

Structural pattern recognition in dissimilarity space

Robert P.W. Duin, Delft University of Technology

Pattern Recognition Lab

Delft University of Technology, The Netherlands

<http://rduin.nl>

Structural pattern recognition

- Shapes
- Sequences
- Graphs

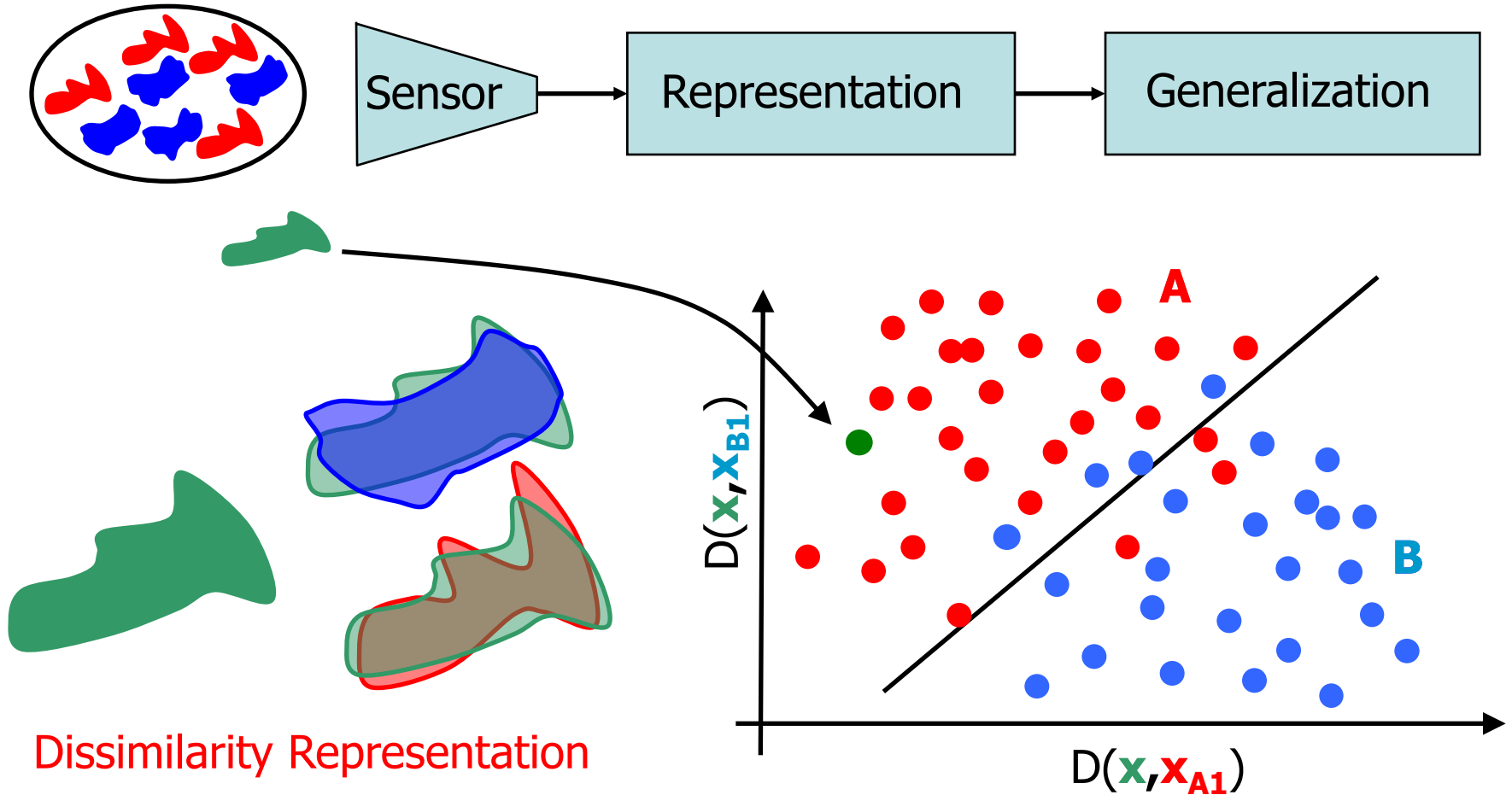
Objects → Feature representation → Classifier

Objects → Similarity / Dissimilarity → Nearest Neighbor Rule

Here:

Objects → Dissimilarities → Dissimilarity Space → Classifier

Dissimilarities \rightarrow True Representation



Dissimilarity Measures

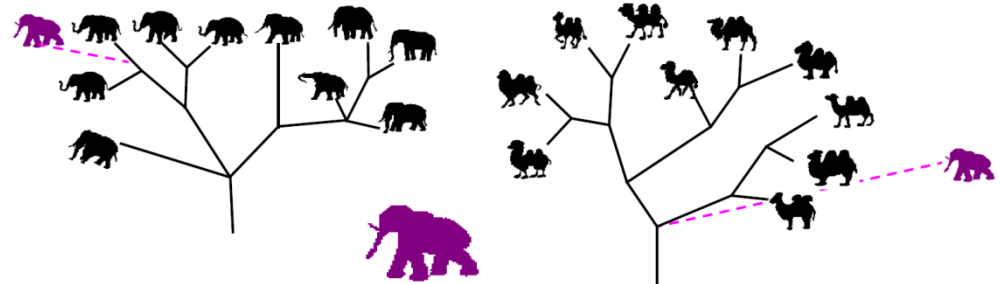
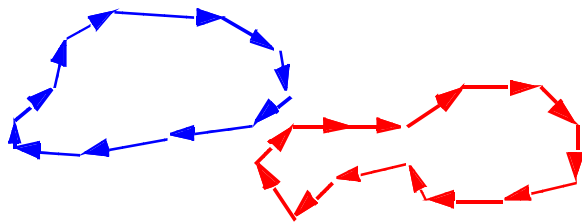
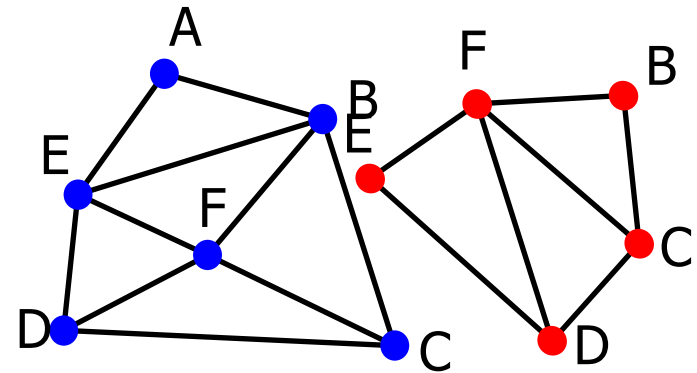
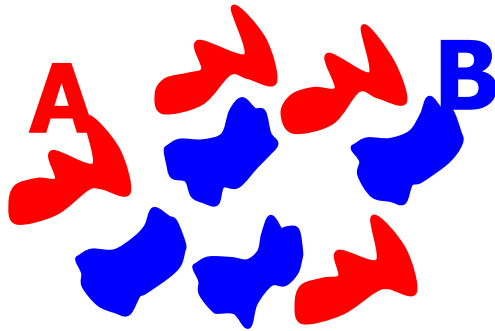
- Shapes : Geometrics, Morphing, Editing
- Sequences: DTW, HMM, Editing
- Graphs: Graph distances based on nodes / edges /attributes

Questions

How to improve a given dissimilarity representation?

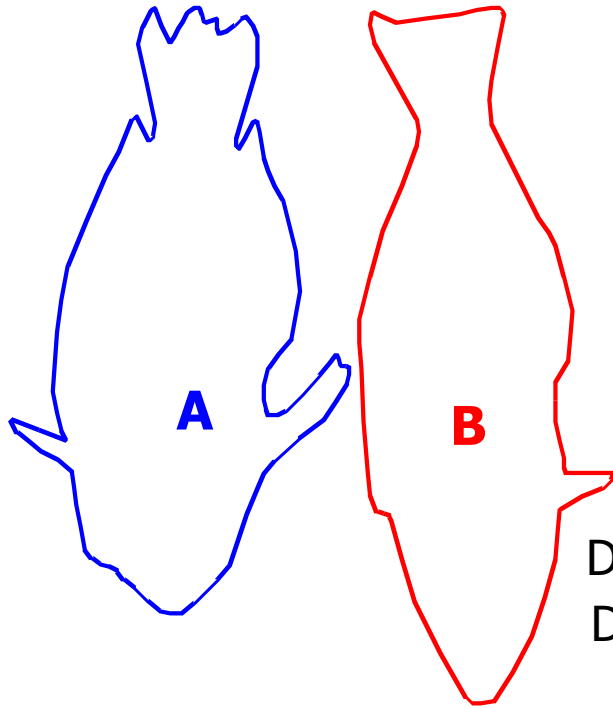
Should it be Euclidean? (\sim Mercer kernels)

Structural Representation



How to generalize? Distances!

Examples Dissimilarity Measures



Dist(**A**,**B**):

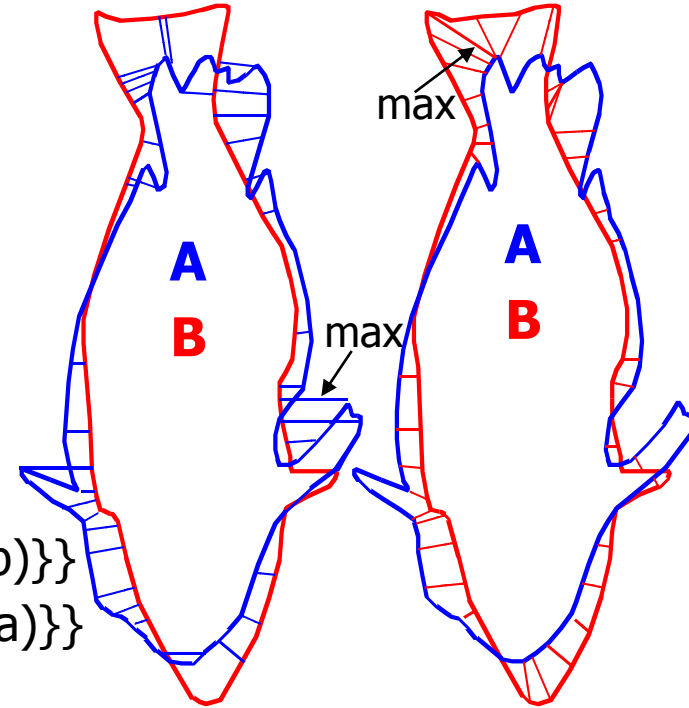
$a \in \mathbf{A}$, points of **A**

$b \in \mathbf{B}$, points of **B**

$d(a,b)$: Euclidean distance

$$D(\mathbf{A},\mathbf{B}) = \max_a \{ \min_b \{ d(a,b) \} \}$$

$$D(\mathbf{B},\mathbf{A}) = \max_b \{ \min_a \{ d(b,a) \} \}$$



Hausdorff Distance (metric):

$$DH = \max \{ \max_a \{ \min_b \{ d(a,b) \} \} , \max_b \{ \min_a \{ d(b,a) \} \} \}$$

$$D(\mathbf{A},\mathbf{B}) \neq D(\mathbf{B},\mathbf{A})$$

Modified Hausdorff Distance (non-metric):

$$DM = \max \{ \text{mean}_a \{ \min_b \{ d(a,b) \} \} , \text{mean}_b \{ \min_a \{ d(b,a) \} \} \}$$

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 .

Class separability

The **identity property**:

- **Definiteness:** $d_{ij} = 0$ iff objects i and j are identical

causes no-overlapping classes if objects are uniquely labeled.

There might be entirely different dissimilarity measures that have this property. Combining helps?

The identity property is sometimes not fulfilled

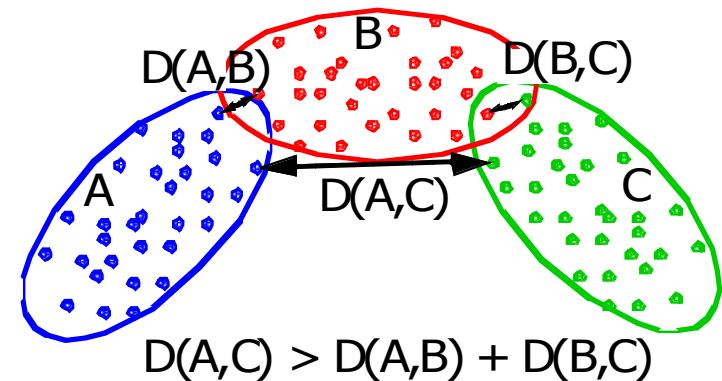


Distance(Table,Book) = 0

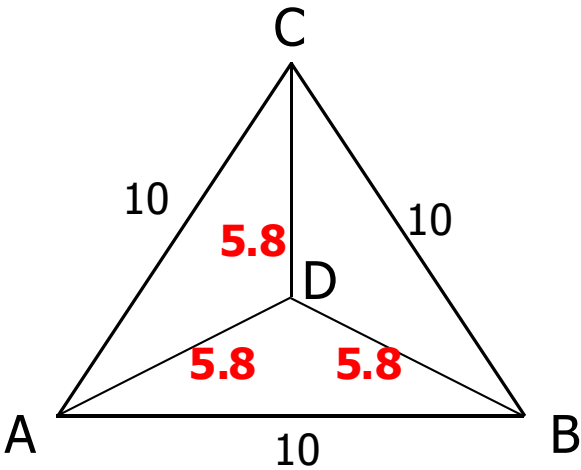
Distance(Table,Cup) = 0

Distance(Book,Cup) = 1

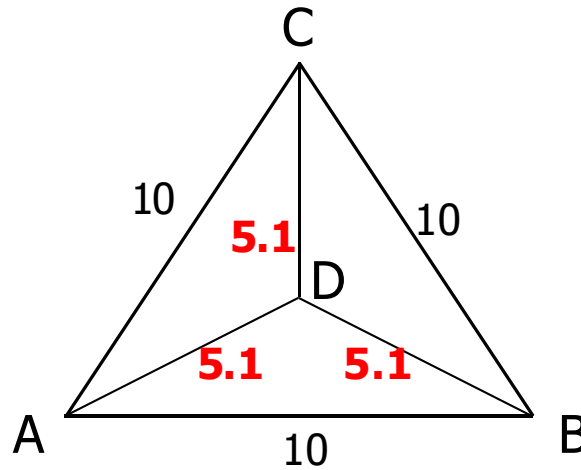
Single-linkage clustering



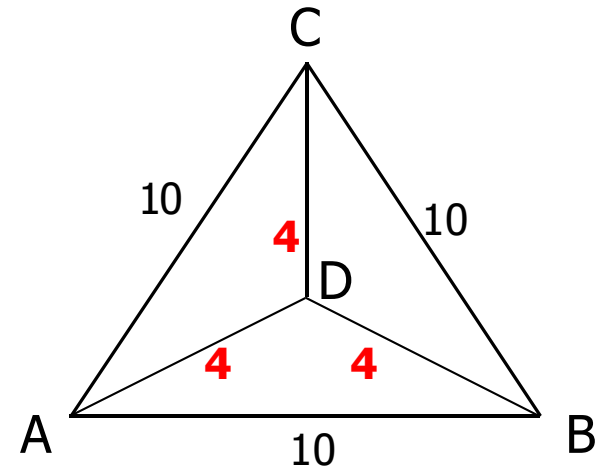
Euclidean - Non Euclidean - Non Metric



Euclidean
metric



non-Euclidean
metric

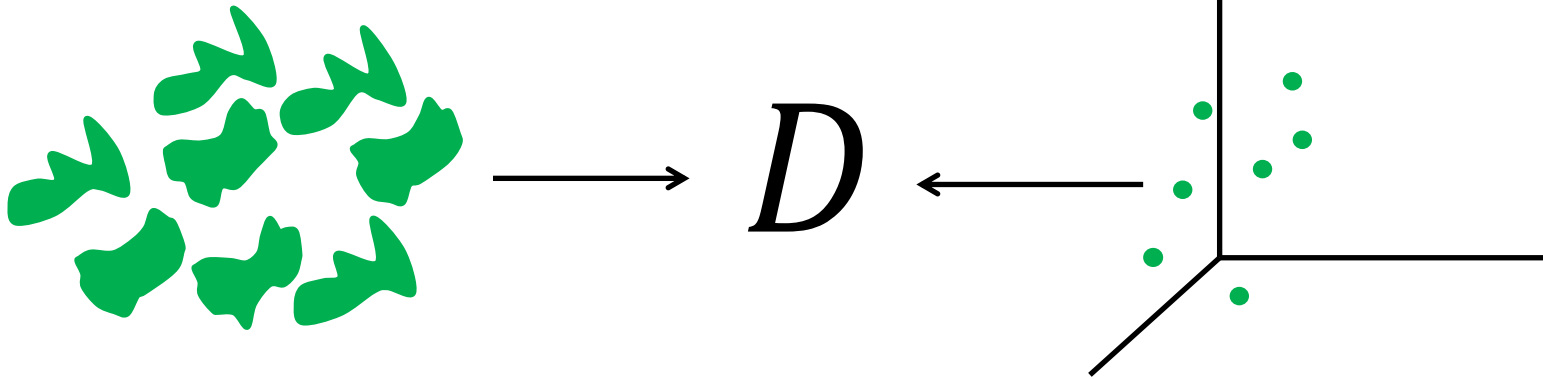


non-Euclidean
non-metric

What is an Euclidean dissimilarity matrix?

Definition

An $n \times n$ dissimilarity matrix between n objects is Euclidean if it can arise as the distances between n points in an Euclidean space.



Note: An Euclidean dissimilarity matrix is **square** and has a **zero diagonal**, but this **insufficient** to be Euclidean.

Euclidean dissimilarities

Theorem I:

Let D_1^2 and D_2^2 be squared Euclidean dissimilarity matrices, then:

$$D^2 = \alpha D_1^2 + \beta D_2^2 \quad (\alpha, \beta \geq 0)$$

is a squared Euclidean dissimilarity matrix as well.

Non-Euclidean Dissimilarities

Theorem II:

Let D^2 be a squared non-Euclidean distance matrix, symmetric and with zero diagonal, then:

$$D^2 = D_p^2 - D_n^2$$

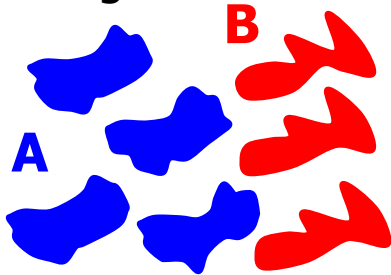
such that

$$D_p^2 \text{ and } D_n^2$$

are both Euclidean

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



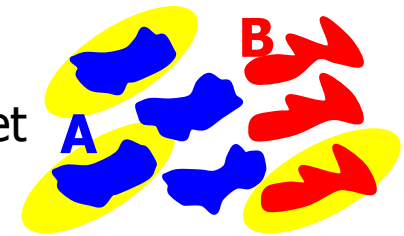
Pekalska, The dissimilarity representation for PR. World Scientific, 2005.

Alternative 1: Dissimilarity Space

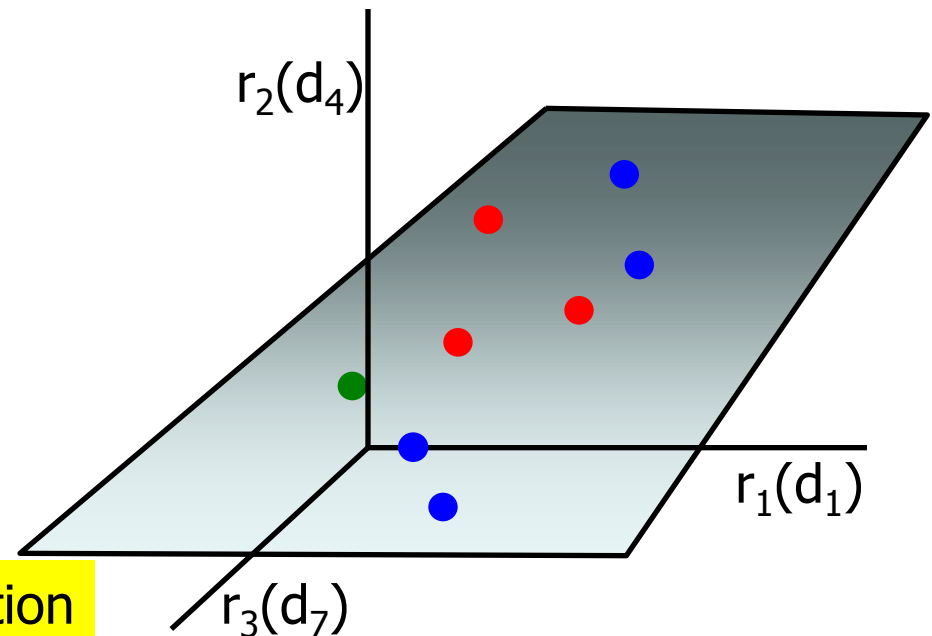
Dissimilarities

$$D_T = \begin{pmatrix} r_1 & & & r_2 & & & r_3 \\ d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} & d_{17} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} & d_{27} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} & d_{37} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} & d_{46} & d_{47} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} & d_{56} & d_{57} \\ d_{61} & d_{62} & d_{63} & d_{64} & d_{65} & d_{66} & d_{67} \\ d_{71} & d_{72} & d_{73} & d_{74} & d_{75} & d_{76} & d_{77} \\ d_x = (d_{x1} & d_{x2} & d_{x3} & d_{x4} & d_{x5} & d_{x6} & d_{x7}) \end{pmatrix}$$

Given labeled training set

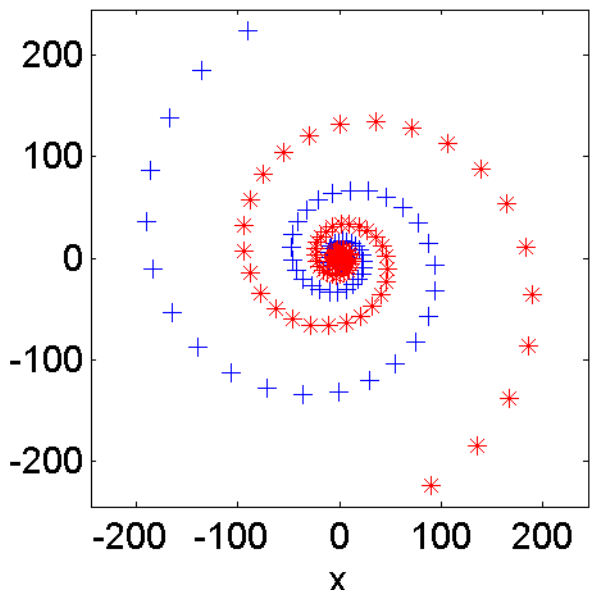


Unlabeled object to be classified

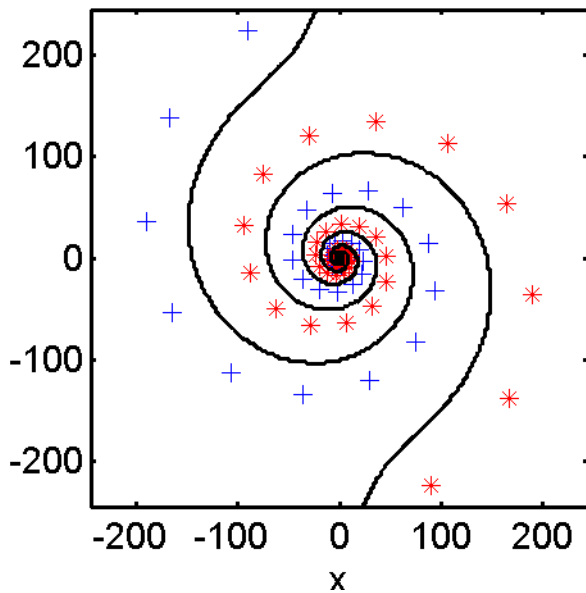


Selection of 3 objects for representation

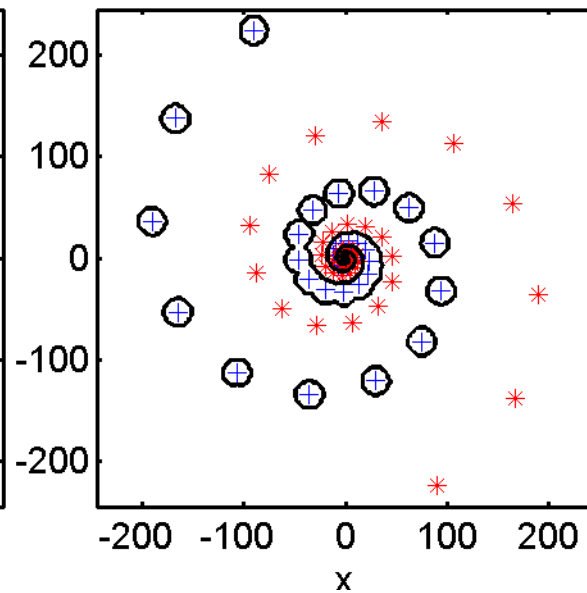
Total dataset



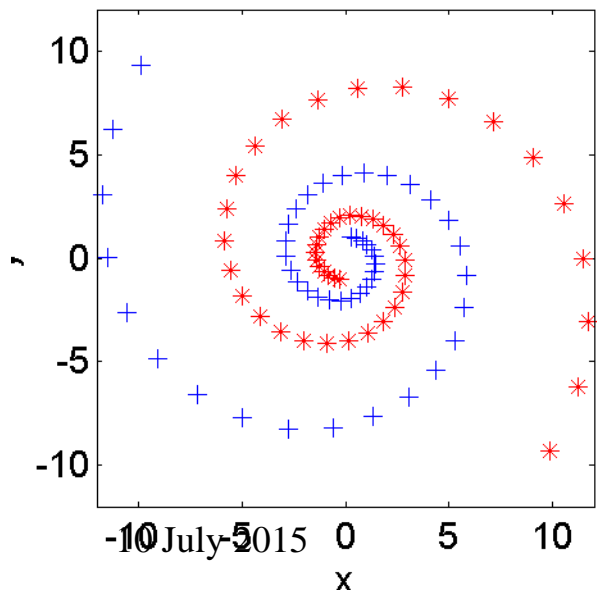
Fisher in dis. space



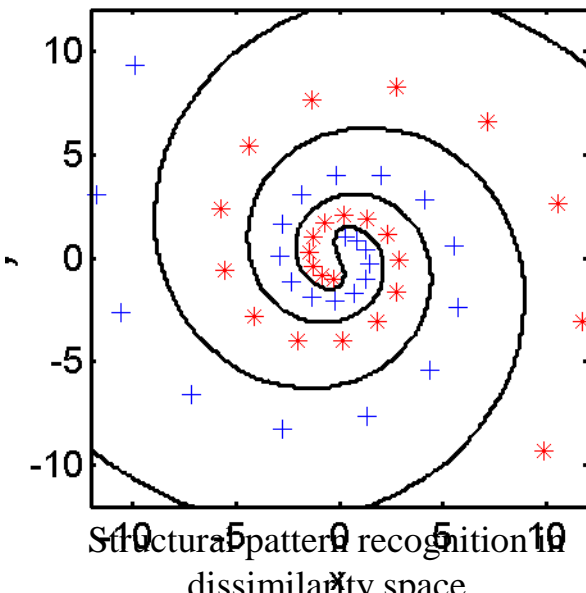
Optimized RB SVM



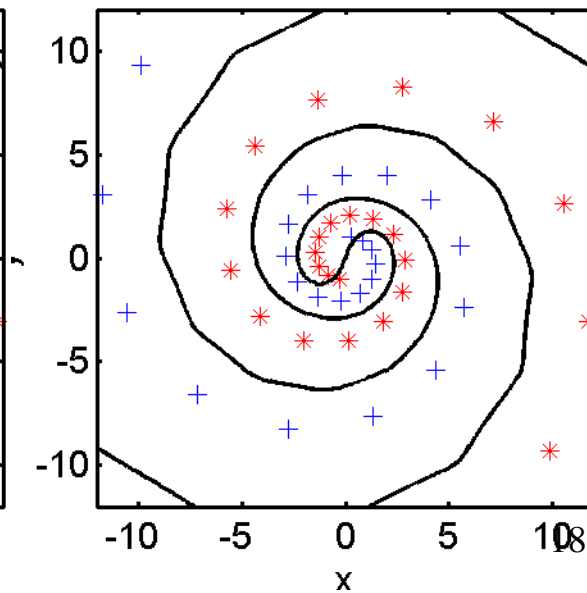
Zoomed dataset



Fisher in dis. space

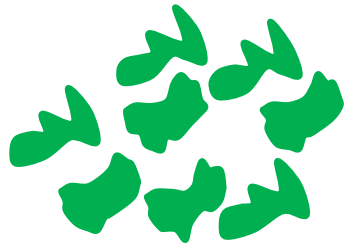


Optimized RB SVM



Structural pattern recognition in dissimilarity space

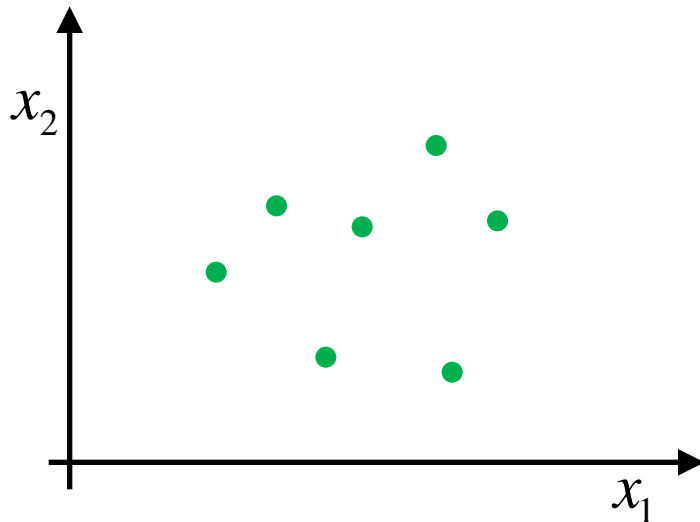
Alternative 2: Embedding



→ Dissimilarity matrix D → X

Training set

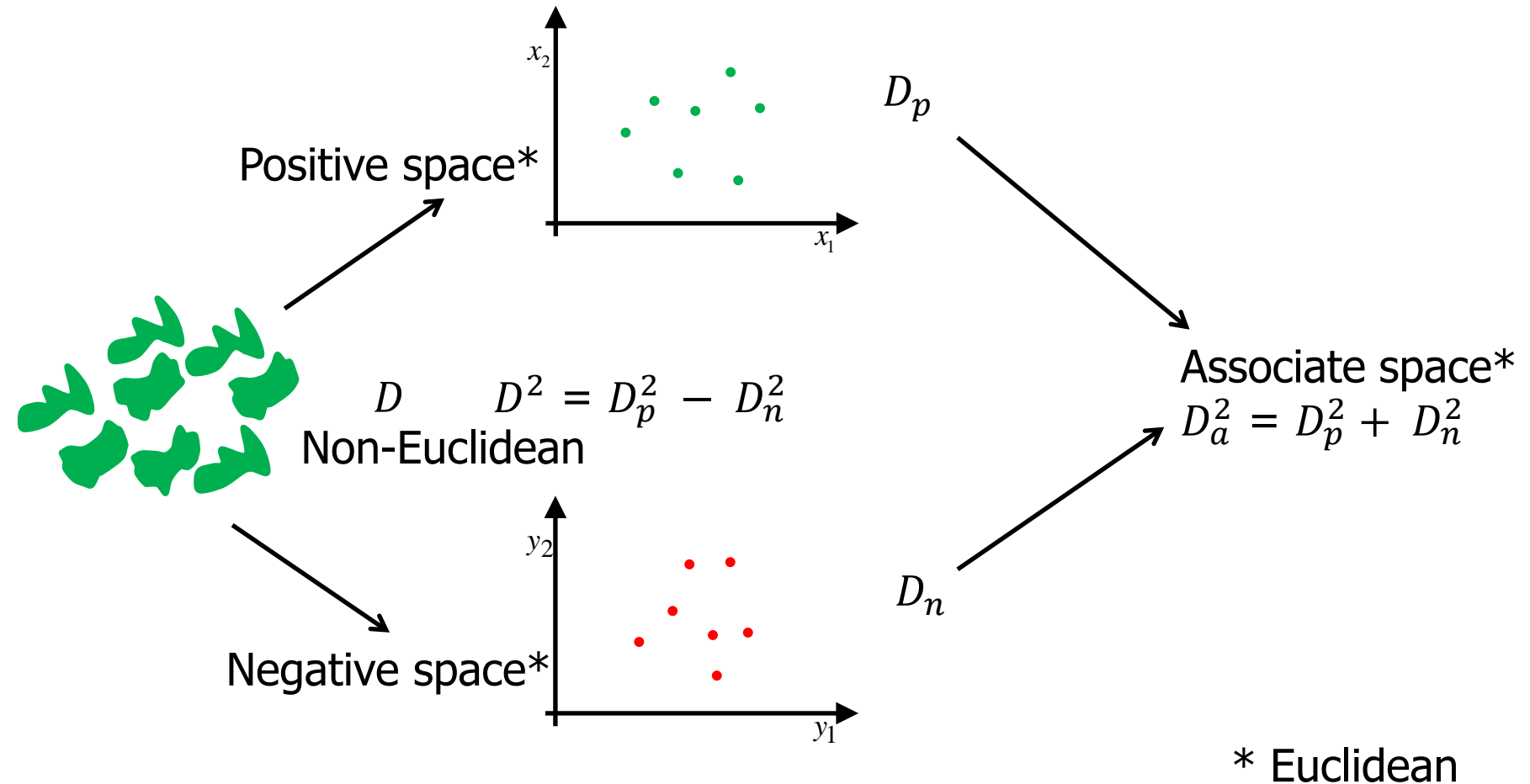
Is there a feature space for which $\text{Dist}(X, X) = D$?



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

Not possible if D is non-Euclidean

Pseudo-Euclidean embedding



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*

The Chickenpieces dissimilarity matrices

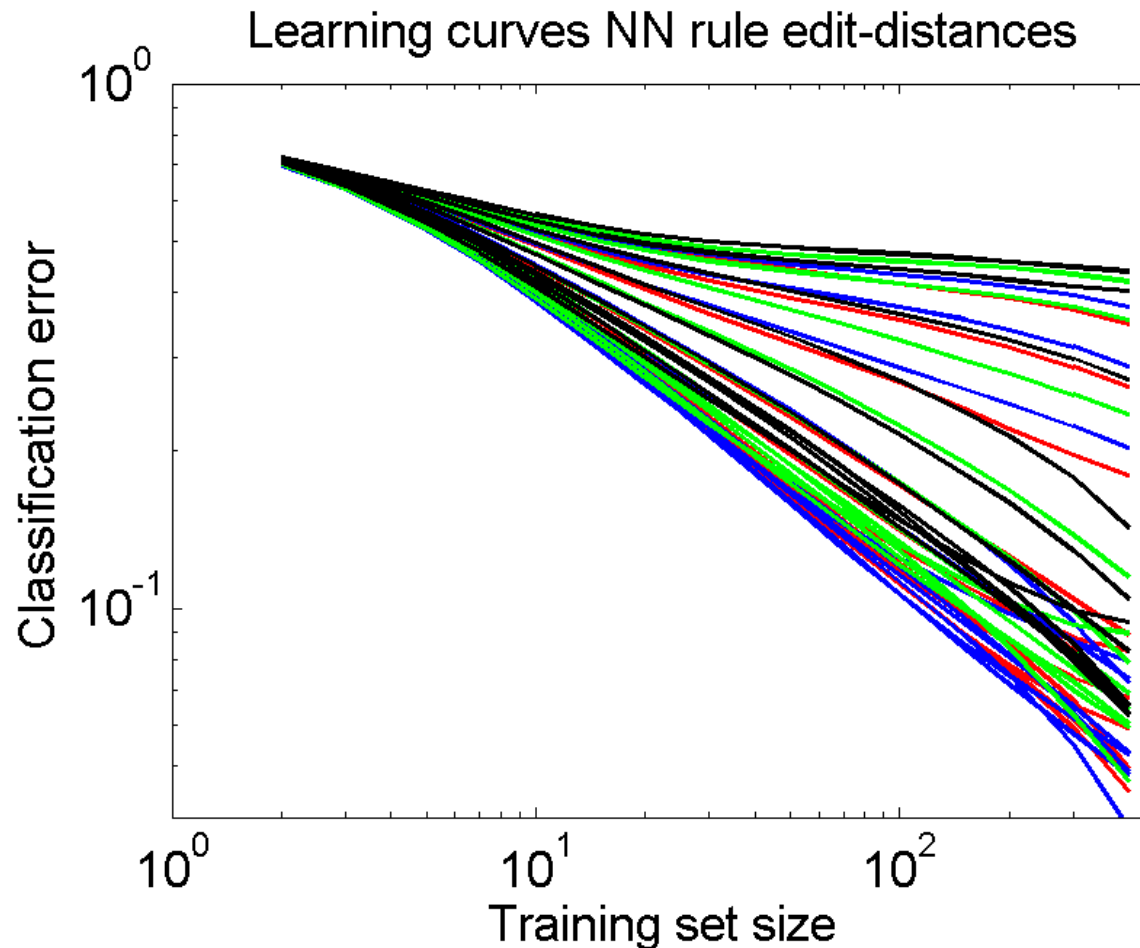


44 Weighted-edit distances measures based on
4 cost functions and
11 string representations.

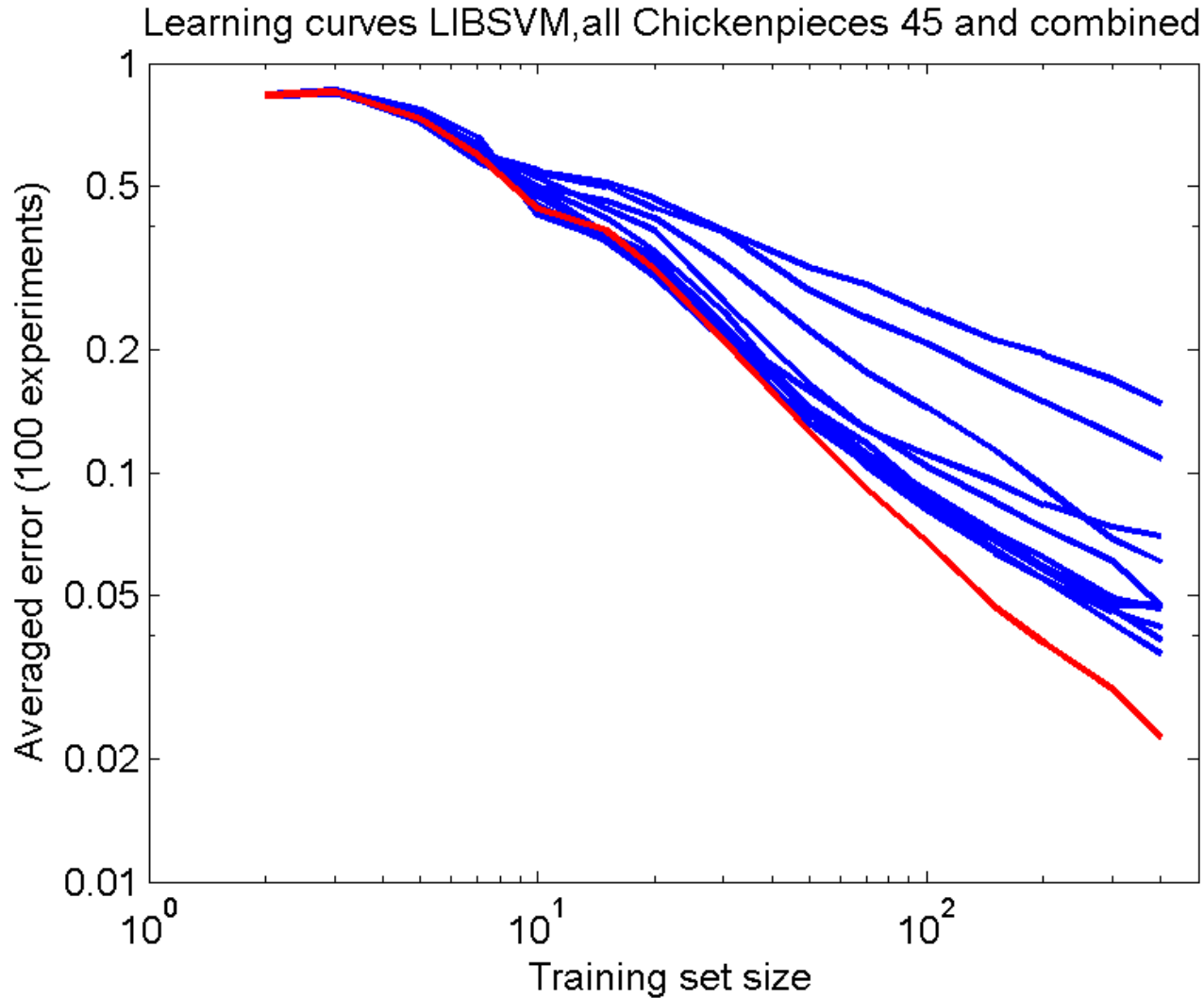
Shape classification by weighted-edit distances (Bunke)

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

The Chickenpieces dissimilarity matrices - performances

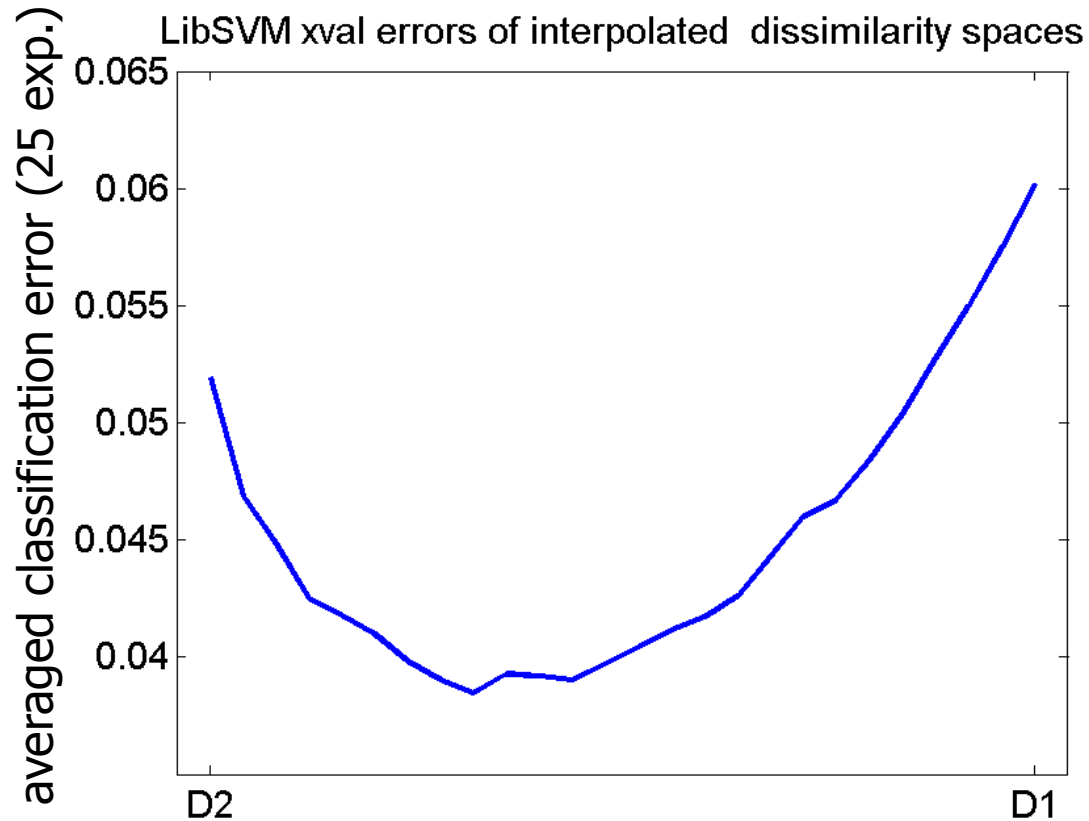


Averaging dissimilarities



Weighted average of two dissimilarity matrices

Chickenpieces-15-45 and Chickenpieces-25-60



Averaging helps!

Chickenpieces: Non-Euclideanness is informative

Average dissimilarity matrices for every cost function: $D_c^2 = \frac{1}{11} \sum_{i=1}^{11} D_{c,i}^2$

Split in Euclidean matrices: $D_c^2 = D_p^2 - D_n^2$

Subtracting helps!



Non-Euclideanness is informative

Cross validation errors

	D_c	D_p	D_n
C=1	0.022	0.137	0.175
C=2	0.020	0.067	0.173
C=3	0.022	0.052	0.148
C=4	0.034	0.108	0.148

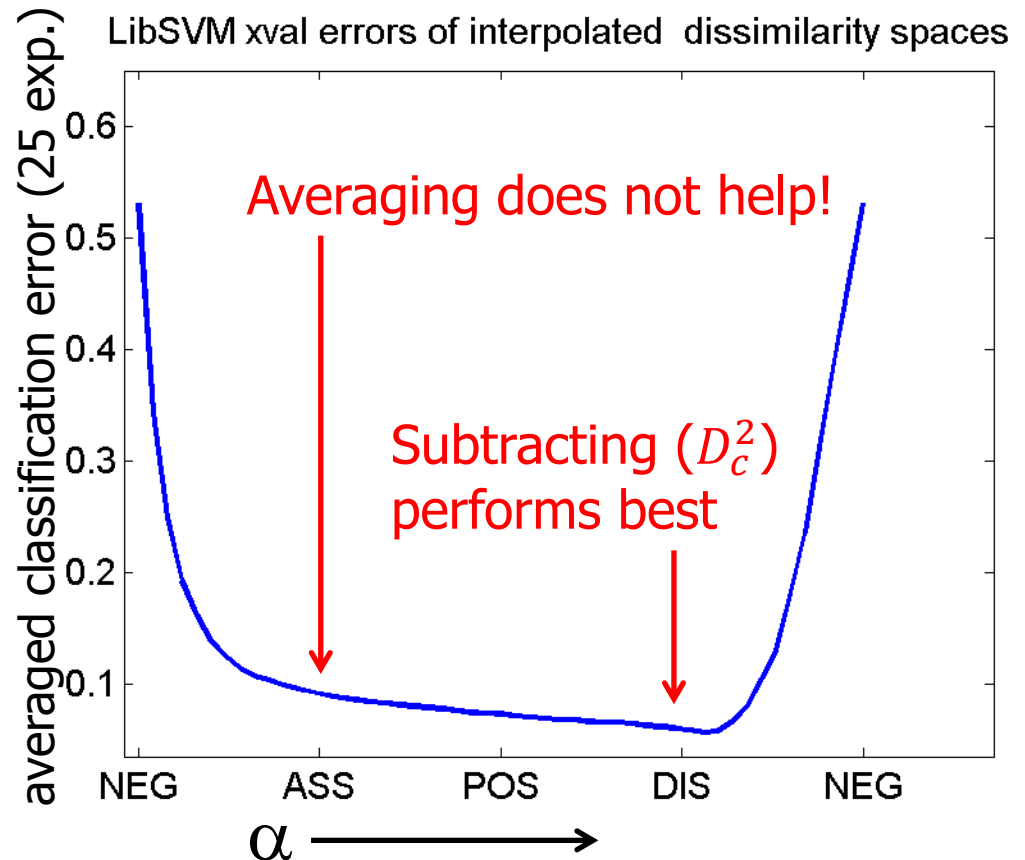
Random assignment error: 0.791

Subtracting dissimilarities

D_c : Chickenpieces-25-60

$$D_c^2 = D_p^2 - D_n^2$$

$$D^2 = \sin(\alpha) D_p^2 + \cos(\alpha) D_n^2$$



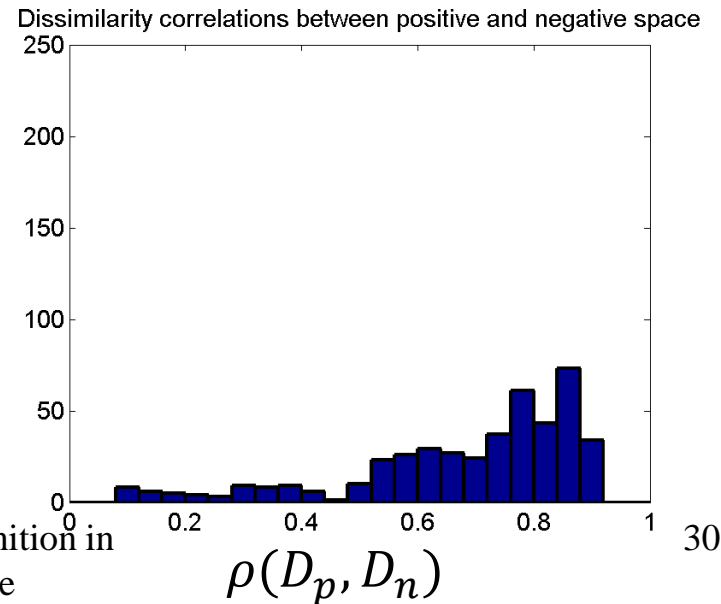
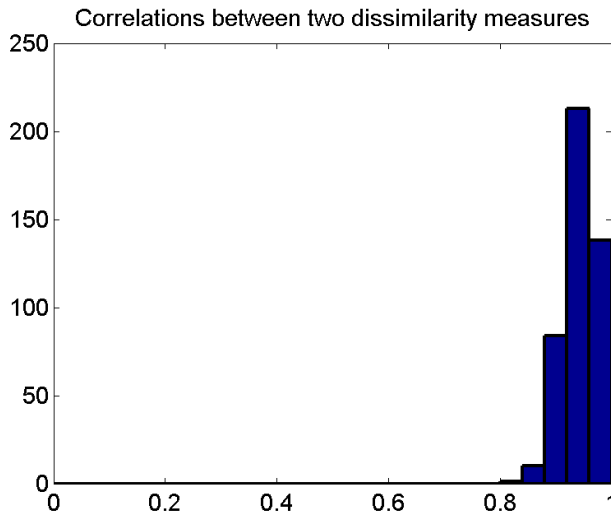
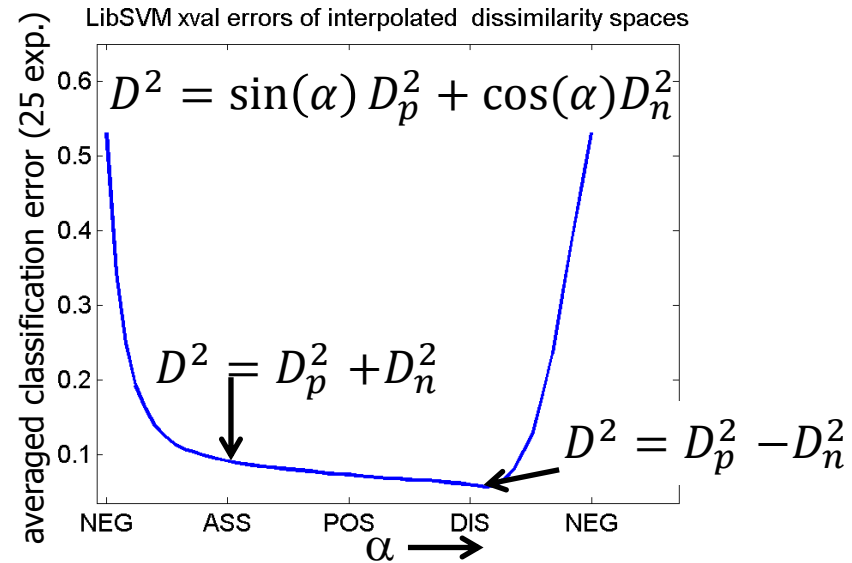
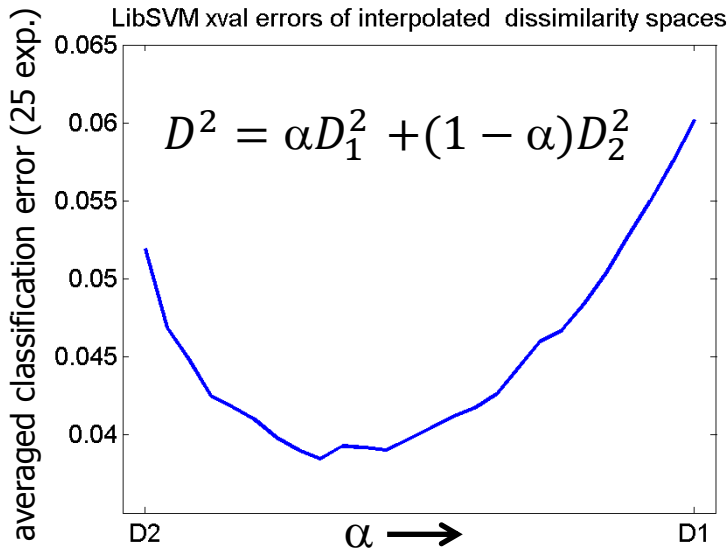
Question

Averaging different (non-Euclidean) dissimilarity measures **may help**.

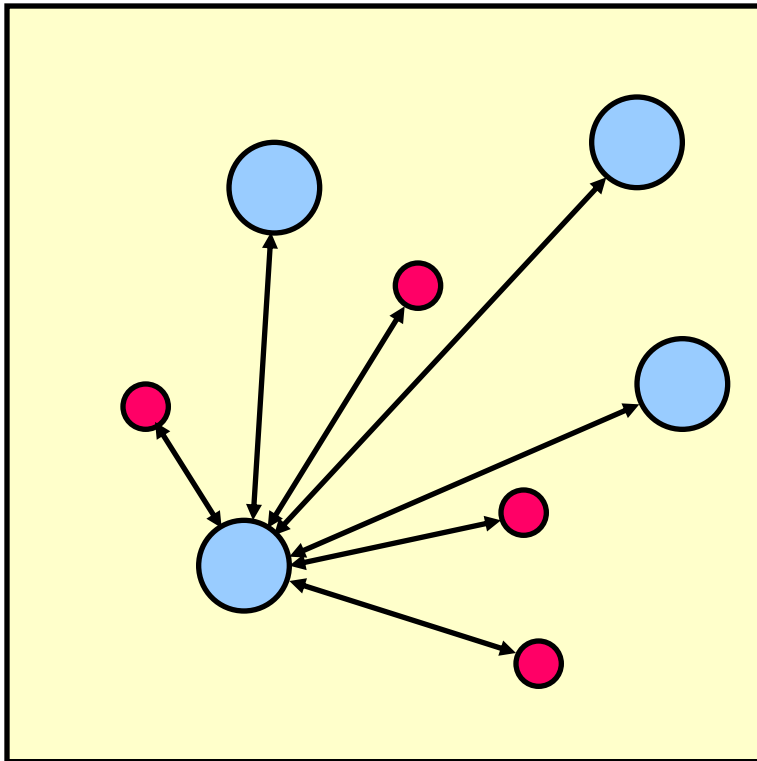
A single non-Euclidean dissimilarity, however, may perform better than the difference of its two constituting Euclidean parts.
So **subtracting may help as well**.

How can we understand this??

Correlations between dissimilarity vectors



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

Ball distances: Non-Euclideanness is very informative

2 x 100 balls with two sizes.
Given are all Euclidean surface distances.

Split in Euclidean matrices: $D^2 = D_p^2 - D_n^2$

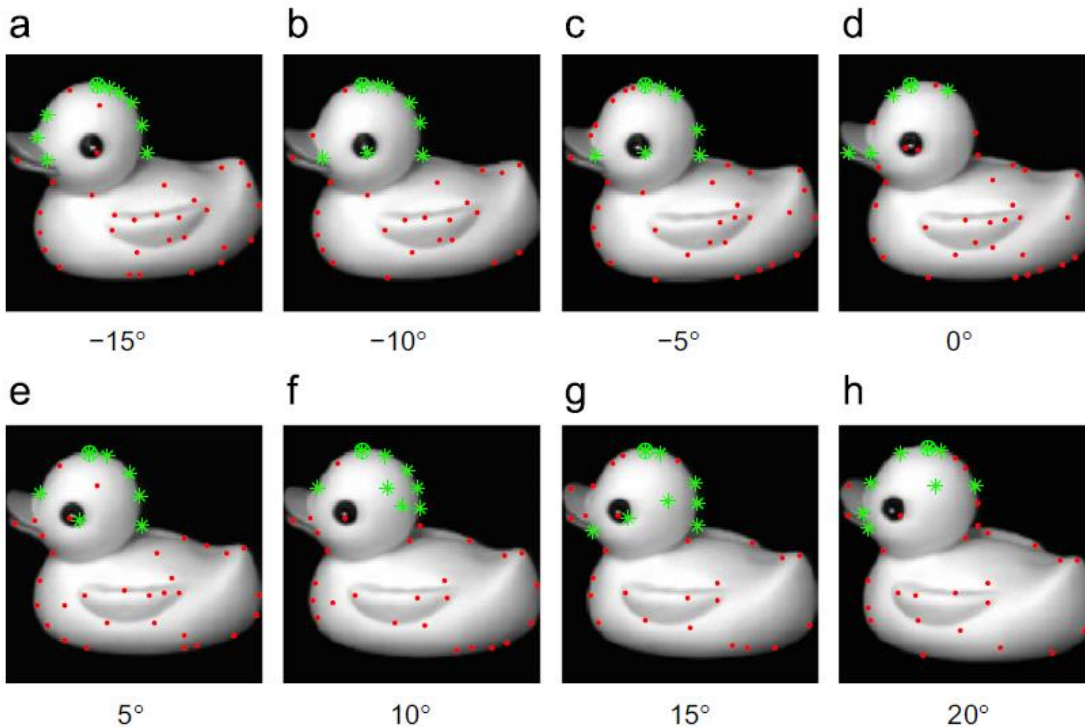
Cross validation errors

D_c	D_p	D_n
0.470	0.405	0.000

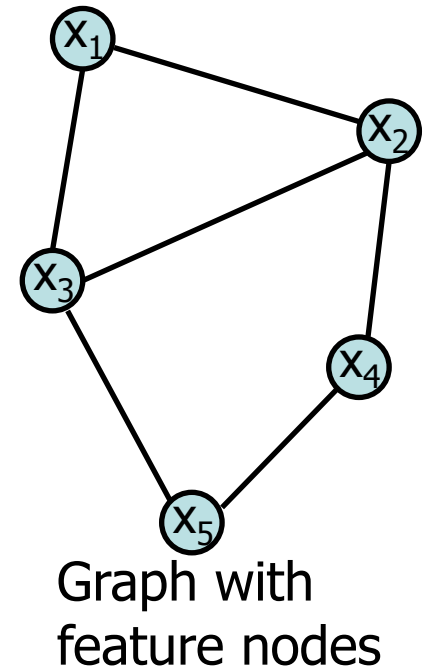
Non-Euclideanness is extremely informative

Random assignment error: 0.50

Application: Graphs



Coil dataset



Coil dataset (100 classes)



Selection of 10 most difficult classes

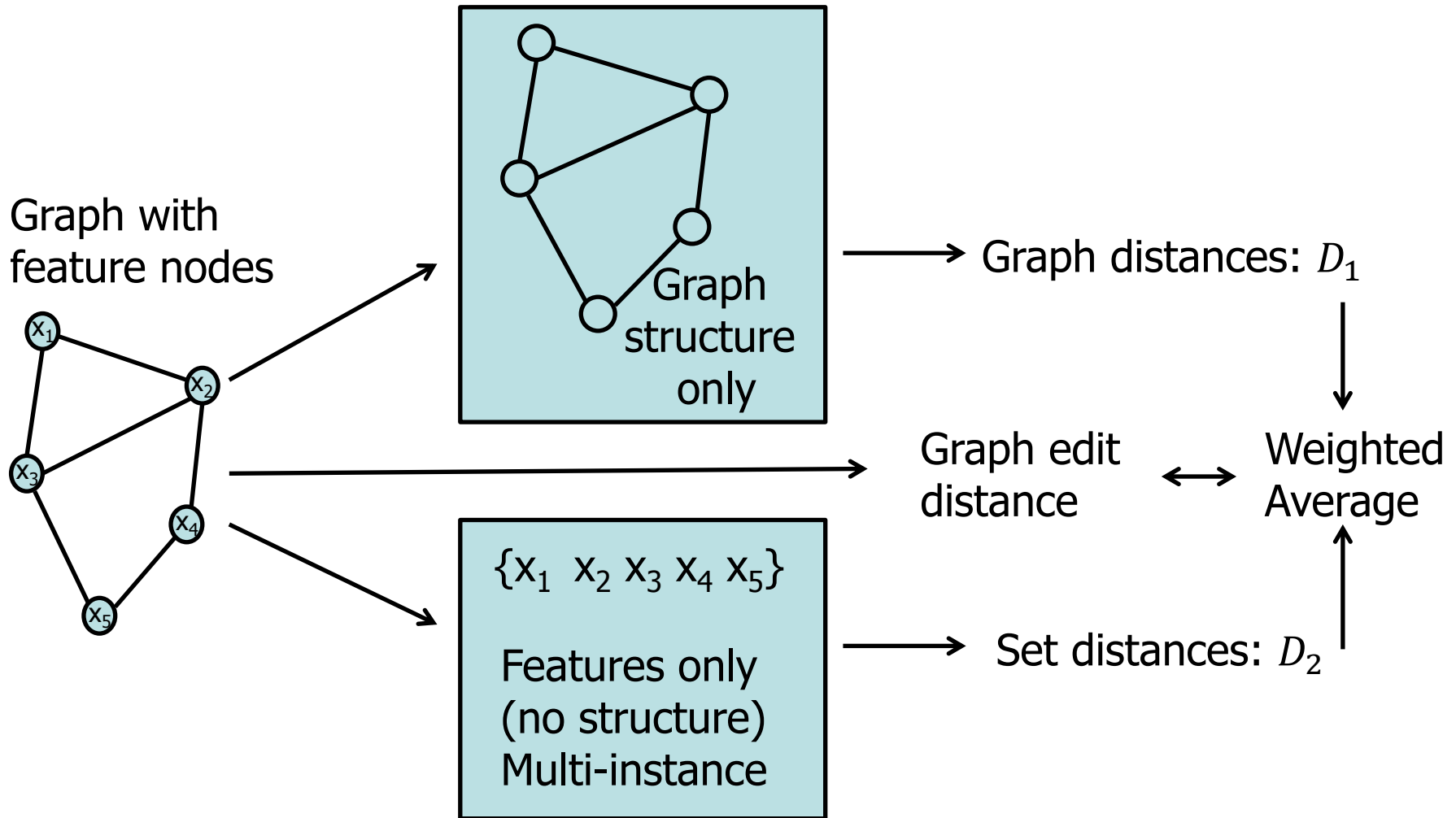
72 objects per class

- Segments
- Sift points
- Harris points

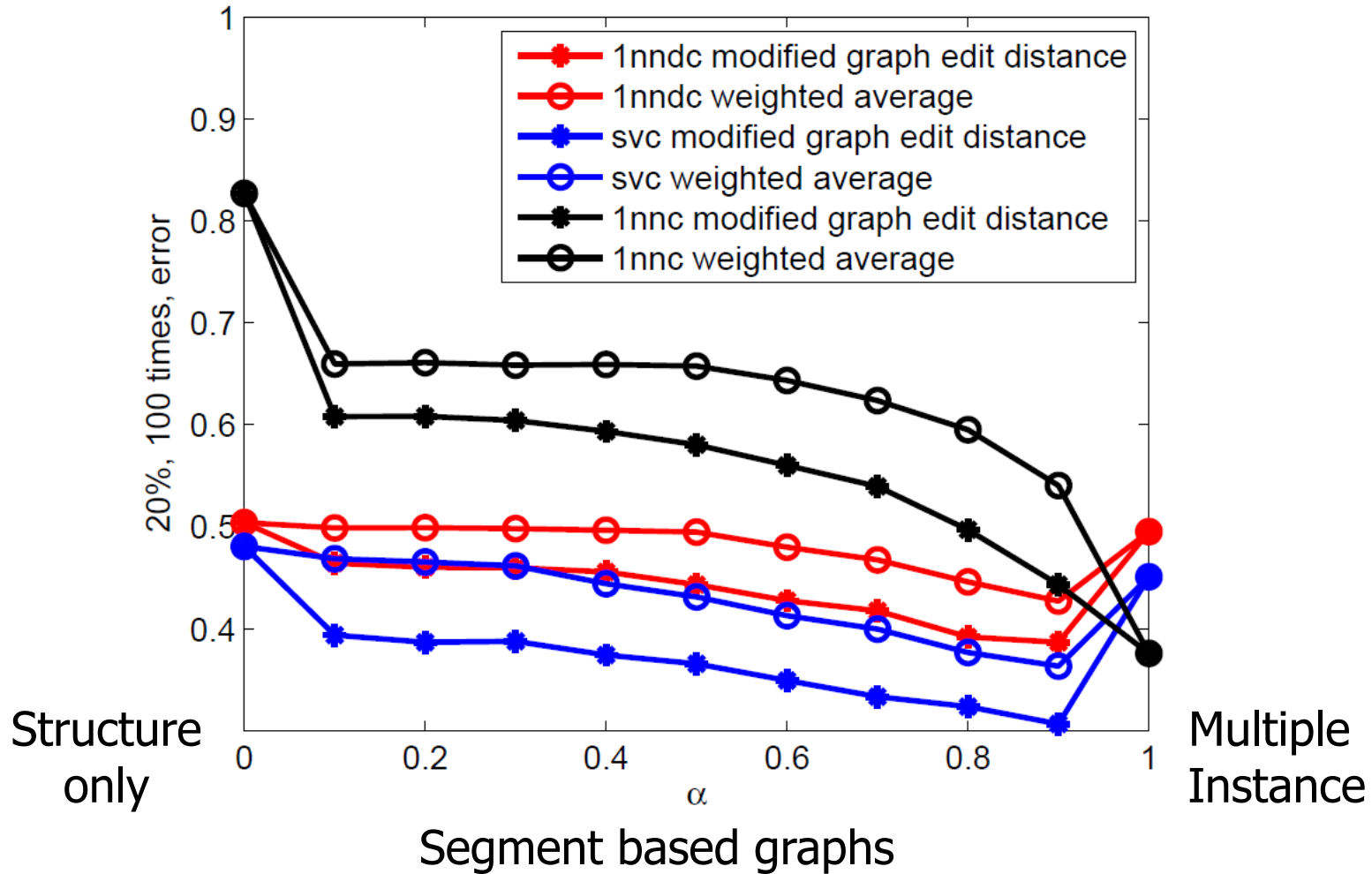


3 sets of attributed graphs

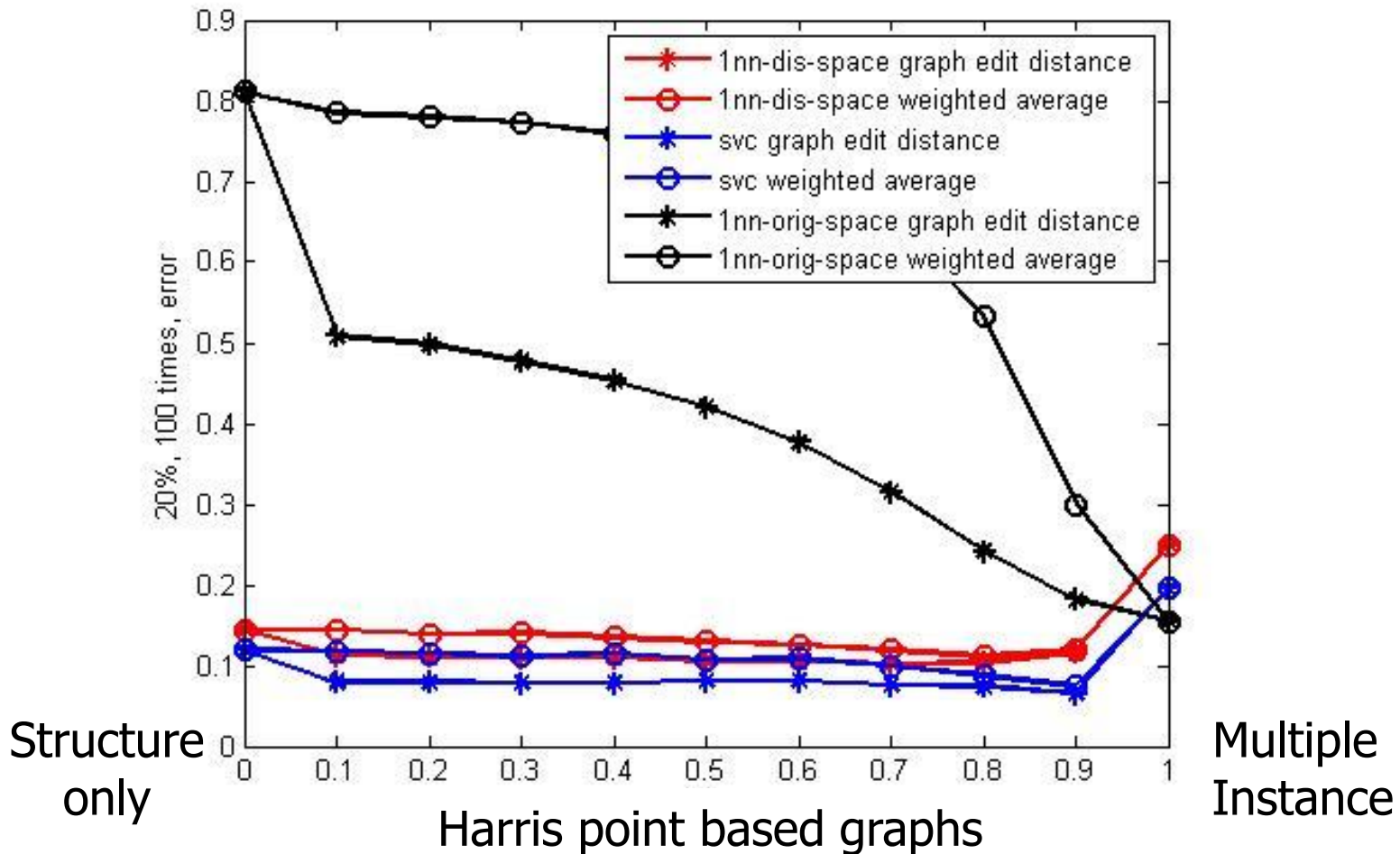
Graphs represented by distance measures



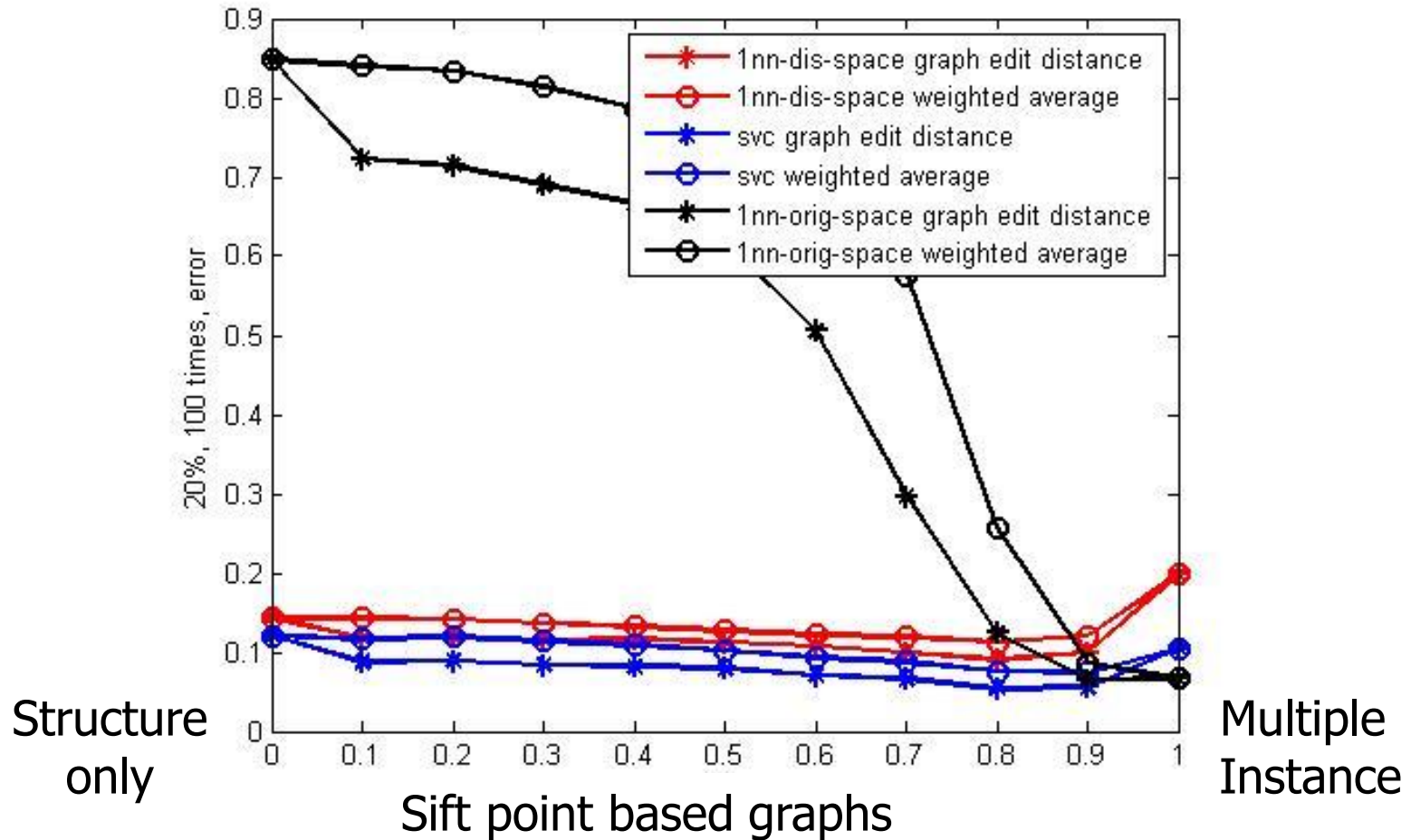
Interpolating structural and feature space dissimilarities



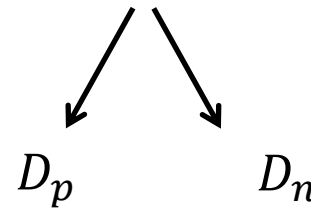
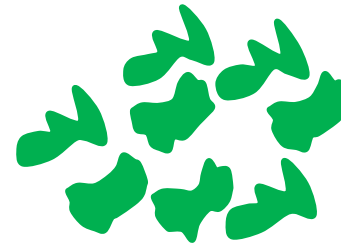
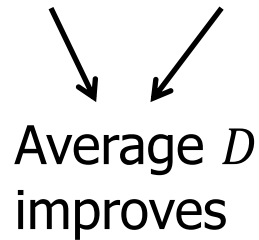
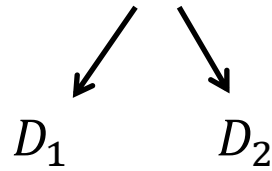
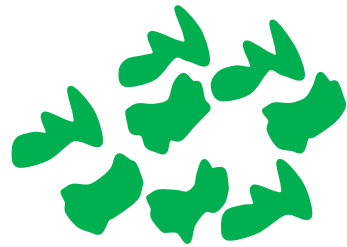
Interpolating structural and feature space dissimilarities



Interpolating structural and feature space dissimilarities



Observations



Non-Euclidean

Euclidean
Decomposition

Euclidean

Average D_e
deteriorates

Both informative
Possibly non-Euclidean

Conclusions

- **Combining** dissimilarity representations based on different measures **may improve** the performance
 - by addition as well as by subtraction
 - for Euclidean as well as for non-Euclidean measures
- Combining the positive and negative Euclidean representations obtained by decomposing a non-Euclidean representation improves the performance just by subtraction
→ **Non-Euclideanness is informative.**
- Can we predict the behavior by just studying the representations before combining?