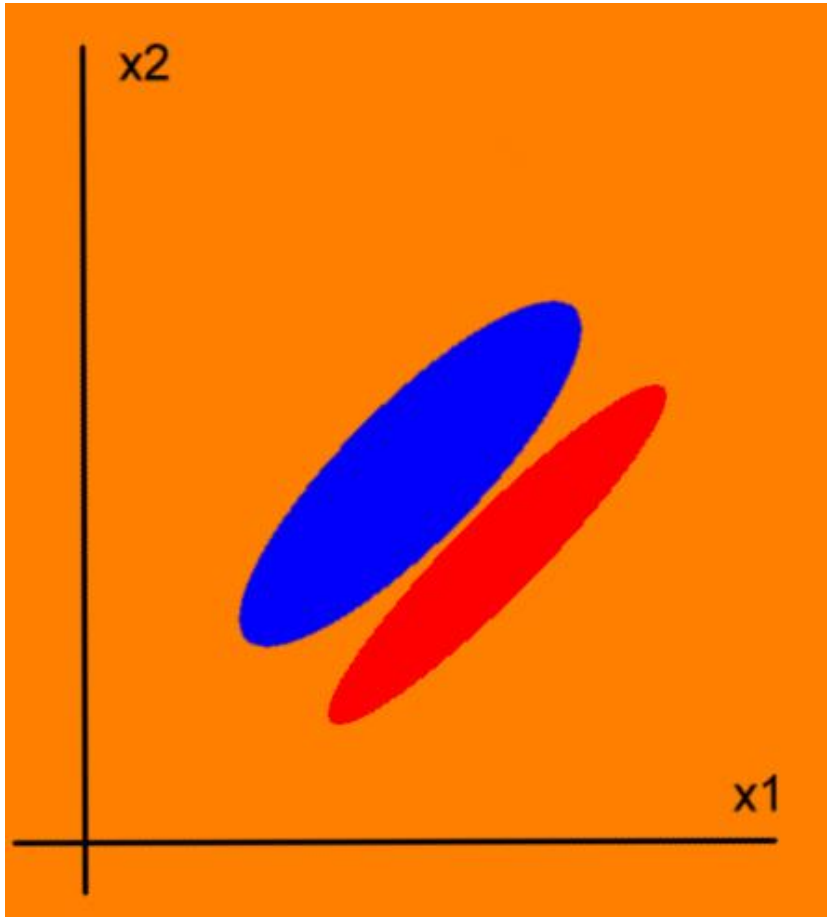
λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
10352	2959	1403	203	94	31

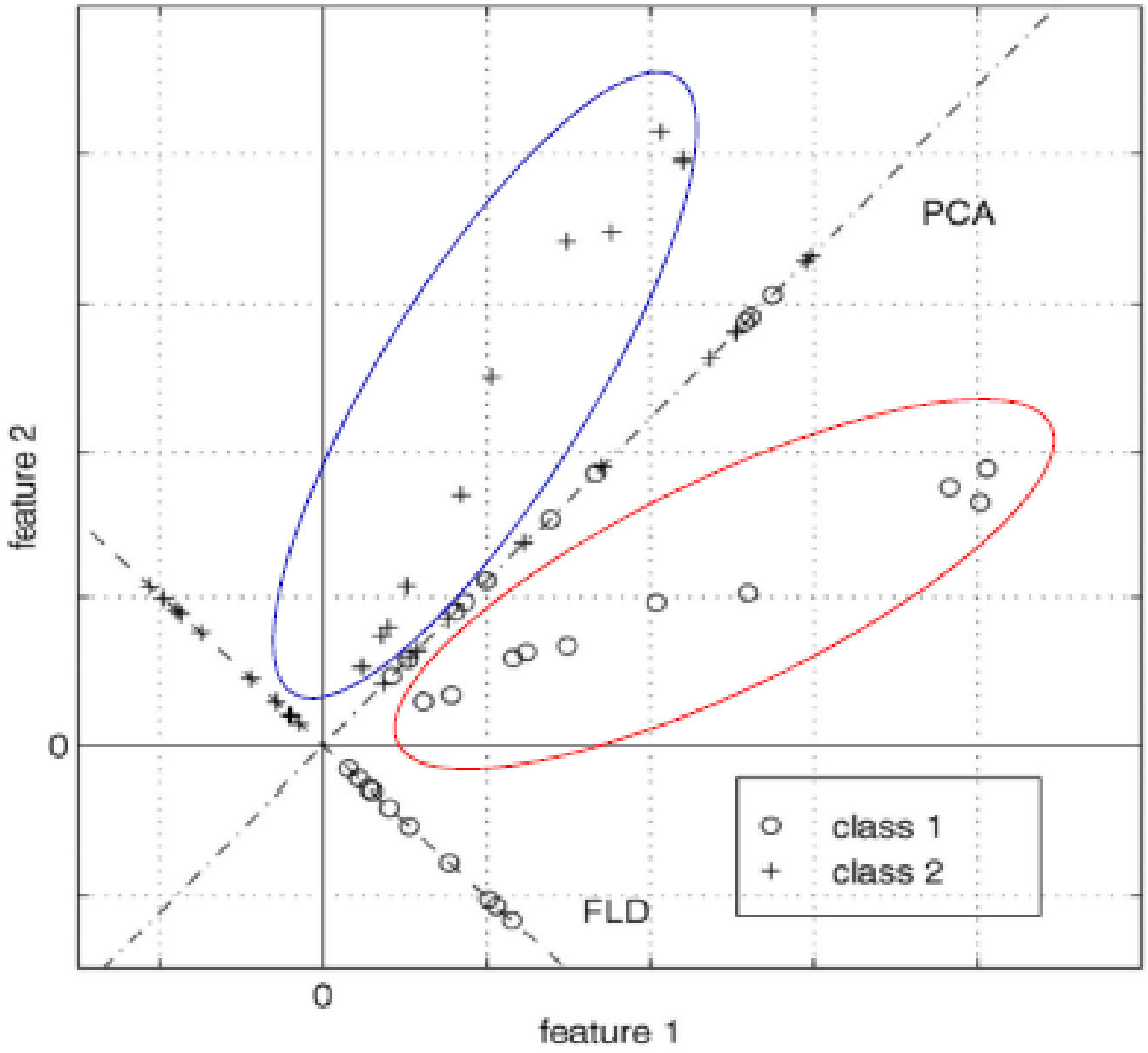
Why is PCT not suitable for classification?

PCT evaluates the contribution of individual features solely by their variances, which may be different from their **discrimination power**.

Why is PCT not suitable for classification?



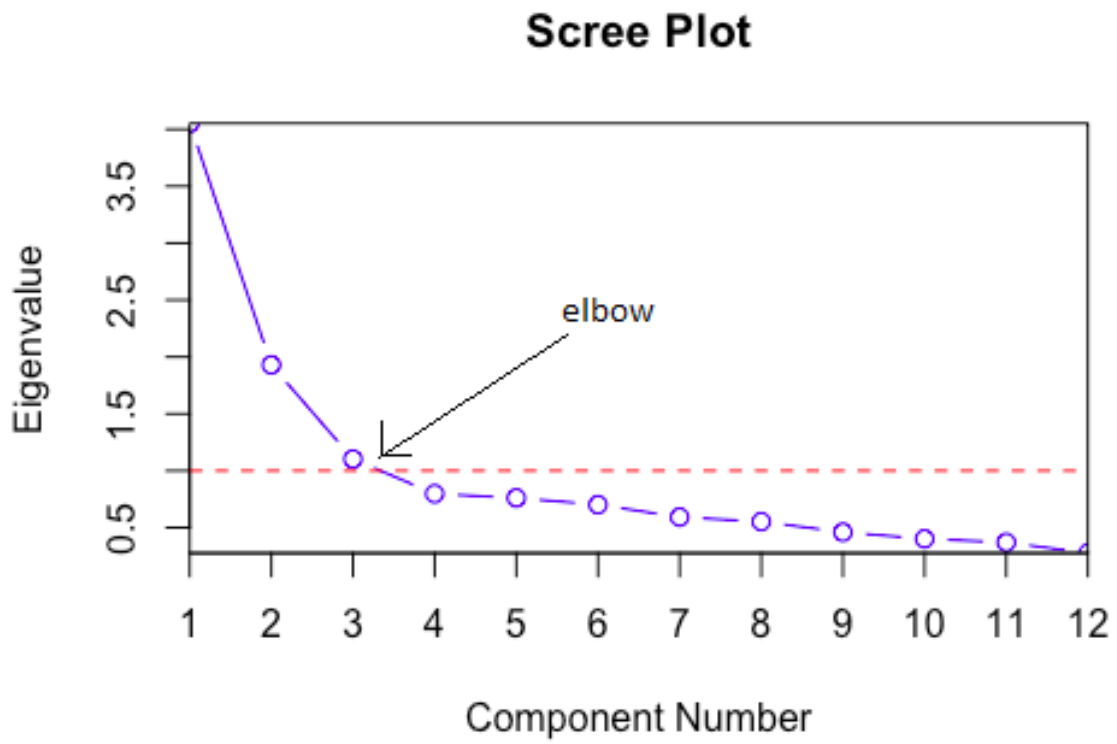



PCA
FLD
class 1
class 2
feature 1
feature 2
0
0

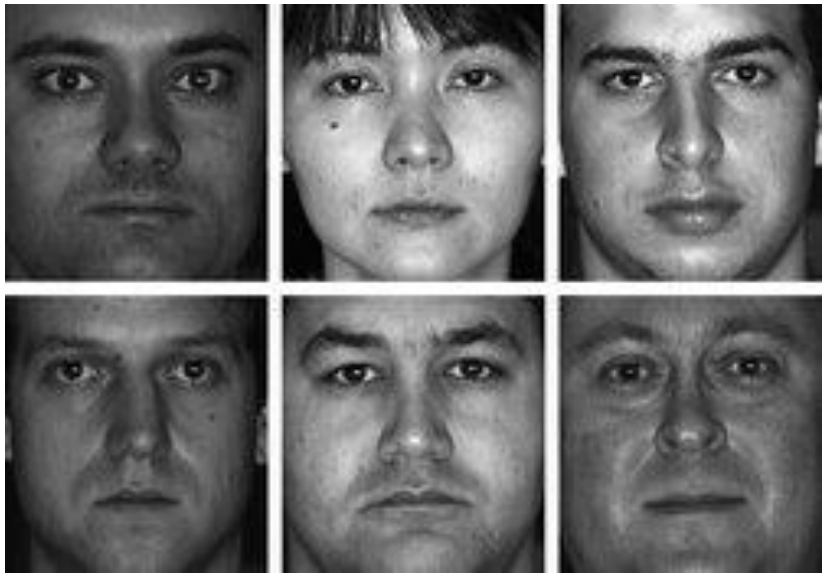
PCT: How many components?

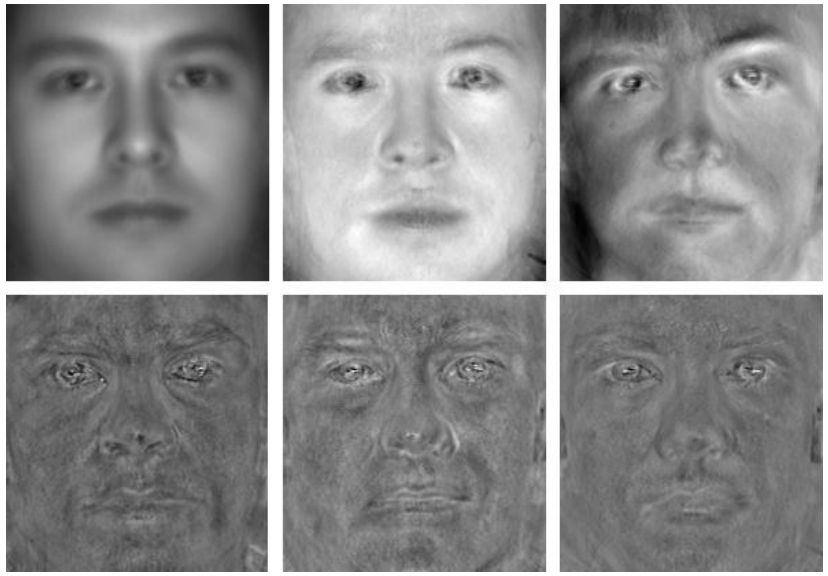
80% of total variation

The “elbow” rule

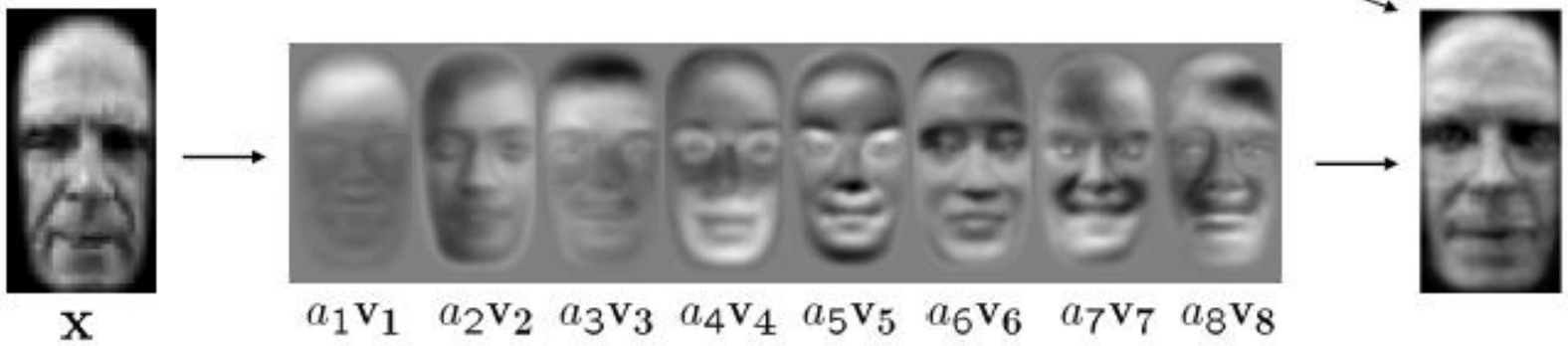


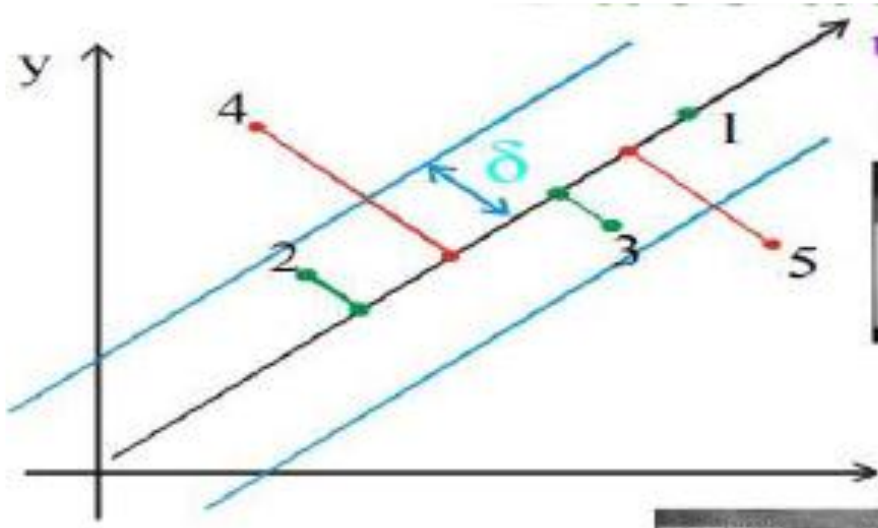
Face recognition by eigenfaces



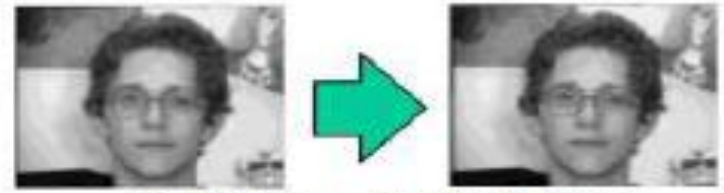


$$\mathbf{x} \approx \overline{\mathbf{x}} + a_1\mathbf{v}_1 + a_2\mathbf{v}_2 + \ldots + a_K\mathbf{v}_\mathbf{K}$$





original projection



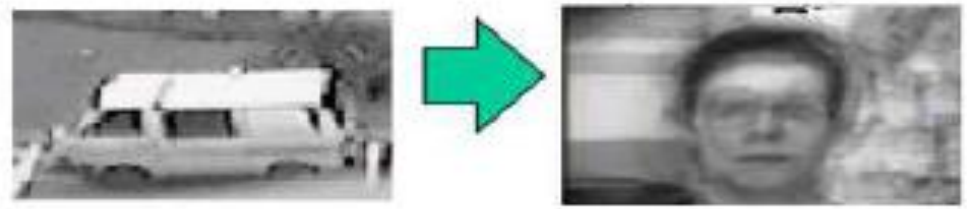
A face, used for training

A face, not used for training

1 *The best case: on the subspace*

2,3 *Close enough*

4,5 *Too far – not a face*



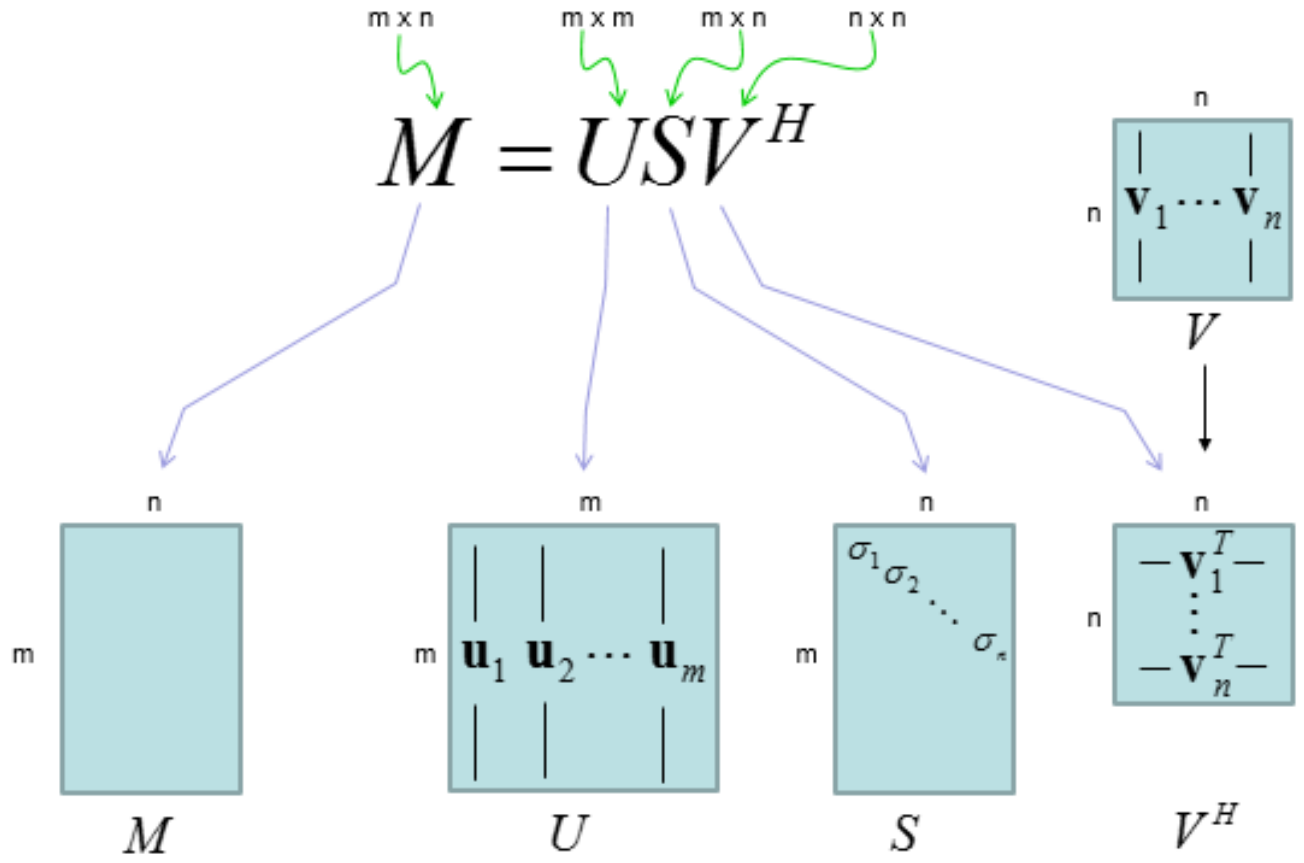
Not a face, not used for training

PCT vs. SVD

M – arbitrary matrix

U, V – orthogonal

S - diagonal

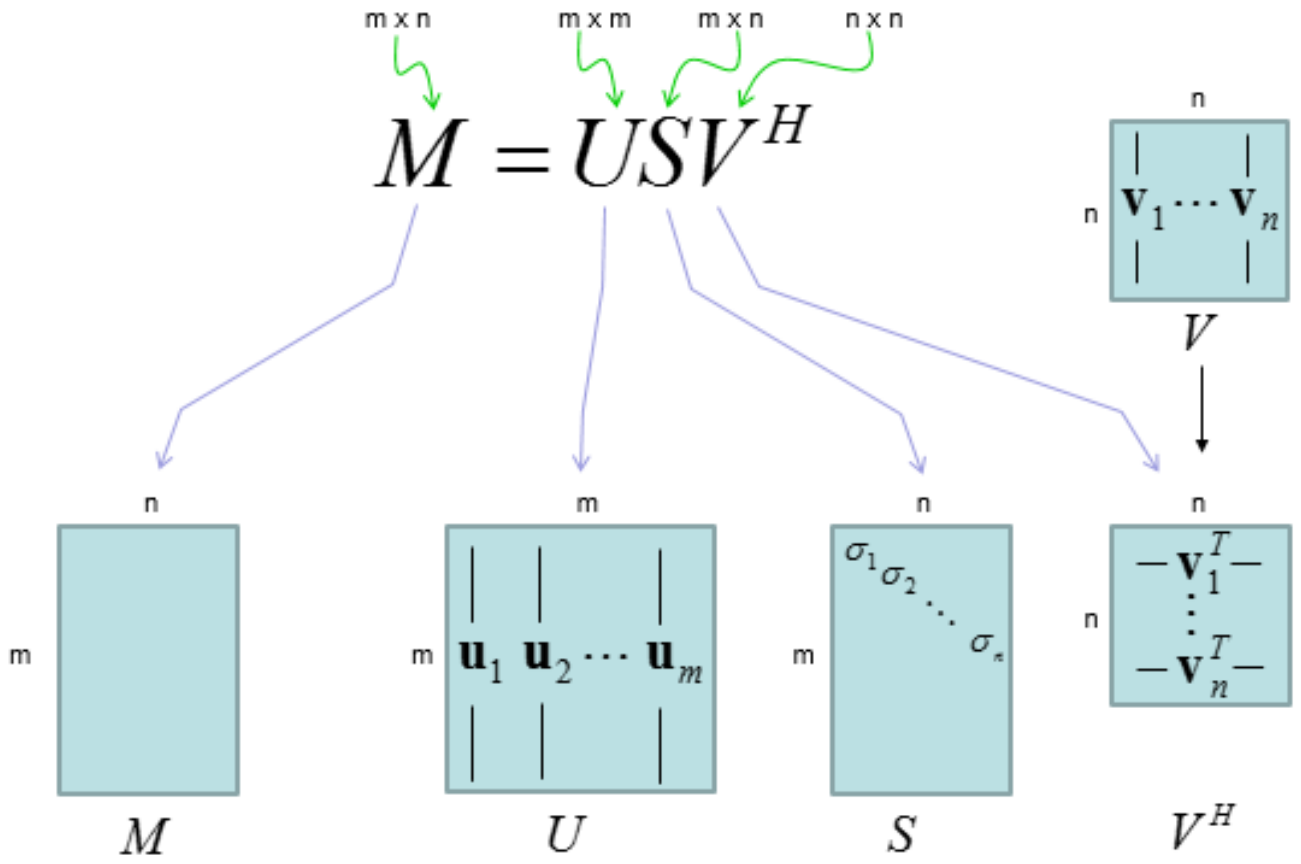


PCT vs. SVD

M – data matrix

C = *M'M* – covariance matrix

SVD of *M* is the same as diagonalization of *C*

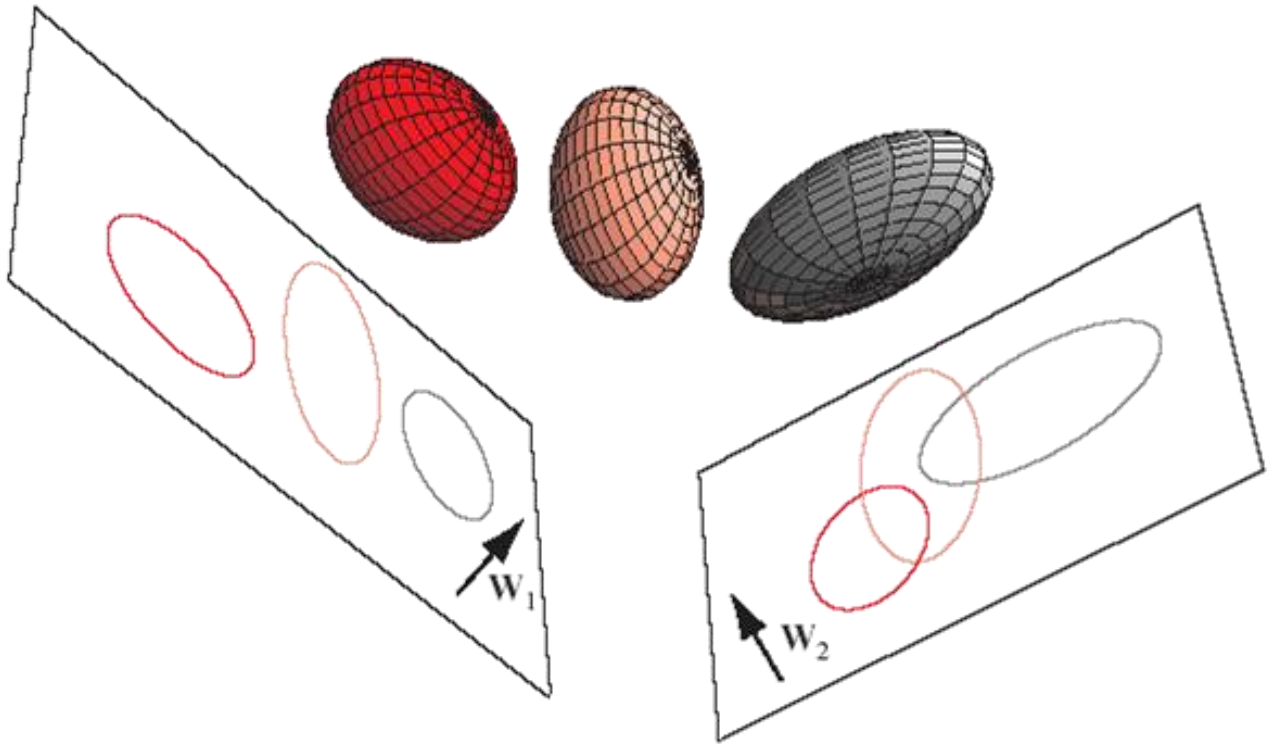


Multi-class problem

- Training sets for each class are available
- Dimensionality reduction methods for classification purposes must consider the discrimination power (separability) of individual features.
- The goal is to maximize the “distance” between the classes.

Example

3 classes, 3D feature space, reduction to 2D



High discriminability

Low discriminability

Feature selection

Two things needed:

- **Discriminability measure** which we want to maximize

- **Selection strategy** (optimization method)

  Feature selection → optimization problem

Measures of discriminability between classes

Analogous to those used in clustering but here “clusters” – training sets – are fixed, while the features are subject to selection.

Ward criterion doesn’t work.

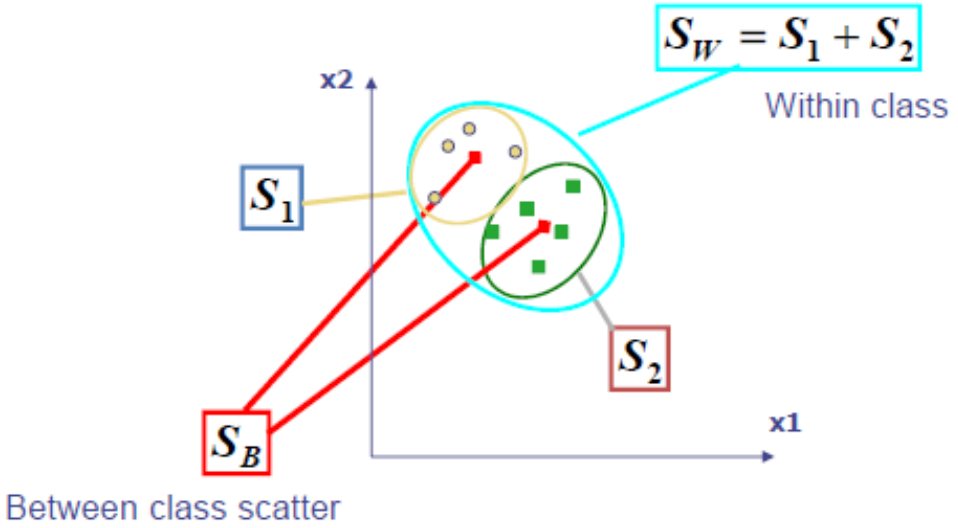
$$J = \sum_{i=1}^{N} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{m}_i\|^2$$

Scatter matrices

- between cluster matrix $$B = \sum_{i=1}^{N} n_i(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t$$

- within cluster matrix $$W = \sum_{i=1}^{N} W_i$$

$$W_i = \sum_{\mathbf{x} \in C_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t$$



The most common discriminability measure

$$\mathrm{tr}(W^{-1}B)$$

If N=2 and both training sets have the same number of elements, then

$$\max \mathrm{tr}(W^{-1}B) \sim \max(\mathbf{m}_1 - \mathbf{m}_2)^t (C_1 + C_2)^{-1} (\mathbf{m}_1 - \mathbf{m}_2)$$

Mahalanobis distance

Bhattacharyya distance

Generalization of the M.D., depends more on the class shapes

$$B = \frac{1}{2}M + \ln \frac{\left|\frac{1}{2}(C_1 + C_2)\right|}{\sqrt{|C_1| \cdot |C_2|}}$$

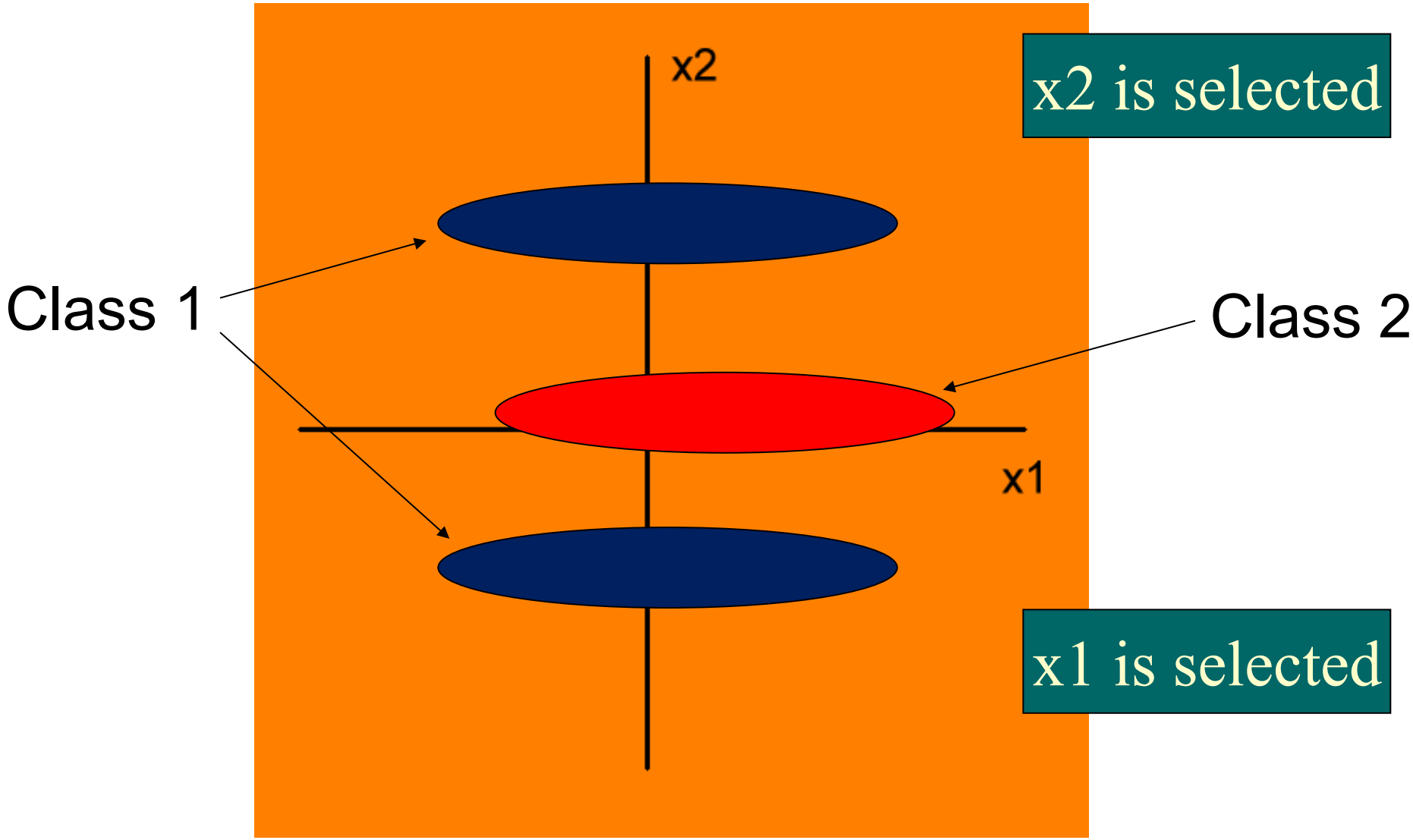
Both *M* and *B* are often used pair-wise
also in a multi-class case.

Prior knowledge in feature selection

- The above discriminability measures require **normally distributed** classes (approximation for some **unimodal** classes).
  They are misleading and inapplicable otherwise.

- The normality should be tested (Pearson's test) before.

A two-class counter-example



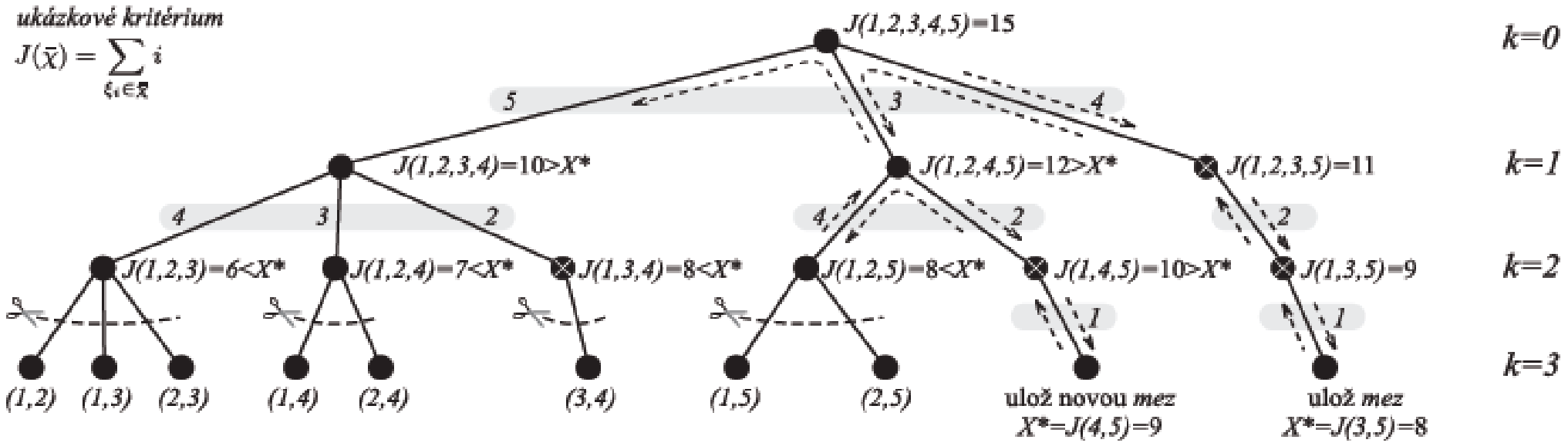
Feature selection algorithms

- **Optimal methods**
  - full search and its modifications
  - complexity *D!/(D-n)!n!*
  - guarantee the global optimum

- **Sub-optimal methods**
  - much faster
  - do not guarantee the global optimum

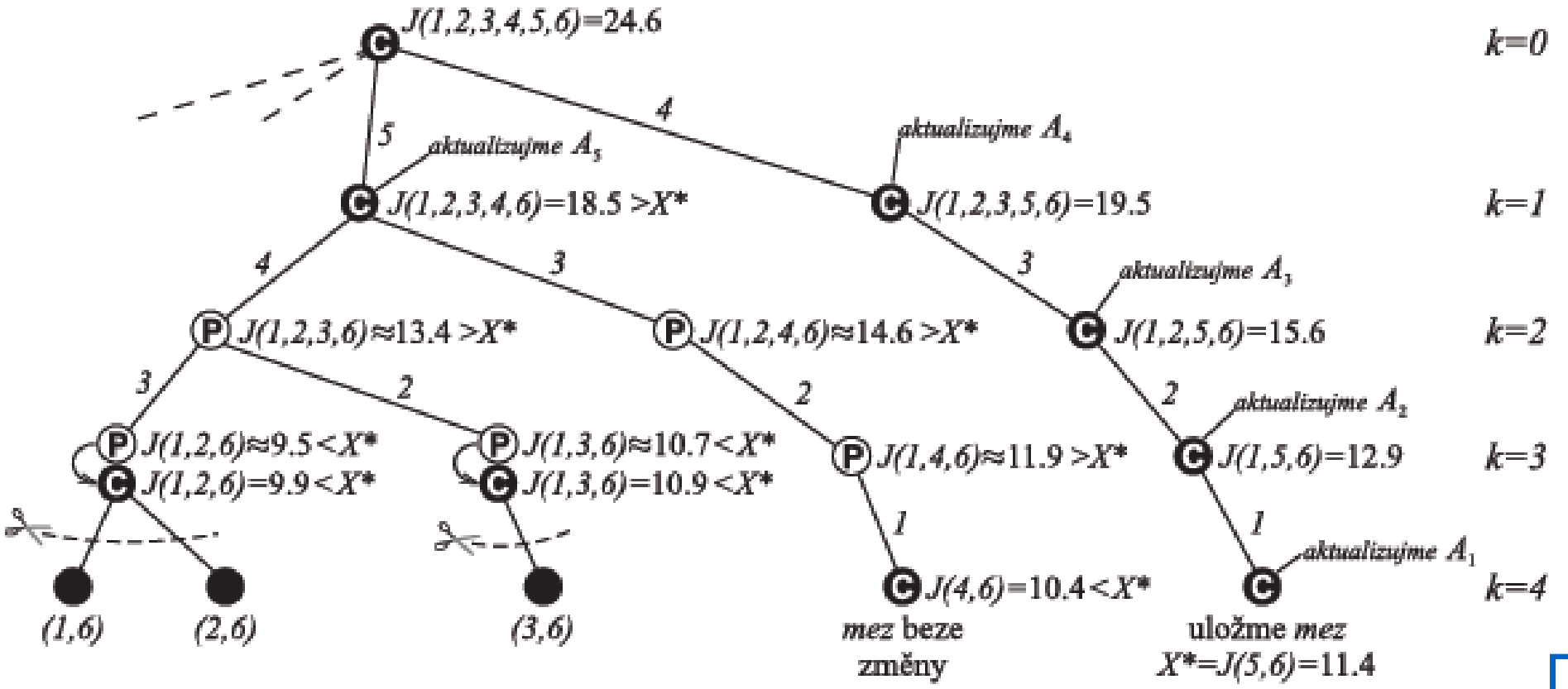
Optimal methods

- Standard full search
- Branch & bound (requires monotonic criteria)



Optimal methods

- Predictive Branch & bound

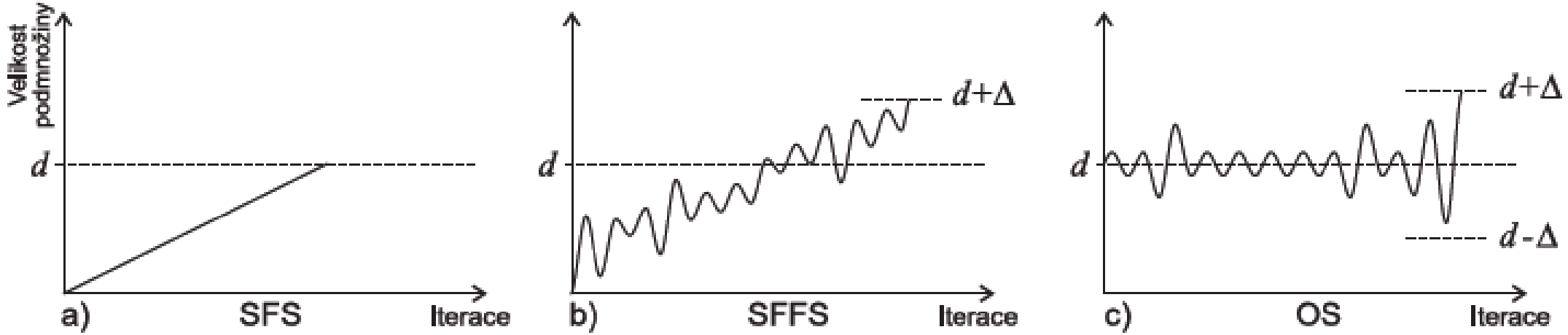


Demos

Sub-optimal methods

- Best individual features
  - optimal for uncorrelated data
- Sequential forward/backward selection (nesting effect!)
- “Plus *k* minus *m*”, $k > m$ (eliminates nesting)
- Floating search
- Oscillating search

Sub-optimal methods

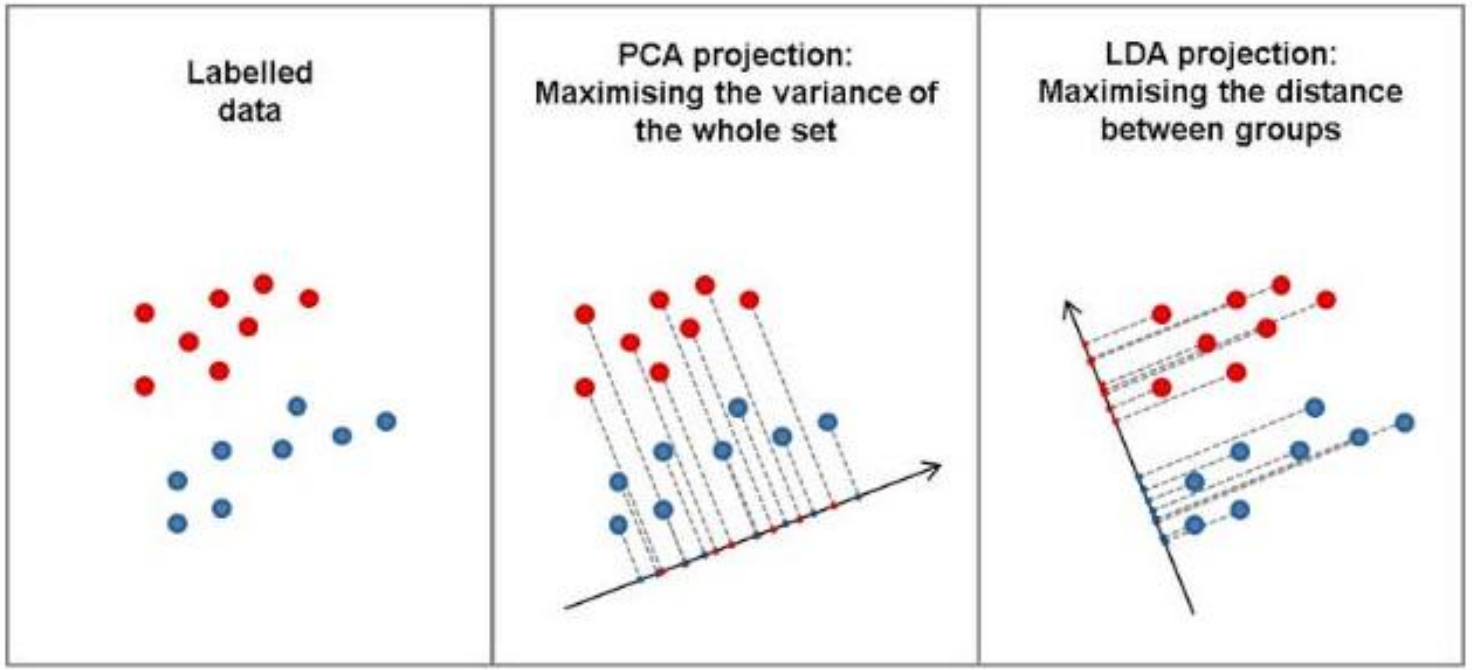


Filters versus Wrappers

- **Filters** optimize the separability of the training set
- **Wrappers** optimize the performance of the particular classifier on the given test set (any selection method can be used, usually much slower)
- Neither filters nor wrappers guarantee optimal performance on independent data but wrappers are believed to be better in this sense

Linear discriminant analysis (LDA)

- Selection of the “best” feature/direction
- Optimal direction is given by the principal eigenvector of $(W^{-1}B)$



Thank you!

Any questions?