

SSSPR 2006

Structural inference of sensor-based measurements

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Robert P.W. Duin

Artsiom Harol, Thomas Landgrebe, Piotr Juszczak, Pavel Paclik, Elzbieta Pekalska,

Dick de Ridder, Marina Skurichina, David M.J. Tax, Serguei Verzakov

Delft University of Technology

The Netherlands

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Structural Inference

How can we learn from structure?

Learning : Input + knowledge $\rightarrow$ more knowledge

Input : Examples, observations

Learning from examples : Generalization

Learning from structure : Generalization from structure

Concepts versus Observations

Plato:

The **concepts live** somewhere **inside** us. We awake them by our observations. It is our **struggle to interpret new observations** in terms of existing concepts.



Aristotle:

We learn the world by observing it. In this process **we struggle with creating concepts**, i.e. generalizations of observations.

Structural versus Statistical Pattern Recognition

Concept of a house

Platonic approach:



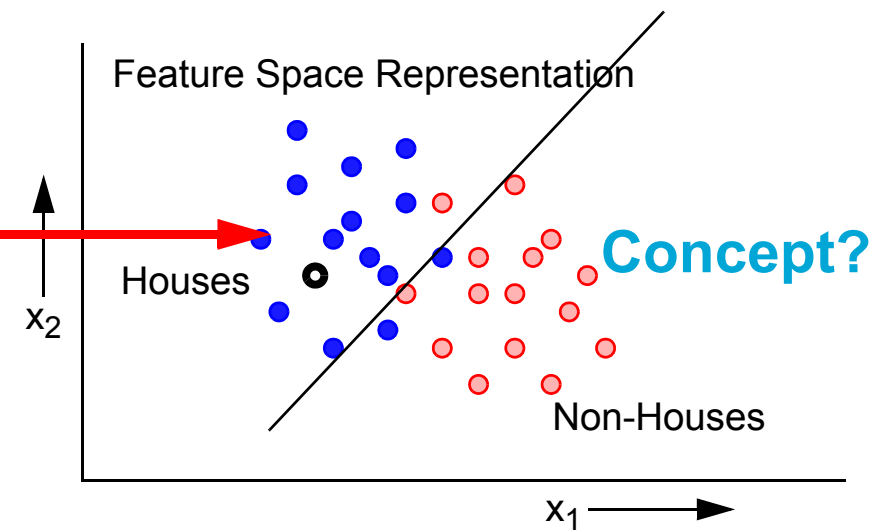
Are these houses?



Aristotalian approach:



Examples of houses



Structural Inference

Logic Inference:	Infer knowledge by means of logic
	All men are mortal
	Socrates is a man
	→ Socrates is mortal
Statistical Inference:	Infer knowledge by means of statistics

Structural Inference

Logic Inference: Infer knowledge by means of logic

All men are mortal

Socrates is a man

→ Socrates is mortal

Statistical Inference: Infer knowledge by means of statistics

Grammatical Inference: Infer a grammar by means of logic

Structural Inference: Infer a structure by means of statistics

Structural Inference

Logic Inference: Infer knowledge by means of logic

All men are mortal

Socrates is a man

→ Socrates is mortal

Statistical Inference: Infer knowledge by means of statistics

Grammatical Inference: Infer a grammar by means of logic

Structural Inference: Infer a structure by means of statistics

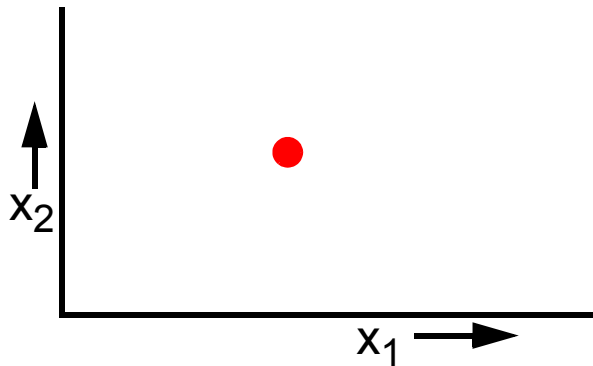
Is there something like:

Structural Inference: Infer knowledge by means of structure?

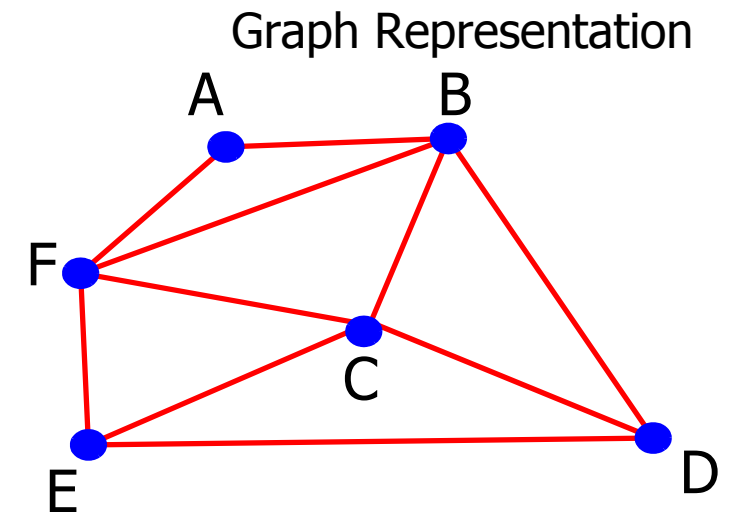
Representations



Feature Space Representation



Features: sizes, colors, angles
Relations: lost
Generalization: easy, many examples needed
overlapping classes



Relations: windows, door, roof
Features: node attributes
Generalization: difficult
often no class overlap

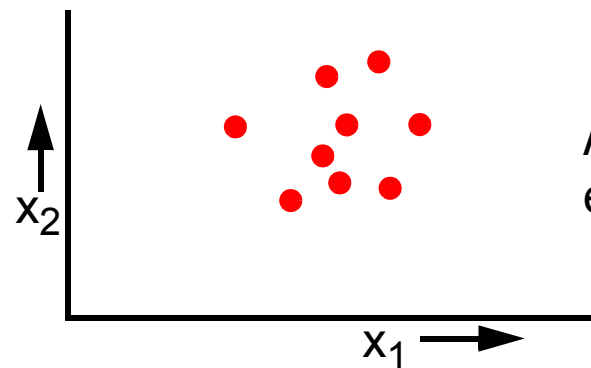
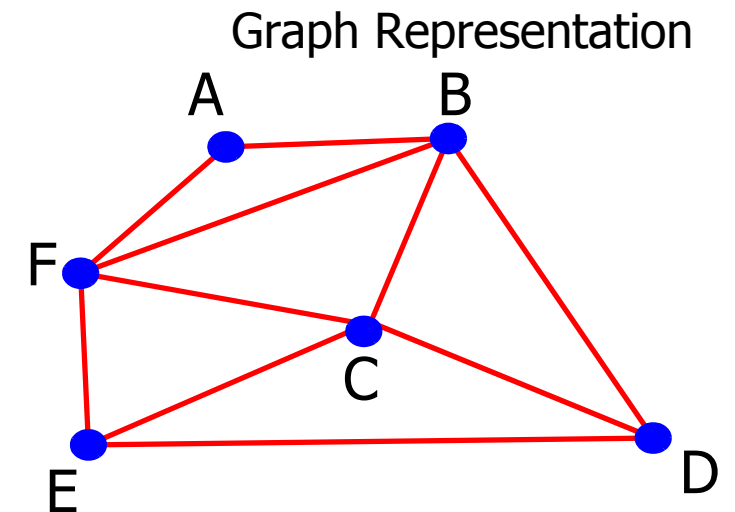
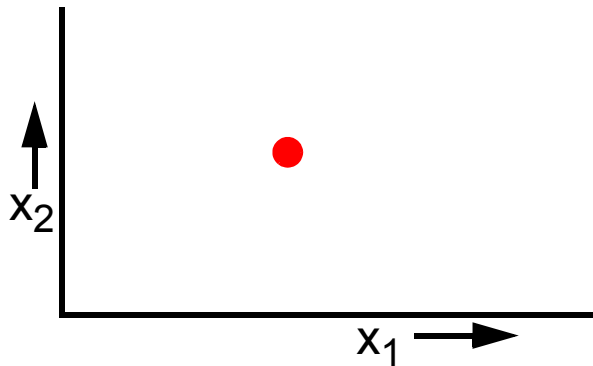
Is there something in between?

If we want to gain something, we should be prepared to lose something

Intermediate Representations?



Feature Space Representation

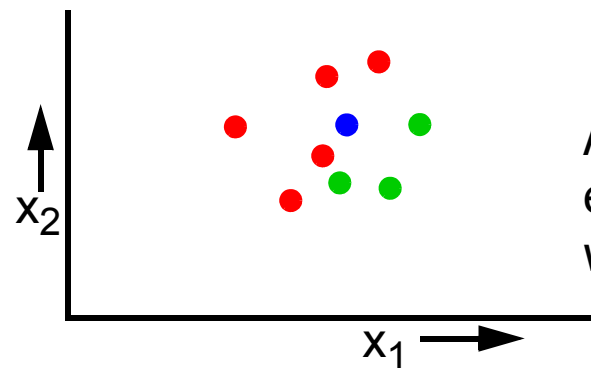
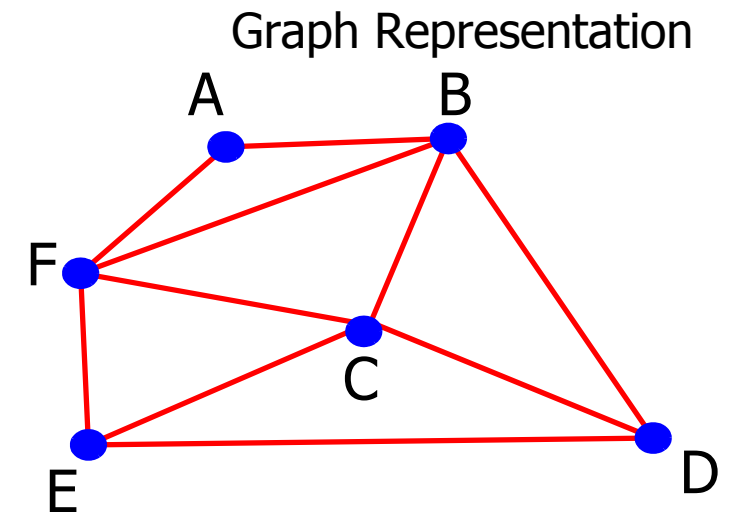
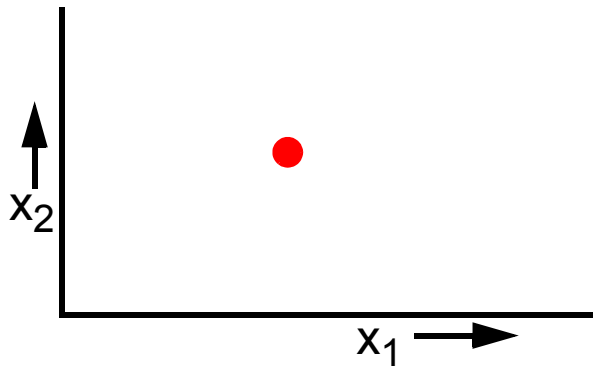


A set of points
e.g. feature representations of all regions

Intermediate Representations?

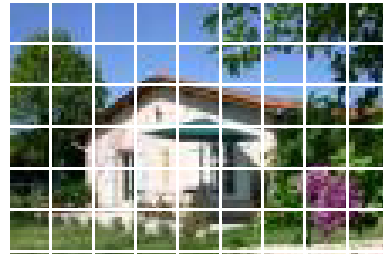


Feature Space Representation

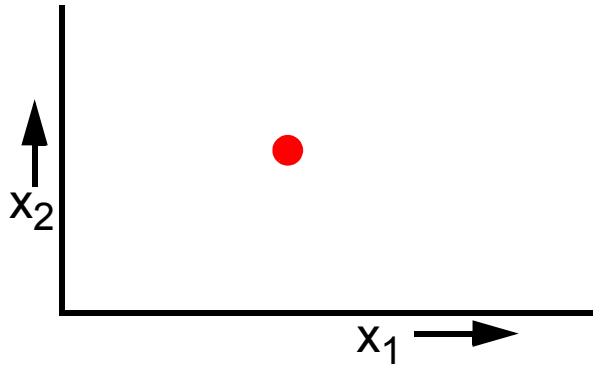


A labeled set of points
e.g. feature representations of
walls, windows, doors, roofs

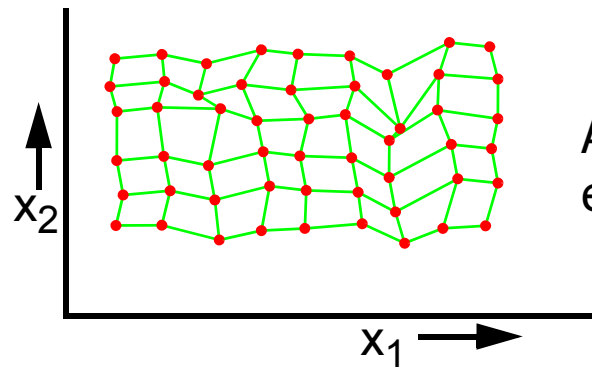
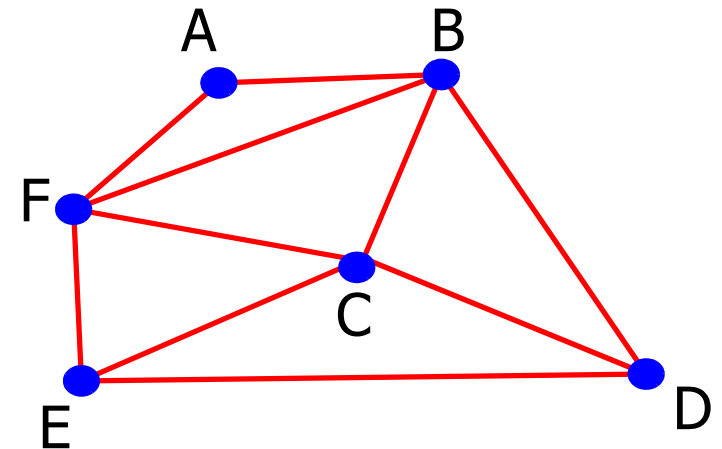
Intermediate Representations?



Feature Space Representation

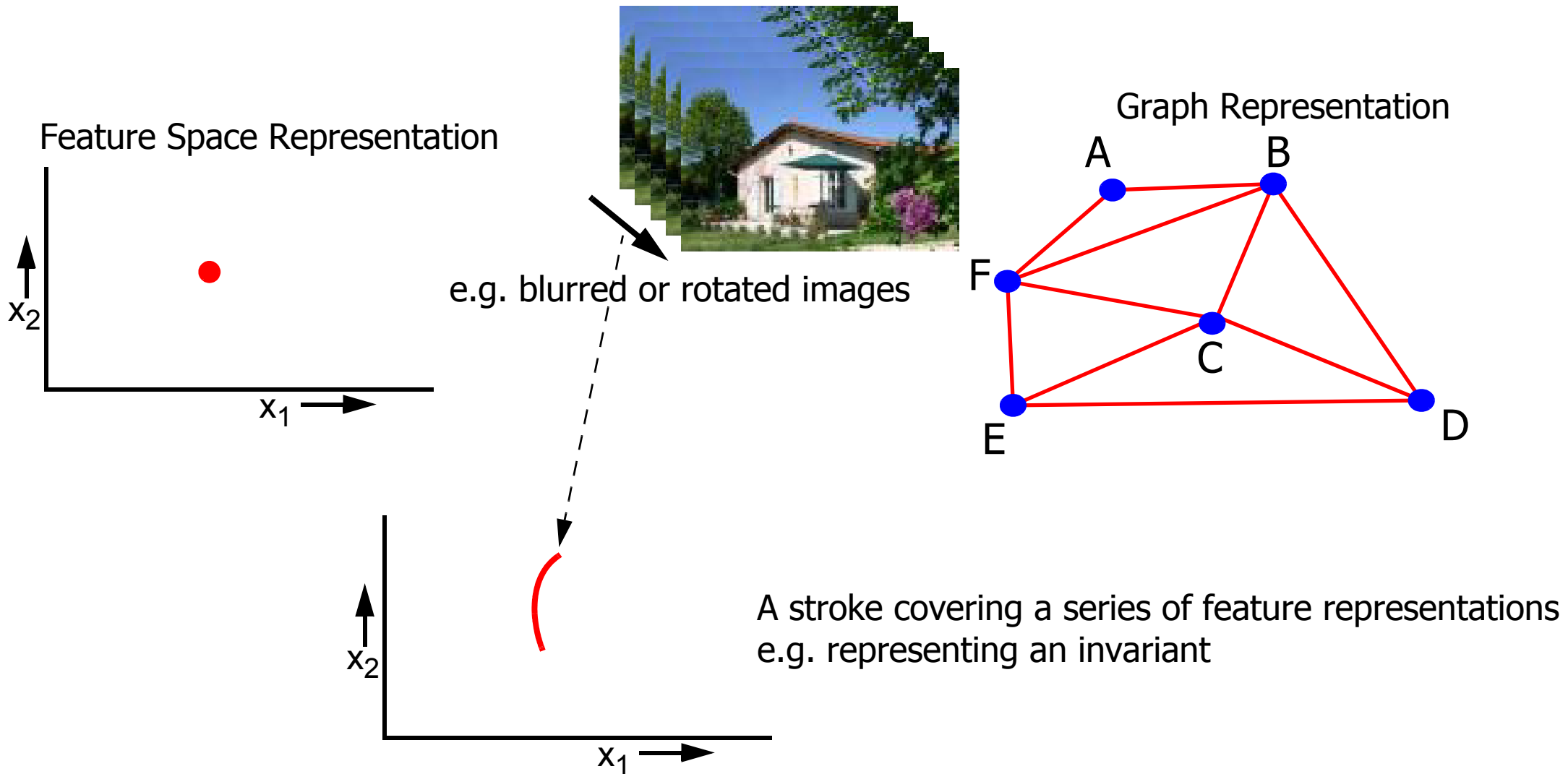


Graph Representation

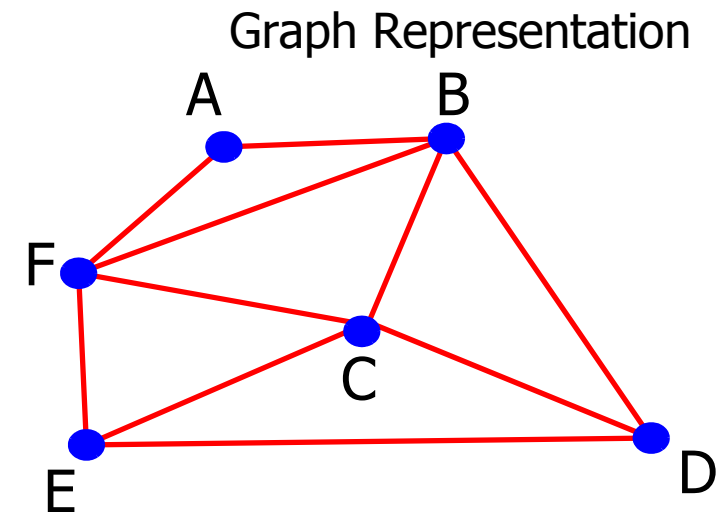
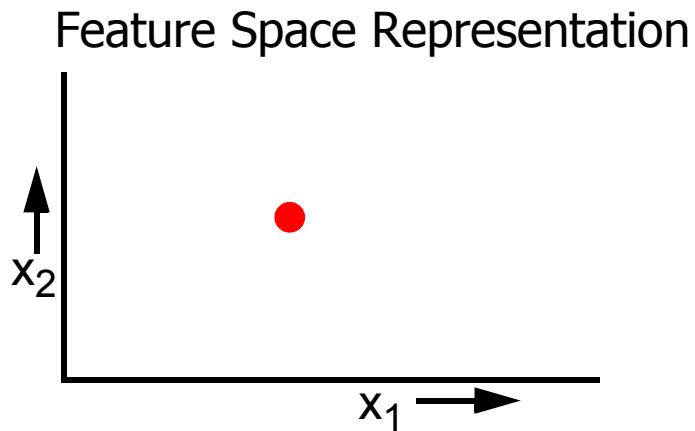


A connected set of points
e.g. feature representations of all image patches

Intermediate Representations?



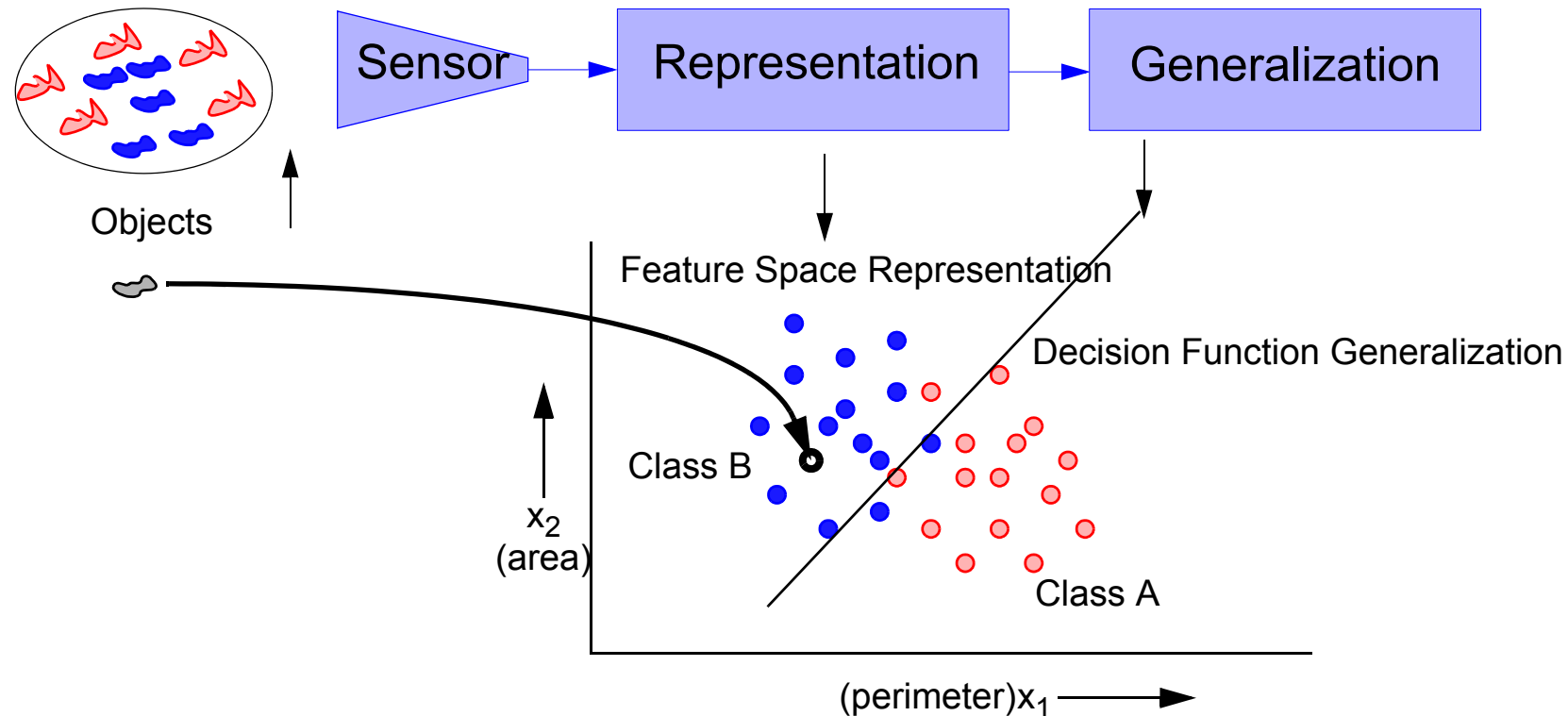
Intermediate Representations?



Single point feature space representations are well supported.
All others directly complicate the representation of classes
and classification functions.

Is a smaller step possible?

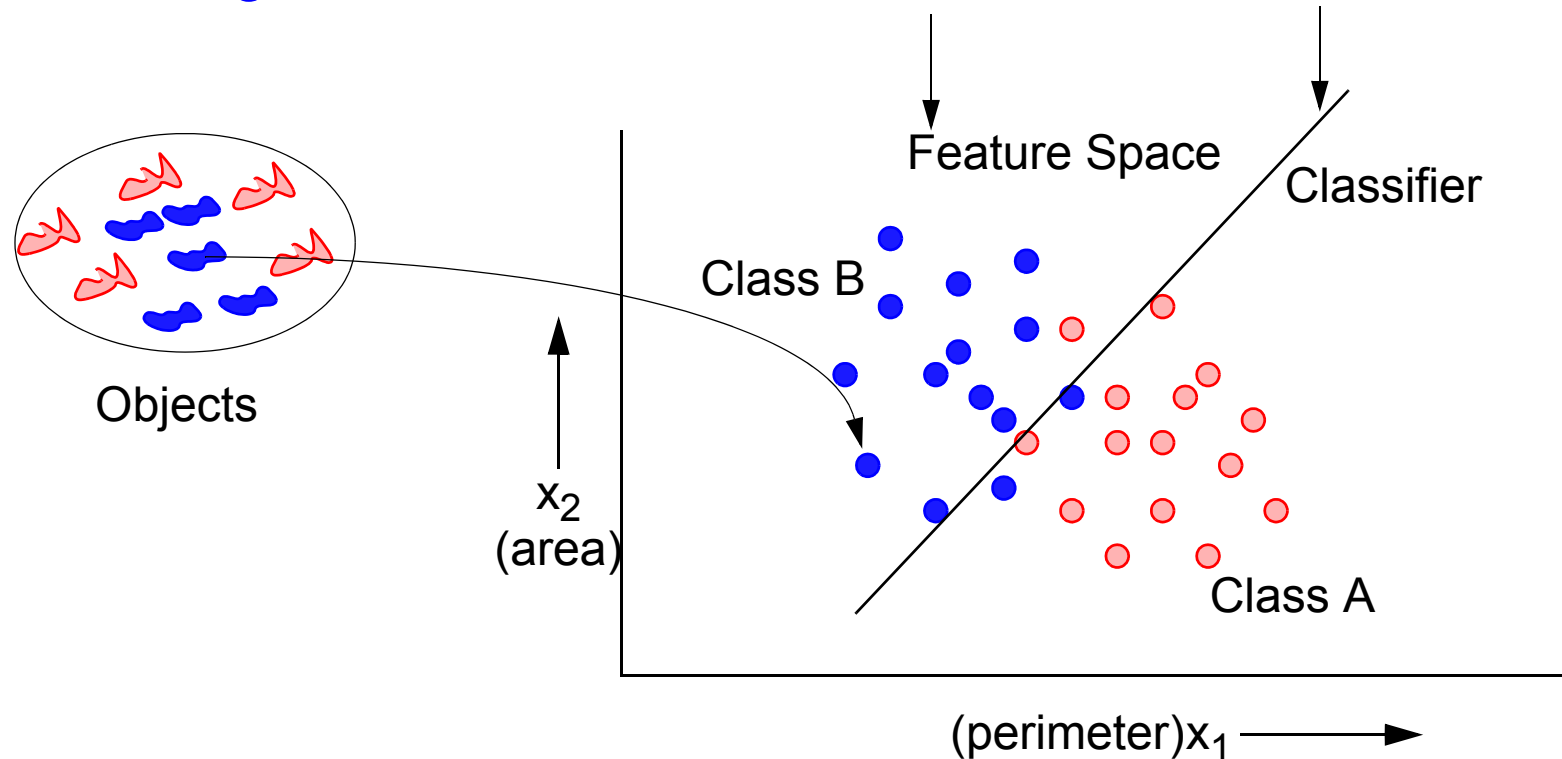
The Pattern Recognition System



Learning from examples
Finding concepts (classes) from observations

Feature Space

Training Set → Representation → Generalization

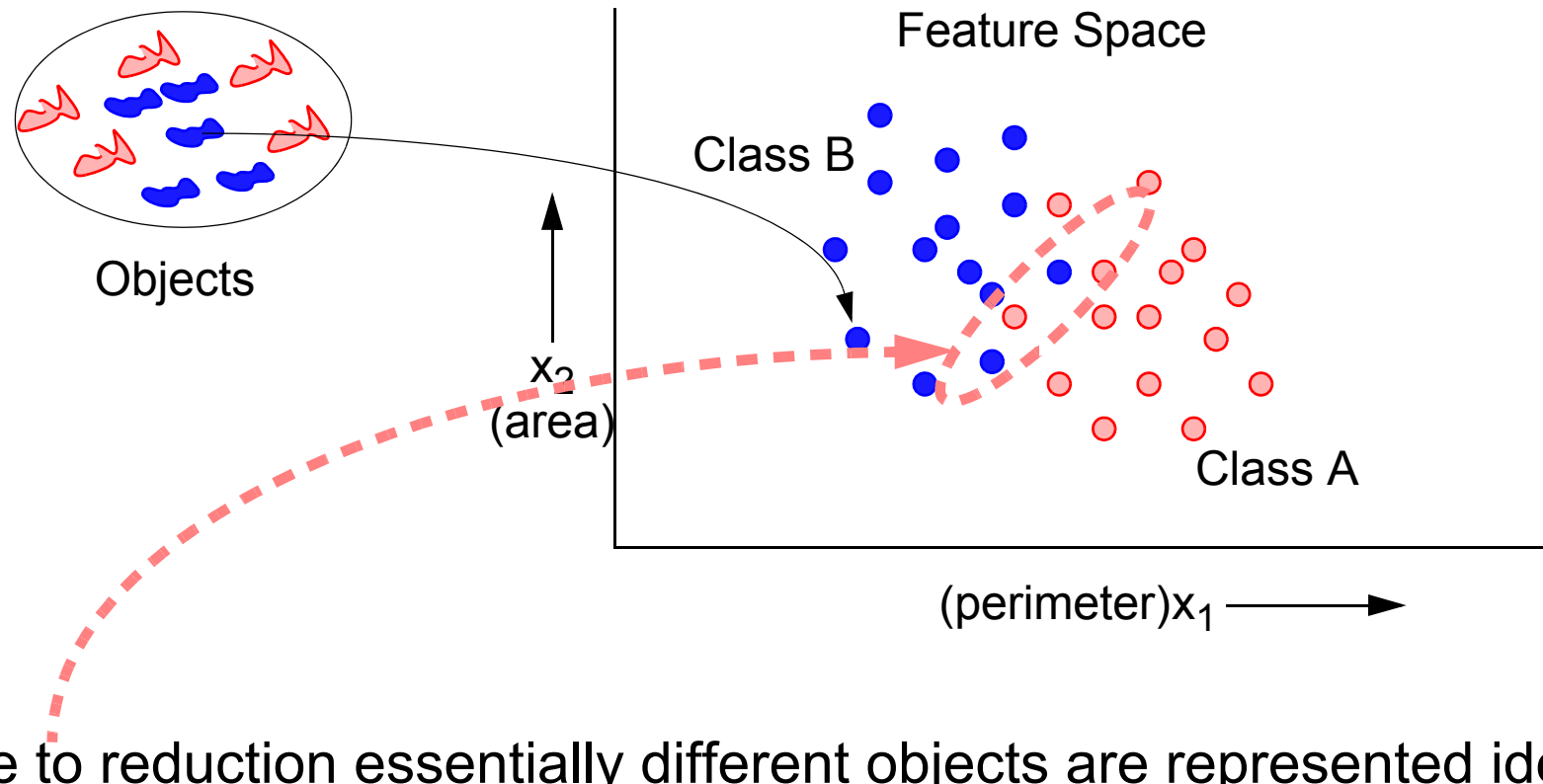


Knowledge → good features → (almost) separable classes

Lack of knowledge → (too many) bad features → hardly separable classes

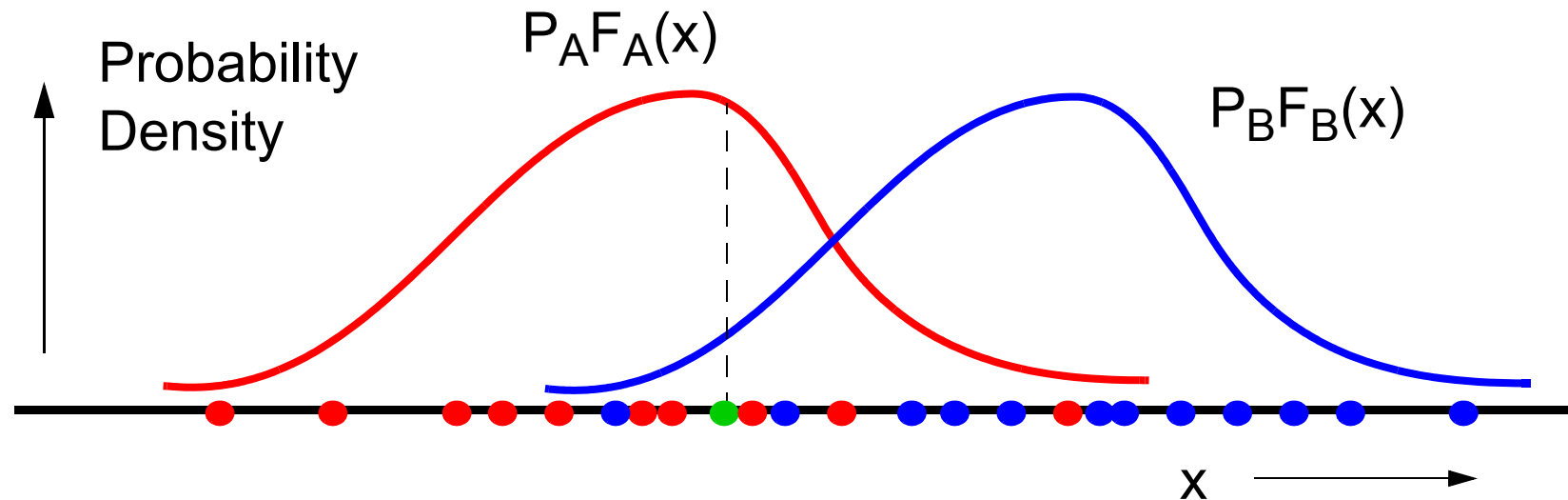
Many features ~ Lack of knowledge, **but objects better represented**

Features Reduce → Overlapping Classes



Due to reduction essentially different objects are represented identically
→ The feature representation needs a statistical (probabilistic) generalization

Features Reduce → Overlapping Classes → Probabilities



Best guess is to choose the most 'probable' class (→ small error).

→ Good for overlapping classes.

→ Assumes

- the existence of a probabilistic class distribution
- a representative set of examples.

No Feature Reduction

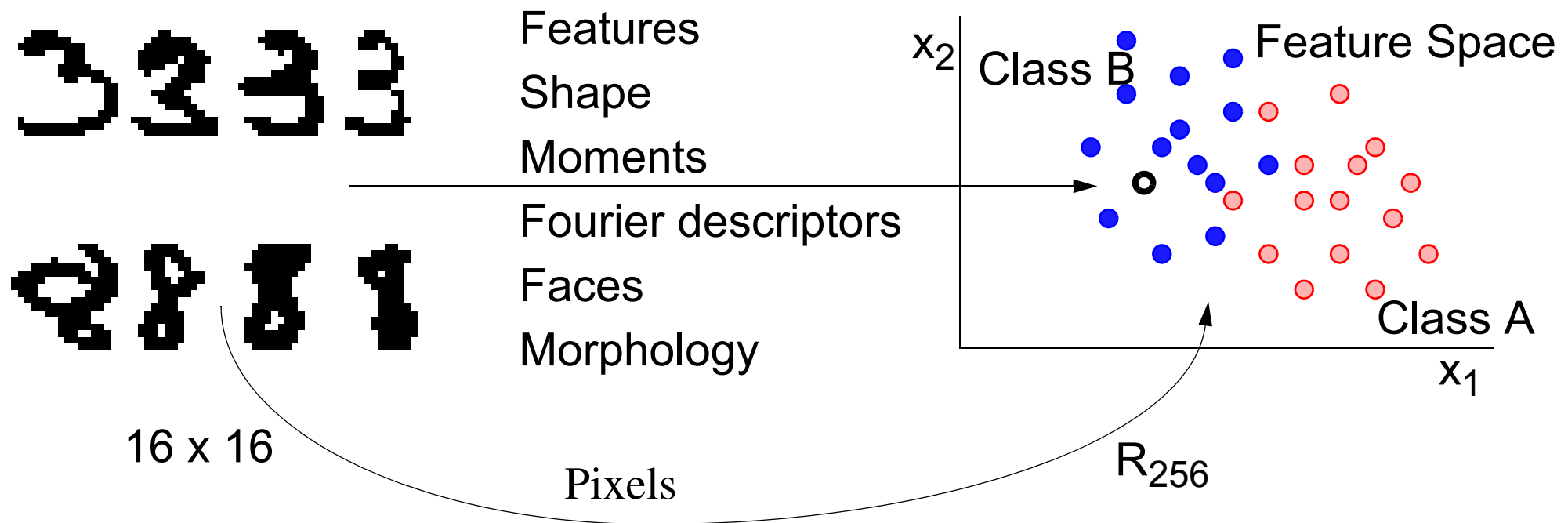
The feature representation enforces class overlap.
To be solved by a probabilistic approach.

However:

Are densities needed in high dimensional spaces?
Are classes densities?

- Objects described by structures
- Classes interpreted by structures

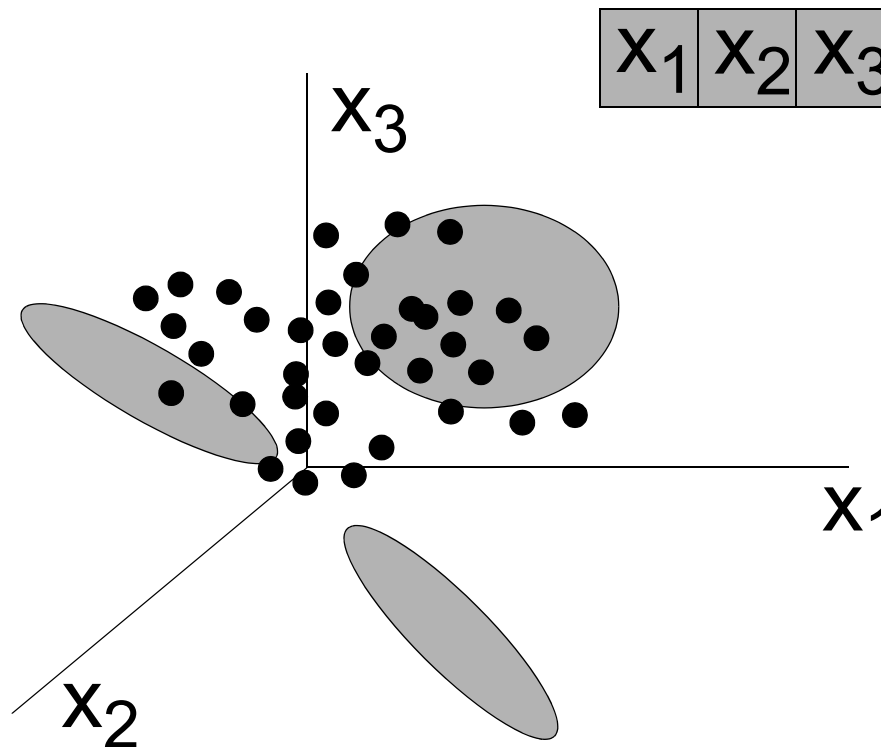
Pixel (Sample) Representation



Pixels are more general, initially complete representation
Large datasets available → good results for OCR

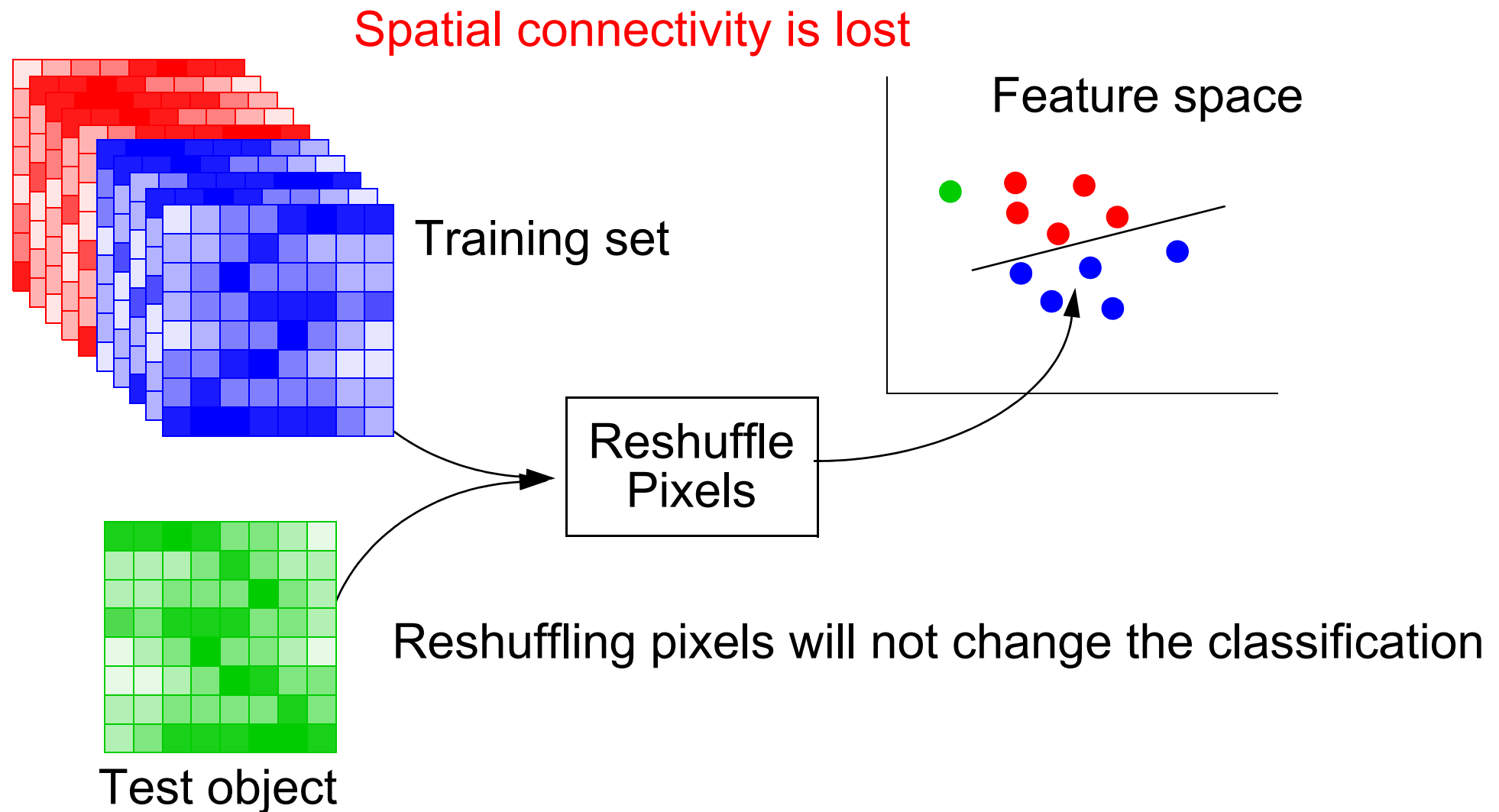
The Connectivity Problem in the Pixel Representation

Spatial connectivity is lost

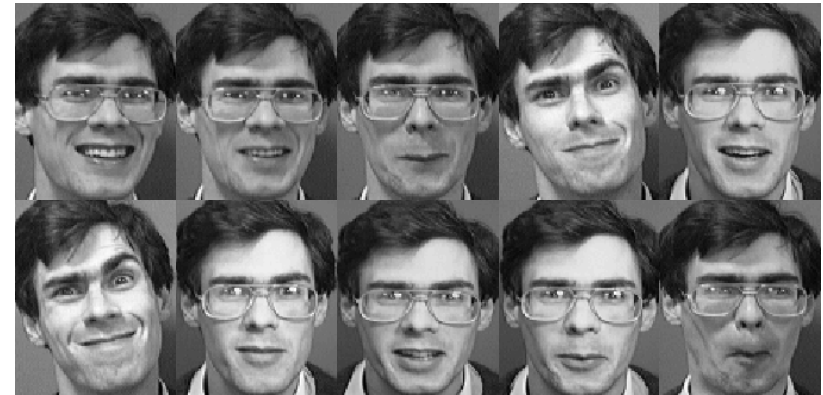


Dependent (connected) measurements are represented independently,
The dependency has to be rediscovered from the data.

The Connectivity Problem in the Pixel Representation



High dimensional data often does not overlap

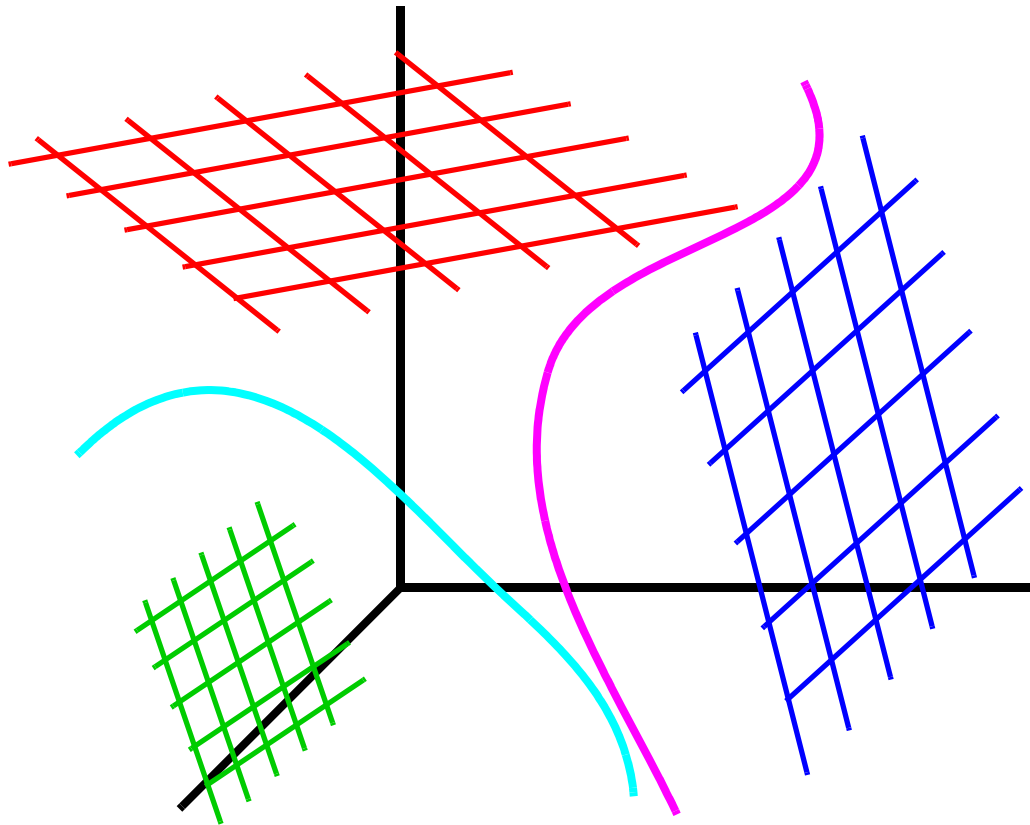


Complete feature representations, which enable the reconstruction of human recognizable, may yield separable classes.

There is no picture that could be member of different classes.

Structural information is not yet there.

Domain based classification

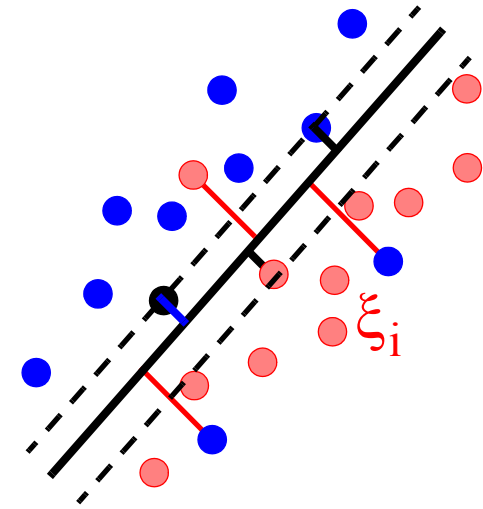


No well sampled training sets are needed.

Classifiers still to be developed.

Class structure $\longleftrightarrow$ Object invariants

SVM



The Support Vector Classifier:

$$\min_{\alpha}: \|W\| + C \sum \xi_i$$

$\min_{\alpha}: \|W\|$: maximize the margin, minimize # support vectors: most simple
(**distance argument, Occam**)

$\min_{\alpha}: \sum \xi_i$: minimize the total error
(**probabilistic argument, Bayes**)

SVM --> Domain based classifier

Objects

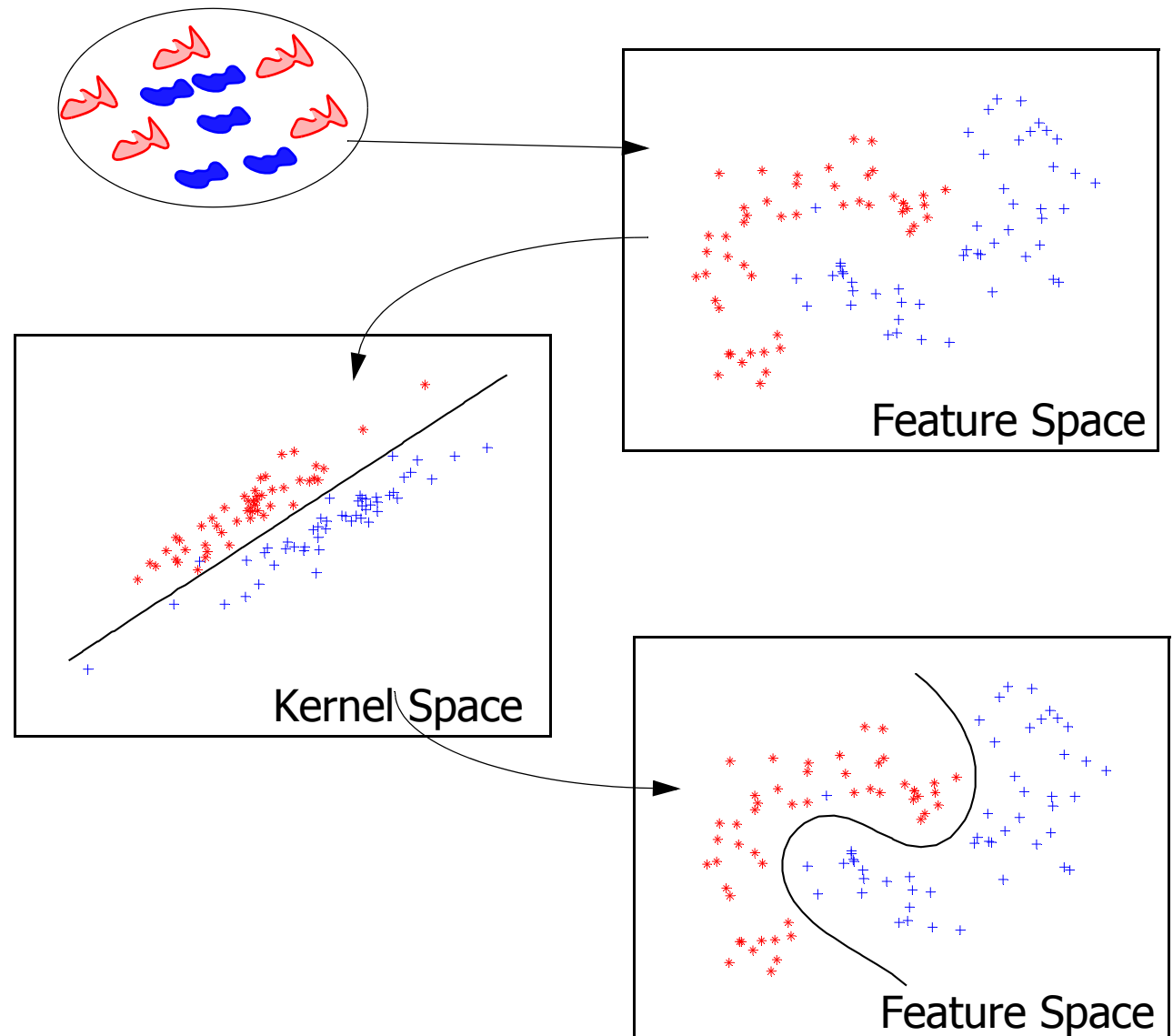
Feature Representation

Kernel: $K(x,y) = N_x(y,\sigma)$

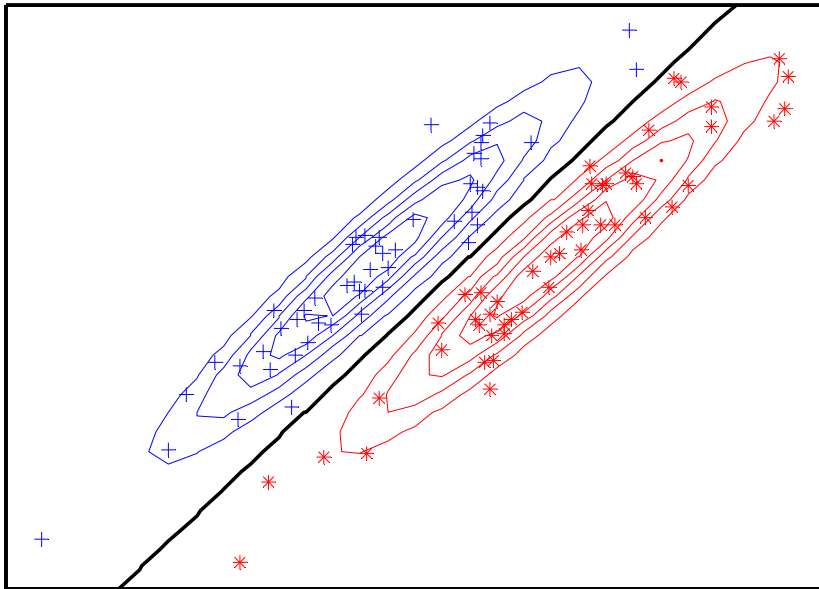
Kernel (Hilbert) Space

Linear SVM

Non-Linear Classifier

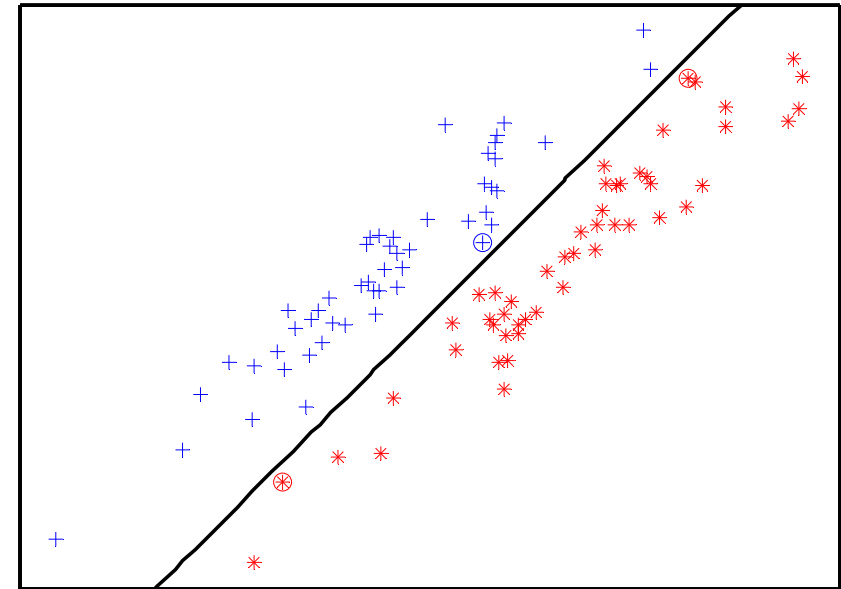


Fisher's LD $\longleftrightarrow$ SVM on Gaussian Data



Fisher's LD

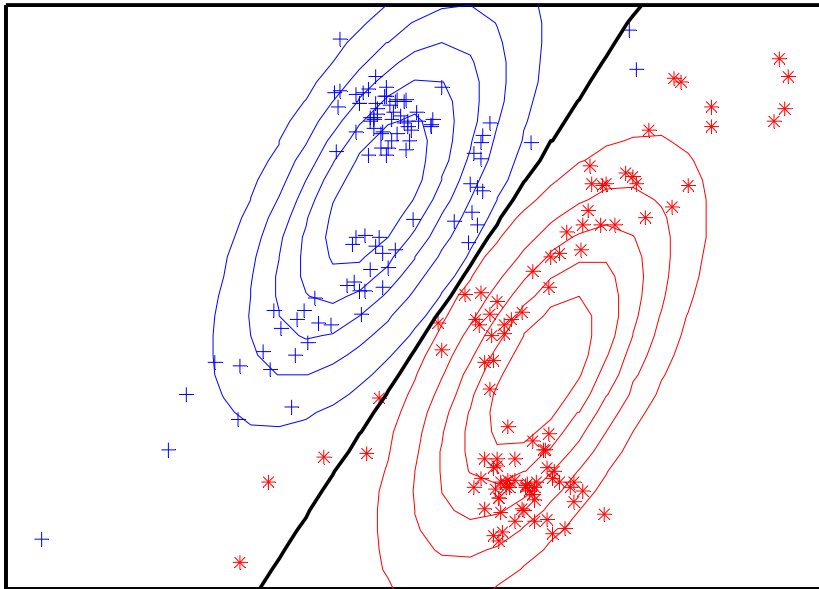
Sensitive for class distributions



SVM

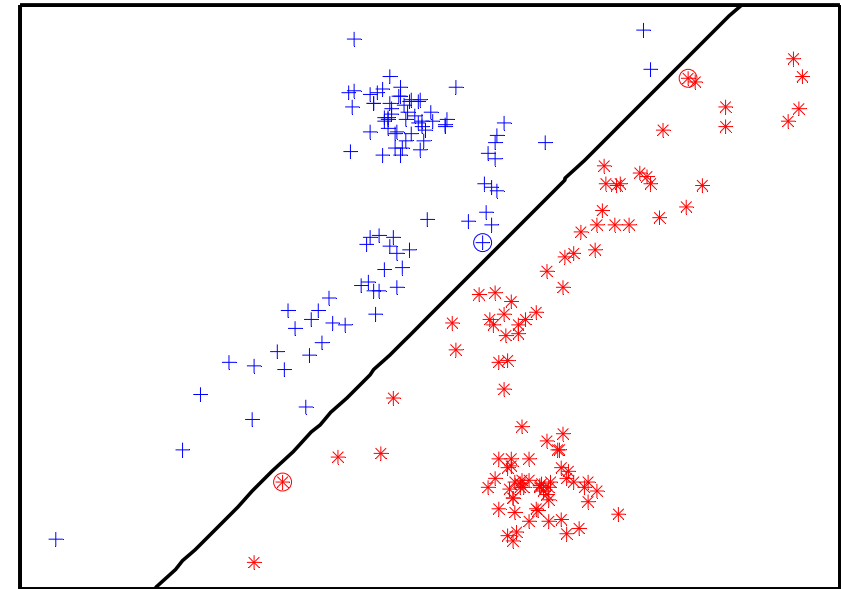
Sensitive for between-class boundaries

Fisher's LD $\leftrightarrow$ SVM on Non-Gaussian Data



Fisher's LD

Sensitive for class distributions



SVM

Sensitive for between-class boundaries

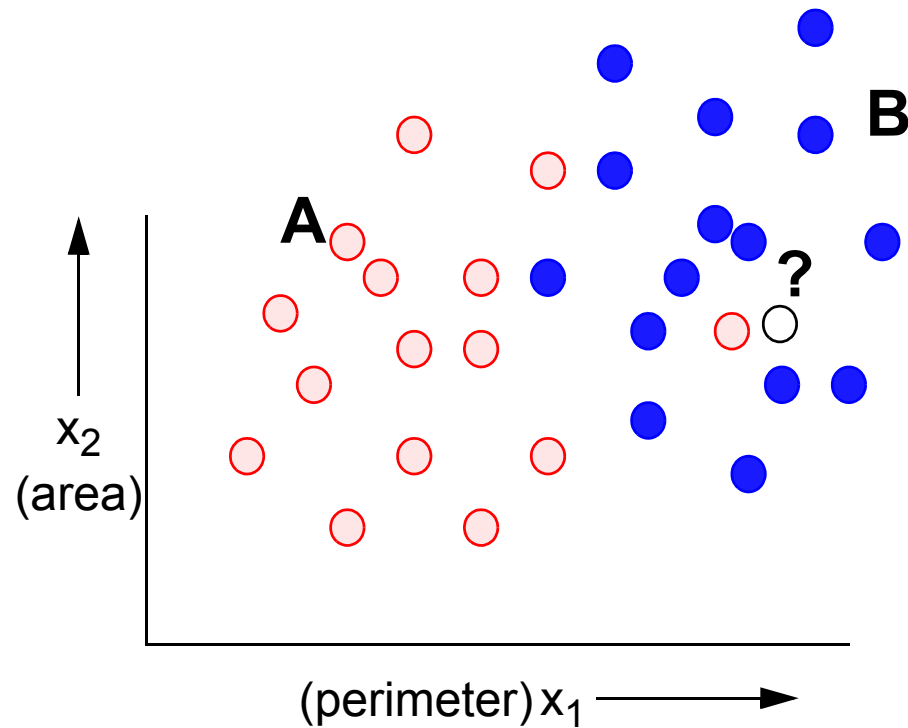
Generalization Strategies: Densities versus Distances



Why is this an apple and not a pear?

1. It is more similar to known apples than to known pears.
2. Most objects that look like this appear to be apples and not pears.

Densities versus Distances



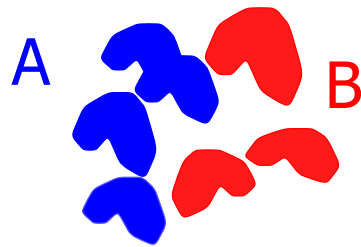
? to be classified as

A - because it is most closest to an object A

B - because the local density of B is larger

Dissimilarity Representation

Define dissimilarity measure d_{ij} between raw data of objects i and j



Given labeled training set T



Unlabeled object x to be classified

$$D_T = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} & d_{17} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} & d_{27} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} & d_{37} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} & d_{46} & d_{47} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} & d_{56} & d_{57} \\ d_{61} & d_{62} & d_{63} & d_{64} & d_{65} & d_{66} & d_{67} \\ d_{71} & d_{72} & d_{73} & d_{74} & d_{75} & d_{76} & d_{77} \end{pmatrix}$$

$$\mathbf{d}_x = (d_1 \ d_2 \ d_3 \ d_4 \ d_5 \ d_6 \ d_7)$$

The traditional Nearest Neighbor rule (template matching) just finds:
 $\text{label}(\arg\min_{\text{trainset}}(d_i)),$
 without using D_T . Can we do any better?

Dissimilarity Space

Dissimilarities

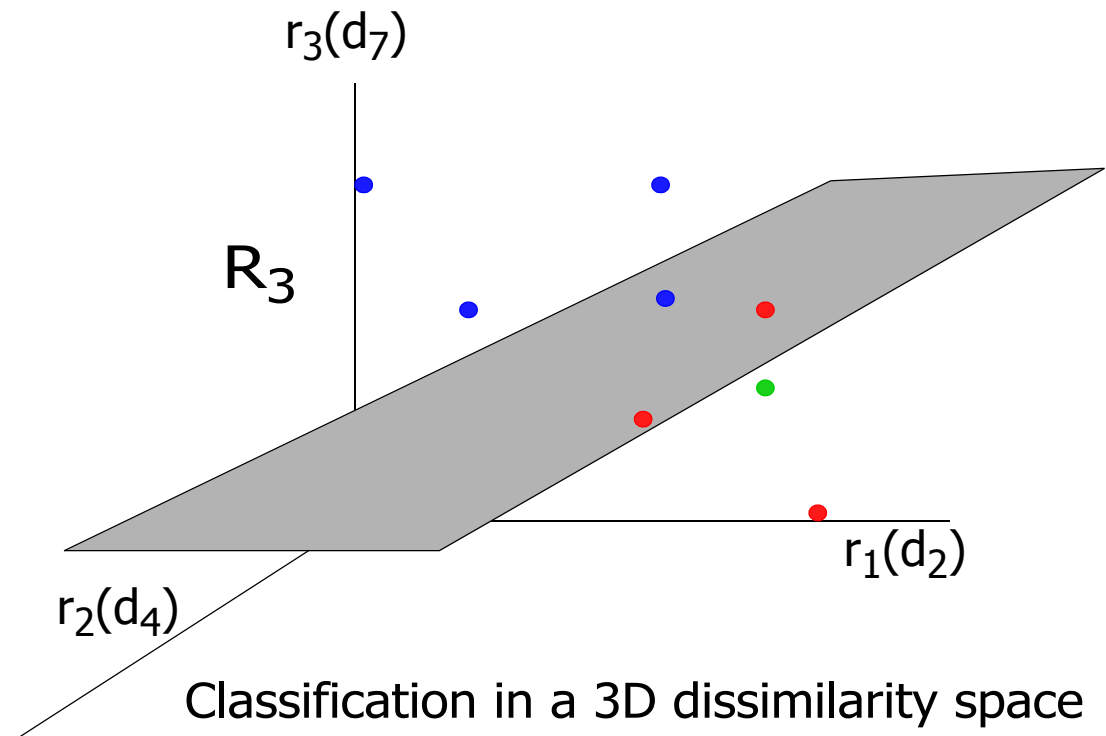
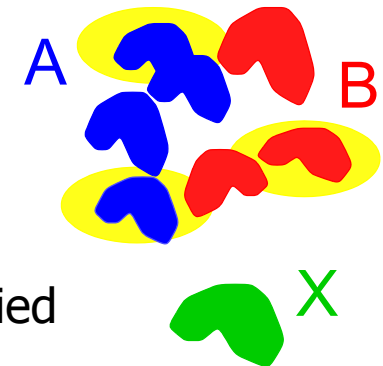
$$D_T = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} & d_{17} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} & d_{27} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} & d_{37} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} & d_{46} & d_{47} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} & d_{56} & d_{57} \\ d_{61} & d_{62} & d_{63} & d_{64} & d_{65} & d_{66} & d_{67} \\ d_{71} & d_{72} & d_{73} & d_{74} & d_{75} & d_{76} & d_{77} \end{pmatrix}$$

Selection of 3 objects for representation

$$\mathbf{d}_x = (d_1 \ d_2 \ d_3 \ d_4 \ d_5 \ d_6 \ d_7)$$

Given labeled training set T

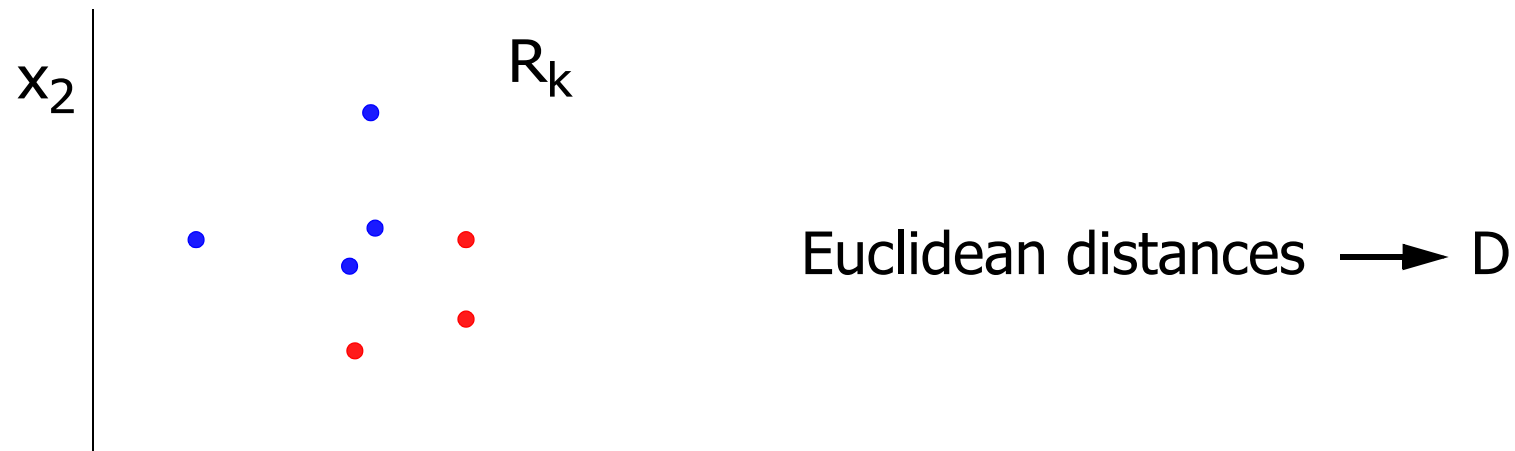
Unlabeled object x to be classified



Embedding



Is there a feature space X for which $\text{Dist}(X, X) = D$?



(Pseudo-)Euclidean Embedding

$m \times m$ D is a given, imperfect dissimilarity matrix of training objects.

Construct inner-product matrix: $B = -\frac{1}{2}JD^{(2)}J$, $J = I - \frac{1}{m}\mathbf{1}\mathbf{1}^T$

Eigenvalue Decomposition ($B = Q\Lambda Q^T$)_p,

Select k eigenvectors: $X = Q_k\Lambda_k^{\frac{1}{2}}$ (problem: $\Lambda_k < 0$)

Let $\mathfrak{I}_k$ be a $k \times k$ diag. matrix, $\mathfrak{I}_k(i,i) = \text{sign}(\Lambda_k(i,i))$ $X = Q_k|\Lambda_k|^{\frac{1}{2}}\mathfrak{I}_k$

$\Lambda_k(i,i) < 0 \rightarrow \text{Pseudo-Euclidean}$

$m \times n$ D_z is the dissimilarity matrix between new objects and the training set.

The inner-product matrix: $B_z = -\frac{1}{2}(D_z^{(2)}J - \frac{1}{n}\mathbf{1}\mathbf{1}^T D^{(2)}J)$

The embedded objects: $Z = B_z Q_k|\Lambda_k|^{\frac{1}{2}}\mathfrak{I}_k$

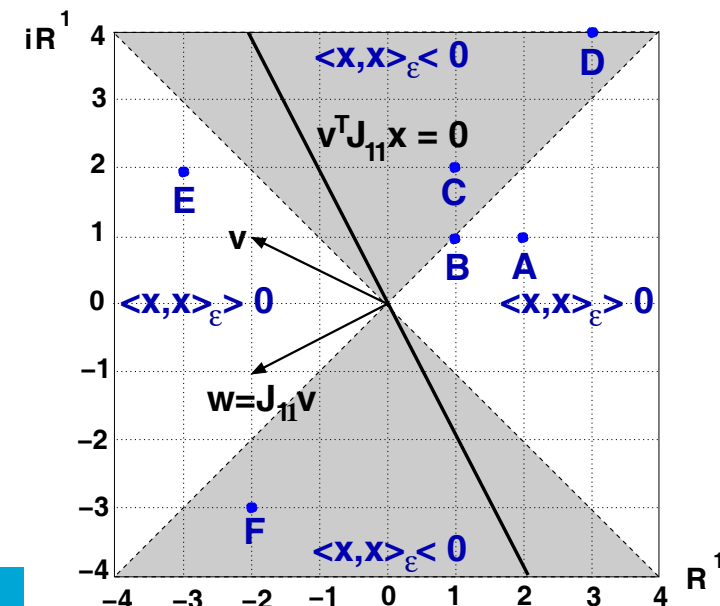
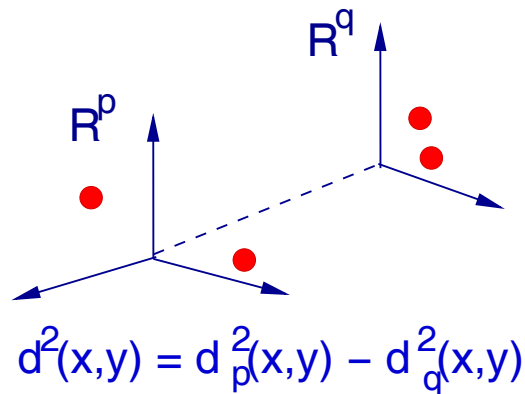
Pseudo-Euclidean Space (Krein Space)

If D is non-Euclidean, B has p positive and q negative eigenvalues.

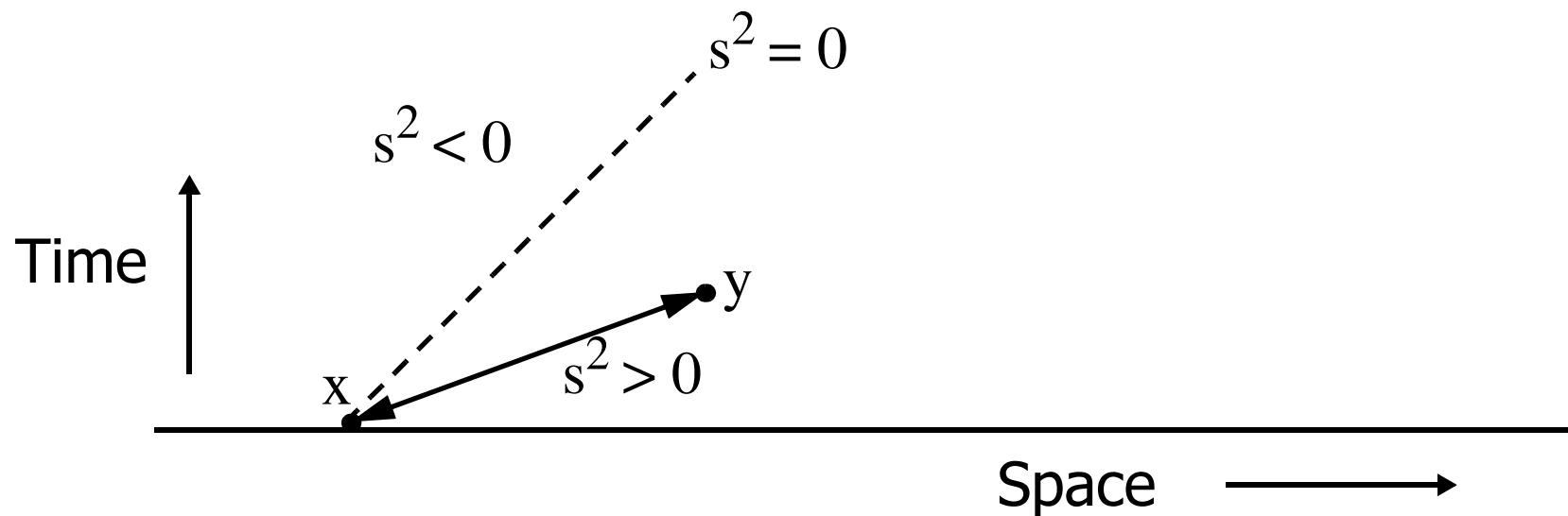
A pseudo-Euclidean space ε with signature (p,q) , $k = p+q$, is a non-degenerate inner product space $\mathfrak{R}^k = \mathfrak{R}^p \oplus \mathfrak{R}^q$ such that:

$$\langle x, y \rangle_\varepsilon = x^T \mathfrak{I}_{pq} y = \sum_{i=1}^p x_i y_i - \sum_{i=p+1}^q x_i y_i, \quad \mathfrak{I}_{pq} = \begin{bmatrix} I_{p \times p} & 0 \\ 0 & -I_{q \times q} \end{bmatrix}$$

$$d_\varepsilon^2(x, y) = \langle x - y, x - y \rangle_\varepsilon = d_p^2(x, y) - d_q^2(x, y)$$



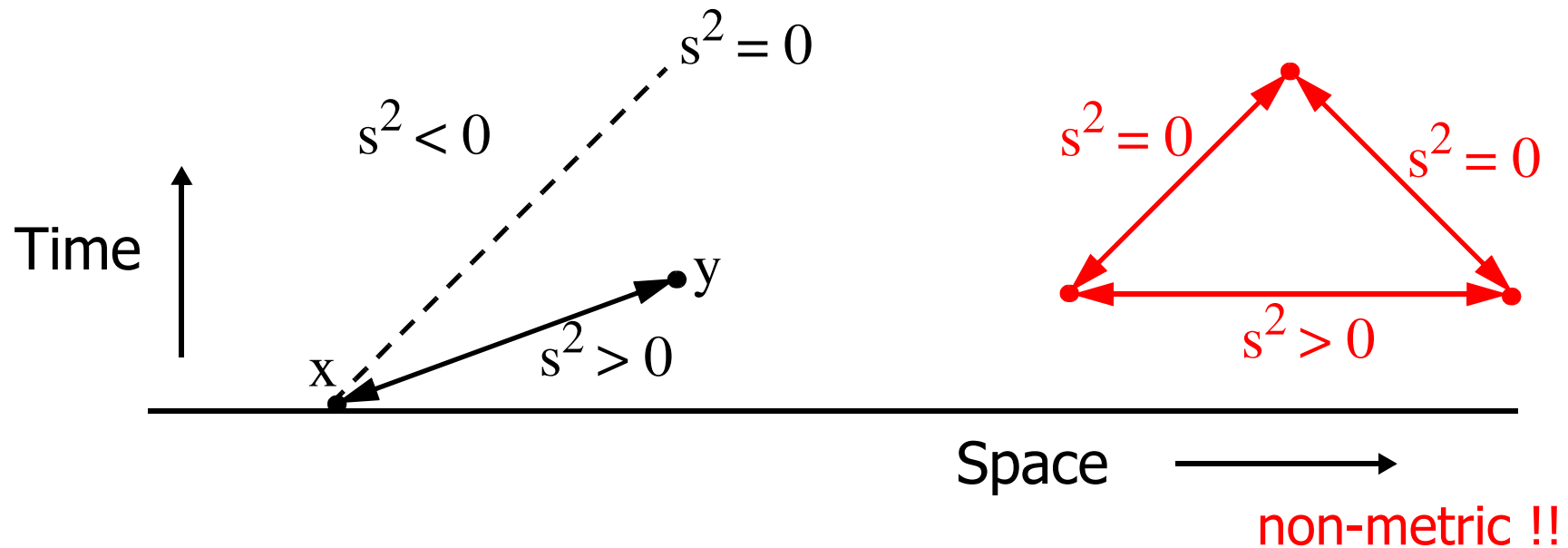
Minkowski Space → Pseudo-Euclidean Space



SpaceTime distance:

$$s^2 = \sum_{i=1}^3 (x_i - y_i)^2 - (t_x - t_y)^2$$

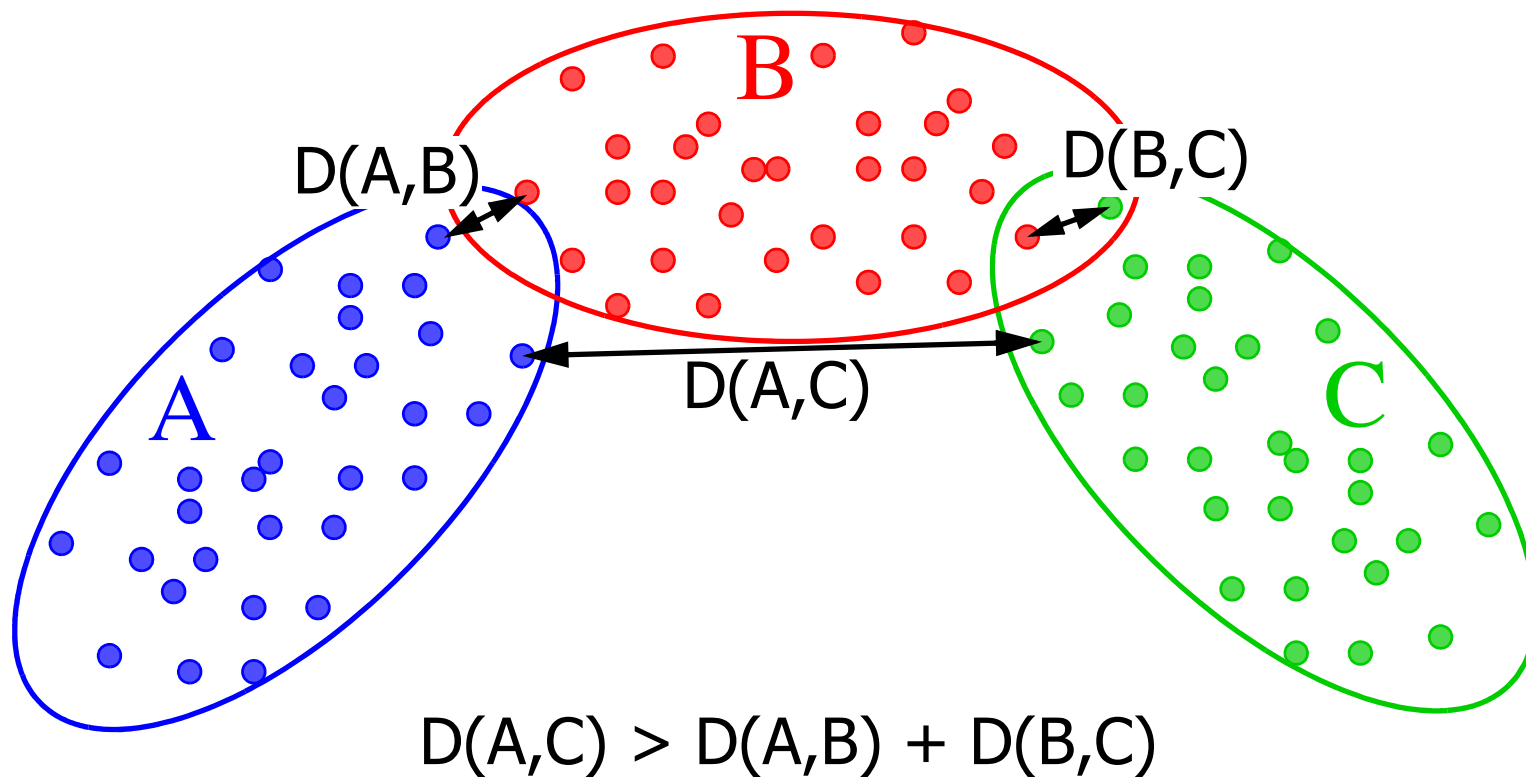
Minkowski Space → Pseudo-Euclidean Space



SpaceTime distance:

$$s^2 = \sum_{i=1}^3 (x_i - y_i)^2 - (t_x - t_y)^2$$

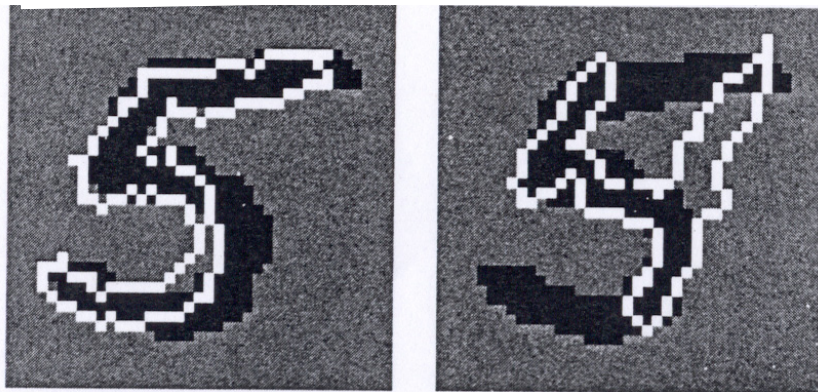
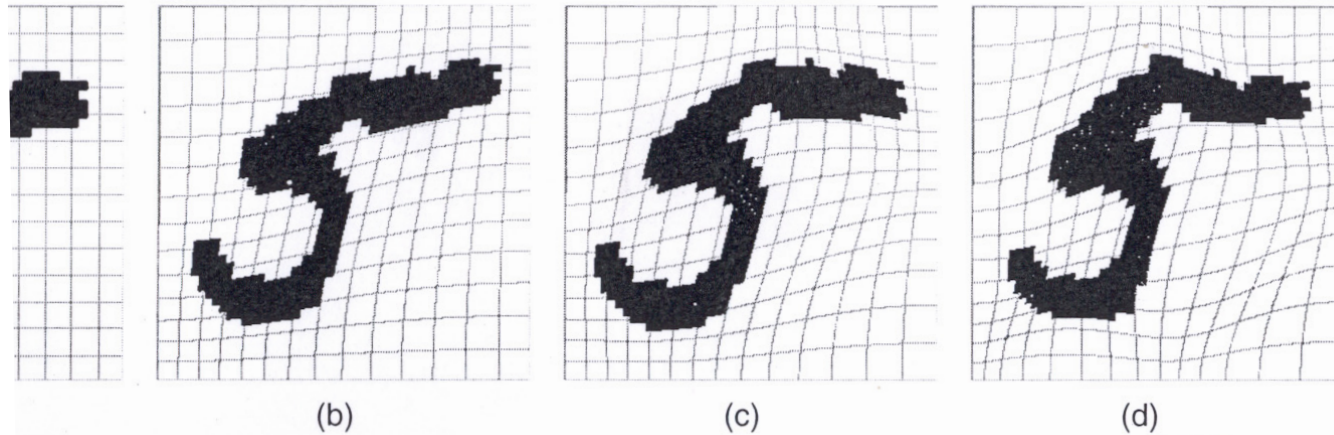
Non-Metric Dissimilarities in Pattern Recognition



The single-linkage cluster distance is non-metric

Dissimilarity based Structural PR - Transformations

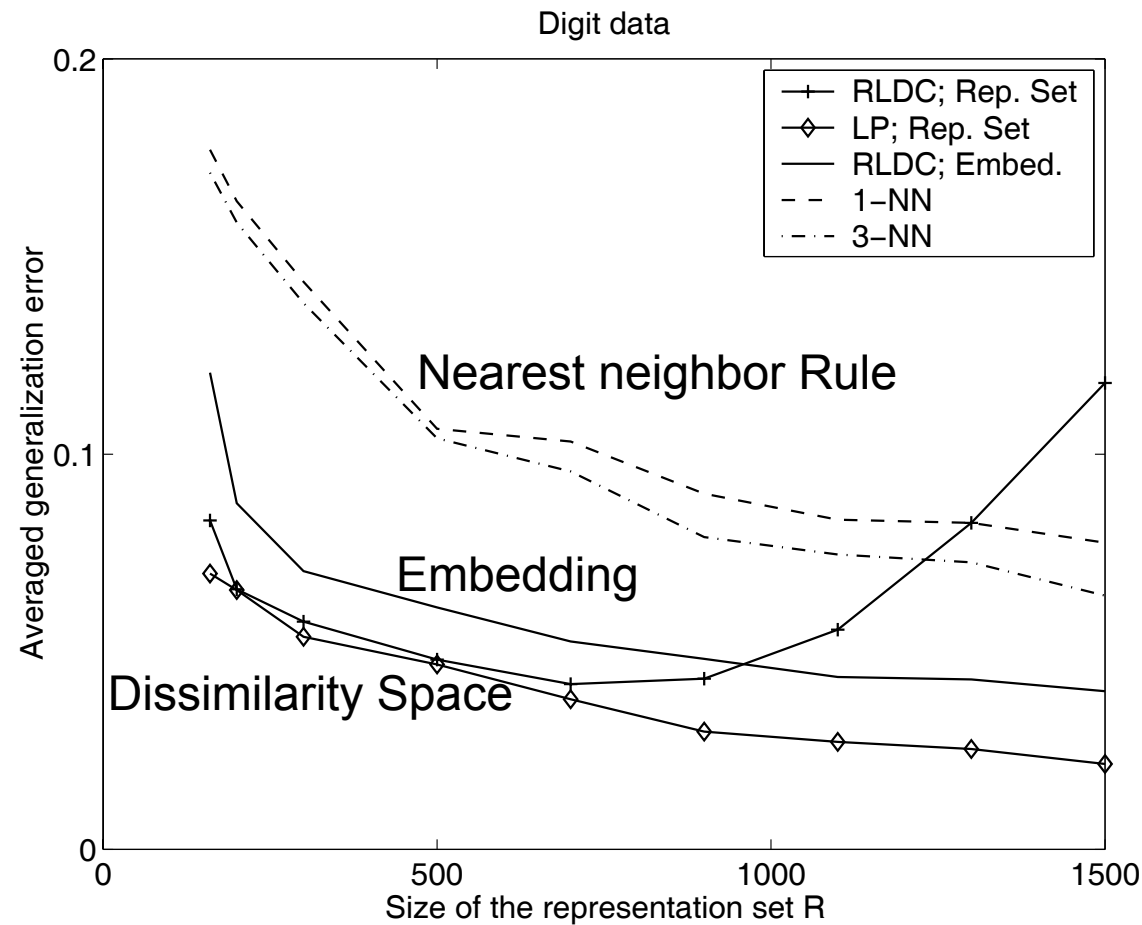
Examples of deformed templates



Matching new objects x to various templates y
 $\text{class}(x) = \text{class}(\arg\min_y(D(x, y)))$

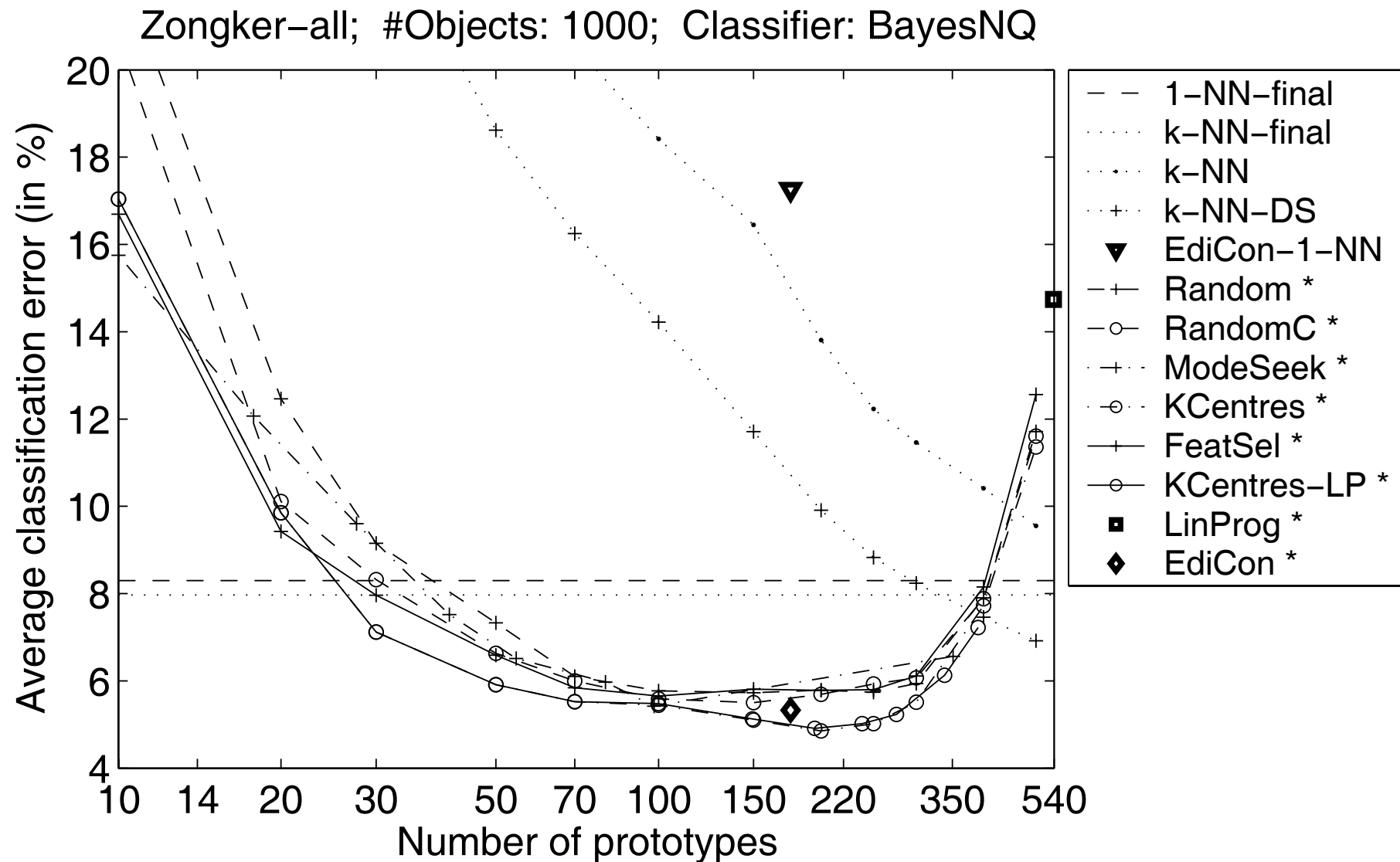
A.K. Jain, D. Zongker, Representation and recognition of handwritten digit using deformable templates, *IEEE-PAMI*, vol. 19, no. 12, 1997, 1386-1391.

Three Approaches Compared for the Zongker Data



Dissimilarity Space better than Embedding better than Nearest Neighbor Rule

Prototype Selection on Zongker Data in Dissimilarity Space

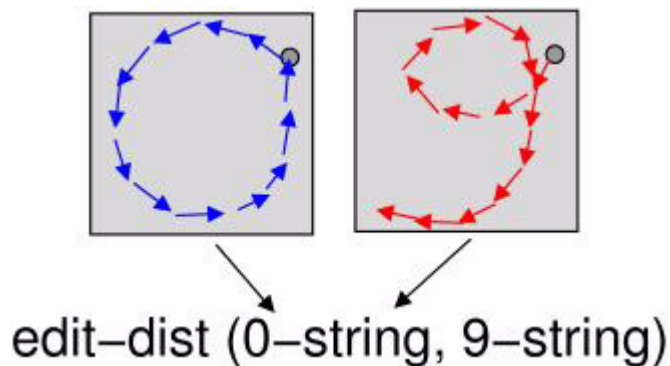


Edit Distances for Strings

Pen-written digits, (H. Bunke, Bern)



An edit distance between the string contours is applied with fixed insertion and deletion costs, and the Euclidean distance substitution cost.



The measure is moderately non-metric and non-Euclidean.

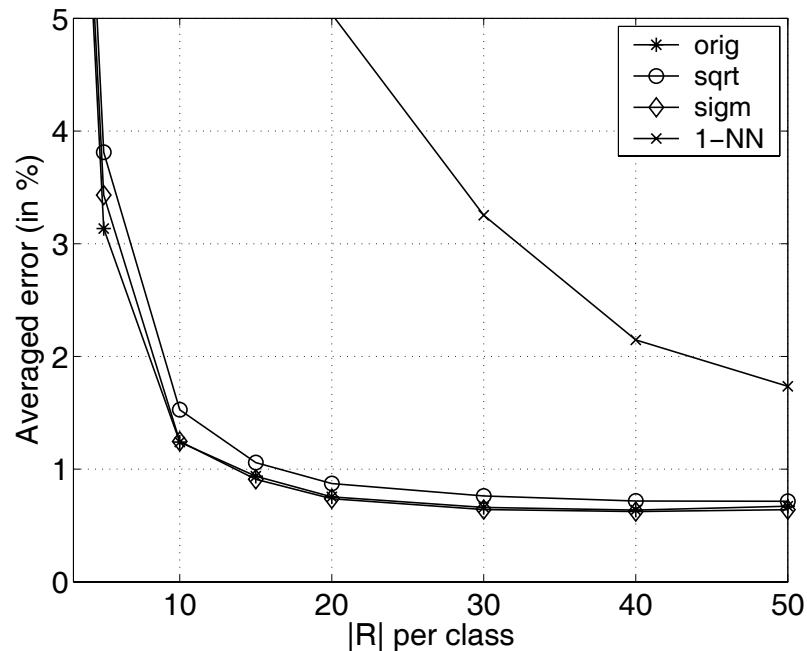
Classification Results for Pen-written Digits

Representation $D(T,R)$,

Fixed training set: $|T| = 10 \times 200$, $R \subset$ changes.

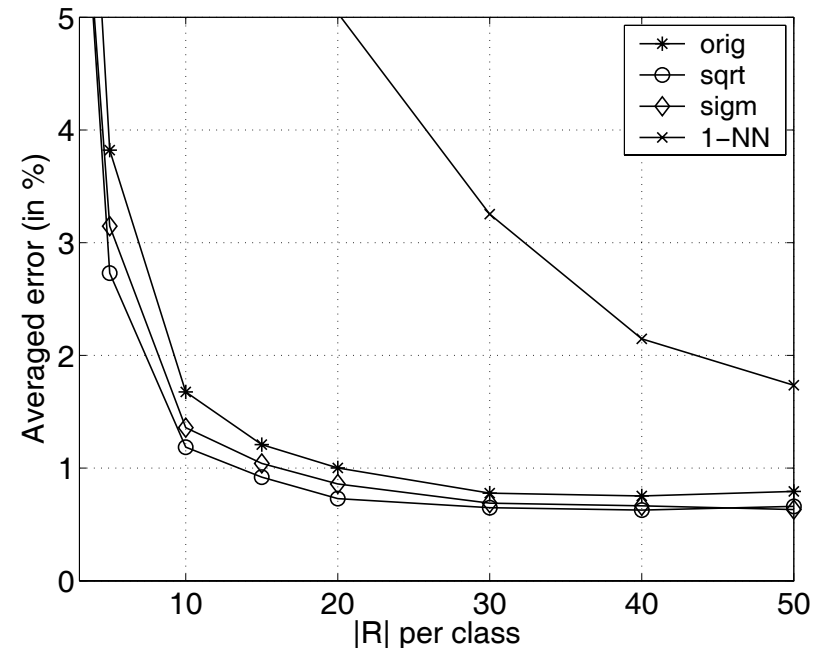
Fixed test set: $|S| = 10 \times 200$. Dimensionalities of the spaces: $0.3 |R|$.

RQDC0.2; PCA-dissimilarity space; $R \subset T$; $|T|=100$; $\dim=0.3|R|$



Dissimilarity Space

RQDC0.2; ps.-Euclidean space; $R \subset T$; $|T|=100$; $\dim=0.3|R|$



Pseudo-Euclidean Space

Quadratic classifiers

Dissimilarity Representation $\longleftrightarrow$ Kernels

Let $R = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$

Kernel classifier: $f(\mathbf{x}) = \mathbf{w}^T K(\mathbf{x}, R) + w_0 = \sum_{w_i \in SV} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$

Linear classifier in a dissimilarity space:

$$f(D(\mathbf{x}, R)) = \mathbf{w}^T D(\mathbf{x}, R) + w_0$$

If D has an **Euclidean behavior**, then

$$K = -\frac{1}{2}JD^{(2)}J \text{ or } K = \exp\{-D^{(2)}/\sigma^2\}$$

are Mercer kernels: SVM can be directly applied, Otherwise:

- Transform D appropriately or regularize K
- Treat K as kernels in pseudo-Euclidean space: indefinite SVM

Dissimilarity Based Classifiers $\longleftrightarrow$ SVMs

Dissimilarity classification

arbitrary dissimilarity measure
full training set
complexity reduction
any classifier

SVM

Mercer kernels
reduced
included
structural risk minimization

Dissimilarity Based Classifiers $\longleftrightarrow$ SVMs

Dissimilarity classification

arbitrary dissimilarity measure

full training set

complexity reduction

any classifier

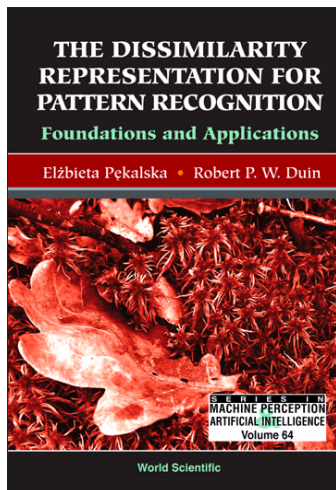
SVM

Mercer kernels

reduced

included

structural risk minimization



E. Pekalska and R.P.W. Duin, *The Dissimilarity Representation for Pattern Recognition, Foundations and Applications*,
World Scientific, Singapore, 2005, 607 p. ISBN 981-256-530-2

Non-Euclidean is the normal

Many measures used in PR are non-Euclidean:

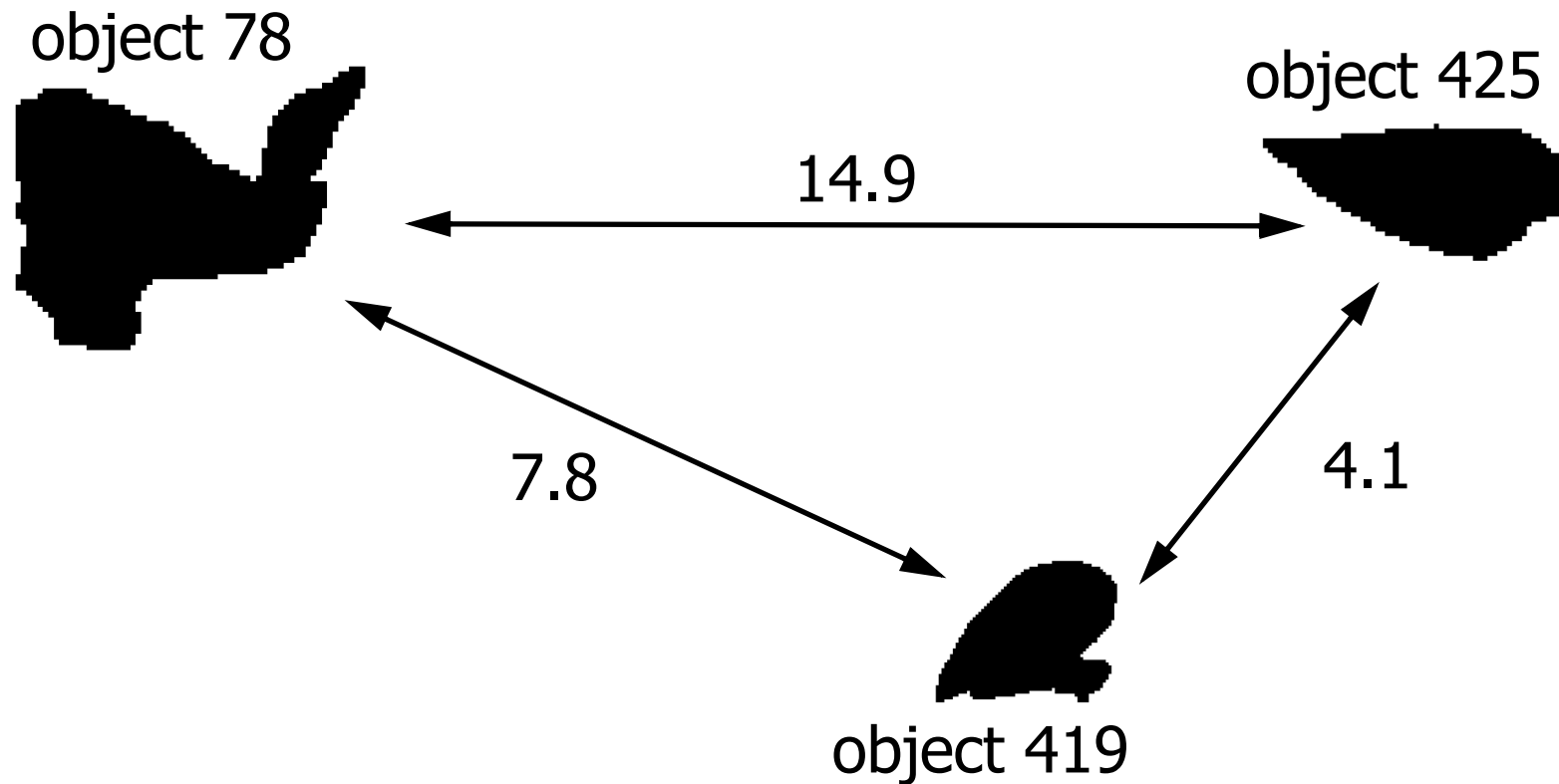
Mahalanobis, Single linkage, Modified Hausdorff, Weighted edit,
City block, Max norm, Cosine, Divergence,

No problem for dissimilarity spaces

Problem for embedding (Pseudo-Euclidean Space)

Problem for SVM (indefinite kernels)

Chicken pieces example



Edit_distance (length = 29, angle = 45)
non-metric result

What is the cause of non-metric data?

1. Distance measure is intrinsically non-metric
2. Some distances are estimated too large
due to suboptimal path minimization (correction?)
3. Some distances are estimated too short
e.g. due to projections or occlusions (correction?)
4. Accidental usage of a non-metric measure
where a metric measure may do well (detectable?)

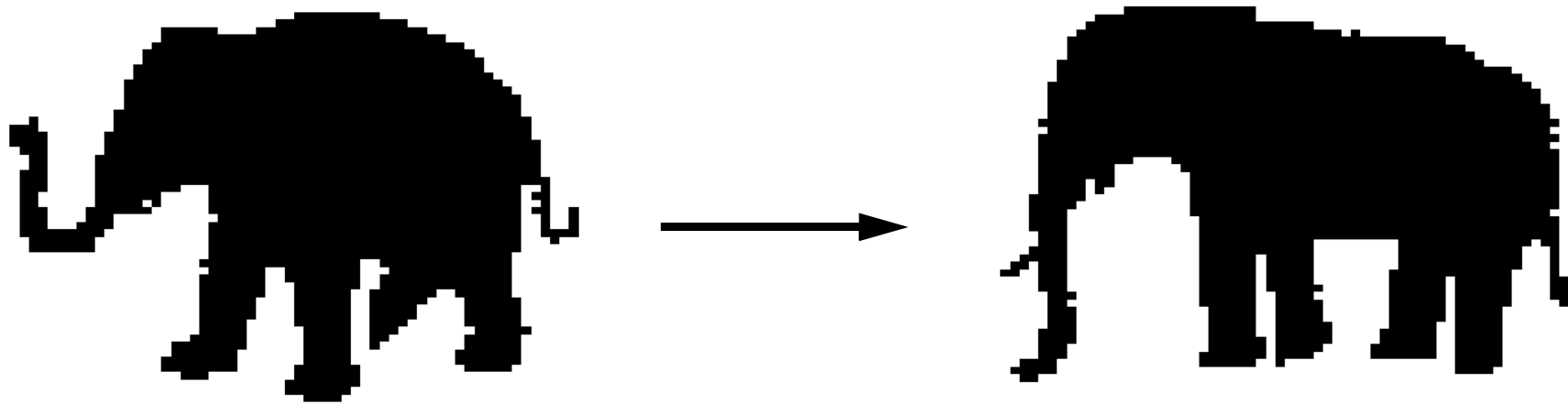
Structural inference by dissimilarity representations

By using dissimilarity representations we can train classifiers based on structural distance measures, but do we really learn from structure?

More should be understood about

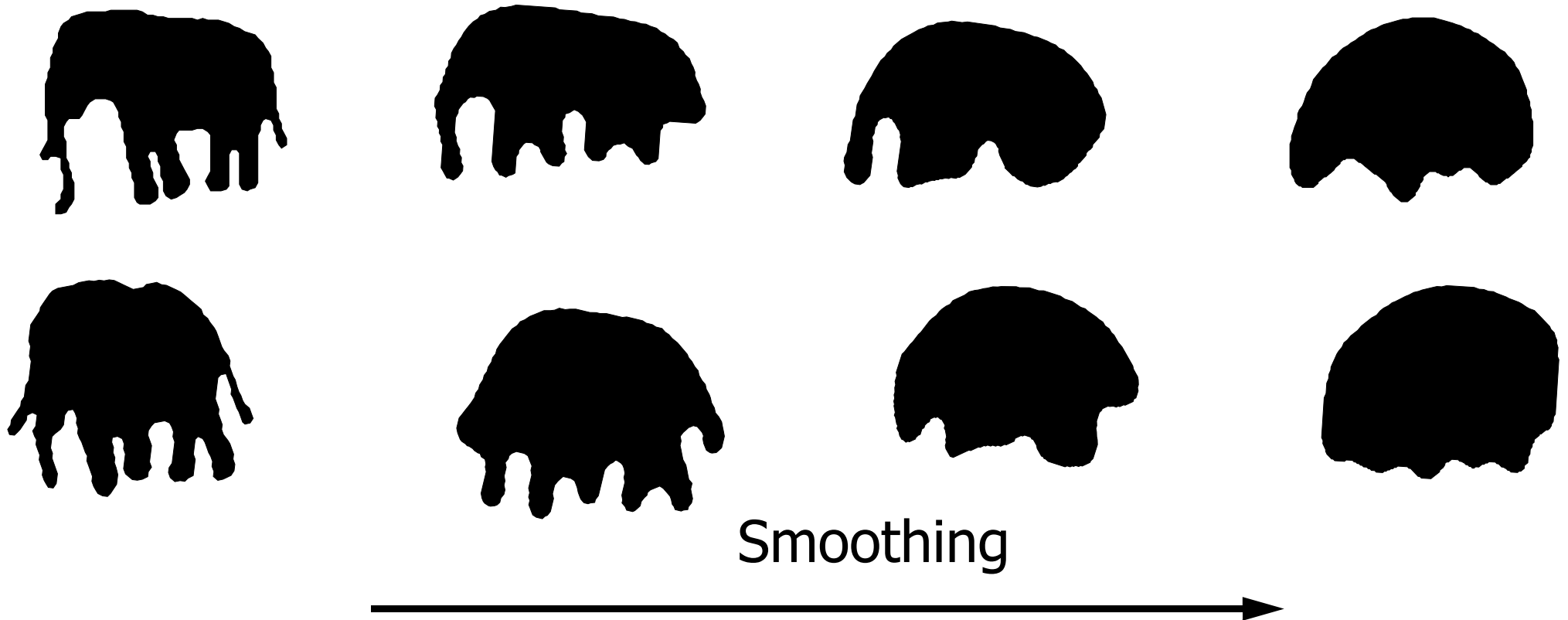
- non-Euclidean topology
- Pseudo-Euclidean embedding
- handling indefinite kernels

Structural inference: morphing



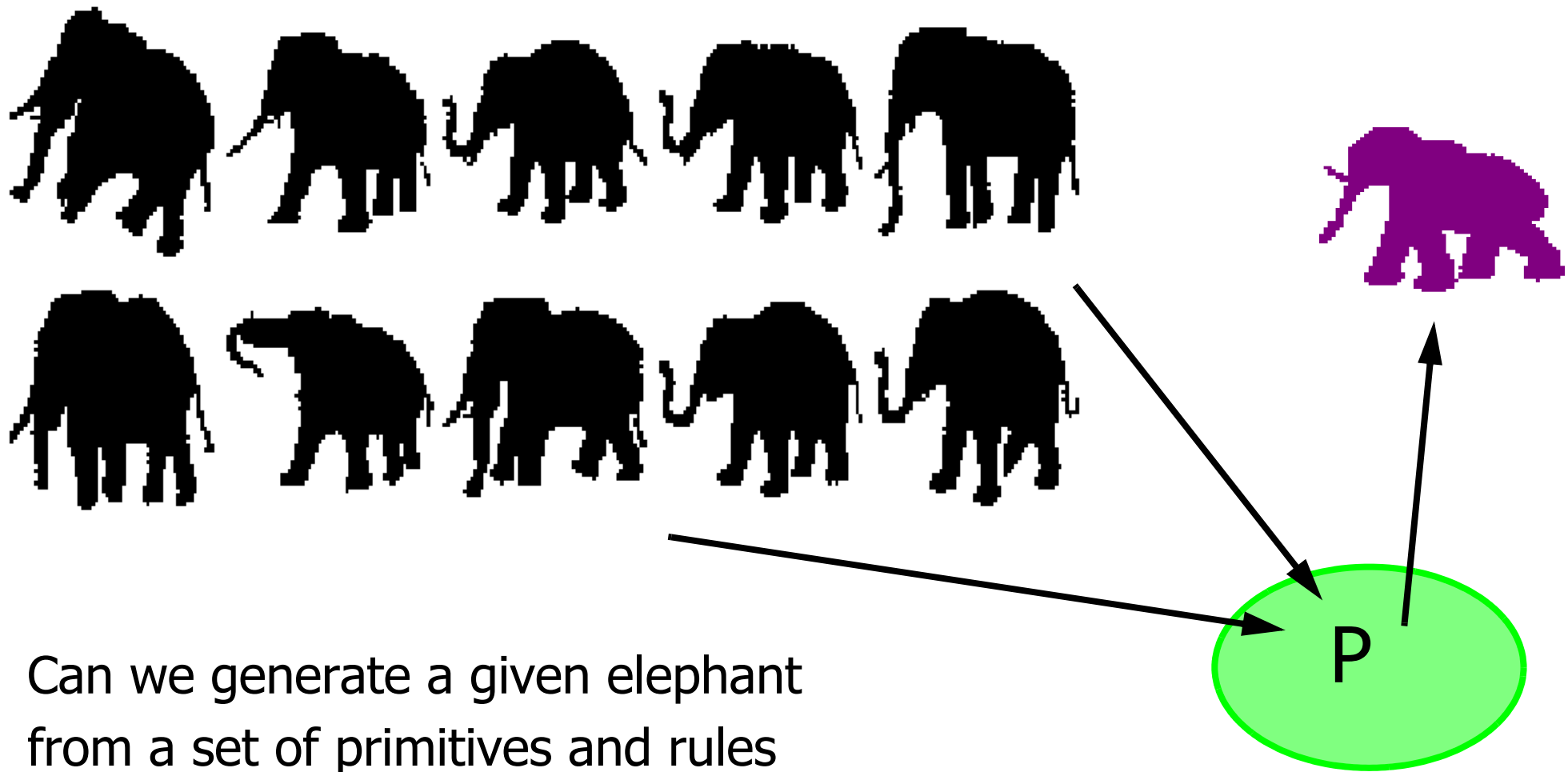
If we know the space of elephants, we can morph (edit) one elephant into another, with only elephants in between.

Structural inference: simplification



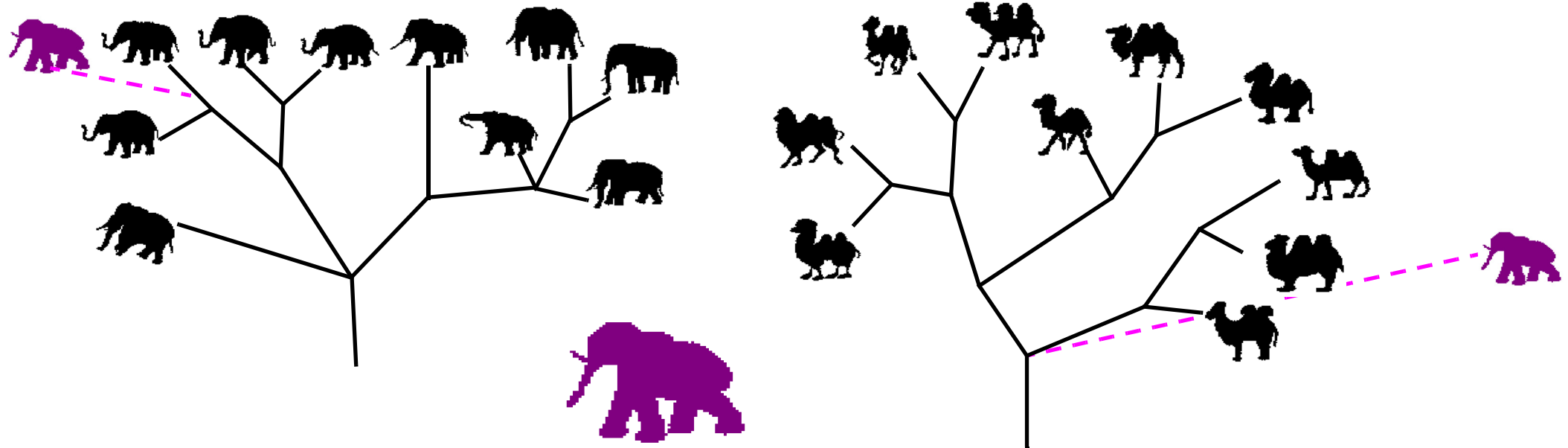
How much smoothing is needed to make shapes similar?

Structural inference: generation



Can we generate a given elephant from a set of primitives and rules induced from a training set?

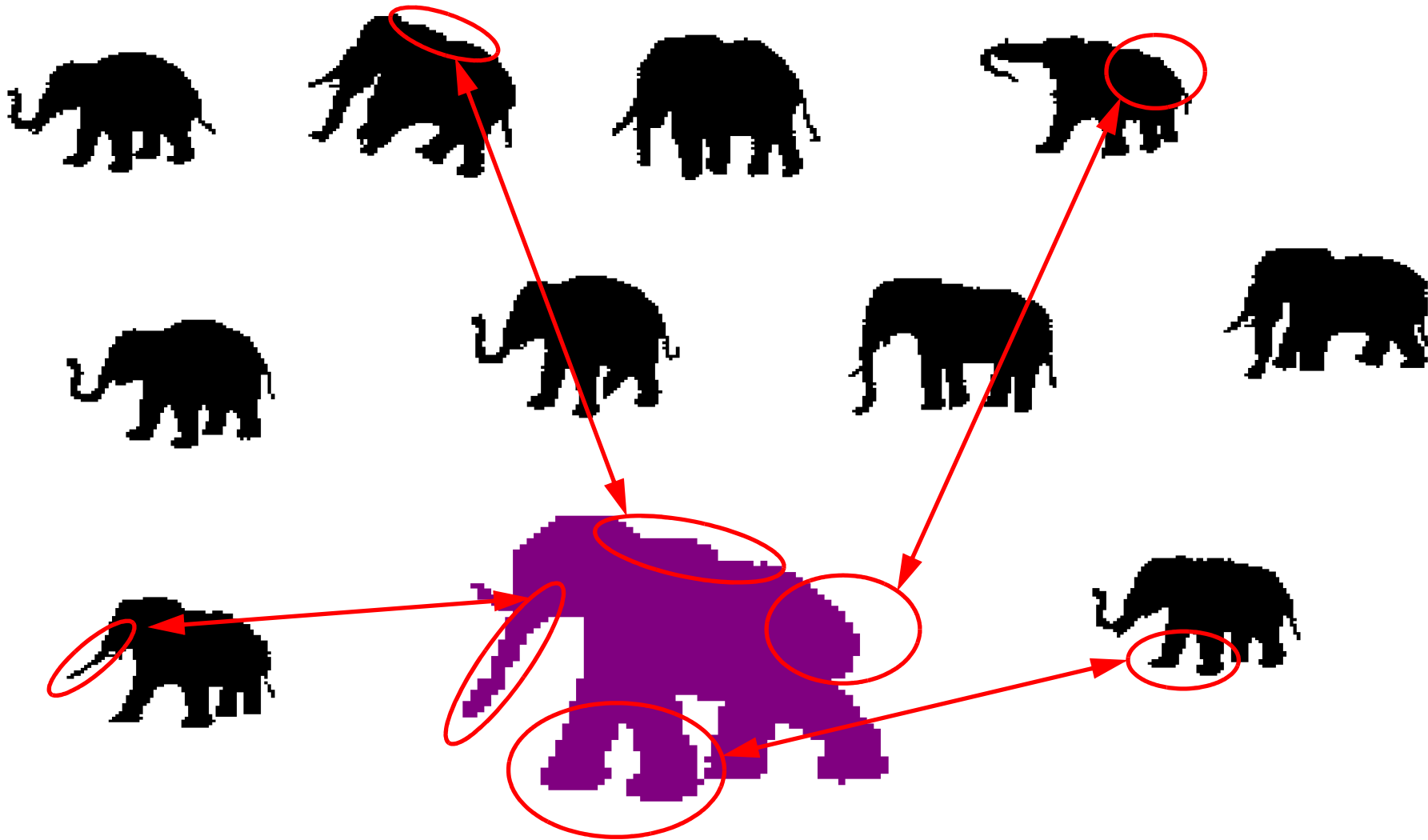
Goldfarb's Evolving Transformation System



Lev Goldfarb's Evolving Transformation System (ETS):

- Generate for each class how the objects could evolve from common primitive objects
- Test how new objects could most easily evolve from the generated trees

Structural inference: part by part



Conclusions

A small feature set reduces, causes overlapping classes, needs a **probabilistic approach** and bears no structural information.

A complete feature set may yield separable classes, so **domain classification** may be possible.

A **dissimilarity based approach** performs this and may use structural information in the dissimilarity measure.
Non-metric problems may have to be solved.

For real structural inference a **similarity based approach** seems more appropriate.

done

under construction

to do