The dissimilarity representation for structural pattern recognition

CIARP, Pucón, Chile, 15-18 November 2011

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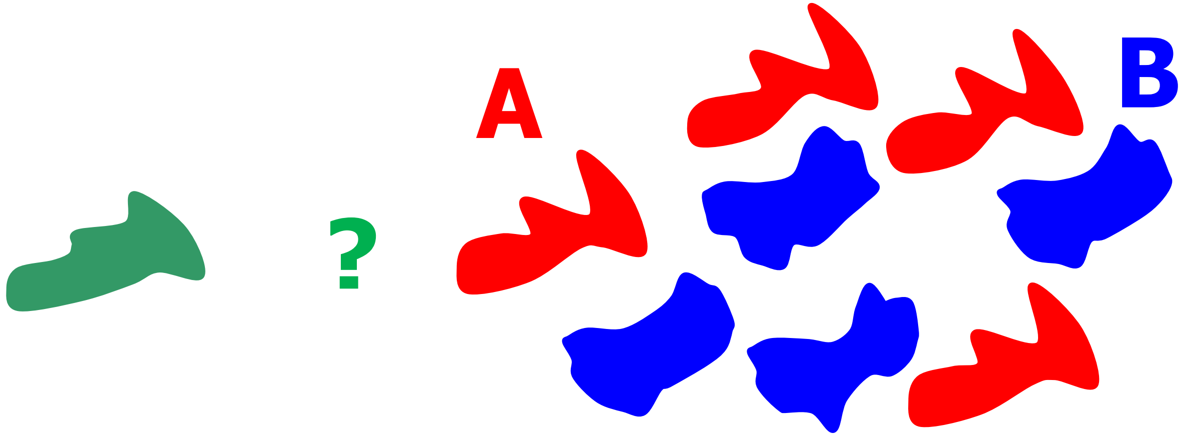
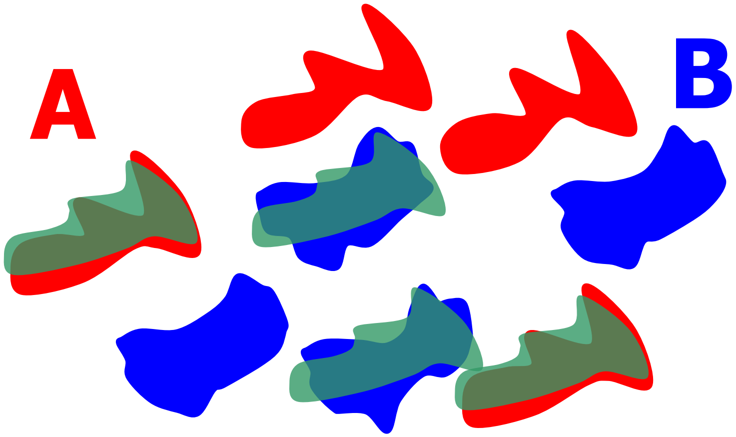
Introduction

Preview



How to classify structures given examples?



By the dissimilarity representation:
An extension of template matching,
based on generalized of kernels

Real world objects and events

Images
Spectra
Time signals
Gestures

→ shapes

How to build a representation?
Features ←→ Structure

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Blob Recognition

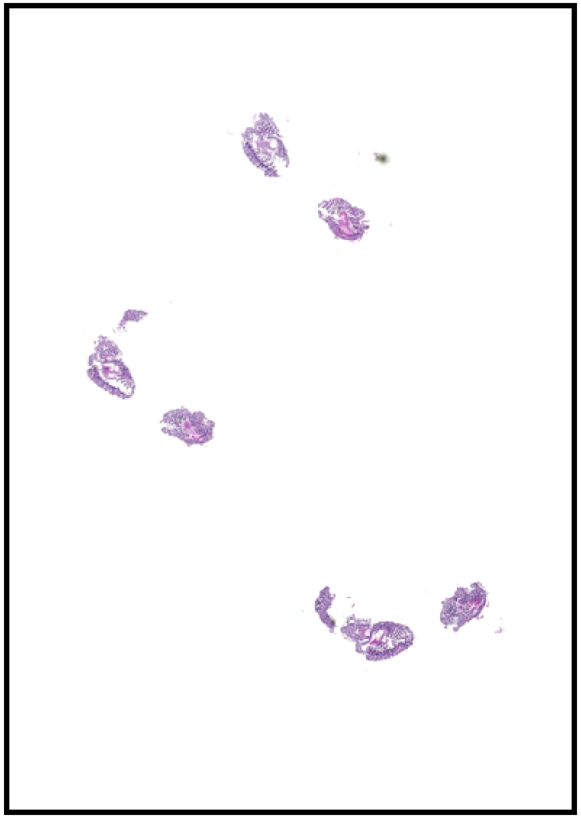
446 binary images, varying size, e.g.: 100 x 130

Andreu, G., Crespo, A., Valiente, J.M.: Selecting the toroidal self-organizing feature maps (TSOFM) best organized to object recogn. In: ICNN. (1997) 1341–1346.

Shape classification by weighted-edit distances (Bunke)

*Bunke, H., Buhler, U.: Applications of approximate string matching to 2D shape recognition. Pattern recognition **26** (1993) 1797–1812*

Colon Tissue Recognition

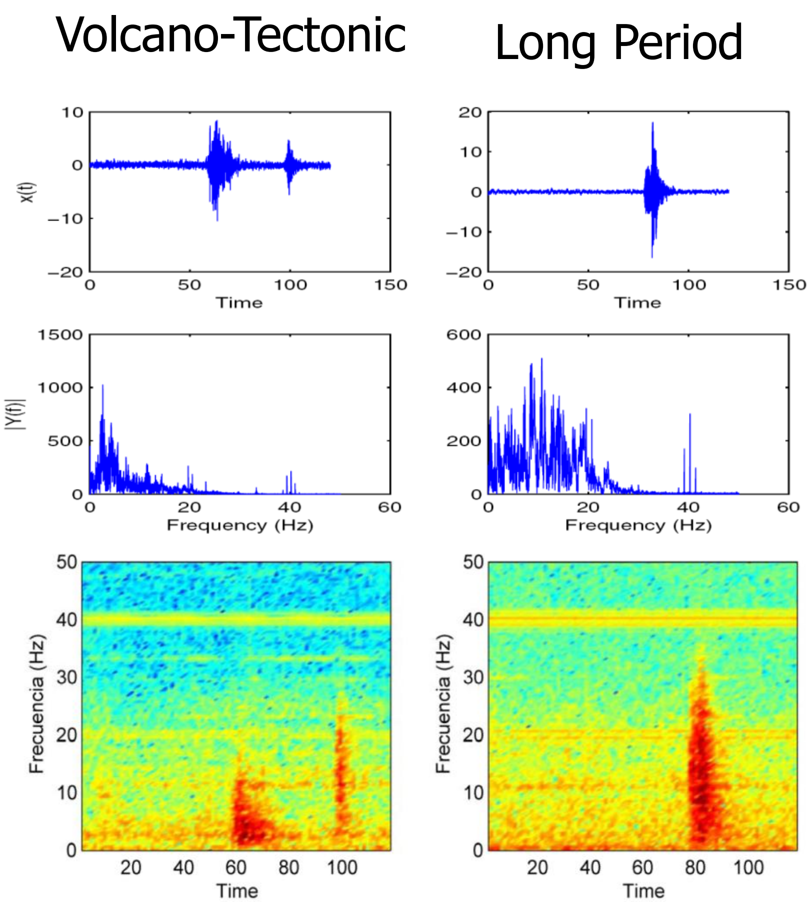


???

normal

pathological

Volcano / Seismic Signal Classification



150 000 events (1994 – 2008)
5 volcanos
40 stations
15 classes

J. Makario,
INGEOMINAS, Manizales, Colombia

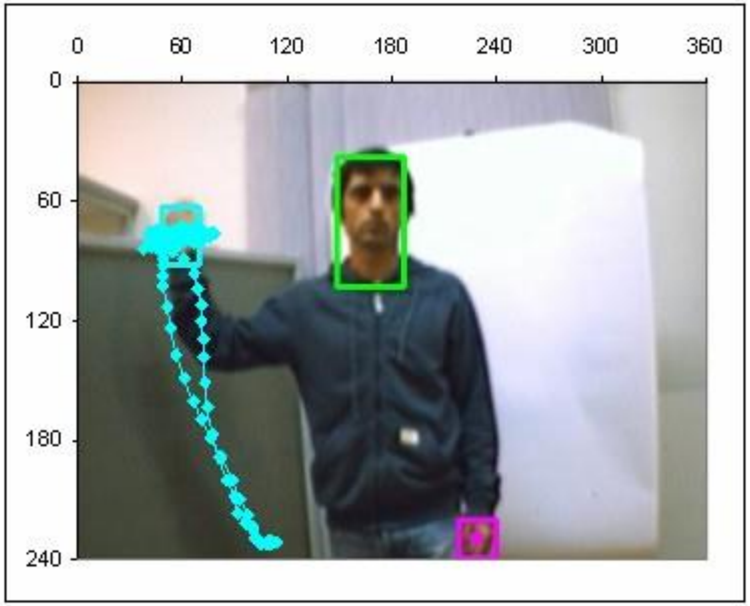
M. Orozco-Alzate,
Nat. Univ. Colombia, Manizales

R. Duin, TUDelft

M. Bicego, Univ. of Verona, Italy

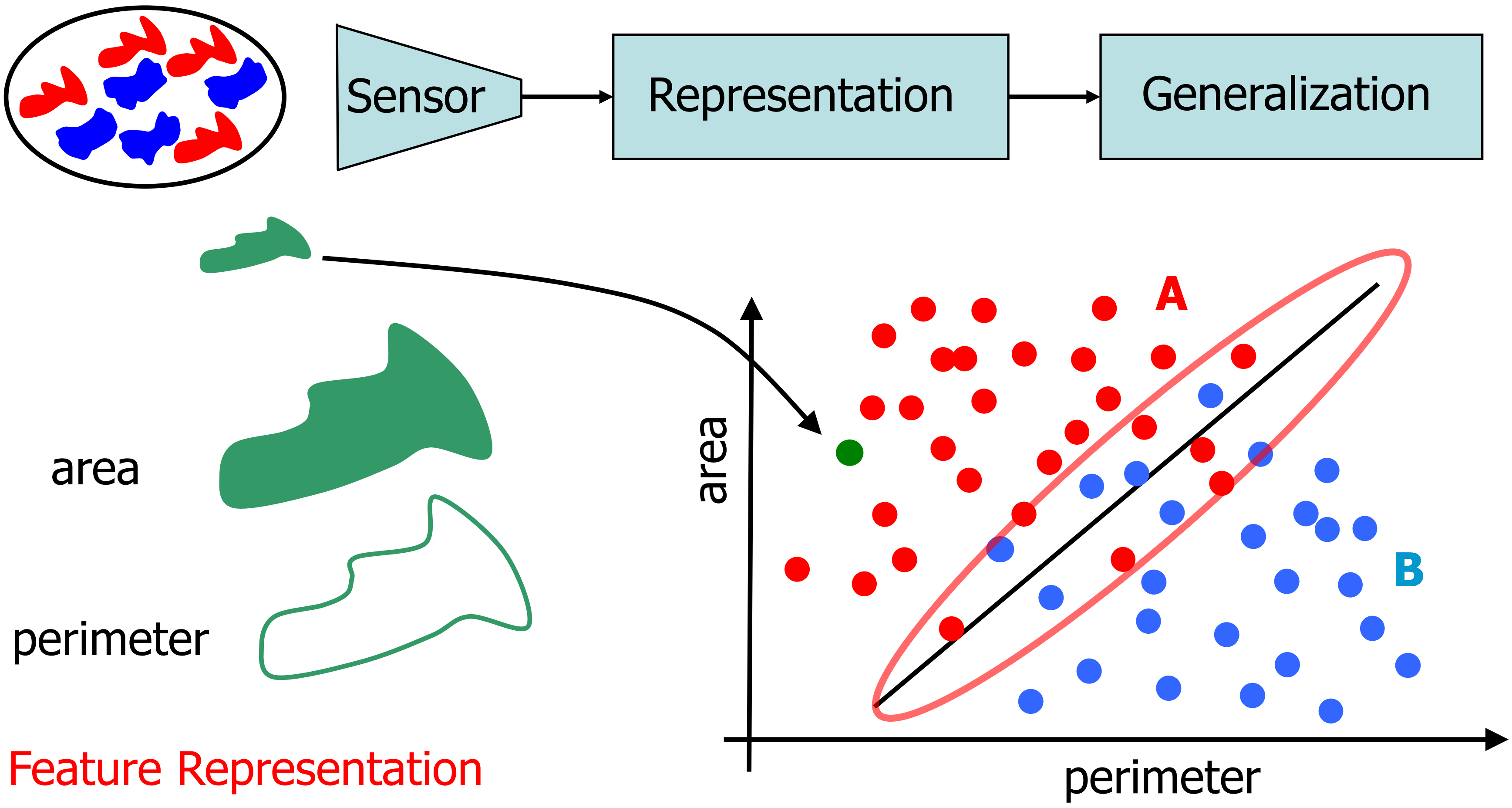
Cenatav, Havana, Cuba

Gesture Recognition



Is this gesture in the database?

Pattern Recognition System

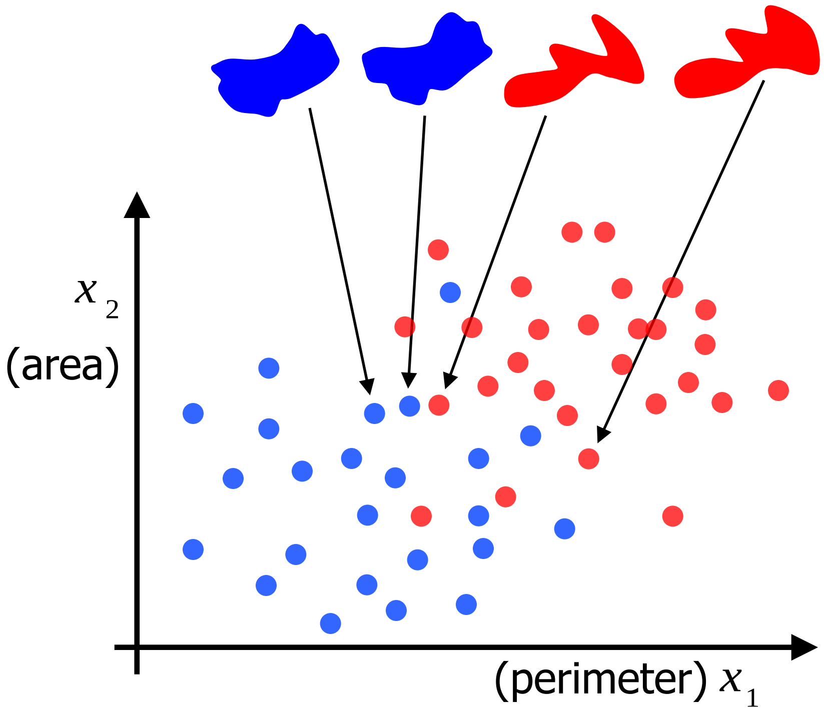


Feature Representation

Representation

Compactness

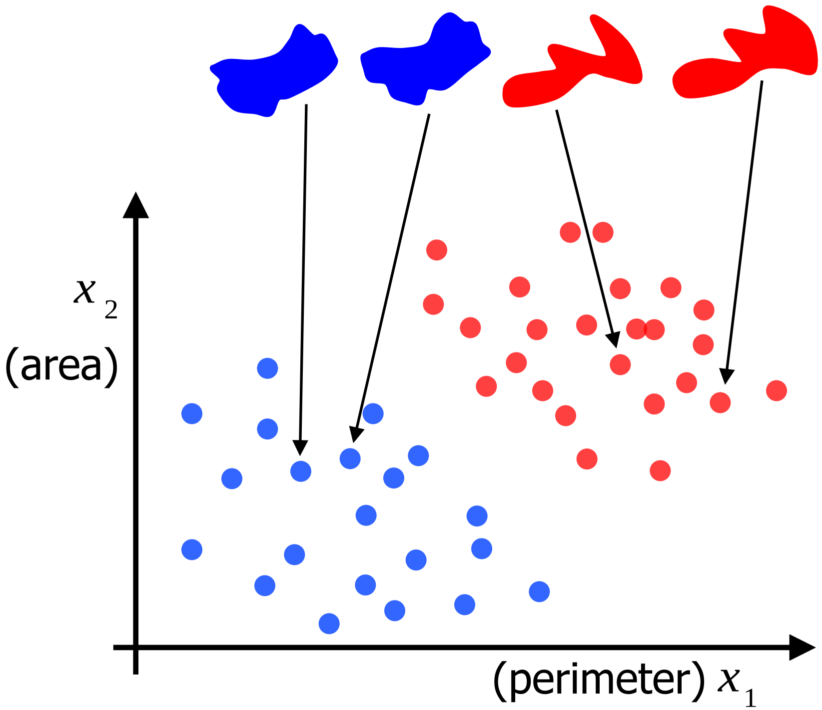
Representations of real world similar objects are close.
There is no ground for any generalization (induction) on representations that do not obey this demand.



The compactness hypothesis is not sufficient for perfect classification as dissimilar objects may be close.
→ class overlap
→ probabilities

A.G. Arkedev and E.M. Braverman, Computers and Pattern Recognition, 1966.

True Representations



Similar objects are close
and
Dissimilar objects are distant.

→ no probabilities needed, domains are sufficient!

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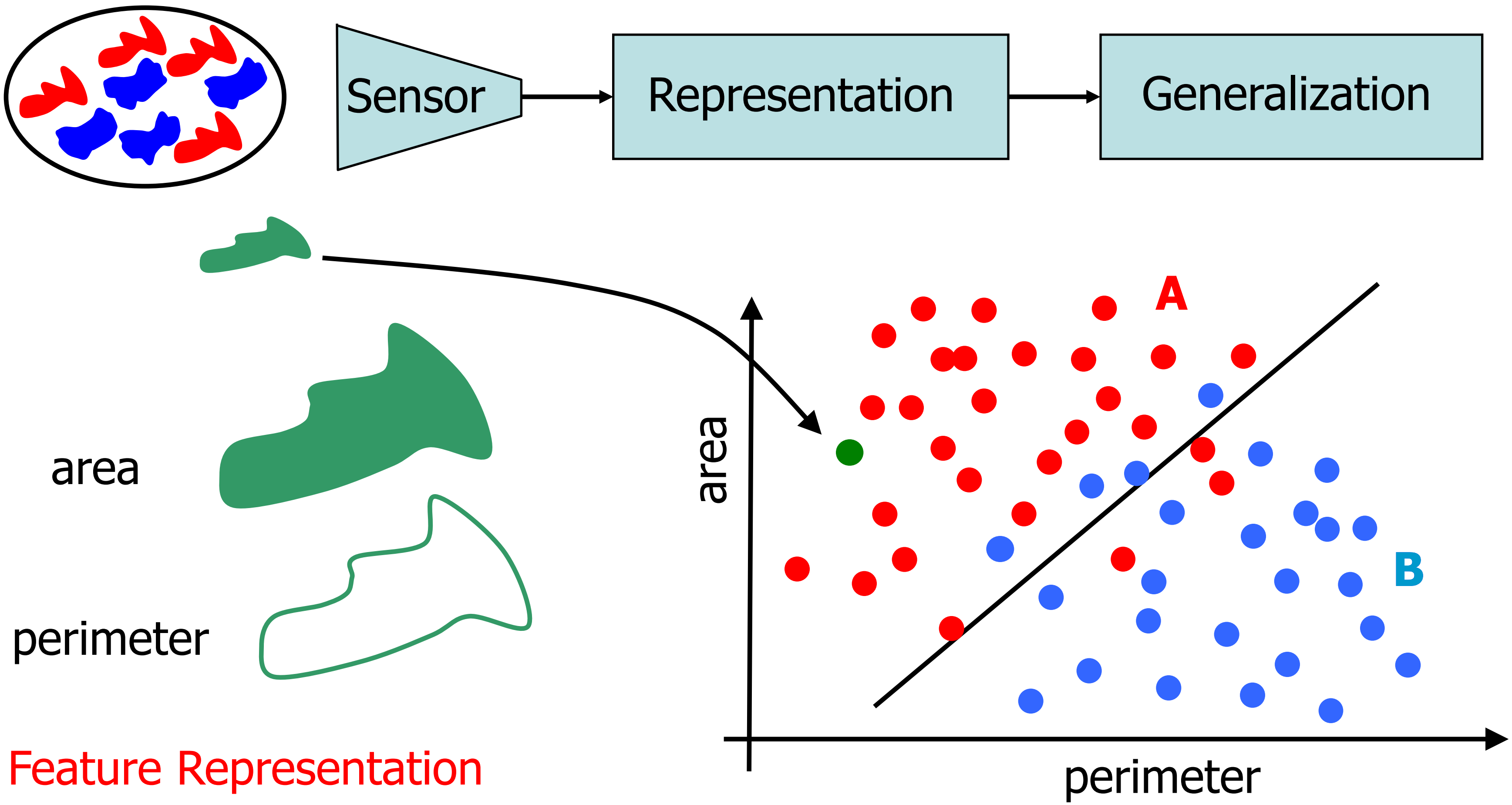
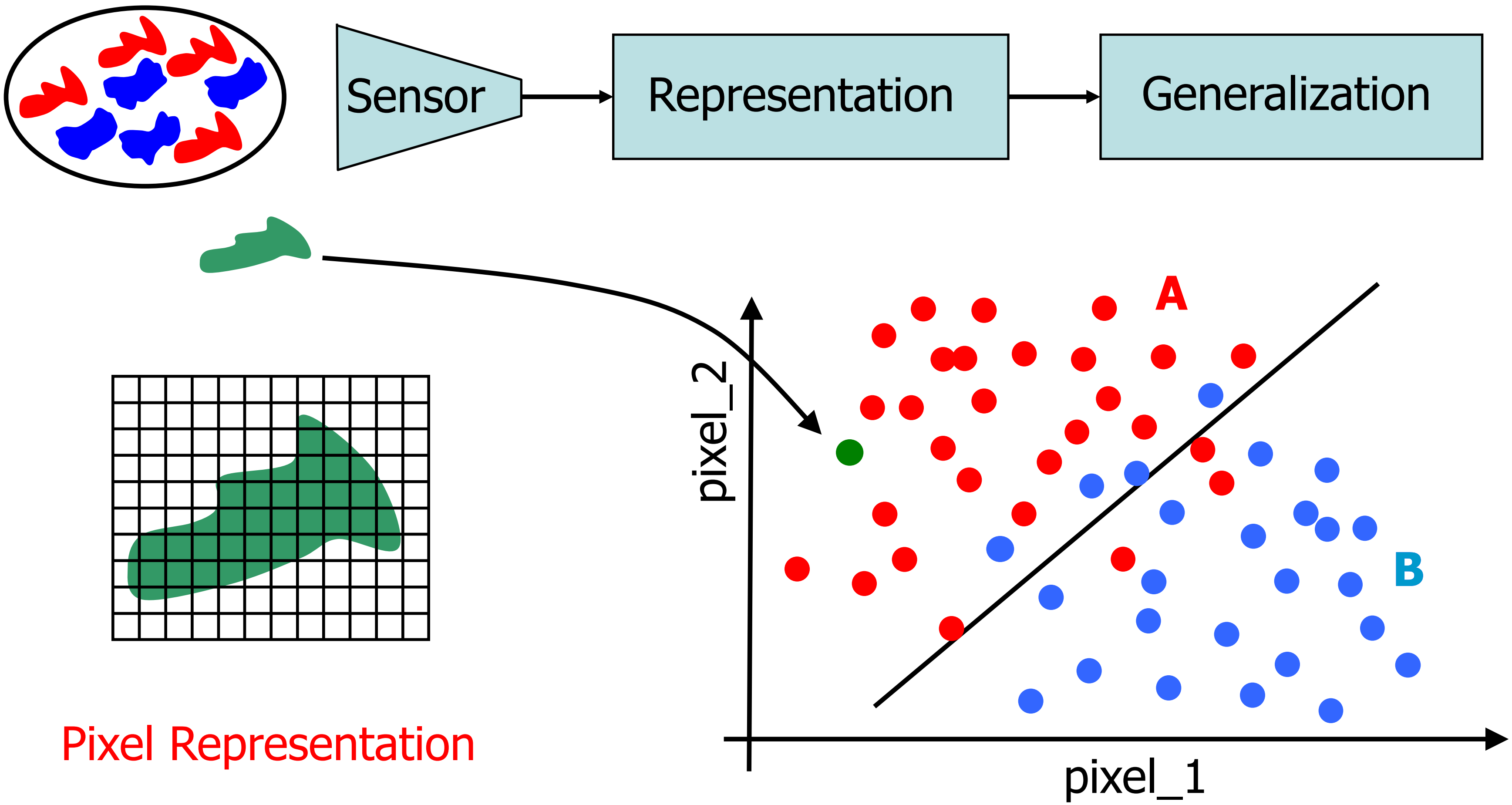
Pattern Recognition System



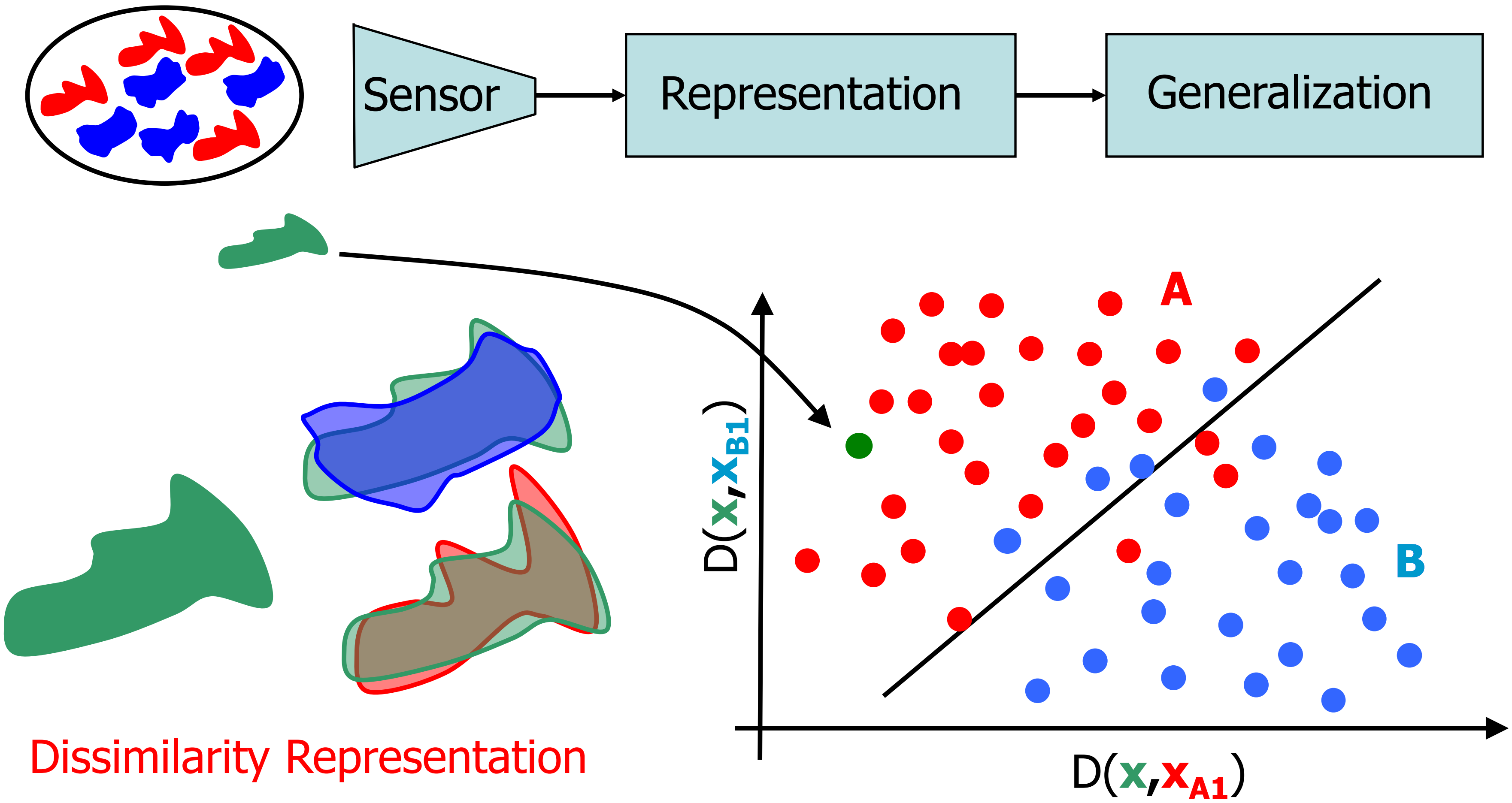
Feature Representation

Pattern Recognition System



Pixel Representation

Pattern Recognition System



Dissimilarity Representation

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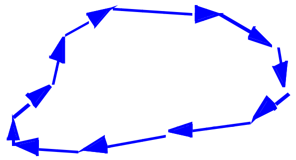
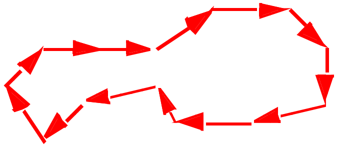
Structural Representation

Strings

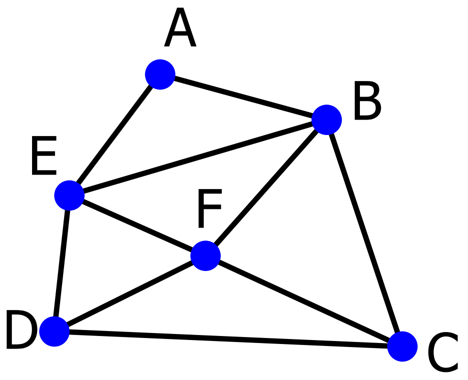


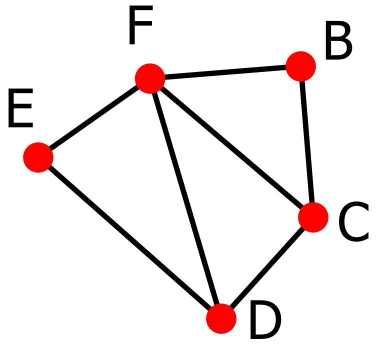
$X = (x_1, x_2, \ldots., x_k)$



$Y = (y_1, y_2, \ldots., y_n)$

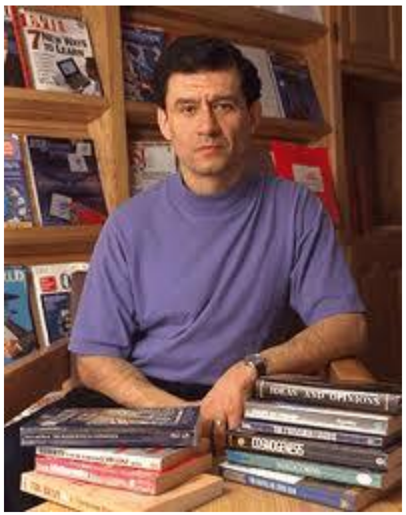
Graphs

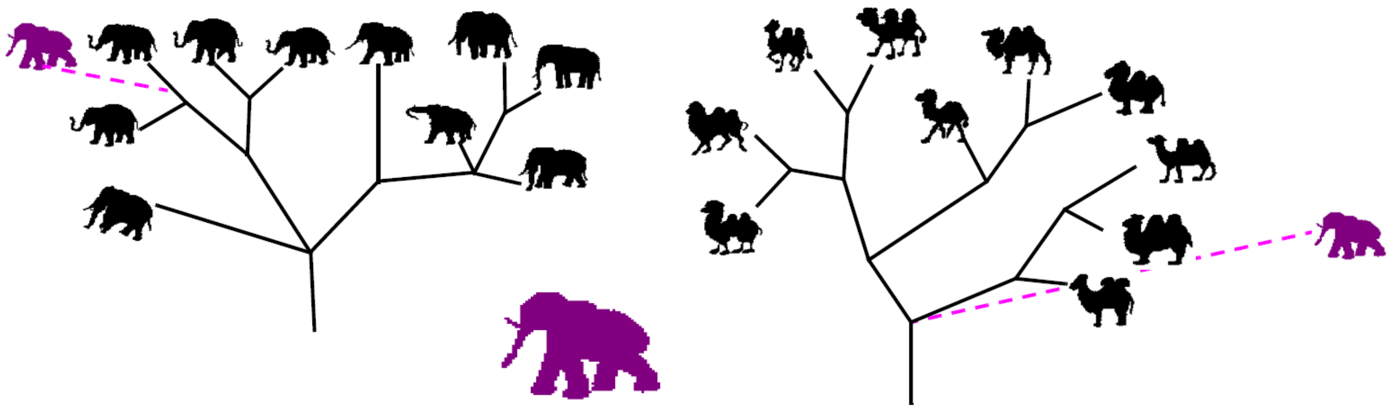




Goldfarb's Evolving Transformation System (ETS)

Lev Goldfarb 1984: features → dissimilarities → PE spaces
1995: vector spaces are not good for representing concepts
concepts need a structural representation





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.

Goldfarb et al., What is a structural representation? Tech. rep. 2004
http://www.cs.unb.ca/tech-reports/documents/tr04-165.pdf

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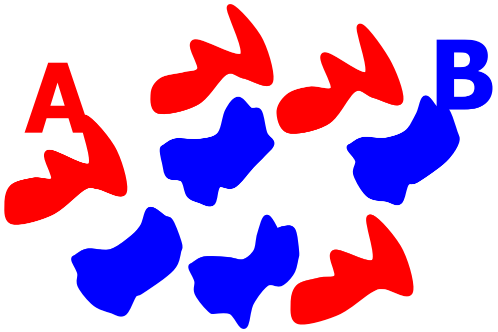
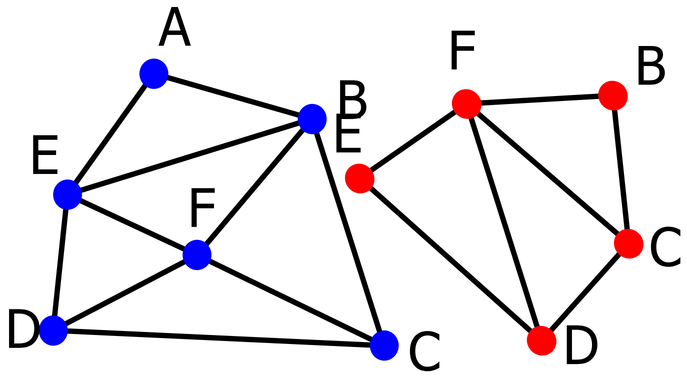
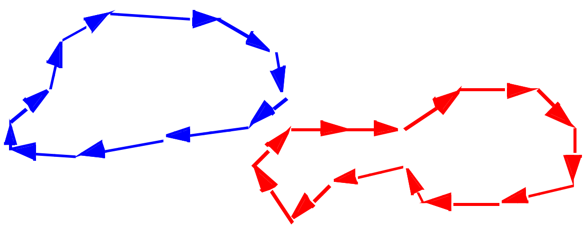
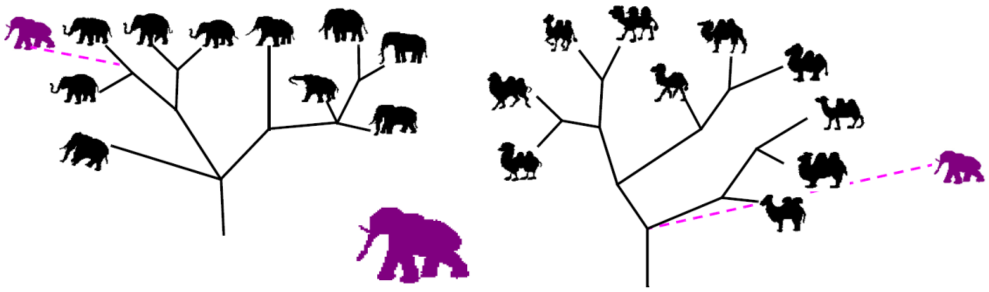
Structural Representation





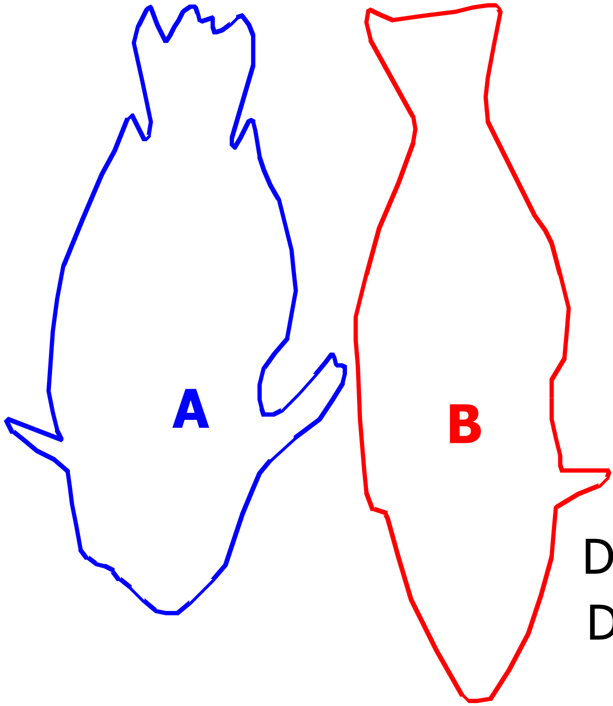




How to generalize? Distances!

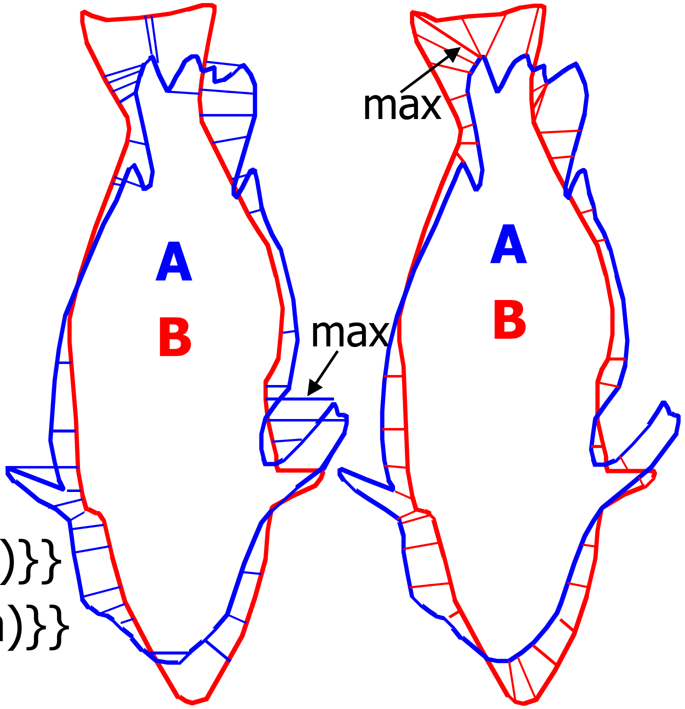
Dissimilarities

Examples Dissimilarity Measures



Dist(**A**,**B**):
a ∈ **A**, points of **A**
b ∈ **B**, points of **B**
d(a,b): Euclidean distance

D(**A**,**B**) = max_a{min_b{d(a,b)}}
D(**B**,**A**) = max_b{min_a{d(b,a)}}



Hausdorff Distance (metric):
DH = max{max_a{min_b{d(a,b)}} , max_b{min_a{d(b,a)}}}

D(**A**,**B**) ≠ D(**B**,**A**)

Modified Hausdorff Distance (non-metric):
DM = max{mean_a{min_b{d(a,b)}},mean_b{min_a{d(b,a)}}}

Dubuisoon & Jain, Modified Hausdorff distance for object matching, ICPR12, 2004,, voll 1, 566-568.

Dissimilarities – Possible Assumptions

Metric

1. Positivity: $d_{ij} \geq 0$
2. Reflexivity: $d_{ii} = 0$
3. Definiteness: $d_{ij} = 0$ iff objects i and j are identical
4. Symmetry: $d_{ij} = d_{ji}$
5. Triangle inequality: $d_{ij} < d_{ik} + d_{kj}$
6. Compactness: if the objects i and j are very similar then $d_{ij} < \delta$.
7. True representation: if $d_{ij} < \delta$ then the objects i and j are very similar.
8. Continuity of d.

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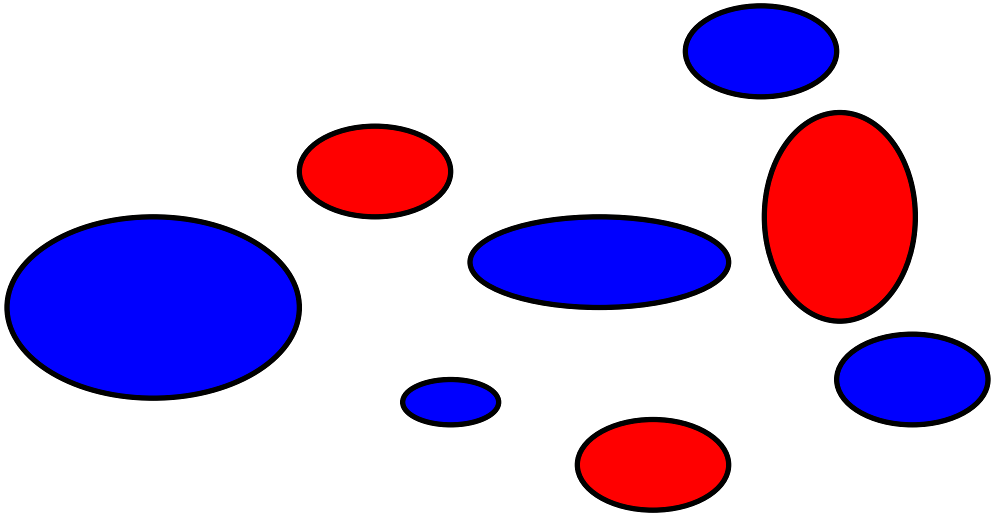
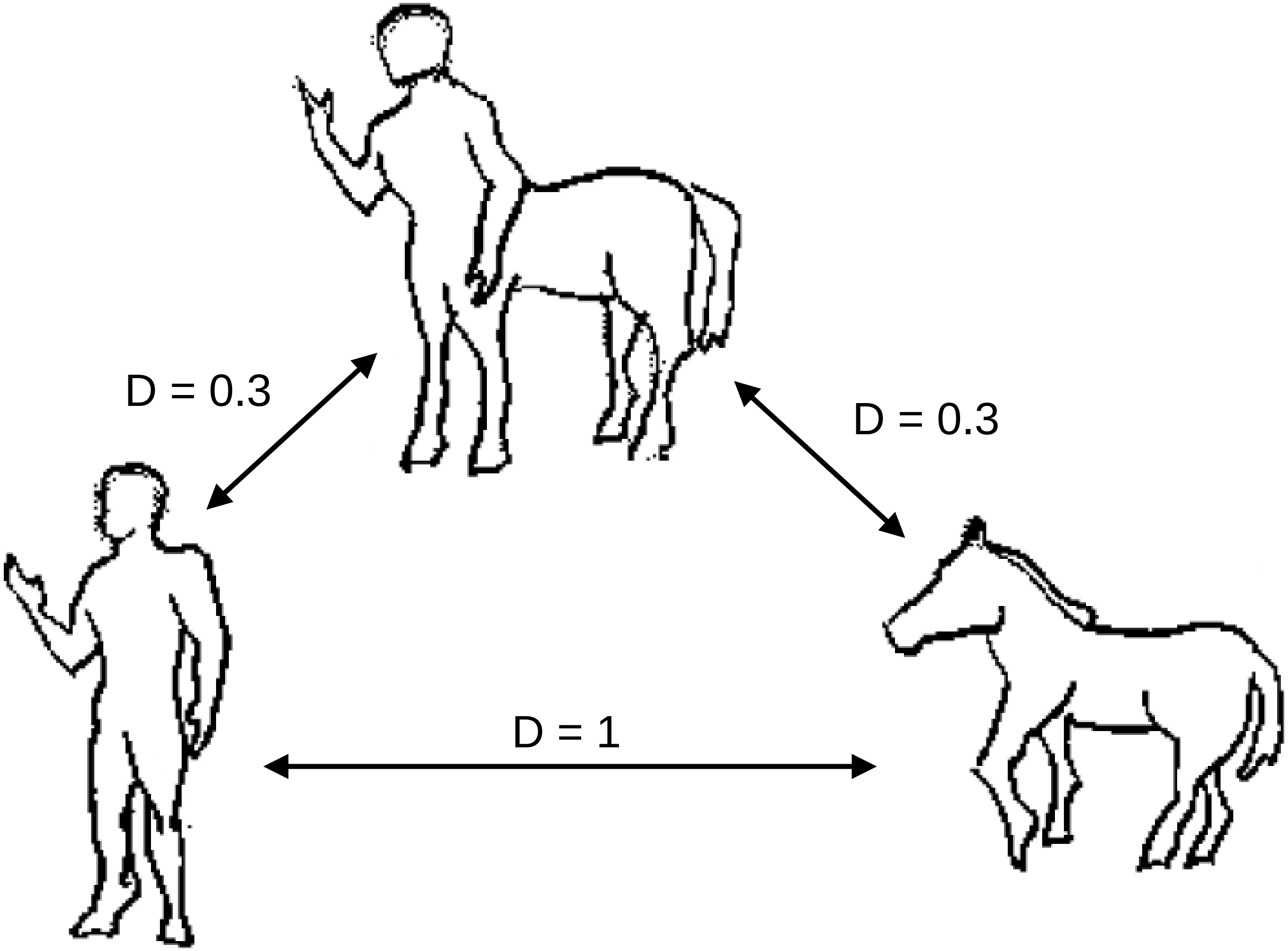
The class of problems

- Compact
- Uniquely labelled

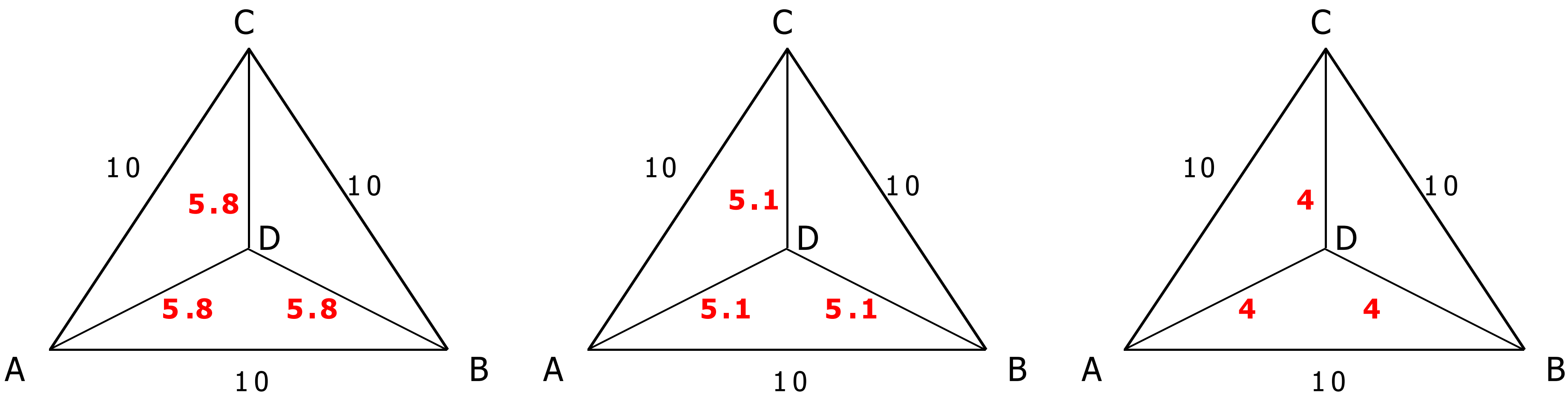


In a dissimilarity representation such classes are separable by any positive definite distance measure



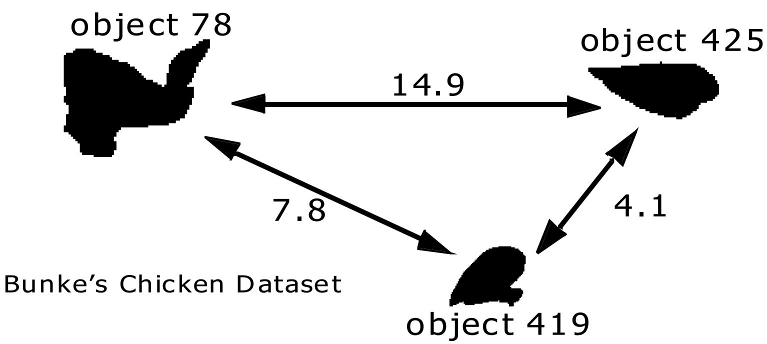
[David W. Jacobs](), [Daphna Weinshall]() and [Yoram Gdalyahu](), Classification with Nonmetric Distances: Image Retrieval and Class Representation, *IEEE Trans. Pattern Anal. Mach. Intell*, 22(6), pp. 583-600, 2000.

Euclidean - Non Euclidean - Non Metric

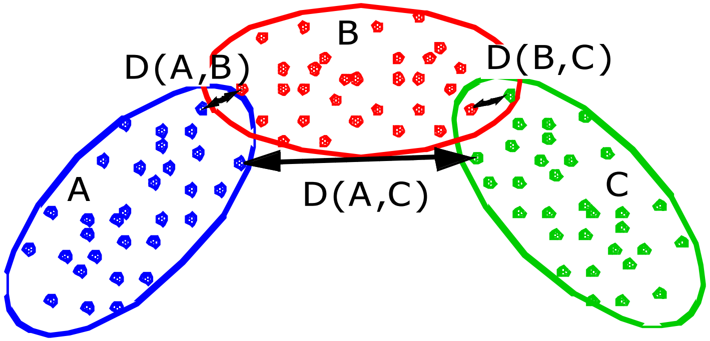


Non-metric distances

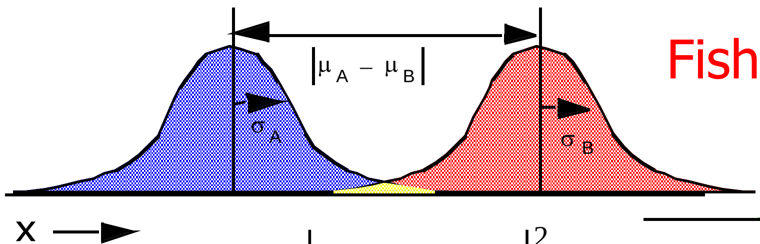
Weighted-edit distance for strings



Single-linkage clustering

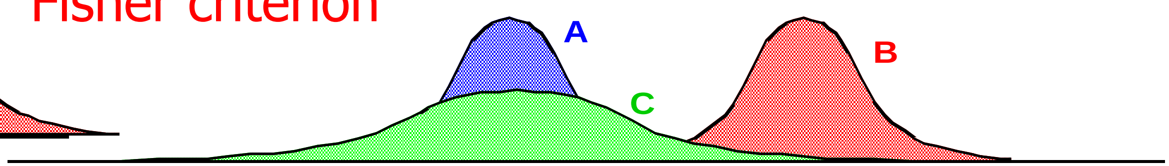


D(A,C) > D(A,B) + D(B,C)



$$J(A, B) = \frac{|\mu_A - \mu_B|^2}{\sigma_A^2 + \sigma_B^2}$$

Fisher criterion



$J(A, C) = 0 \quad J(A, B) = \text{large}$

$J(C, B) = \text{small} \neq J(A, B)$

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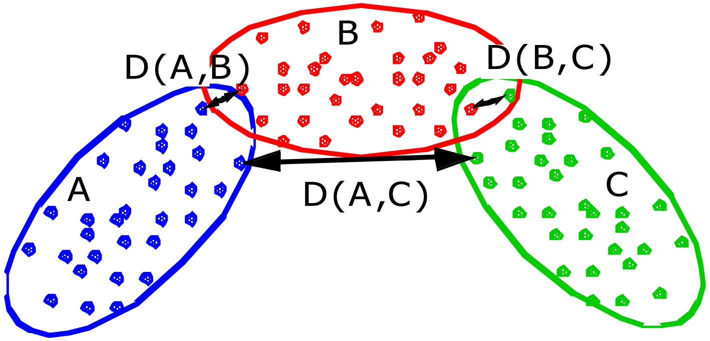
Intrinsicly Non-Euclidean Dissimilarity Measures
Single Linkage

Distance(Table,Book) = 0

Distance(Table,Cup) = 0

Distance(Book,Cup) = 1

Single-linkage clustering



D(A,C) > D(A,B) + D(B,C)

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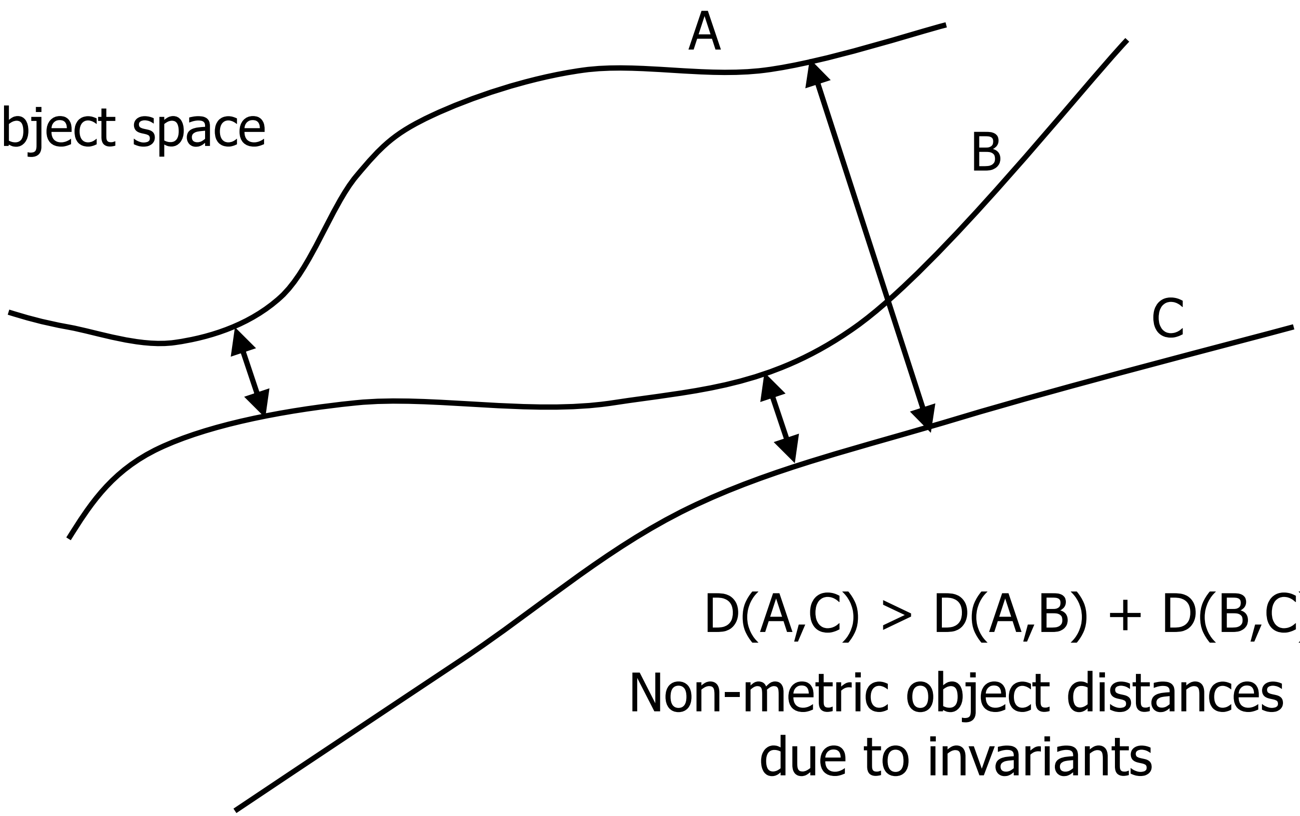
Intrinsicly Non-Euclidean Dissimilarity Measures
Invariants

Object space



D(A,C) > D(A,B) + D(B,C)

Non-metric object distances
due to invariants

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Indefinite Metric and the 1NN rule

Indefinite metric: $d_{ij} = 0$ for objects i and j that are not identical

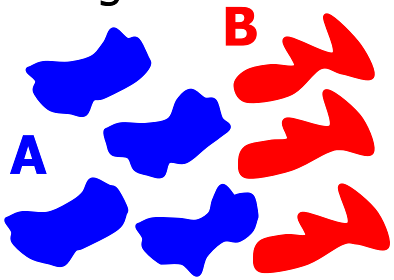
→ Possibly different labels

→ Template matching and 1-NN rule may fail!

Dissimilarity Representation

Alternatives for the Nearest Neighbor Rule

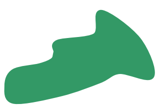
Training set



Dissimilarities d_{ij} between all training objects

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

Unlabeled object **x** to be classified



$$d_x = (d_{x1} \; d_{x2} \; d_{x3} \; d_{x4} \; d_{x5} \; d_{x6} \; d_{x7})$$

1. Dissimilarity Space
2. Embedding

Pekalska, The dissimilarity representation for PR. World Scientific, 2005.

Alternative 1: Dissimilarity Space

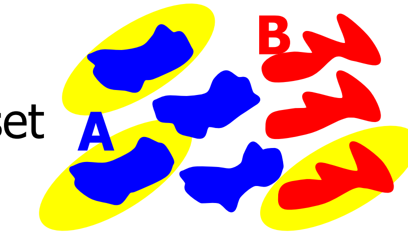
Dissimilarities

$r_1 \quad r_2 \quad r_3$

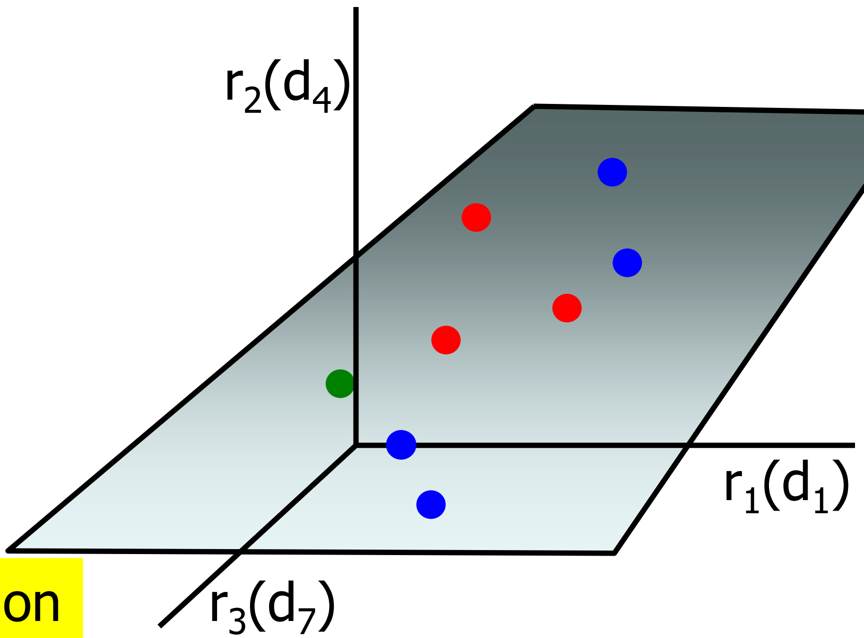
$$D_T = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} & d_{17} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} & d_{27} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} & d_{37} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} & d_{46} & d_{47} \\ d_{51} & d_{52} & d_{53}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

$$d_x = (d_{x1} \; d_{x2} \; d_{x3} \; d_{x4} \; d_{x5} \; d_{x6} \; d_{x7})$$

Given labeled training set

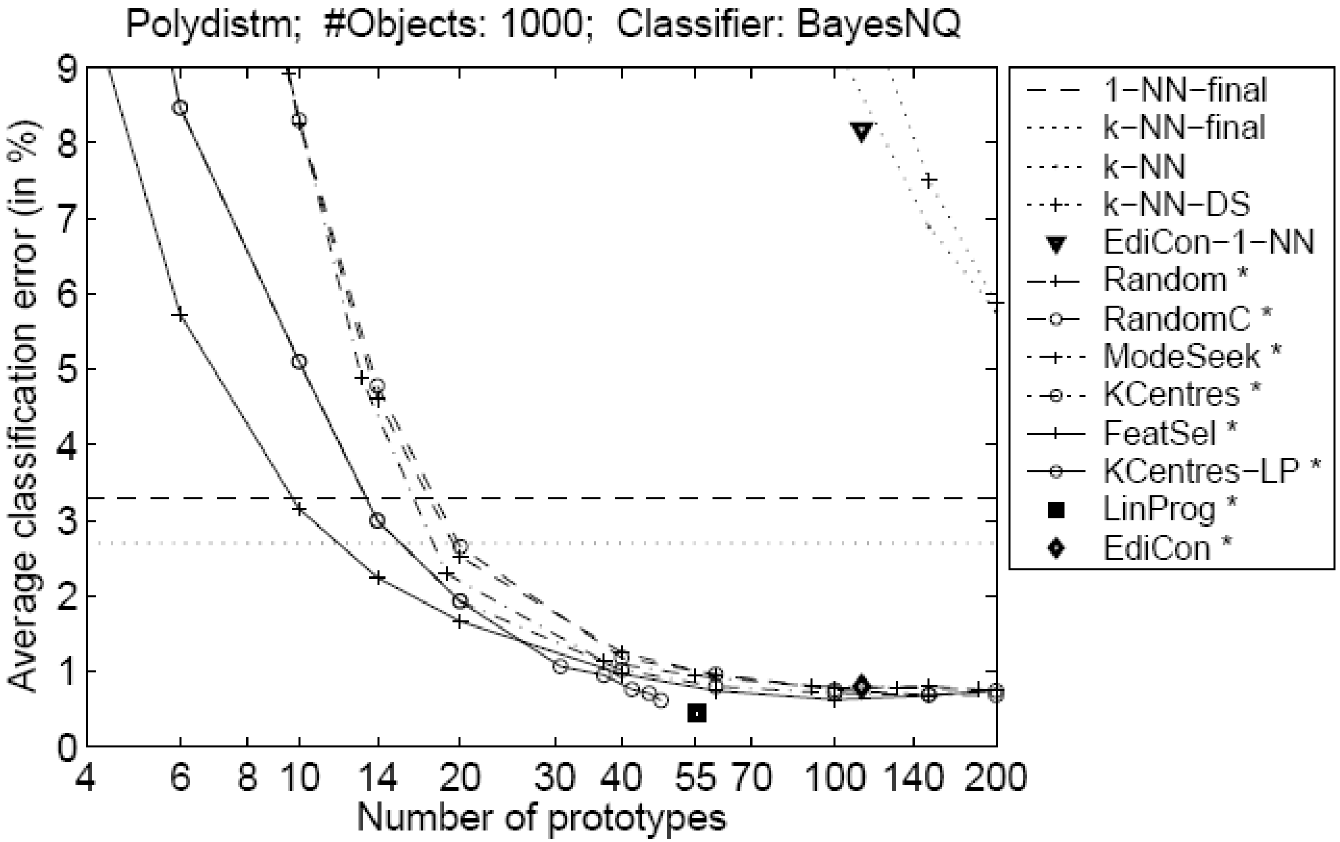


Unlabeled object to be classified



Selection of 3 objects for representation

Prototype Selection: Polygon Dataset



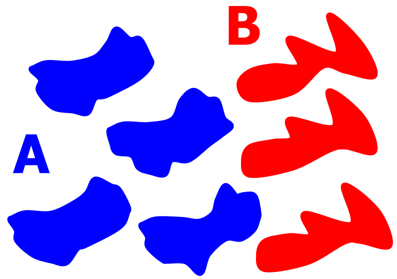
The classification error as a function of the number of selected prototypes. For 10-20 prototypes results are already better than by using 1000 objects in the NN rules.

Pekalska et al., Prototype selection for dissimilarity-based classification, Pattern Recognition, 2006, 189-208.

Dissimilarity space properties

- Euclidean by postulation
- Dissimilarity character not used
- Any classifier may be used
- May be filled by additional training objects
- (just a limited set of objects needed for representation)
- Control of computational complexity

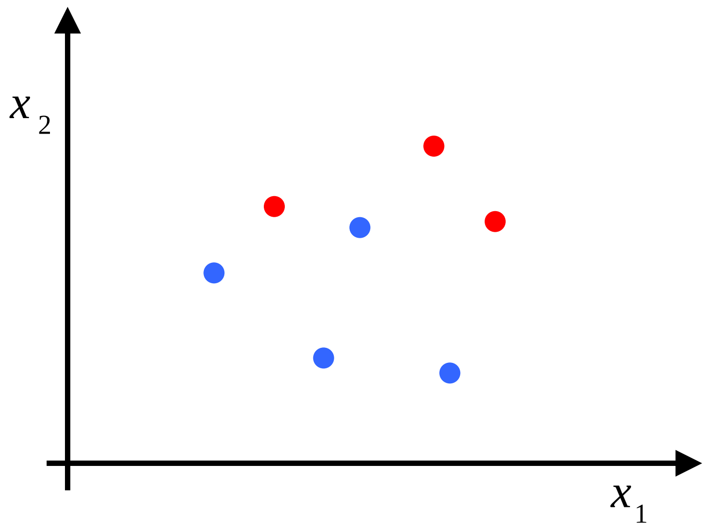
Alternative 2: Embedding



Training set

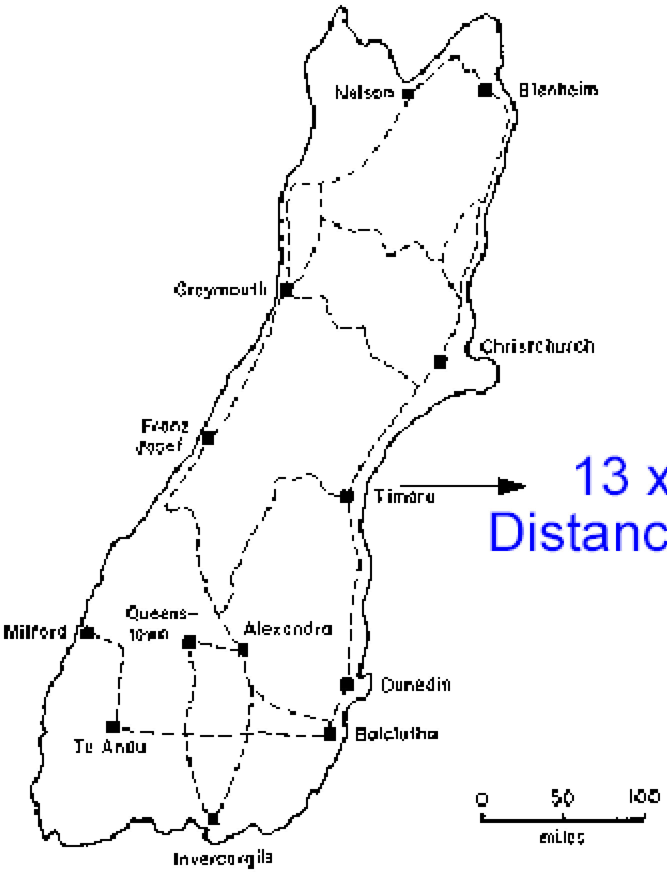
→ Dissimilarity matrix D → X

Is there a feature space for which Dist(X,X) = D ?

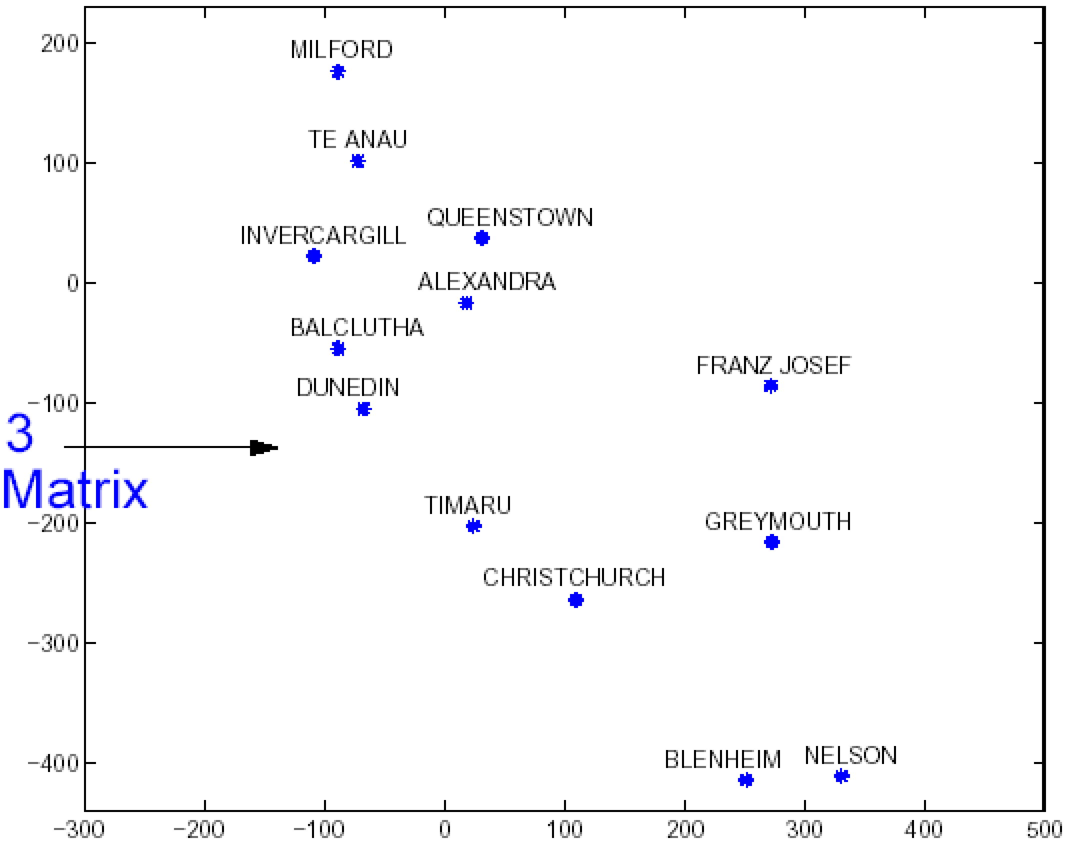


Position points in a vector space such that their Euclidean distances → D

Embedding



13 x 13
Distance Matrix



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(Pseudo-)Euclidean Embedding

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

Construct inner-product matrix: $B = -\frac{1}{2} J D^{(2)} J \qquad J = I - \frac{1}{m}\mathbf{11}$

Eigenvalue Decomposition , $B = Q \Lambda Q^T$

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

Let $\Im_k$ be a k x k diag. matrix, $\Im_k(i,i)$ = sign($\Lambda_k(i,i)$)

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

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

The inner-product matrix: $B_z = -\frac{1}{2}(D_z^{(2)} J - \frac{1}{n}\mathbf{11}^T D^{(2)} J)$

The embedded objects: $Z = B_z Q_k \left|\Lambda_k\right|^{-\frac{1}{2}} \Im_k$

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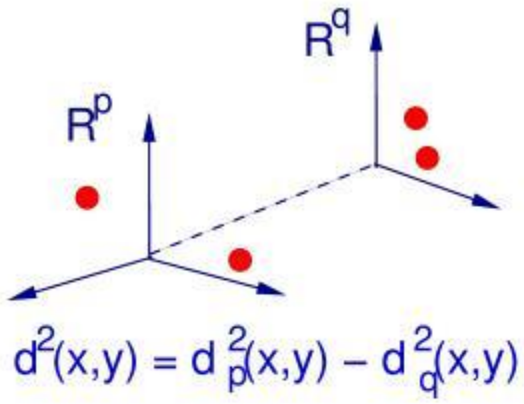
PES: Pseudo-Euclidean Space (Krein Space)

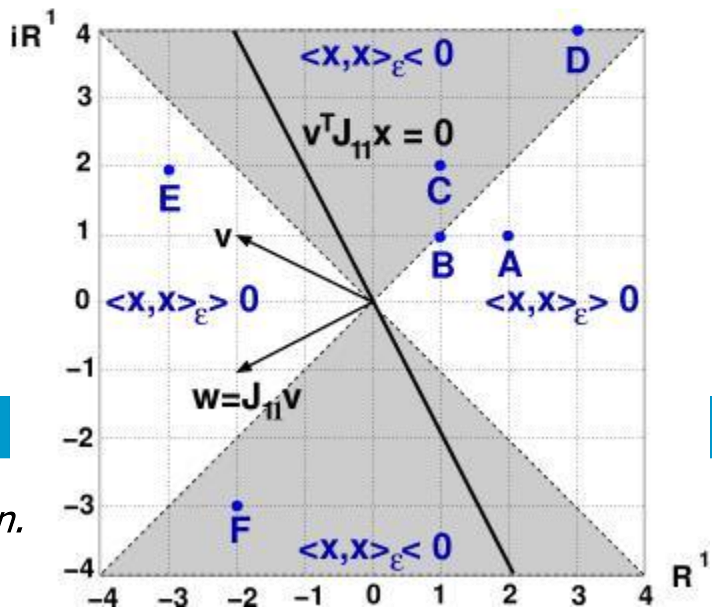
If D is non-Euclidean, B has p positive and q negative eigenvalues.

A pseudo-Euclidean space $\mathcal{E}$ with signature (p,q), $k = p+q$, is a non-degenerate inner product space $\Re_k = \Re_p \oplus \Re_q$ such that:

$$\langle x, y \rangle_\varepsilon = x^T \Im_{pq} y = \sum_{i=1}^{p} x_i y_i - \sum_{j=p+1}^{q} x_j y_j \qquad \Im_{pq} = \begin{bmatrix} I_{p\times p} & 0 \\ 0 & -I_{q\times q} \end{bmatrix}$$

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





Pekalska, The Dissimilarity Representation for Pattern Recognition. Foundations and Applications. World Scientific, Singapore , 2005

Pseudo Euclidean Space

Euclidean embedding D → X

$$d_{ij}^2 = \left\| \mathbf{x}_i - \mathbf{x}_j \right\|^2$$

Pseudo Euclidean embedding D → $\{X^p, X^q\}$

$$d_{ij}^2 = \left\| \mathbf{x}_i^p - \mathbf{x}_j^p \right\|^2 - \left\| \mathbf{x}_i^q - \mathbf{x}_j^q \right\|^2$$

'Positive' and 'negative' space,
Compare Minkowsky space in relativity theory

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PE-space embedding properties

- A square matrix with dissimilarities is needed
  (all training (+ test objects) needed for representation)
- Projection of new objects is difficult
- Densities are not (yet) well defined
- Distance to a classifier is inappropriate for classification

PE-Space classifiers

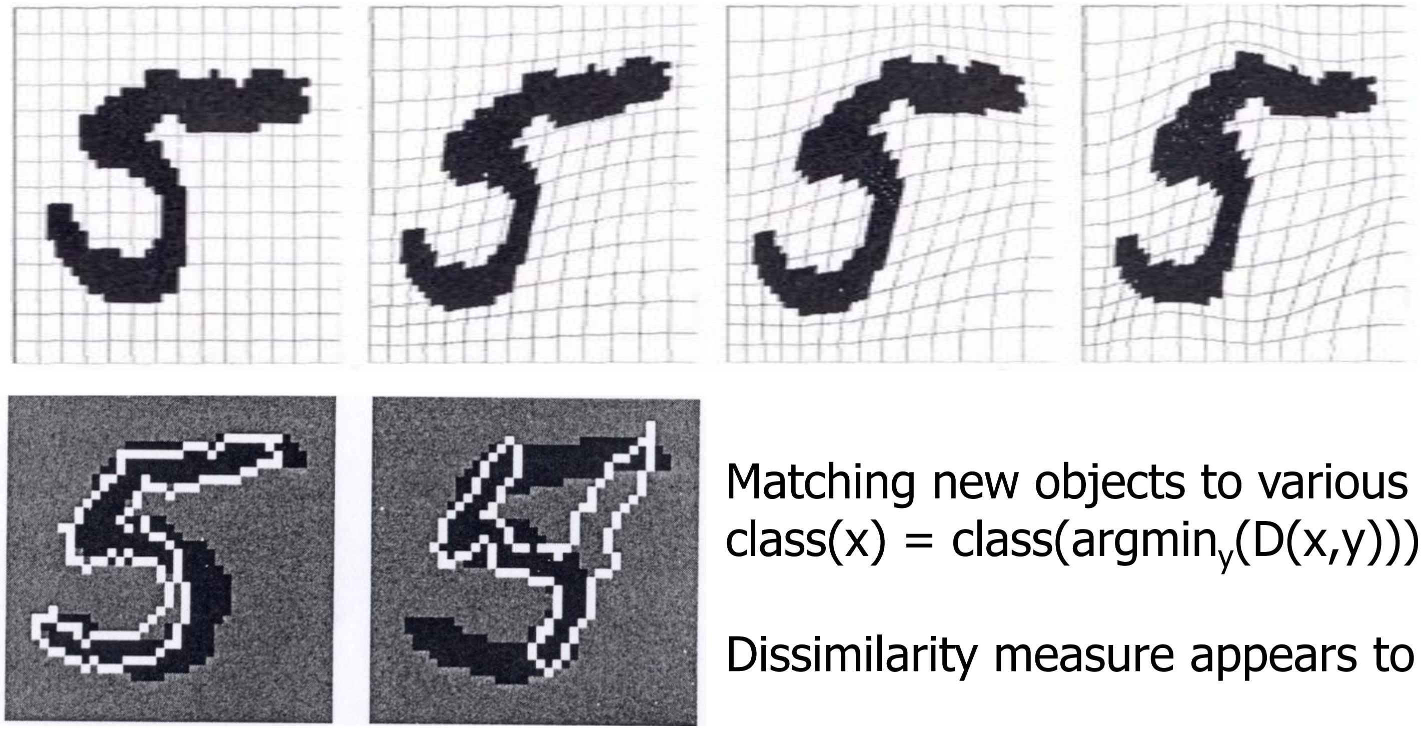
- kNN, Parzen, Nearest Mean
  As object distances can be computed (are known)

- LDA, QDA
  As PE inner possibly product definitions cancel they can be computed, interpretation … ?

- SVM
  May get a result (indefinite kernel), possibly not optimal

- Others ??

Examples Dissimilarity Measures

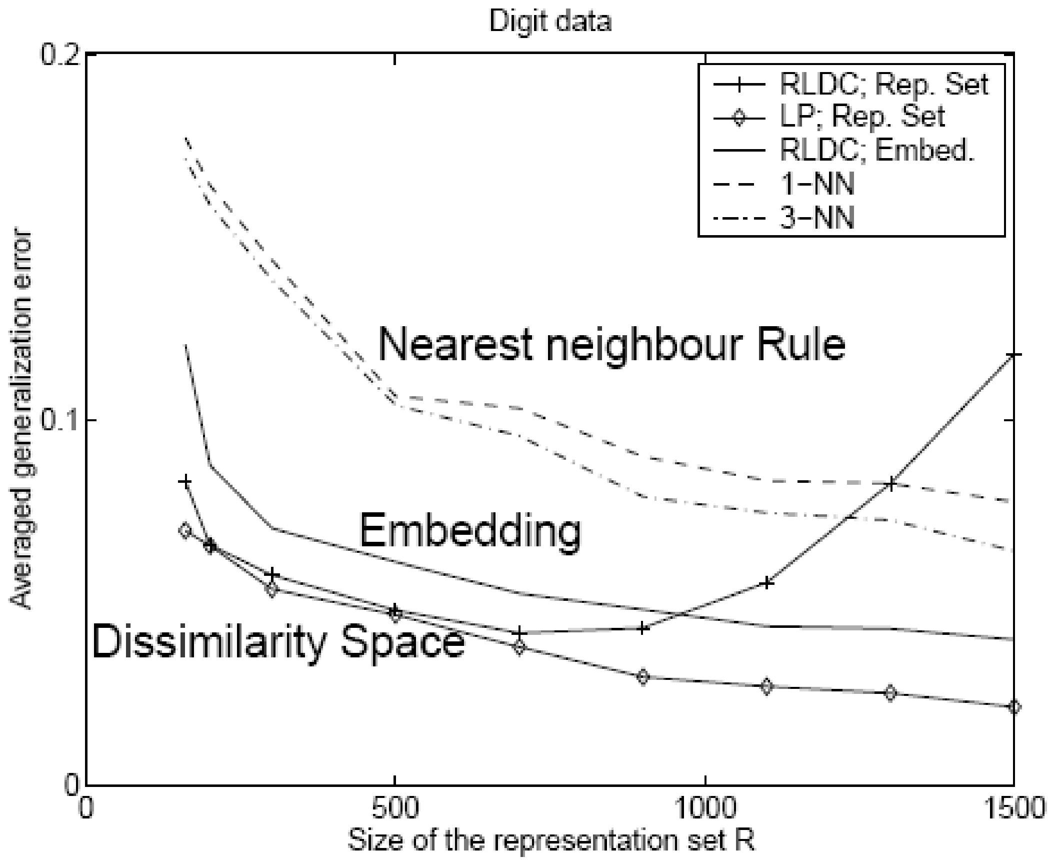


Matching new objects to various templates:
class(x) = class(argmin$_y$(D(x,y)))

Dissimilarity measure appears to be non-metric.

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 equivalent to Embedding better than Nearest Neighbour Rule

Pekalska, The Dissimilarity Representation for Pattern Recognition. Foundations and Applications. World Scientific, Singapore , 2005

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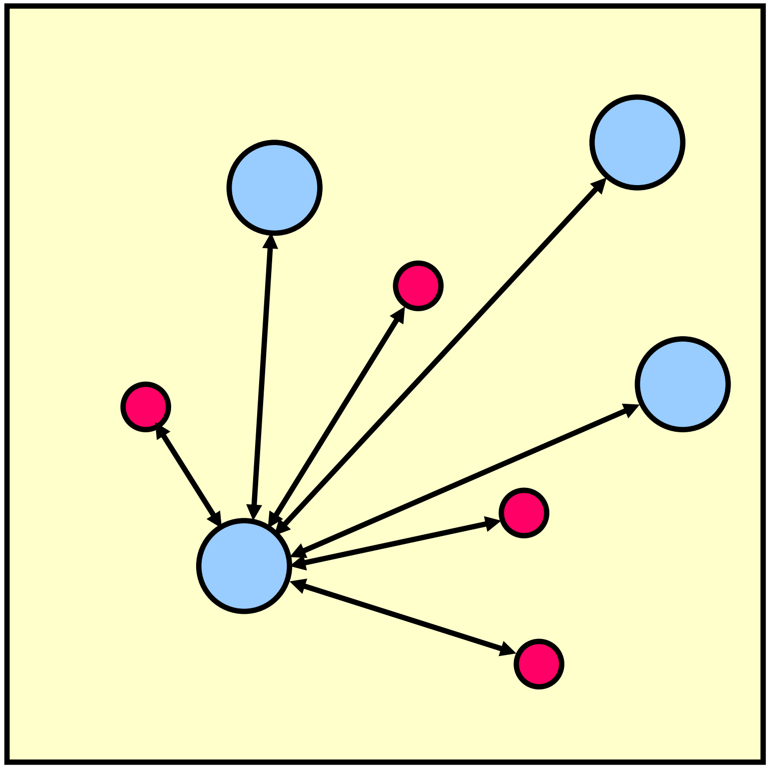
Ball Distances



- Generate sets of balls (classes) uniformly, in a (hyper)cube; not intersecting.
- Balls of the same class have the same size.
- Compute all distances between the ball surfaces.

-> Dissimilarity matrix D

Duin et al., Non-Euclidean dissimilarities: Causes and informativeness, SSSPR 2010, 324-333.

Balls3D

Classifier	PE Sp	Ass Sp	Pos Sp	Neg Sp	Cor Sp
1-NN	47.4 (2.0)	47.4 (2.0)	47.4 (2.0)	44.2 (1.5)	47.4 (2.0)
Parzen	45.7 (1.7)	45.5 (1.6)	45.6 (1.7)	35.5 (1.7)	45.7 (1.7)
NM	47.5 (2.0)	47.7 (2.0)	47.6 (1.9)	49.6 (0.2)	48.1 (1.8)
SVM-1	50.7 (2.2)	50.0 (2.7)	50.0 (2.5)	62.1 (1.7)	50.1 (2.0)

Classifier	PE Dis Sp	Ass Dis Sp	Pos Dis Sp	Neg Dis Sp	Cor Dis Sp
1-NN	49.8 (2.2)	49.8 (2.2)	49.8 (2.2)	5.1 (0.8)	49.7 (2.2)
Parzen	47.9 (2.2)	47.9 (2.2)	47.9 (2.2)	4.6 (0.5)	47.9 (2.2)
NM	49.8 (2.2)	49.8 (2.2)	49.8 (2.2)	5.0 (0.8)	49.9 (2.2)
SVM-1	50.2 (1.6)	50.8 (1.7)	50.7 (1.7)	1.9 (0.5)	49.8 (1.5)

10 x (2-fold crossvalidation of 50 objects per class)

Representation Strategies

Avoiding the PE space

Dissimilarity Space: $X = D$

Correcting

Associated space	$X = \{[X_p, X_q], \varnothing\}$	$\tilde{d}_{ij}^2 = d_p^2(x_i, x_j) + d_q^2(x_i, x_j)$
Positive space	$X = X_p$	$\tilde{d}_{ij}^2 = d_p^2(x_i, x_j)$
Negative space	$X = X_q$	$\tilde{d}_{ij}^2 = d_q^2(x_i, x_j)$
Additive Correction	$\tilde{d}_{ij}^2 = d_{ij}^2 + c, i \neq j$	$X = \mathrm{Embedding}(\tilde{D})$

As it is

Pseudo Euclidean Space $X = \{X_p, X_q\}$ $d_{ij}^2 = d_p^2(x_i, x_j) - d_q^2(x_i, x_j)$

Classifiers to be developed further

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Is the PE Space Informative?

	size	classes	Non-Metric	NEF	Rand Err	+ - Original, D	+ Positive, D_p	- Negative, D_q
Chickenpieces45	446	5	0	0.156	0.791	**0.022**	0.132	0.175
Chickenpieces60	446	5	0	0.162	0.791	**0.020**	0.067	0.173
Chickenpieces90	446	5	0	0.152	0.791	**0.022**	0.052	0.148
Chickenpieces120	446	5	0	0.130	0.791	**0.034**	0.108	0.148
FlowCyto	612	3	1e-5	0.244	0.598	0.103	**0.100**	0.327
WoodyPlants50	791	14	5e-4	0.229	0.928	**0.075**	0.076	0.442
CatCortex	65	4	2e-3	0.208	0.738	**0.046**	0.077	0.662
Protein	213	4	0	0.001	0.718	0.005	[illegible]	0.034
Balls3D	200	2	3e-4	0.001	0.500	**0.470**	0.495	0.000
GaussM1	500	2	0	0.262	0.500	**0.202**	**0.202**	0.228
GaussM02	500	2	5e-4	0.393	0.500	0.204	**0.174**	0.252
CoilYork	288	4	8e-8	0.258	0.750	**0.267**	0.313	0.618
CoilDelftSame	288	4	0	0.027	0.750	**0.413**	0.417	0.597
CoilDelftDiff	288	4	8e-8	0.128	0.750	**0.347**	0.358	0.691
NewsGroups	600	4	4e-5	0.202	0.733	**0.198**	0.213	0.435
BrainMRI	124	2	5e-5	0.112	0.499	0.226	**0.218**	0.556
Pedestrians	689	3	4e-8	0.111	0.348	**0.010**	0.015	0.030

Informative

Extremely Informative

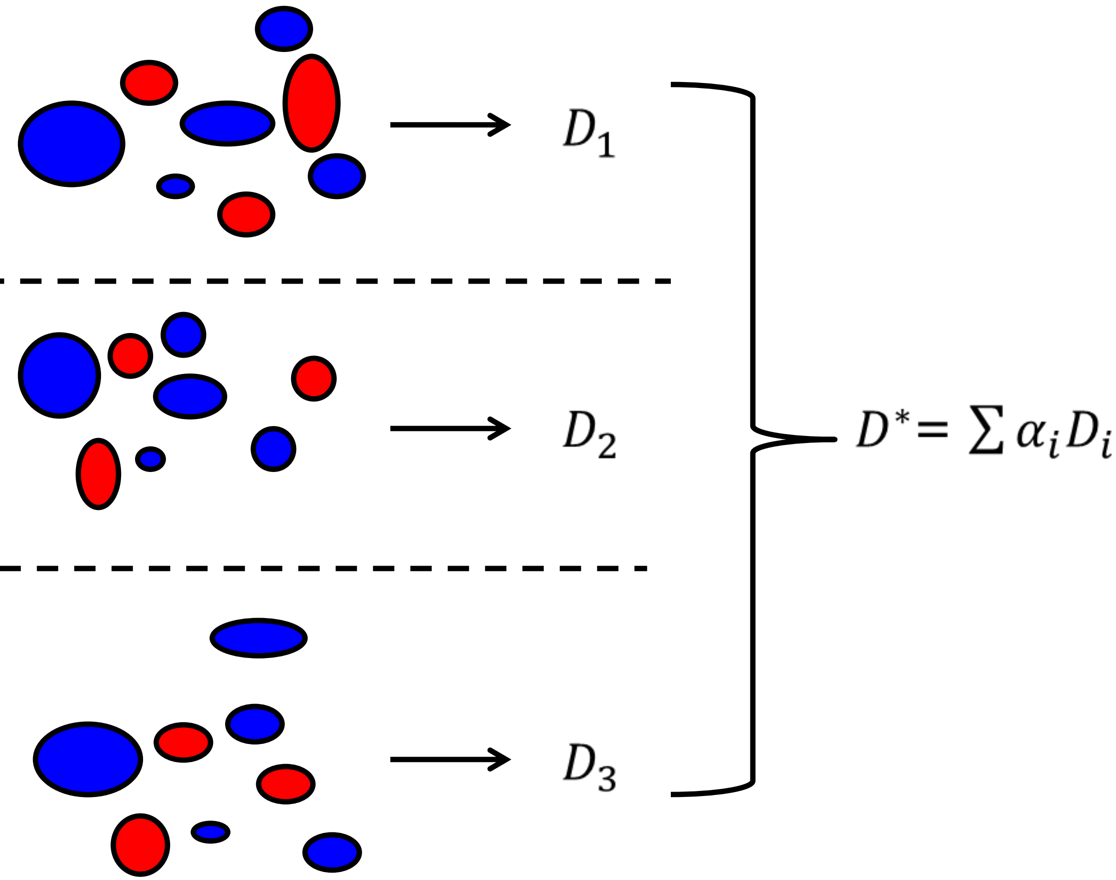
Not Informative

Multiple Dissimilarity Matrices

Dissimilarity Measure 1:

Dissimilarity Measure 2:

Dissimilarity Measure 3:



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Averaging of dissimilarity matrices

Dissimilarity space

Data	NEF	1-NN	1-NND	SVM-1
CoilDelftDiff	0.13	0.48	0.44	0.40
CoilDelftSame	0.03	0.65	0.41	0.39
CoilYork	0.26	0.25	0.37	0.33
Averaged		0.37	0.22	0.24

- Three procedures for **graph matching** compared on the Coil dataset: 4 classes (objects), 72 images per class.
- Classification errors for 25 times 10-fold crossvalidation.

CoilDelftDiff Graphs are compared in the eigenspace with a dimensionality determined by the smallest graph in every pairwise comparison by the JoEig Approach [1].
CoilDelftSame Dissimilarities in 5D eigenspace derived from the two graphs by the JoEig approach [1].
CoilYork Dissimilarities are found by graph matching, using the algorithm of Gold and Ranguranjan [2]

[1] Lee & Duin, An inexact graph comparison approach in joint Eigenspace, SSSPR 2008.
[2] Gold & Rangarajan, A graduated assignment algorithm for graph matching. PAMI 18(4), 1996

Examples

Example: Chickenpieces (H. Bunke, Bern)

BACK

BREAST

DRUMSTICK

THIGH-AND-BACK

WING

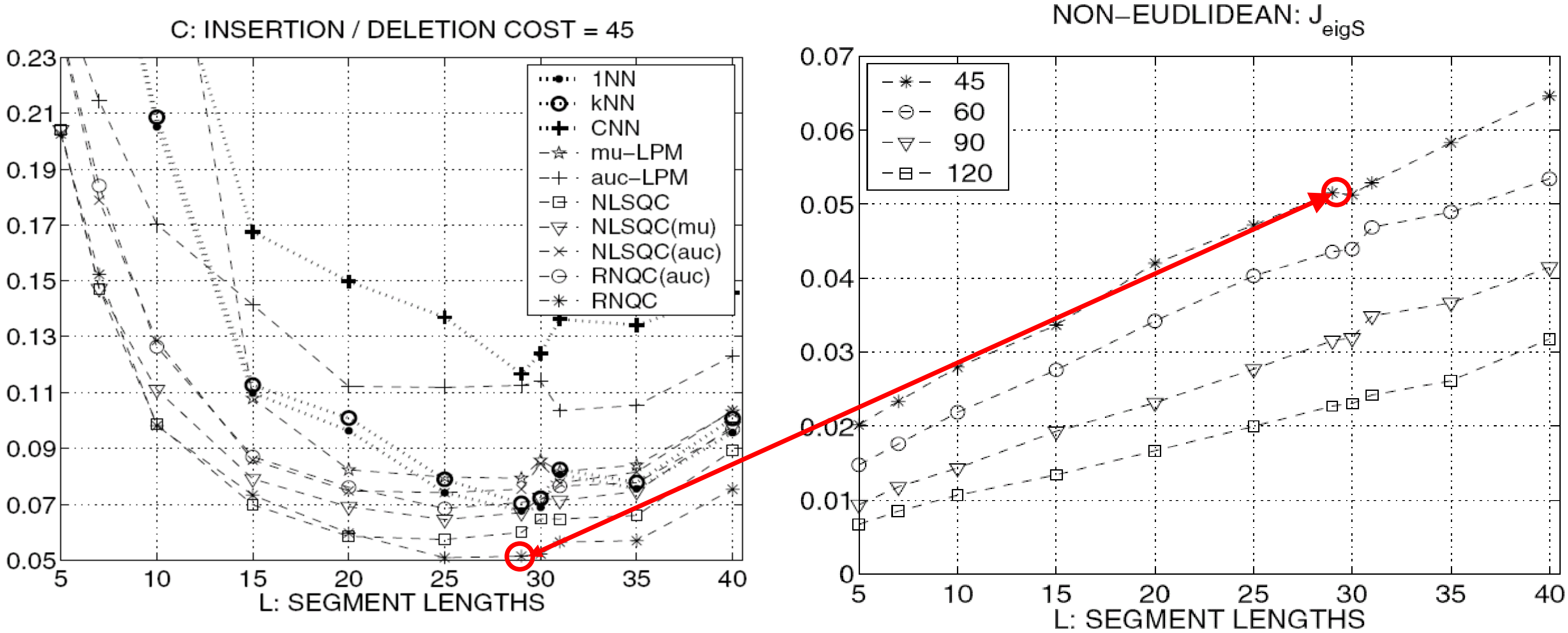
446 binary images, varying size, e.g.: 100 x 130

Andreu, G., Crespo, A., Valiente, J.M.: Selecting the toroidal self-organizing feature maps (TSOFM) best organized to object recogn. In: ICNN. (1997) 1341–1346.

Shape classification by weighted-edit distances (Bunke)

Bunke, H., Buhler, U.: Applications of approximate string matching to 2D shape recognition. Pattern recognition ***26*** *(1993) 1797–1812*

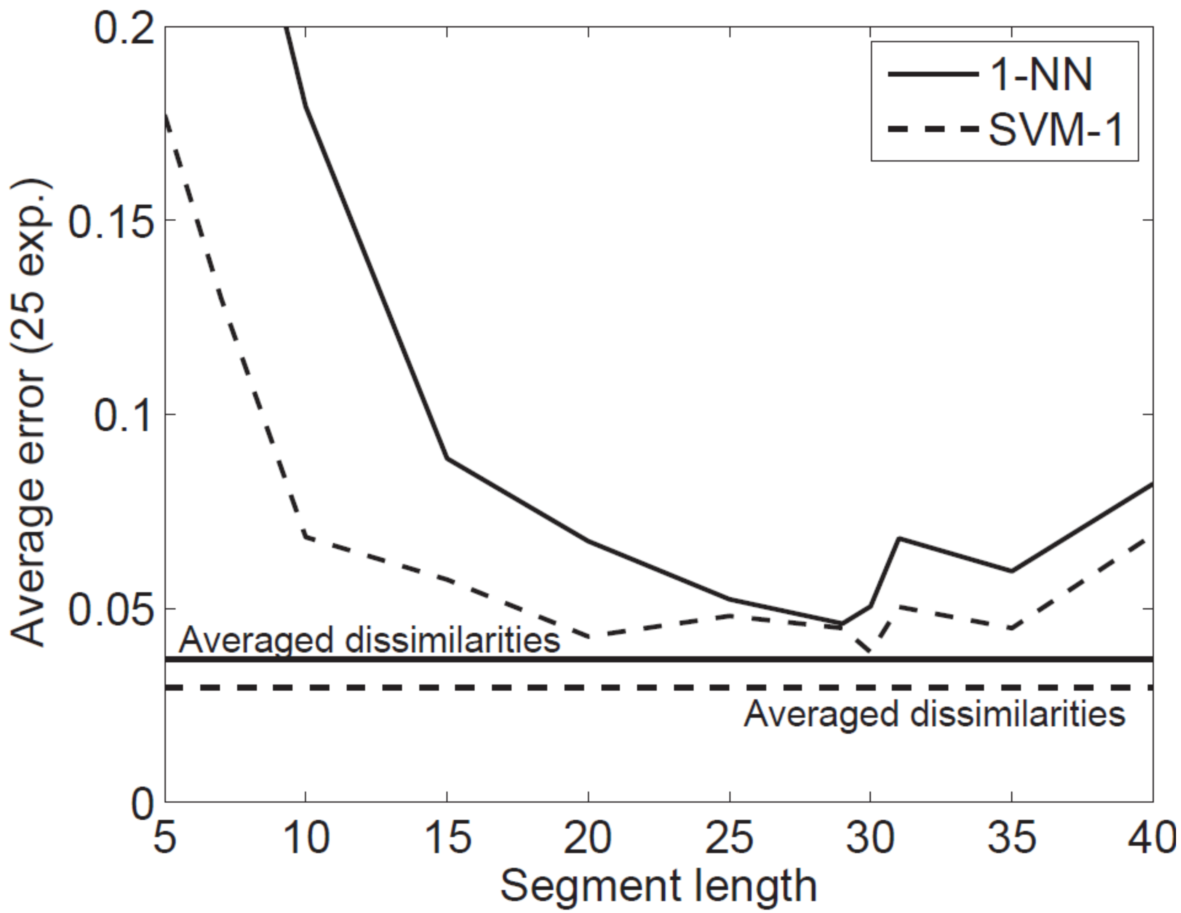
Chickenpieces: Various Dissimilarity Measures



<u>Best classification result is for a very non-Euclidean dissimilarity measure !</u>

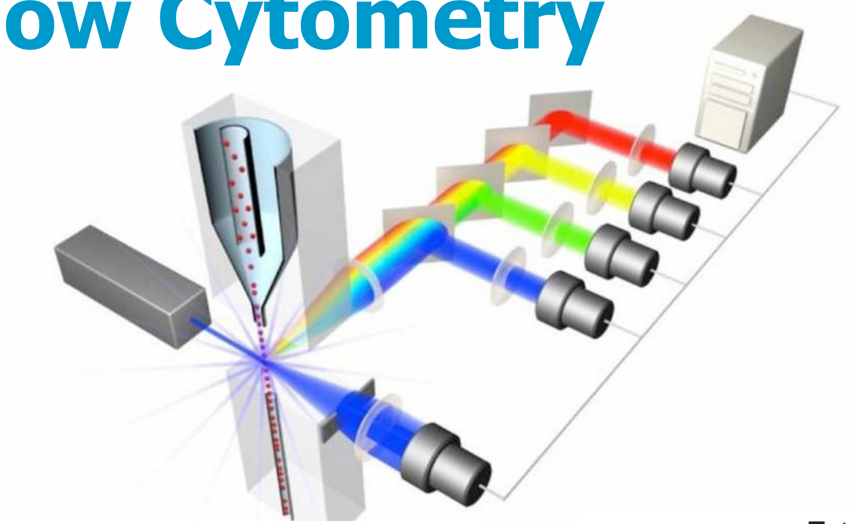
Pekalska et al., On not making dissimilarities Euclidean, SSSPR 2004, 1145-1154.

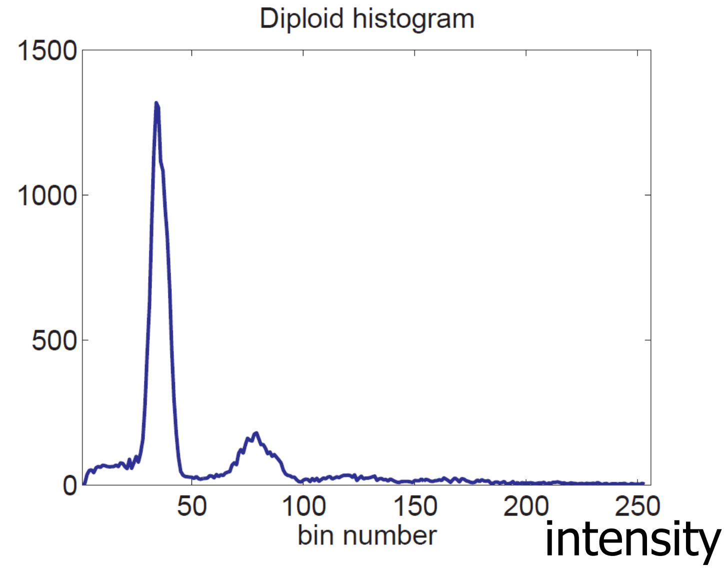
Chickenpieces: classification errors

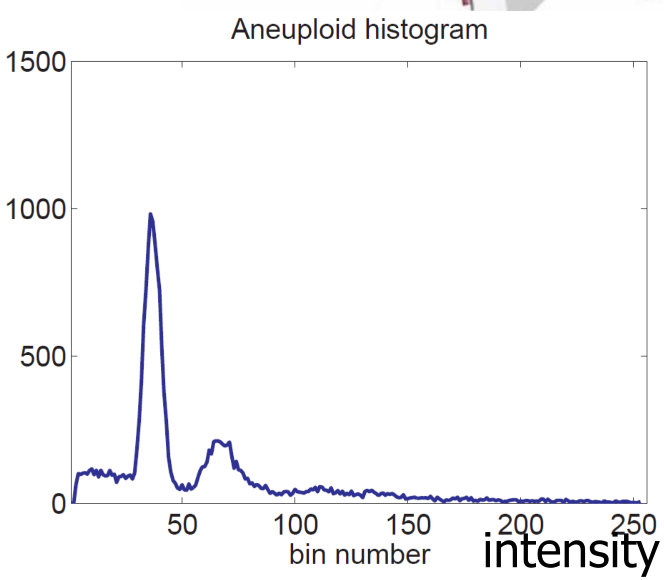


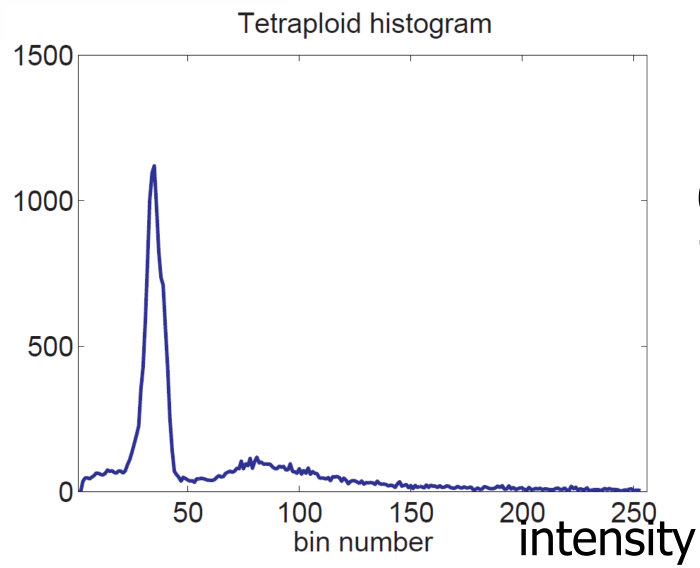
← Different dissimilarity measures →

Flow Cytometry









612 histograms in 3 classes

Nap & van Rodijnen, Atrium Hospital, Heerlen

Flow Cytometry: classification errors

Pairwise, horizontal (intensity calibration):
D(hist1,hist2) = $min_\alpha L_1$(hist1,hist2(α))

⟵ Dissimilarity space ⟶

Data Source	NEF	1-NN	1-NND	SVM-1
Tube 1	0.27	0.38	0.38	0.30
Tube 2	0.27	0.37	0.37	0.29
Tube 3	0.27	0.38	0.40	0.27
Tube 4	0.27	0.42	0.42	0.30
Averaged	0.24	0.27	0.20	0.11

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Bio-crystallization

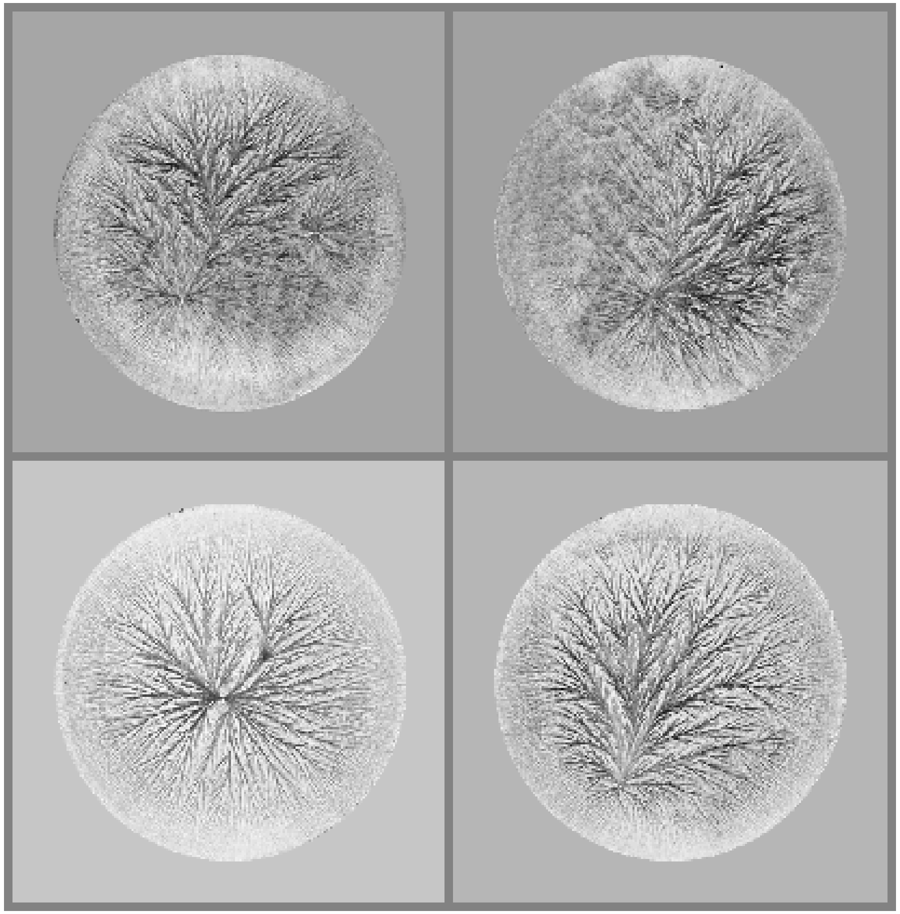
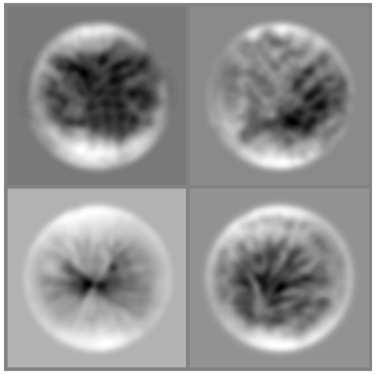


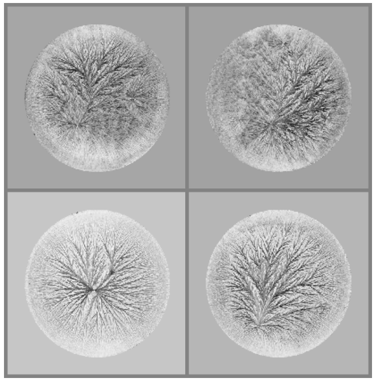
image size: 2114 x 2114
Different food products / quality
2 classes, 54 examples/class

Busscher et al., Standardization of the iocrystallization Method for Carrot Samples, Biological Agriculture and Horticulture, 2010, Vol. 27, pp. 1–23

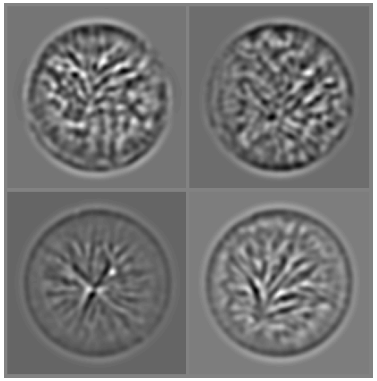
Bio-crystallization: Dissimilarity Measures



Gauss → L2



Originals



Laplace → L2

Laplace → Abs → Histogram → L1

Bio-crystallization: classification errors

Dissimilarity space

Dissimilarity Measure	NEF	1-NN	1-NND	SVM-1
Gauss	0	0.329	0.266	0.106
Laplace	0	0.229	0.313	0.125
Laplace Histogram	0.067	0.107	0.172	0.072
Averaged	0.004	0.114	0.166	0.057

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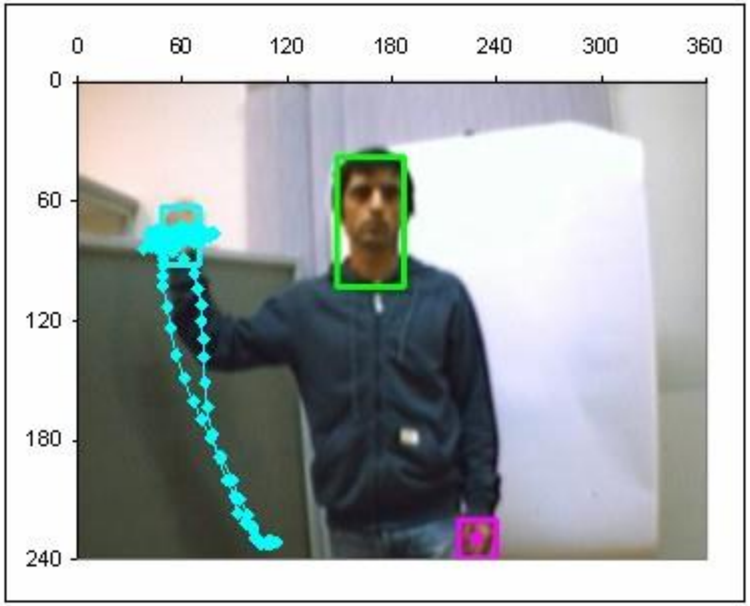
Gesture Recognition



Is this gesture in the database?

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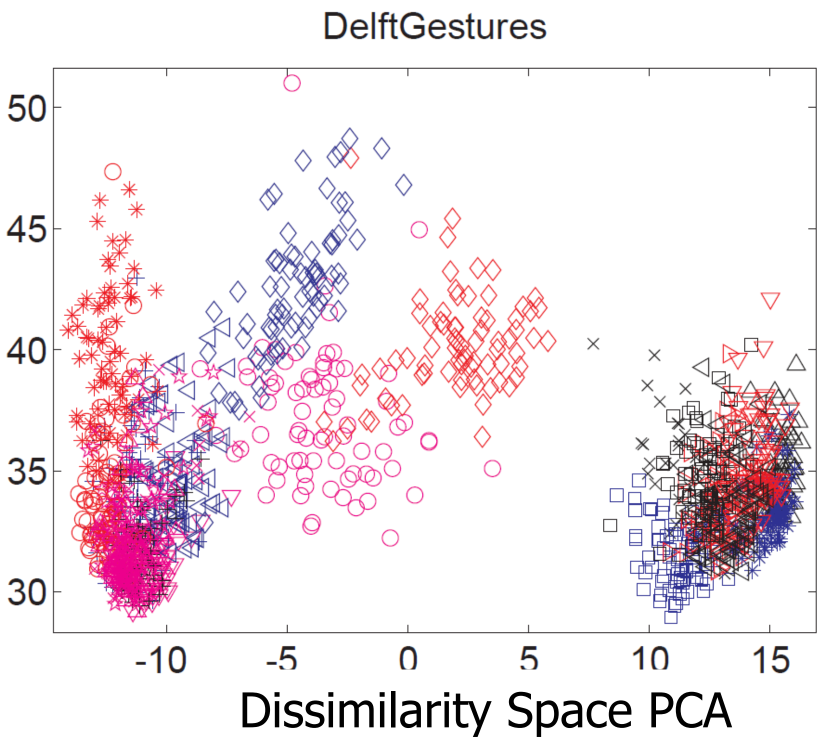
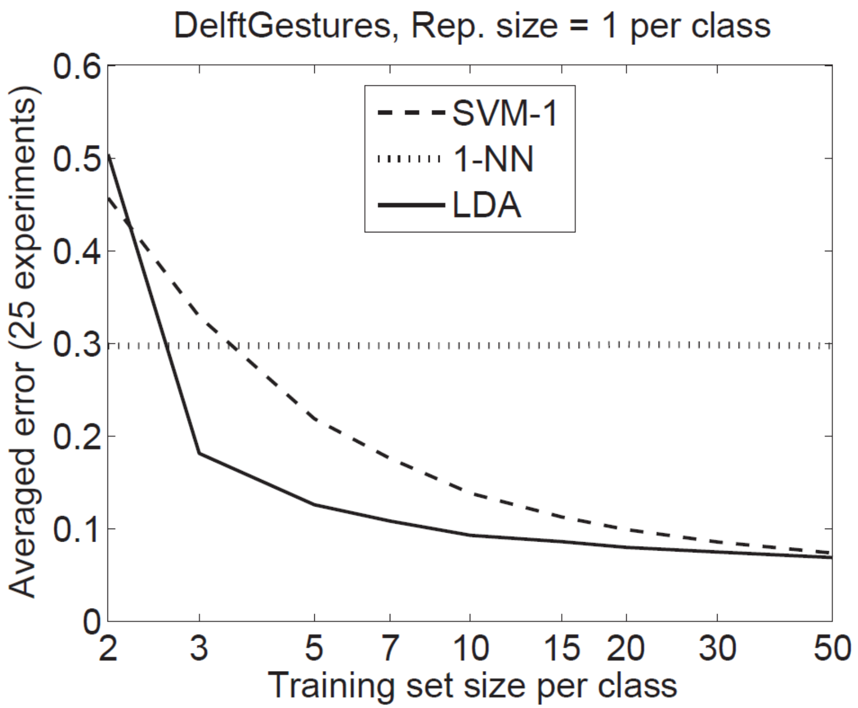
Gesture Recognition

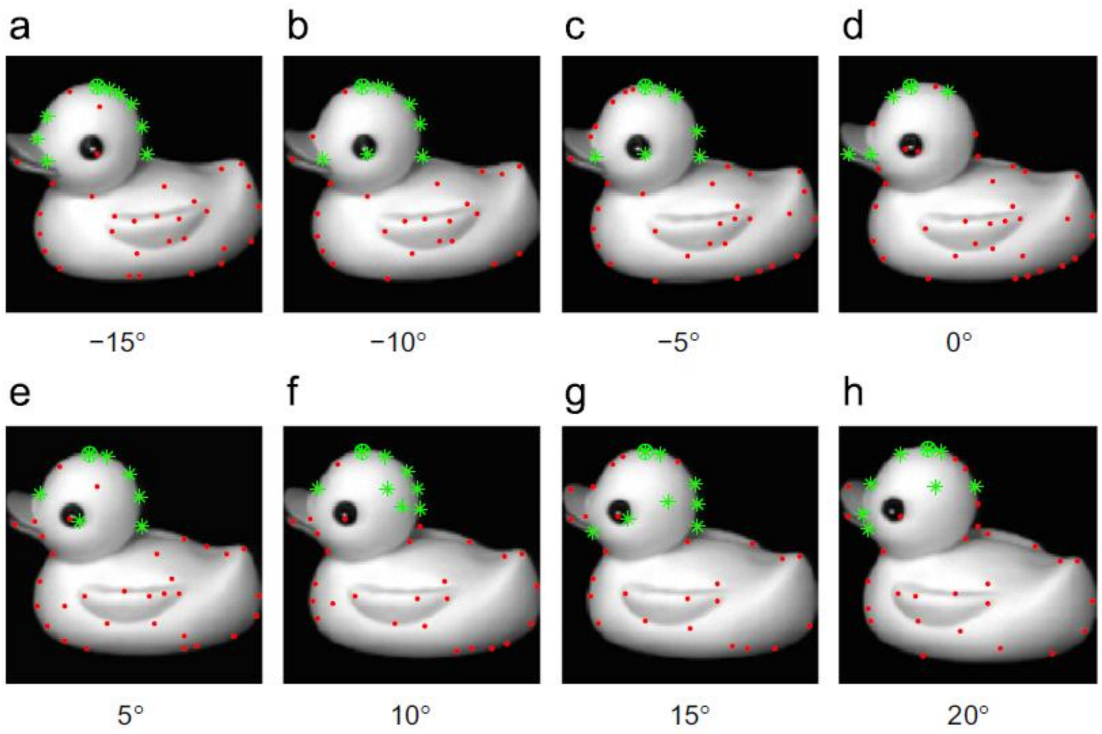


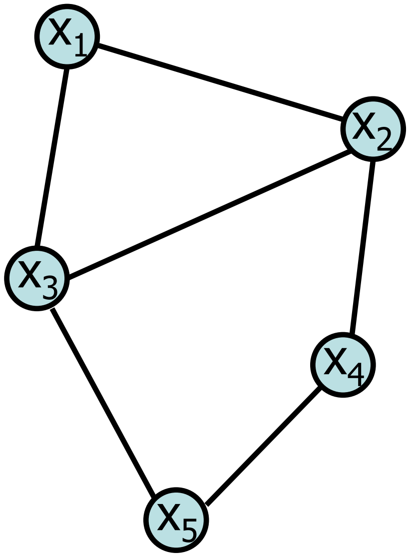


20 signs (classes), 75 examples/sign
Distance measure: DTW

Lichtenauer et al. Sign language recognition by combining statistical DTW and independent classification. PAMI 2008, 2040–2046.

Application: Graphs

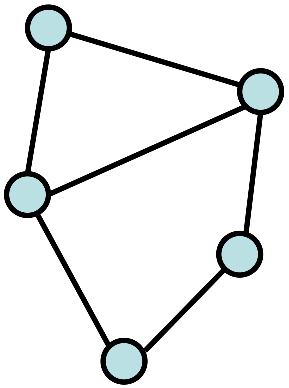




Graph with feature nodes

Taken from: Ren, Aleksic, Wilson, Hancock,
A polynomial characterization of hypergraphs using the Ihara zeta function,
Pattern Recognition, 2011, 1941-1957

Interpolating structural and feature space dissimilarities



Structure only
(no features)

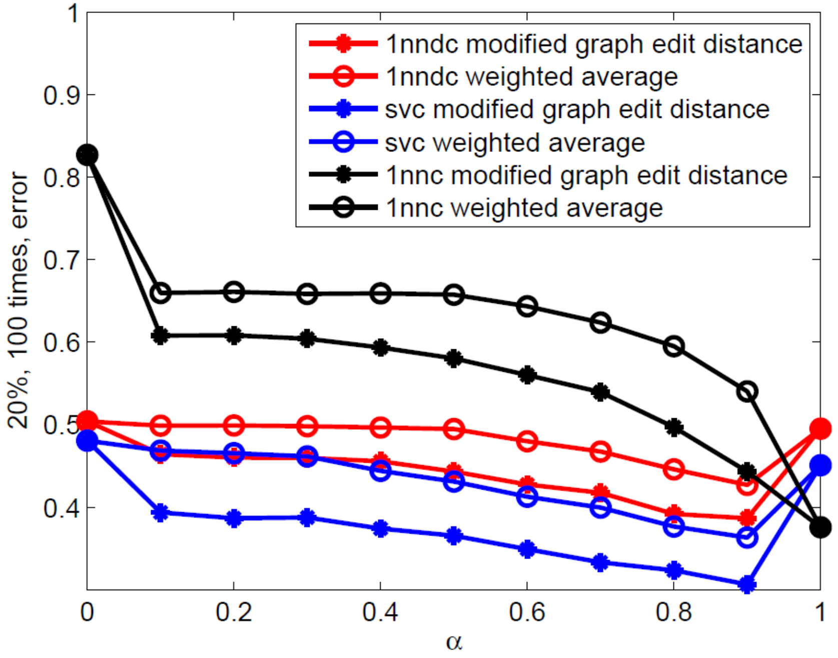


Fig. 5. Results of coil-segment for modified graph edit distance.

$\{x_1 \ x_2 \ x_3 \ x_4 \ x_5\}$

Features only
(no structure)

W.R.Lee et al., Bridging Structure and Feature Representations in Graph Matching, IJPRAI,2011, accepted

Conclusion

The Bridge
The Toll Bridge

between **structural** and **statistical** pattern recognition offered by the **dissimilarity** representation

………

is a **toll bridge**,

to be paid by solving the **non-Euclidean** problem

………

The dissimilarity space may settle the fare