The Dissimilarity Representation for Pattern Classification

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Topics

- Pattern recognition system
- Representation issues
- Dissimilarity Representation
  - Dissimilarity Space
  - Embedding
  - Comparison
- Non-Euclidean data
- Conclusions

Measuring Human Relevant Information

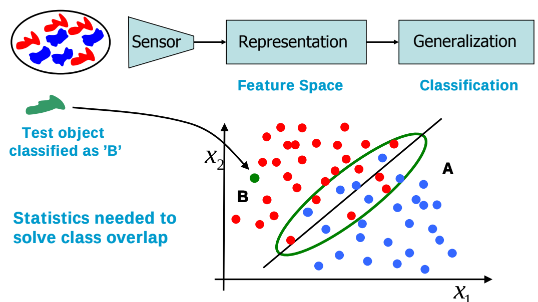
A

B

Nearest neighbours sorted:

B A A A B A A B A B

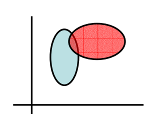
Pattern Recognition System



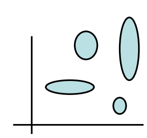
Representation Issues

Good Representations

- Class specific
  Different classes should be represented in different positions in the representation space.



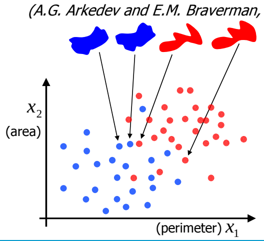
- Compact
  Every class should be represented in a small set of finite domains.



Compactness

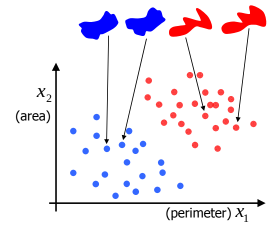
Representations of real world similar objects are close.
There is no ground for any generalization (induction) on representations that do not obey this demand.

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



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

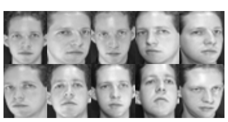
True Representations



Similar objects are close
and
Dissimilar objects are distant.

→ no probabilities needed, domains are sufficient!

High dimensional data often does not overlap

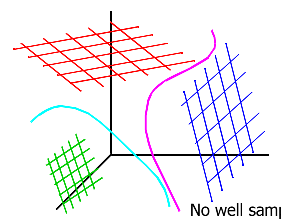


Complete feature representations, which enable the reconstruction of human recognizable objects, may yield separable classes.

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

In some representations classes are separable.

Domains instead of Densities

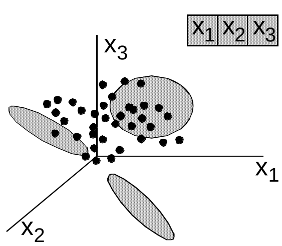


No well sampled training sets are needed.

Statistical classifiers have still to be developed.

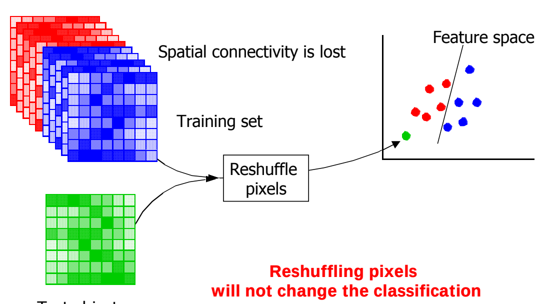
Class structure ←→ Object invariants

The Connectivity Problem in the Pixel Representation



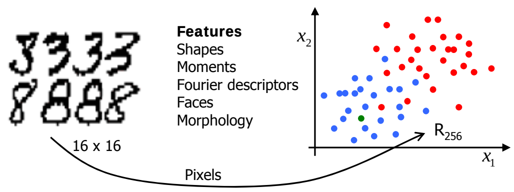
Dependent (connected) measurements are represented independently.
The dependency has to be refound from the data.

The Connectivity Problem in the Pixel Representation



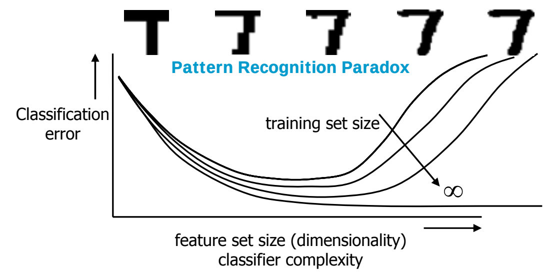
Reshuffling pixels will not change the classification

Pixel Representation



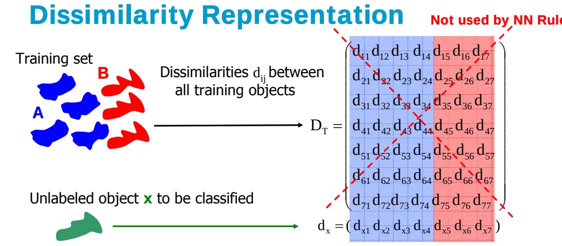
Pixels are more general, initially complete representation
Large datasets are available → good results for OCR

Peaking Phenomenon, Overtraining
Curse of Dimensionality, Rao's Paradox



Dissimilarity Representation

Dissimilarity Representation



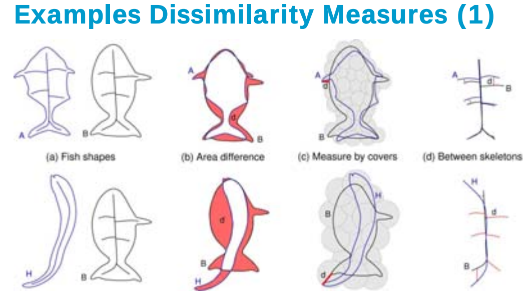
The traditional Nearest Neighbor rule (template matching) finds:
label(argmin$_{trainset}\{d_{xi}\}$) ,
without using D_T. Can we do any better?

Dissimilarities – Possible Assumptions

Metric

1. Positivity: $d_{ij} \geq 0$
2. Reflexivity: $d_{ii} = 0$
3. Definiteness: $d_{ij} = 0$ 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.

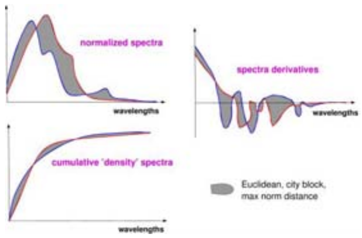
Examples Dissimilarity Measures (1)



The measure should be descriptive. If there is no preference, a number of measures can be combined.

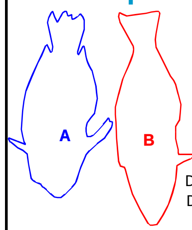
Examples Dissimilarity Measures (2)

Comparison of spectra: some examples



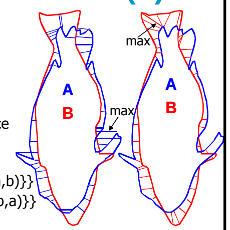
In real applications, the dissimilarity measure should be robust to noise and small aberrations in the (raw) measurements.

Examples Dissimilarity Measures (3)



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)}}

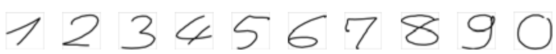


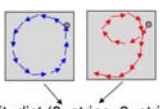
Hausdorff Distance (metric):
DH = max{max_a{min_b{d(a,b)}} , max_b{min_a{d(b,a)}}}

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)}}}

Examples Dissimilarity Measures (4)

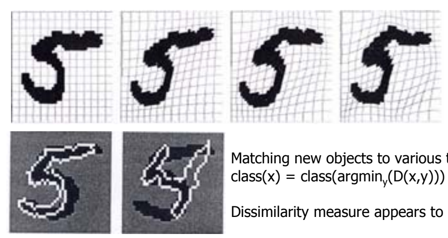




weighted edit distance: non-Euclidean!

edit–dist (0–string, 9–string)

Examples Dissimilarity Measures (5)



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

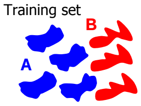
Dissimilarity measure appears to be non-metric.

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

Classification of Dissimilarity Data

Alternatives for the Nearest Neighbor Rule

Training set



Dissimilarities d_{ij} between all training objects

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

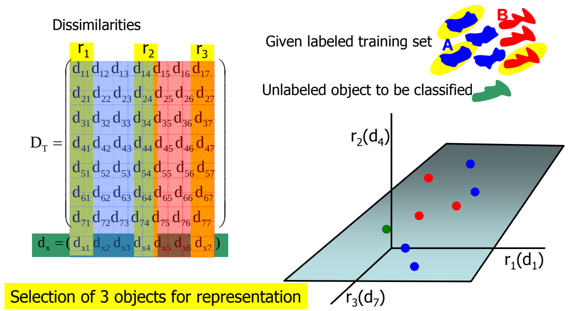
Unlabeled object **x** to be classified

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

1. Dissimilarity Space
2. Embedding

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

Alternative 1: Dissimilarity Space



Selection of 3 objects for representation

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Example Dissimilarity Space: NIST Digits 3 and 8

Example of raw data

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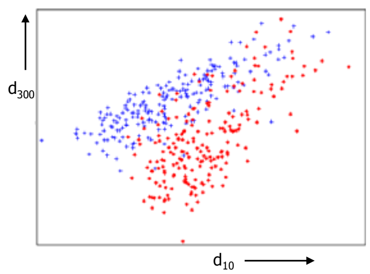
Example Dissimilarity Space: NIST Digits 3 and 8

NIST digits: Hamming distances of 2 x 200 digits



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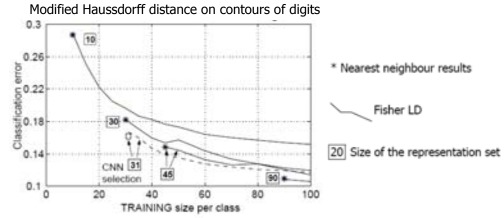
Dissimilarity Space Classification ←→ Nearest Neighbor Rule

Modified Haussdorff distance on contours of digits



Dissimilarity based classification outperforms the nearest neighbor rule.

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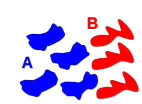
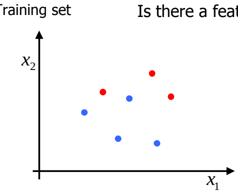
Embedding



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

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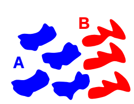
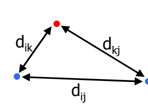
Embedding of non-metric measurements



→ Dissimilarity matrix D → X



If the dissimilarity matrix cannot be explained from a vector space,
(e.g. for Hausdorff and Hamming distance of images)
or if $d_{ij} > d_{ik} + d_{kj}$ (triangle inequality not satisfied)
embedding in Euclidean space not possible
→ Pseudo-Euclidean embedding

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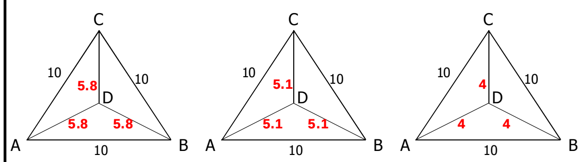
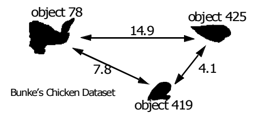
Euclidean - Non Euclidean - Non Metric

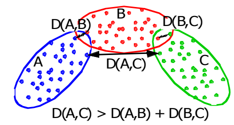


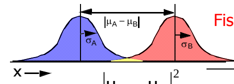
Non-metric distances

Weighted-edit distance for strings

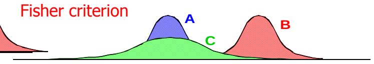


Single-linkage clustering





Fisher criterion



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

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

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

Embedding of non-Euclidean Dissimilarities

(Pseudo-)Euclidean Embedding

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

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

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 $k \times k$ diag. matrix, $\Im_k(i,i) = \text{sign}(\Lambda_k(i,i))$

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

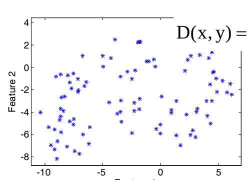
$n \times m$ D_z is the dissimilarity matrix between new objects and the training set.

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

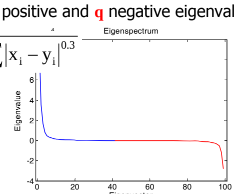
The embedded objects: $Z = B_z Q_k |\Lambda_k|^{-\frac{1}{2}} \Im_k$

Pseudo-Euclidean Embedding

If D is non-Euclidean then B has $\mathbf{p}$ positive and $\mathbf{q}$ negative eigenvalues



$$D(x,y) = \sqrt[0.3]{\sum |x_i - y_i|^{0.3}}$$



Solutions:

- Remove all eigenvectors with small and negative eigenvalues
- or, take absolute values of eigenvalues and proceed
- or, construct a pseudo-Euclidean space

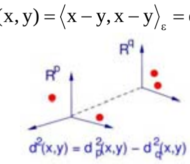
PES: Pseudo-Euclidean Space (Krein Space)

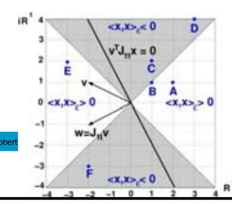
If D is non-Euclidean, B has p positive and q negative eigenvalues.

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:

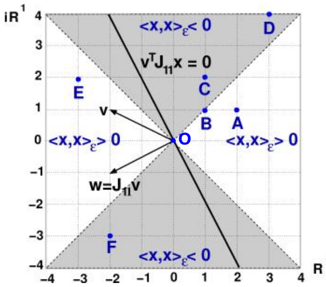
$$\langle x,y \rangle_\varepsilon = x^T \Im_{pq} y = \sum_{i=1}^{p} x_i y_i - \sum_{j=p+1}^{q} x_j y_j \qquad \Im_{pq} = \begin{bmatrix} I_{p \times p} & 0 \\ 0 & -I_{q \times q} \end{bmatrix}$$

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





Distances in PES



$d^2(O,A) > 0$
$d^2(O,E) > 0$
$d^2(O,B) = 0$
$d^2(O,D) < 0$

All points in the grey area are closer to O than O itself !?

Any point has a negative square distance to some points on the line $v^TJx=0$.
Can it be used as a classifier?
Can we define a margin as in the SVM?

PE Space ←→ Kernels

$$K(x,y) = -\tfrac{1}{2} J D(x,y)^{(2)} J \qquad J = I - \tfrac{1}{m}\mathbf{11}$$

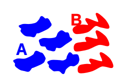
may by considered as a kernel. If

$$K(x,y) = < L(x), L(y) >$$

- The **kernel trick** may be used: operations defined on inner products in kernel space can be operated directly on K(x,y) **without embedding**!
- True for **Mercer kernels** (all eigenvalues ≥ 0).
- Difficult for **indefinite kernels**.
- Studying classifiers in **PE space** is studying the indefinite **kernel space**.
- Dissimilarities are more informative than kernels (due to normalization).

Dissimilarity based classifiers compared

Dissimilarity based classification procedured compared

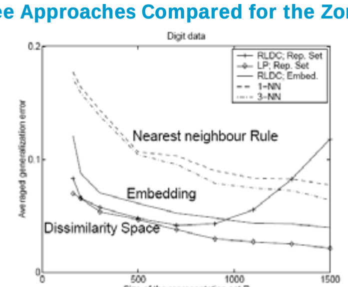
Training set  → Dissimilarity matrix D

Test object x  → Dissimilarities d_x with training set

1. Nearest Neighbour Rule
2. Reduce training set to representation set
⇒ dissimilarity space
3. Embedding:Select large Λ_{ii} > 0 ⇒ Euclidean space
Select large $|\Lambda_{ii}|$ > 0 → pseudo-Euclidean space

} discriminant function

Three Approaches Compared for the Zongker Data



Dissimilarity Space equivalent to Embedding better than Nearest Neighbour Rule

Polygon Data

Convex Pentagons

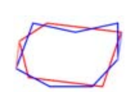
Heptagons

no class overlap
zero error

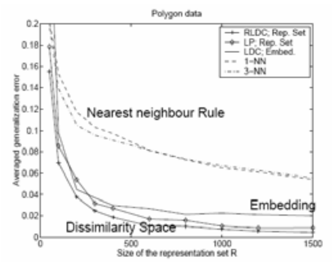
Minimum edge length: 0.1 of maximum edge length

Distance measures: Hausdorff D = max { $\max_i(\min_j(d_{ij}))$, $\max_j(\min_i(d_{ij}))$ }.
Modified Hausdorff D = max {$\mathrm{mean}_i(\min_j(d_{ij}))$, $\mathrm{mean}_j(\min_i(d_{ij}))$ }. (no metric!)
d_{ij} = distance between vertex i of polygon_1 and vertex j of polygon_2.
Polygons are scaled and centered.

Find the largest of the smallest vertex distances



Dissimilarity Based Classification of Polygons



Zero error difficult to reach!

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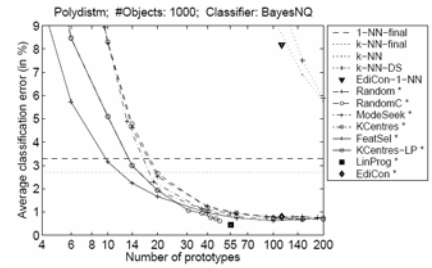
Prototype Selection: Polygon Dataset



The classification performance of the quadratic Bayes Normal classifier and the k-NN in dissimilarity spaces and the direct k-NN, as a function of the number of selected prototypes. Note that for 10-20 prototypes already better results are obtained than by using 1000 objects in the NN rules.

An Analysis of Causes of Non Metric Data

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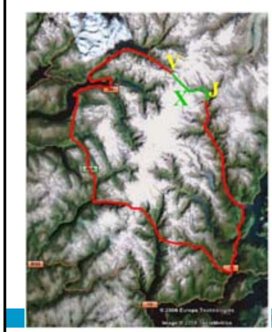
Lack of information



1800:
Crossing the Jostedalsbreen was impossible.
Travelling around (200 km) lasted 5 days.
Untill the shared point X was found.
People could visit each other in 8 hours.

D(V,J) = 5 days
D(V,X) = 4 hours
D(X,J) = 4 hours

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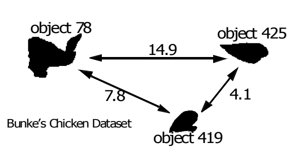
Computational Problems

Large distances are overestimated due to computational problems



Weighted edit distance for strings

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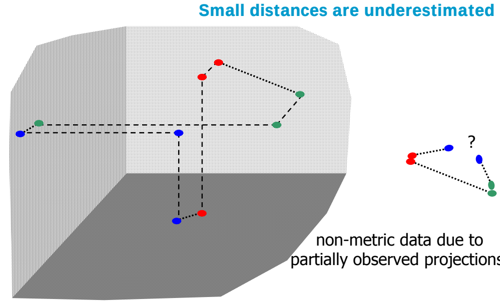
Projections - Occlusions

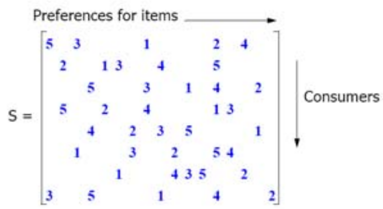
Small distances are underestimated



non-metric data due to partially observed projections

TUDelft

Projections - Occlusions

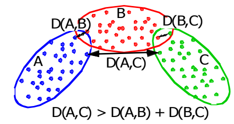


Example: consumer preferences for recommendation systems

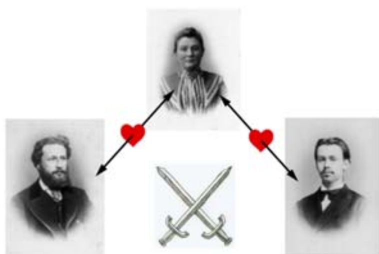
Intrinsicly Different Dissimilarity Measures

Distance(Table,Book) = 0
Distance(Table,Cup) = 0
Distance(Book,Cup) = 1

Single-linkage clustering



Intrinsicly Different Dissimilarity Measures



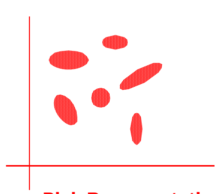
Non-Euclidean human relations

Causes of Metric Dissimilarities

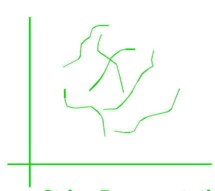
- Overestimated large distances (too difficult to compute)
- Underestimated small distances (one-sided view of objects)
  caused by the construction of complicated measures, needed to correspond with human observations.
- Essential non-metric distance definitions
  as the human concept of distance differs from the mathematical one.

Perspective

Human defined patterns do not fit in a Euclidean space.
Objects cannot be represented by points as they have an inner life.
Respect it.



Blob Representation



String Representation