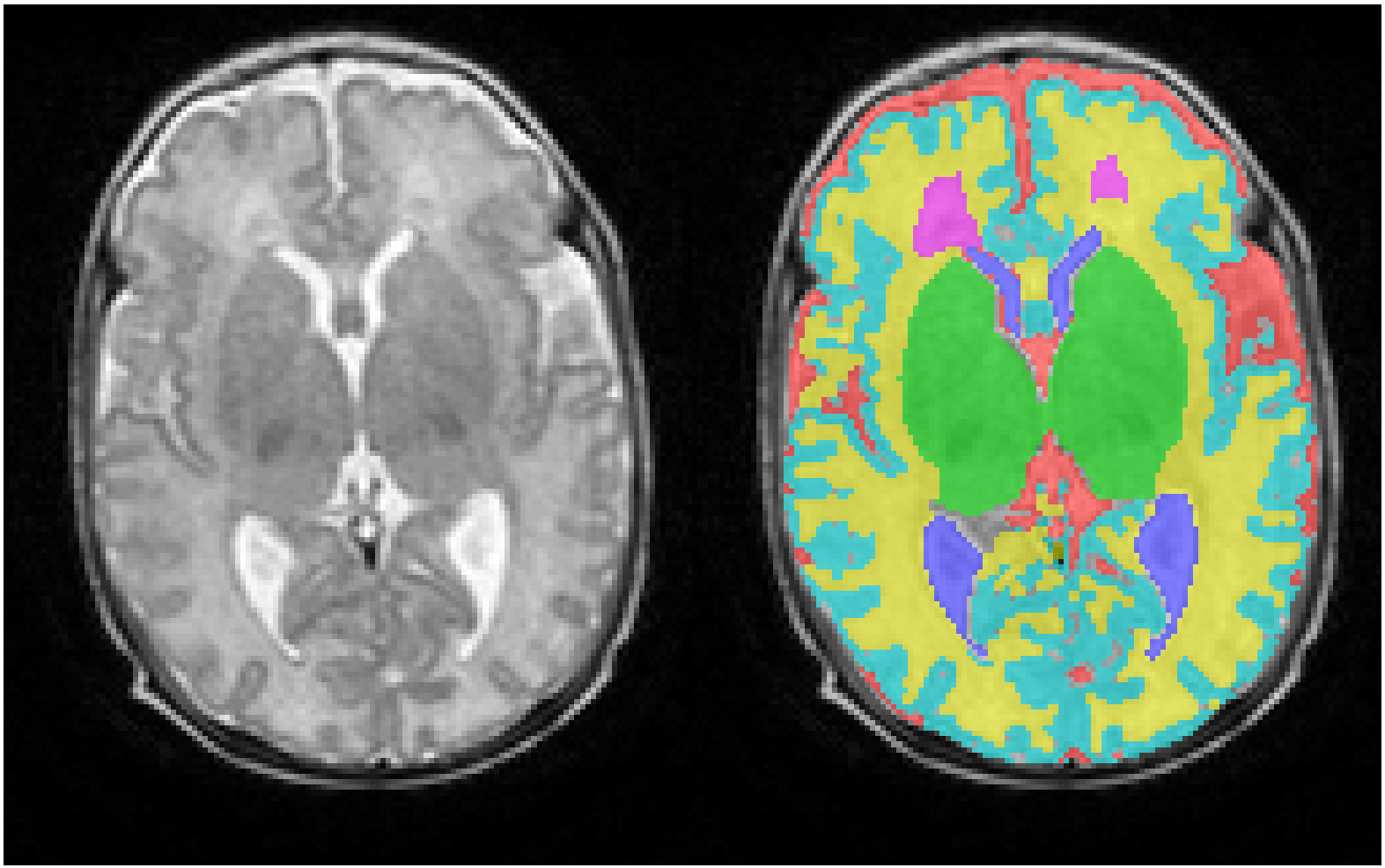
Classification and clustering: a few approaches

Isabelle Bloch

LTCI, Télécom Paris

isabelle.bloch@telecom-paris.fr

Objective: example



Content

A few approaches for classification and clustering with applications to images:

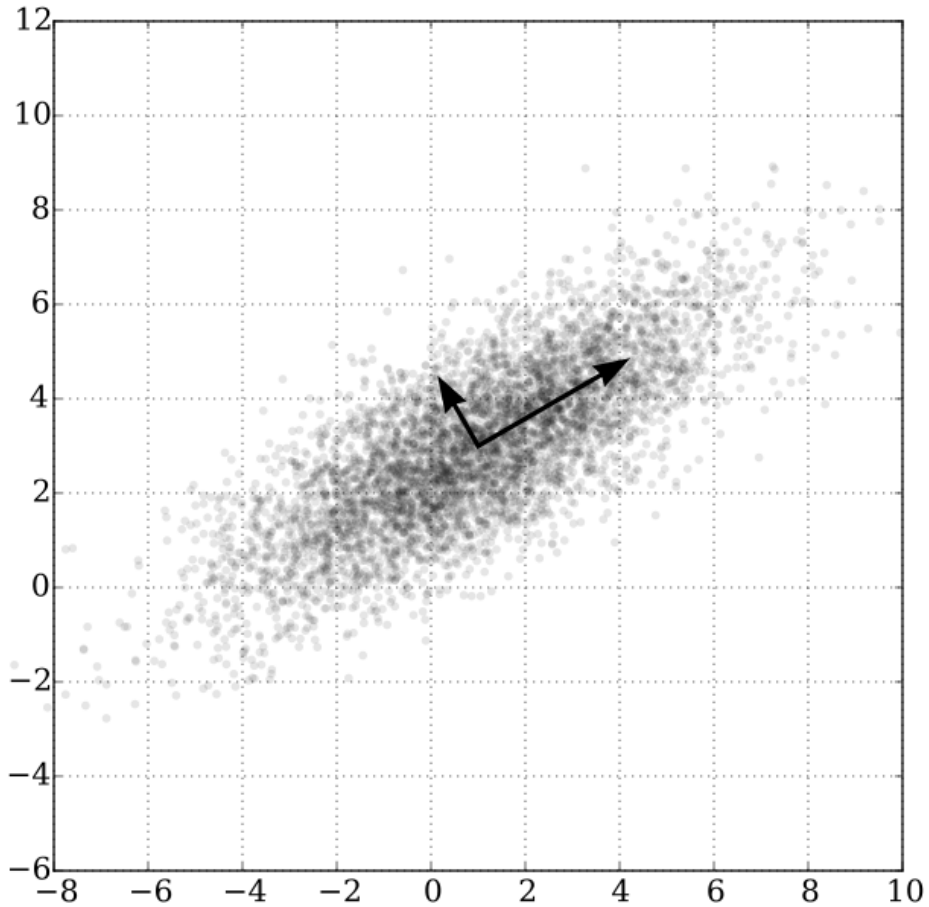
- Principal component analysis.
- Automatic clustering: k-means.
- Bayesian classification.
- Hierarchical clustering.
- SVM.
- Artificial neural networks.

Aim: data (images) $\rightarrow$ features $\rightarrow$ classes or clusters.

Feature space = characteristics of data on which classification will rely.
Decision space = classes, clusters.

Principal component analysis (PCA)

Find uncorrelated variables in the feature space



Reminder on covariance:
$A = (a_1 ... a_n), B = (b_1 ... b_n)$ with 0 mean ("centered").
Variance of A and B:

$$\sigma_A^2 = \frac{1}{n-1} \sum_{i=1}^{n} < a_i a_i > \quad \sigma_B^2 = \frac{1}{n-1} \sum_{i=1}^{n} < b_i b_i >$$

Covariance between A and B:

$$\sigma_{AB}^2 = \frac{1}{n-1} \sum_{i=1}^{n} < a_i b_i > = \frac{1}{n-1} AB^t$$

Properties of covariance:

- $\sigma_{AB}^2 = 0$ iff A and B are entirely decorrelated.
- $\sigma_{AB}^2 = \sigma_A^2$ iff $A = B$.

m samples of dimension $n \rightarrow$ matrix X of size $m \times n$.

- row of X = all measurements of a particular type
- column of X = measurements of a particular sample

Covariance $= S_X = \frac{1}{n-1} XX^t$ (square matrix $m \times m$).

- diagonal terms = variance of particular measurement types
- off-diagonal terms = covariance between measurement types

Diagonalization

$$Y = PX \text{ such that } S_Y = \frac{1}{n-1} YY^t \text{ is diagonal}$$

with P orthonormal ($p_i p_j = \delta_{ij}$),
Rows p_i of P = principal components = eigenvectors of XX^t.
ith diagonal value of S_Y = variance of X along p_i.

PCA algorithm:

1. centering data (subtracting the mean for each measurement type);
2. computing the eigenvectors of XX^t.

Underlying assumptions:

- Linearity (extension to apply non-linearity before PCA: kernel PCA).
- Mean and variance sufficient $\Rightarrow$ Gaussian distributions.
- Principal components with larger associated variances represent interesting dimensions, while those with lower variances represent noise $\Rightarrow$ dimension reduction.
- Principal components are orthogonal.

Example: face recognition

e.g. http://www.cs.toronto.edu/~guerzhoy/320/lec/pca.pdf
http://dhoiem.cs.illinois.edu/courses/vision_spring10/lectures/Lecture15-FaceRecognition.ppt

Automatic clustering: k-means

- k classes $C_1 \ldots C_k$.
- Class center = prototype (in the feature space) = $m_1 \ldots m_k$.
- Distance d in the feature space: for sample x, $d(x, m_i)$ (Euclidean, Mahalanobis...)

Minimization of an objective function J:

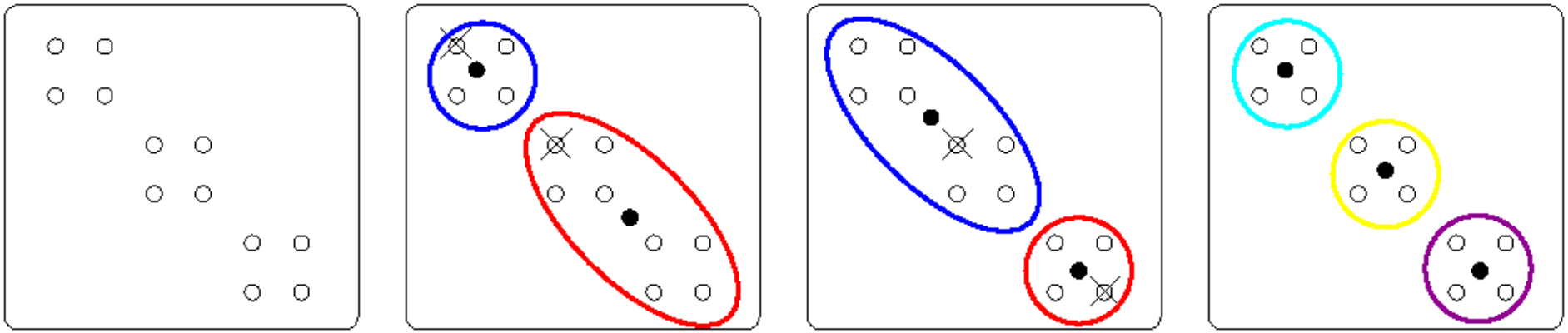
$$J = \sum_{i=1}^{k} \sum_{x \in C_i} d(x, m_i)^2$$

Solution:

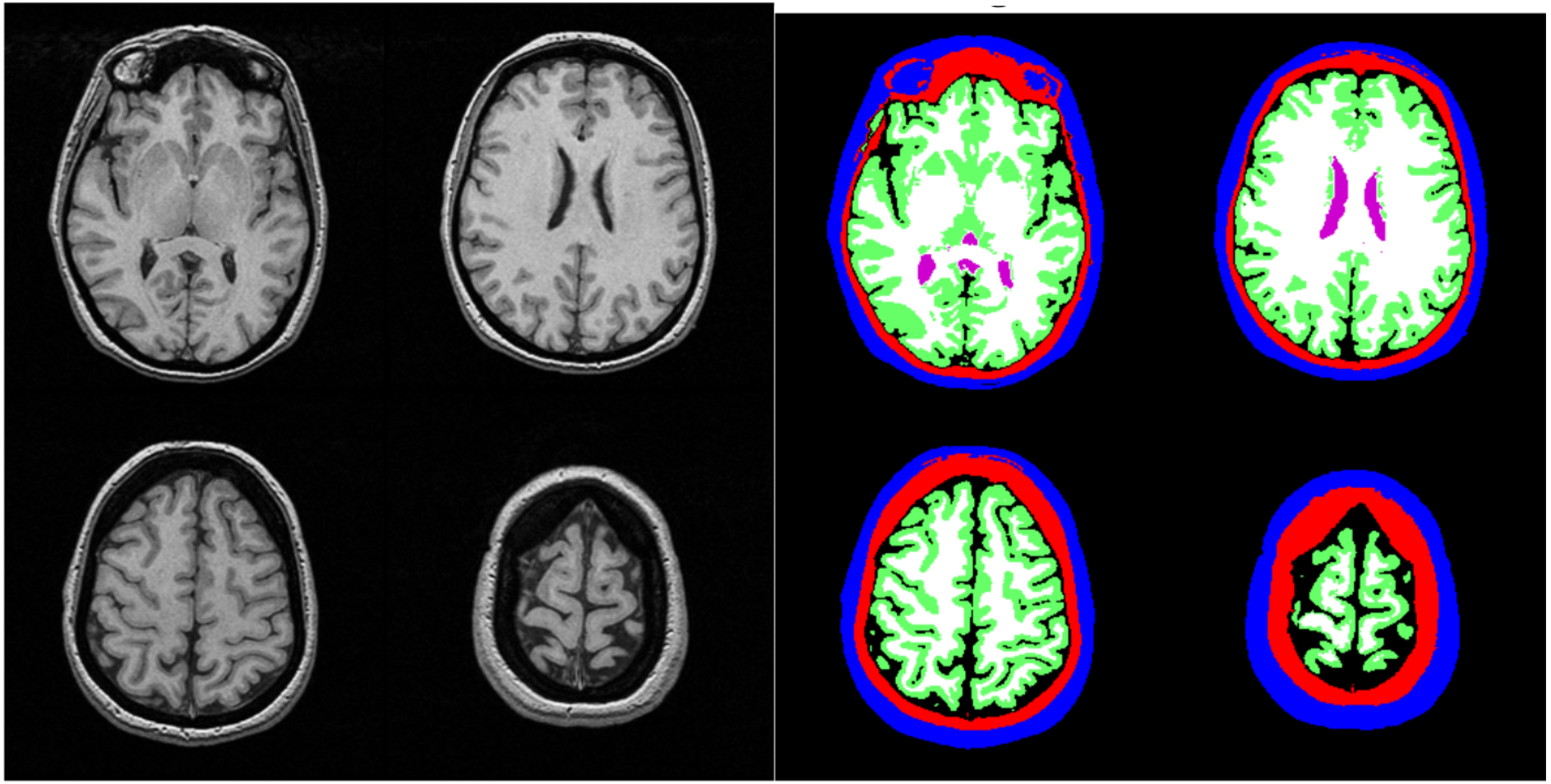
1. m_i fixed $\Rightarrow x \in C_i$ iff $\forall j, d(x, m_i) \leq d(x, m_j)$.
2. class assignment fixed $\Rightarrow m_i = \frac{\sum_{x \in C_i} x}{|C_i|}$.

Algorithm:

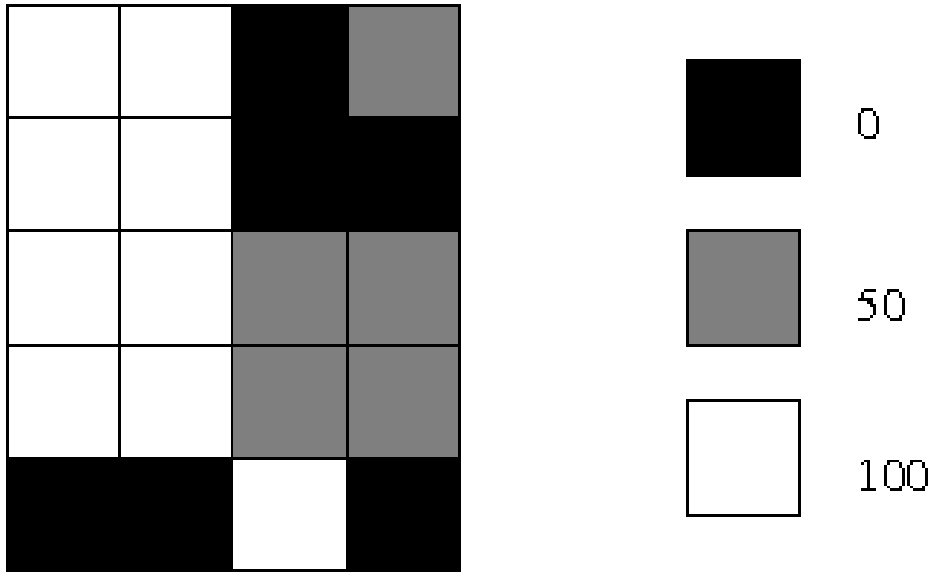
- Choose k and set initial class centers.
- Iterate steps 1 and 2.
- Until convergence... towards a local minimum of J!


a
b
c
d
= centres initiaux
= centres finaux

Example: MRI brain images



Exercise: which classification result for $k = 2$?



ISODATA

Extends k-means algorithm with splitting and grouping steps:

- adaptation of class number,
- more parameters,
- splitting along the direction of maximal variance,
- grouping if class centers are closed to each other.

Bayesian clustering

Probabilistic modeling of an image

- $\Omega = \{\omega_1, \omega_2, ...\}$ = set of classes
- s = site (pixel) and $S = \{s\}$ = set of sites
- Y_s = random variable associated with each site
- y_s gray level (realization of Y_s) – or more generally a feature vector

MAP decision:

s assigned to ω_i such that:

$$P(\omega_i|y_s) \text{ maximal}$$

Bayes rule:

$$P(\omega_i|y_s) = \frac{p(y_s|\omega_i)P(\omega_i)}{p(y_s)}$$

Estimating $p(y_s|\omega_i)$ (likelihood):

- learning from annotated data (supervised)
- histogram $\Rightarrow$ distribution of gray levels (unsupervised)
  - parametric methods
  - non parametric methods

Estimating $P(\omega_i)$ (prior):

- prior knowledge on class occurrences
- learning on a significant sample set
- otherwise equiprobable classes

$$P(\omega_i) = \frac{1}{Card(\Omega)}$$

$$\Rightarrow p(y_s|\omega_i) \text{ maximal}$$

= classification in the sense of maximum likelihood

Usual hypotheses:

- independence of features conditionnally to the classes
- Gaussian distributions
- Markov hypothesis on the class field $\Rightarrow$ included in the prior

Markovian regularization

- Minimization of an energy defined globally on the image:

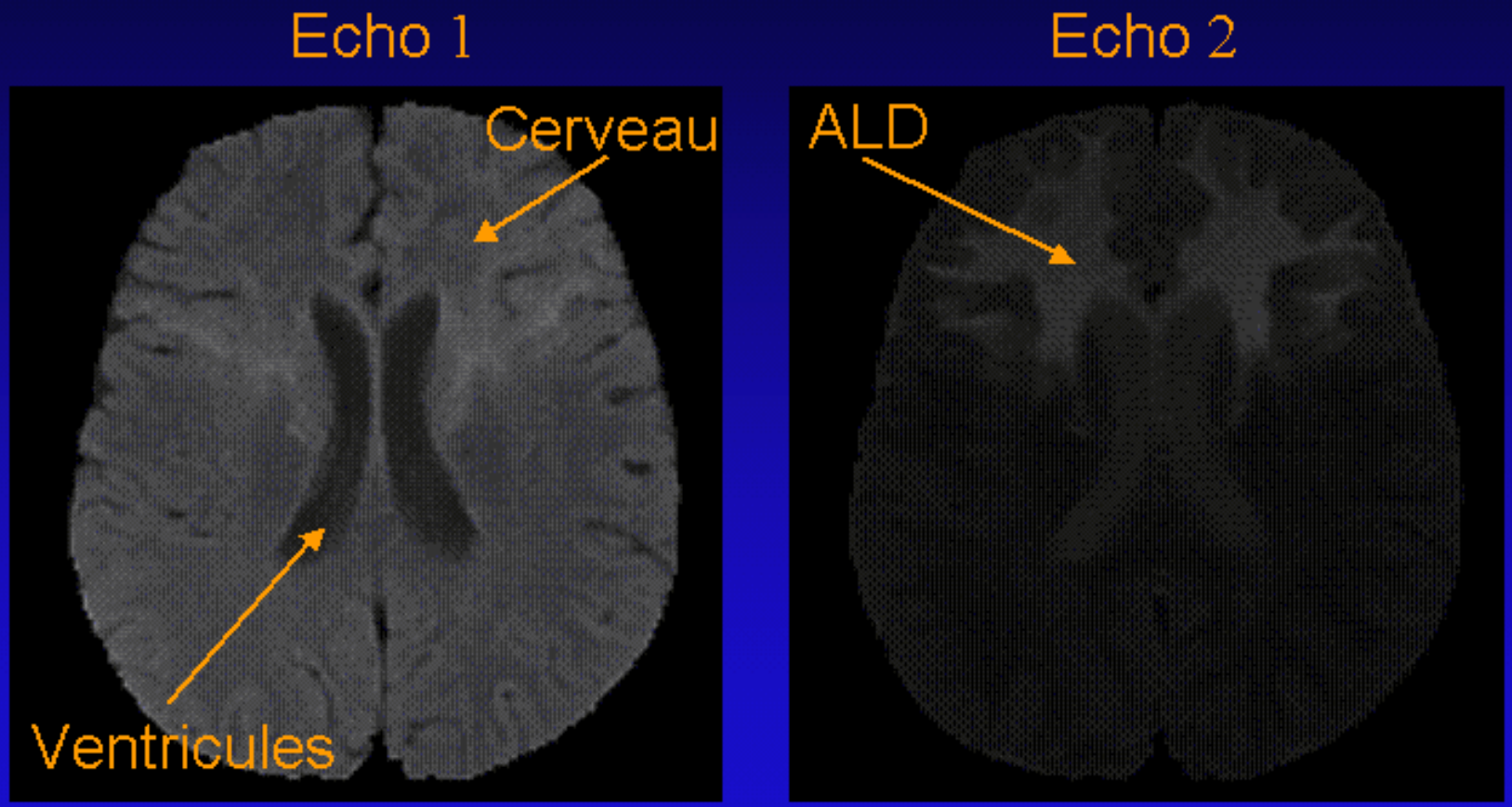
$$U(x) = U(x, y) + U_{prior}(x)$$

with

$$U(x) = \sum_s \frac{(\mu_{x_s} - y_s)^2}{\sigma^2} - \beta \sum_{s,t} \delta(x_s, x_t)$$

  - $U(x, y)$ = data fidelity
  - $U_{prior}(x)$ = contextual term
- No analytical solution
- Iterative and stochastic optimization (simulated annealing) or iterative conditional modes if the initialization is good enough s

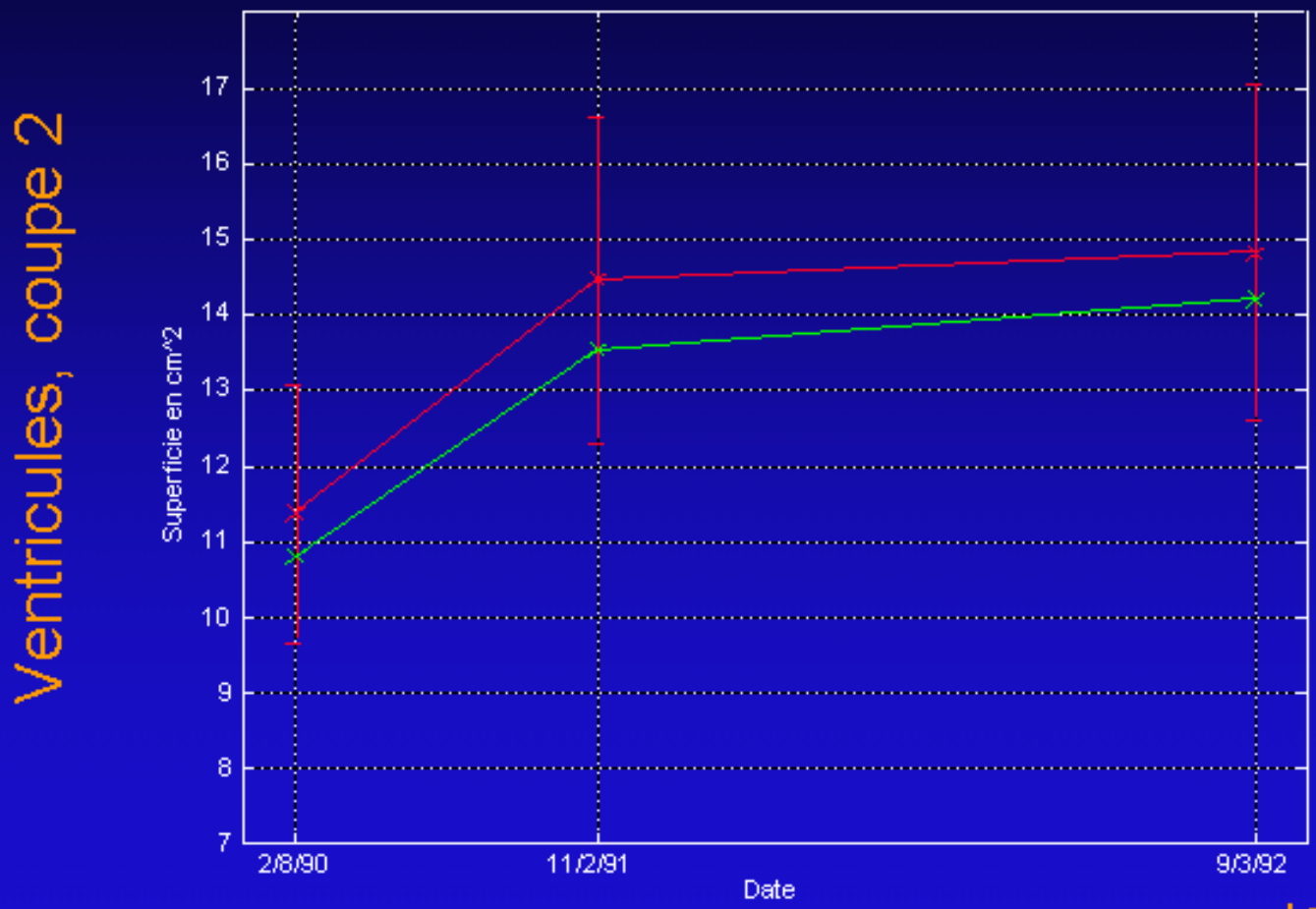
L'adrénoleukodystrophie



Etiquettes discrètes, résultats pour l'ALD

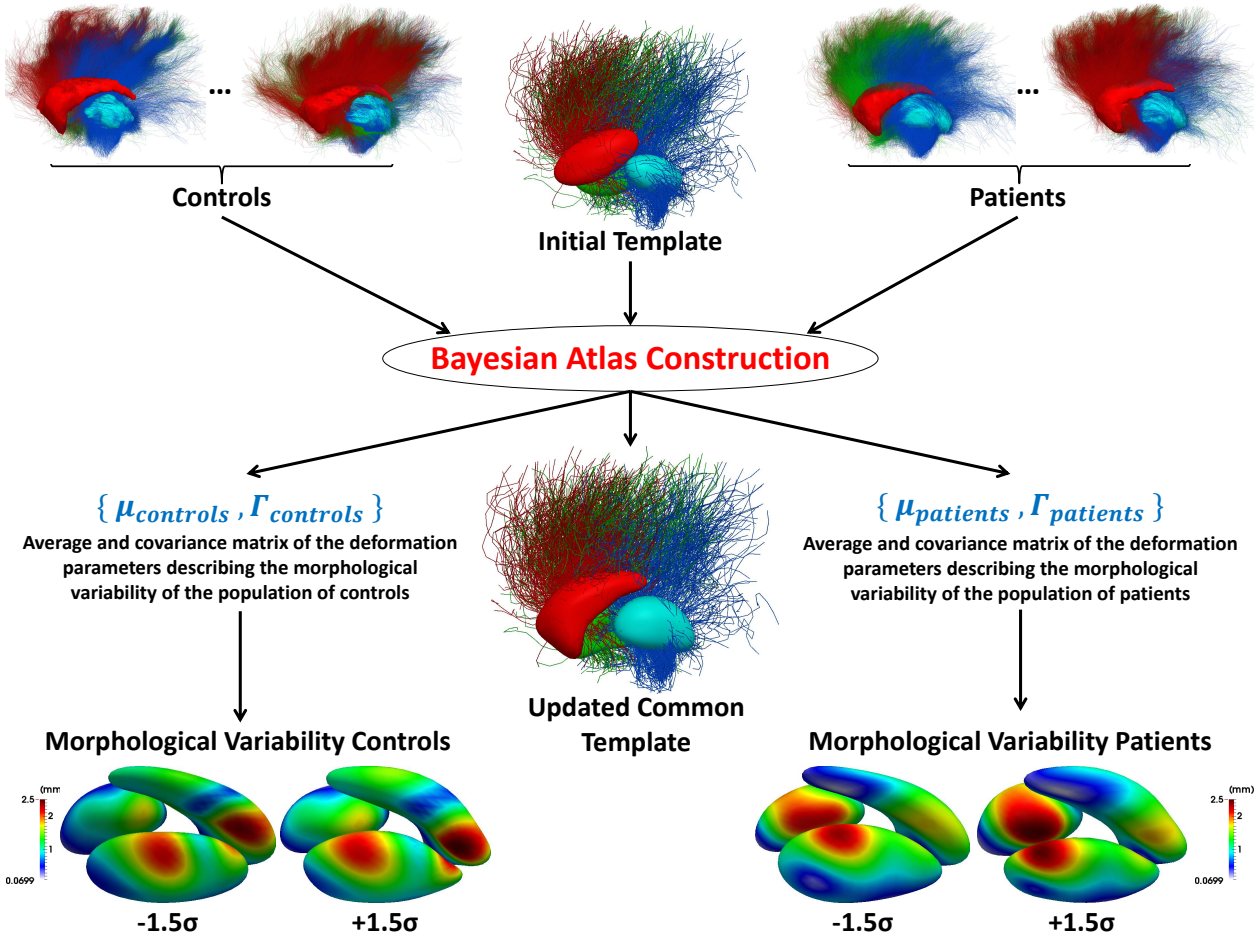
Lars Aurdal, ENST

Etiquettes discrètes, suivi d'un cas d'ALD



Etiquettes discrètes, suivi d'un cas d'ALD

Pietro Gori et al.



Exercise:

Landcover classification in a satellite image:

- wheat (class C_1) which covers 60 % of the region of interest,
- forest (class C_2) which covert 10% of the region of interest,
- remaining: man-made objects, etc.

A large zone Z has been detected, which is homogeneous, with a mean gray level $m = 80$.

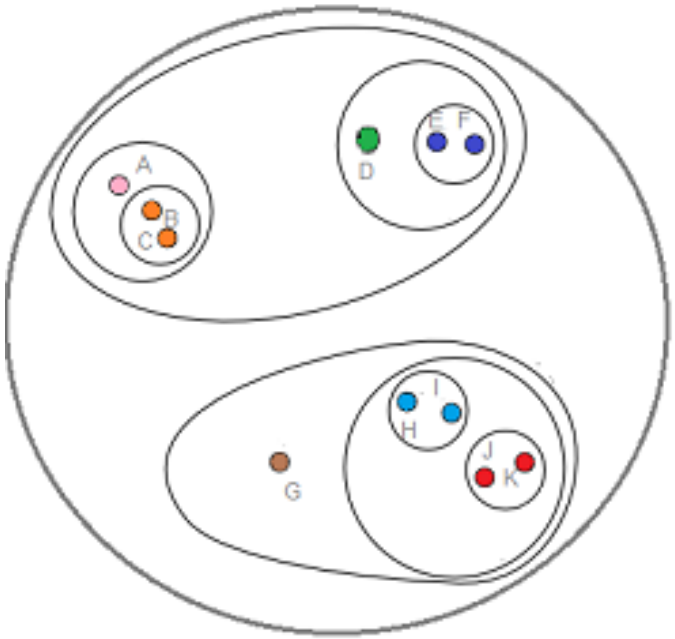
After a learning phase, conditional probabilities $P(n|C_1)$ et $P(n|C_2)$ (for a gray level n) are estimated as Gaussian distributions of parameters:

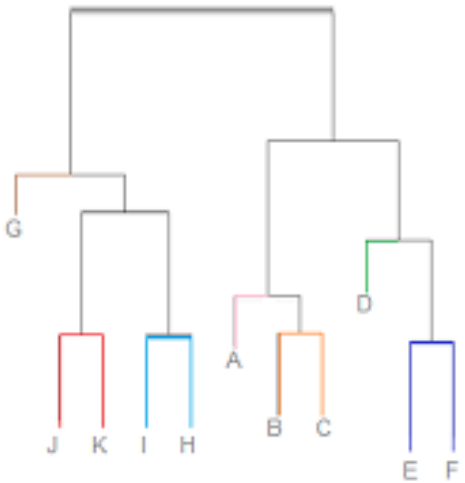
- for wheat: $m_1 = 100$, $\sigma_1 = 20$,
- for forest: $m_2 = 85$, $\sigma_2 = 5$.

1. To which class should Z be assigned according to the maximum likelihood criterion?
2. To which class should Z be assigned according to the maximum a posteriori criterion?
3. Actually, the estimation of forest coverage is not known precisely and can vary between 8% à 20% of the region of interest. Would this change the decision?

Hierarchical clustering

Set of nested clusterings (ex: taxonomy).





http://www.statisticshowto.com

Equivalence between indexed hierarchy in the sample space E and ultra-metric on E.

Ultra-metric: $\delta : E \times E \rightarrow \mathbb{R}^+$ such that

$$\forall (x_1, x_2) \in E^2,\ \delta(x_1, x_2) = 0 \Leftrightarrow x_1 = x_2,$$

$$\forall (x_1, x_2) \in E^2,\ \delta(x_1, x_2) = \delta(x_2, x_1),$$

$$\forall (x_1, x_2, x_3) \in E^3,\ \delta(x_1, x_2) \leq \max(\delta(x_1, x_3), \delta(x_3, x_2)).$$

$\Rightarrow$ any triangle is isocele.

Chain (path) distance:

- path from x_1 to x_2: sequence $c = \{c_1 = x_1, c_2, ...c_n = x_2\}$
- step $P(c) = \max_{i=1}^{n-1} d(c_i, c_{i+1})$
- chain distance: $\delta(x_1, x_2) = \inf_{c \in CH(x_1,x_2)} P(c)$
  $(CH(x_1, x_2) =$ set of all paths from x_1 to $x_2)$

$\Rightarrow \delta$ is an ultra-metric

Ordering property: $\forall \Delta$ ultra-metric, $\Delta \leq d \Rightarrow \Delta \leq \delta$,
for the ordering $d_1 \leq d_2 \Leftrightarrow \forall (x, y) \in E^2,\ d_1(x, y) \leq d_2(x, y)$.

Equivalence relation from an ultra-metric δ:

$$\forall \delta_0 \in \mathbb{R}^+,\ xR_{\delta_0}y \ \Leftrightarrow\ \delta(x,y) \leq \delta_0$$

Partition $P(\delta_0) = E/R_{\delta_0}$ = set of classes

- Within a class: path from any sample to any other sample by steps of length $\leq \delta_0$.
- From a sample of a class to a sample of another class: at least one step of length $> \delta_0$.

Hierarchy on E: $\mathcal{H} \subseteq \mathcal{P}(E)$ such that:

- $E \in \mathcal{H}$,
- $\forall x \in E,\ \{x\} \in \mathcal{H}$,
- $\forall (h, h') \in \mathcal{H}^2,\ \begin{cases} h \cap h' = \emptyset, \\ \text{or } h \subseteq h', \\ \text{or } h' \subseteq h. \end{cases}$.

Example: $\mathcal{H} = \bigcup_{\delta_0 \in \mathbb{R}^+} P(\delta_0)$

Indexed hierarchy: $(\mathcal{H}, f)$ such that $\mathcal{H}$ is a hierarchy and f is a mapping $\mathcal{H} \to \mathbb{R}^+$ such that:

- $\forall x \in E,\ f(\{x\}) = 0$,
- $\forall (h, h') \in \mathcal{H}^2, h \subset h',\ h \neq h' \ \Rightarrow\ f(h) < f(h')$.

Fundamental result

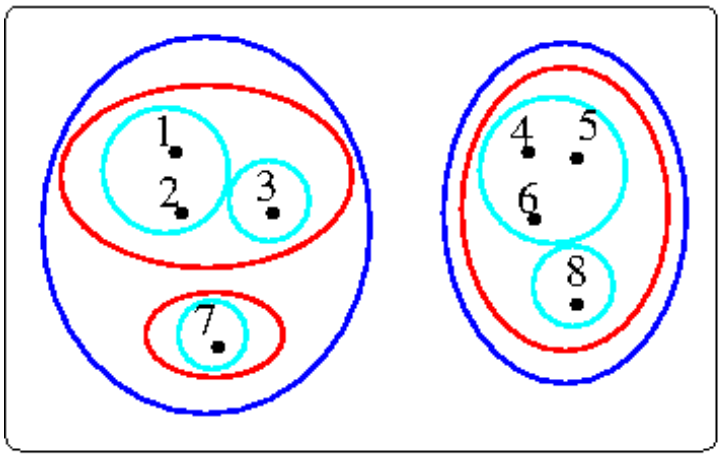
- Let $\mathcal{H} = \bigcup_{\delta_0 \in \mathbb{R}^+} P(\delta_0)$. $(\mathcal{H}, f)$ is an indexed hierarchy for:

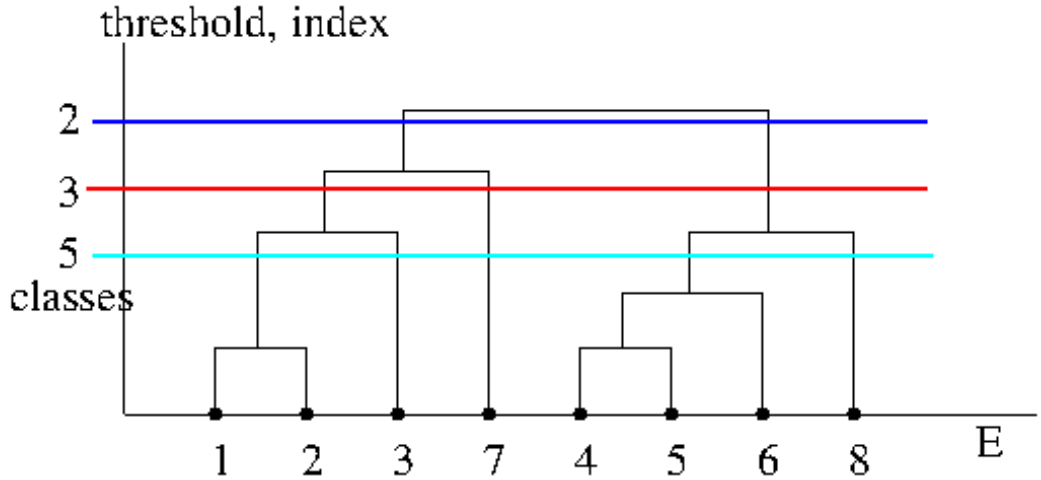
$$\forall h \in \mathcal{H},\ f(h) = \min\{\delta_0 \mid h \in P(\delta_0)\}.$$

- Conversely, let $(\mathcal{H}, f)$ be an indexed hierarchy. Then δ defined as:

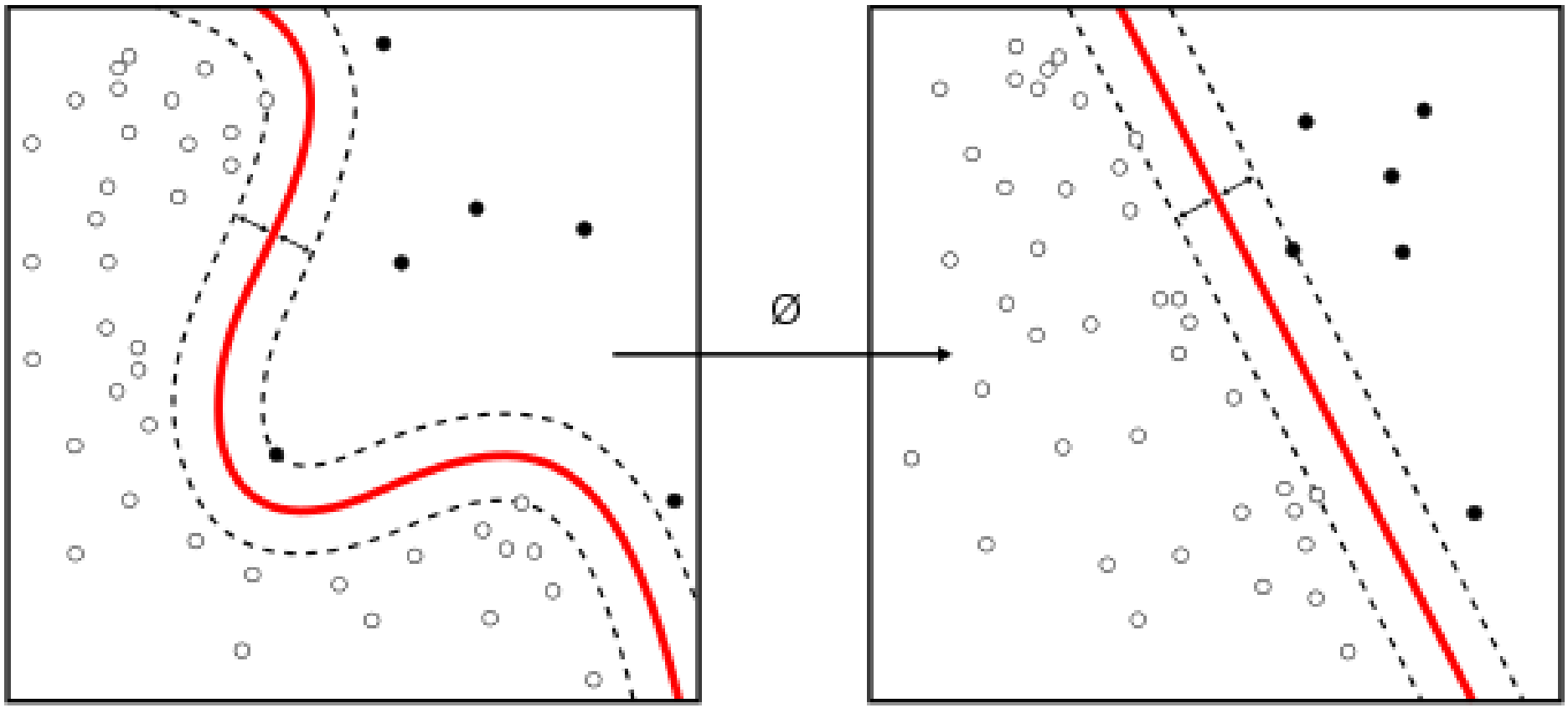
$$\delta(x, y) = \min_{h \in \mathcal{H}} \{f(h) \mid (x, y) \in h^2\}.$$

is an ultra-metric.

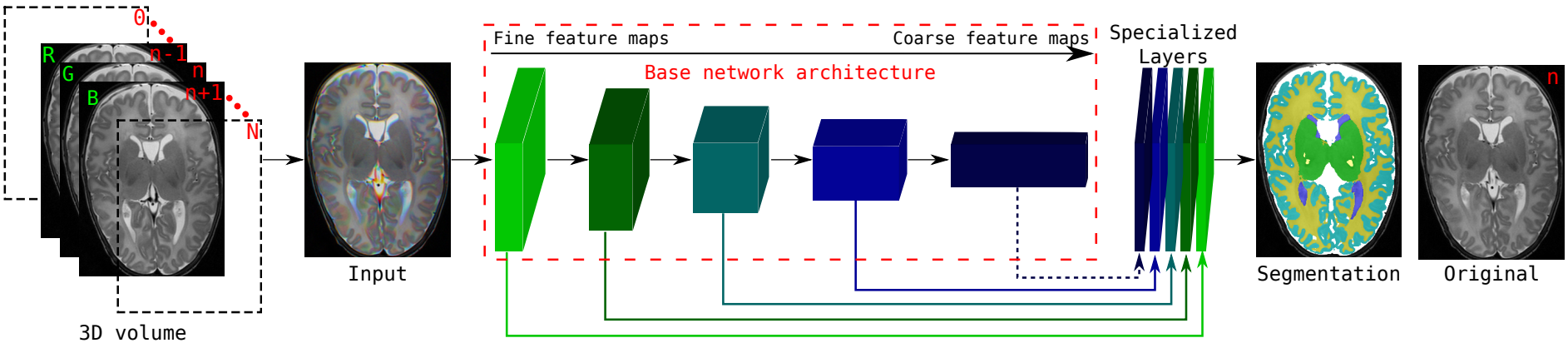


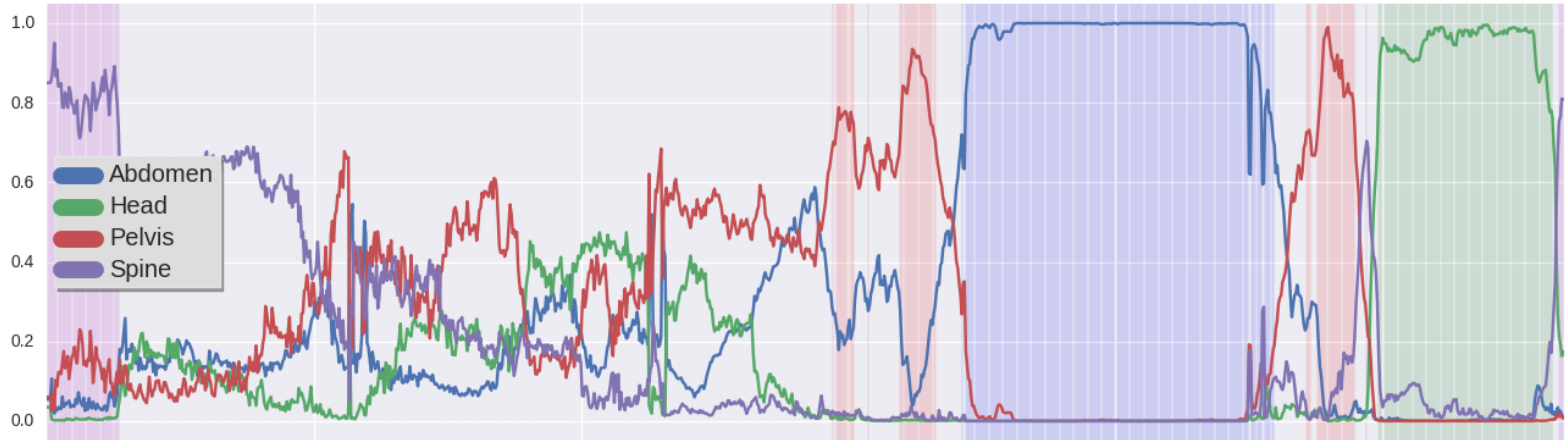


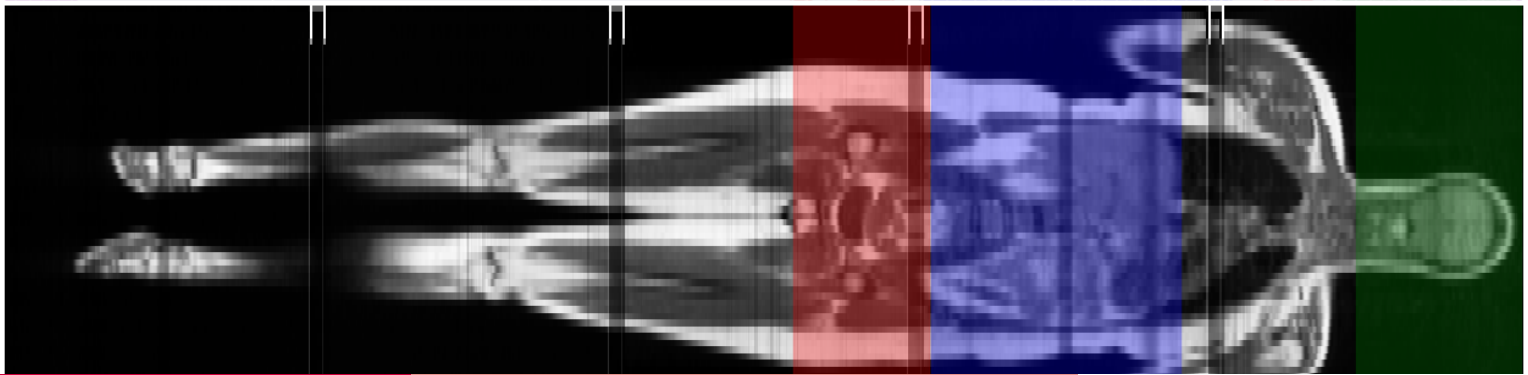
SVM



Artificial neural networks







To know more:
C. Bishop: Pattern Recognition and Machine Learning, Springer, 2006.
(among others!)