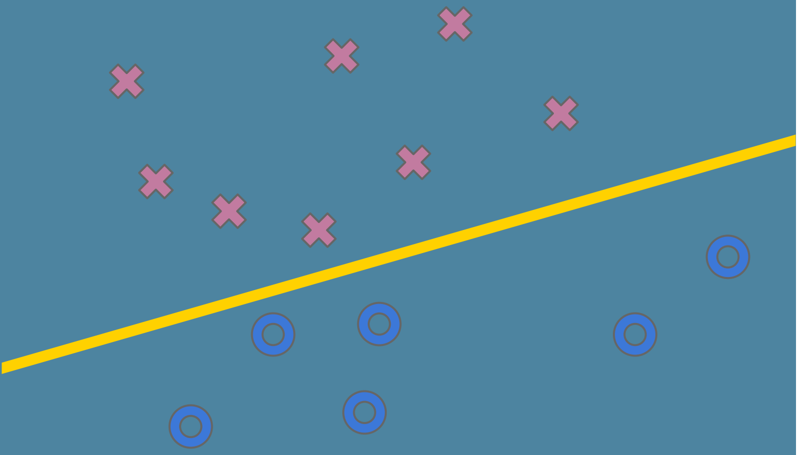
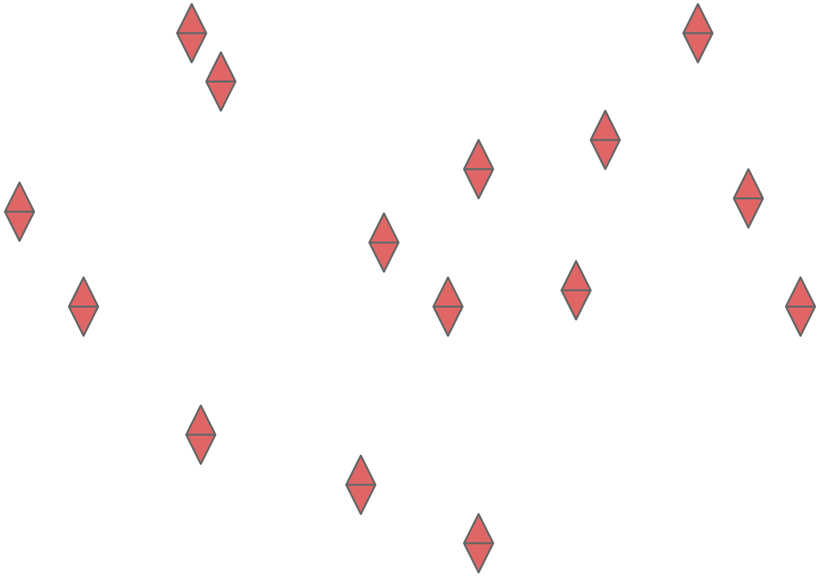
Outline

1. Geometrical machine learning
    a. Dimensionality curse
    b. Manifold assumption
2. Dimensionality reduction
    a. Feature selection
    b. Multidimensional Scaling (MDS)
    c. Isomap
    d. Locally linear embedding (LLE)
    e. t-SNE
3. Clustering
    a. k-means
    b. DBSCAN
    c. Hierarchical clustering
    d. metrics
4. Density estimation
    a. Kernel density estimation

Supervised learning



Unsupervised learning



Geometrical machine learning

girafe ai

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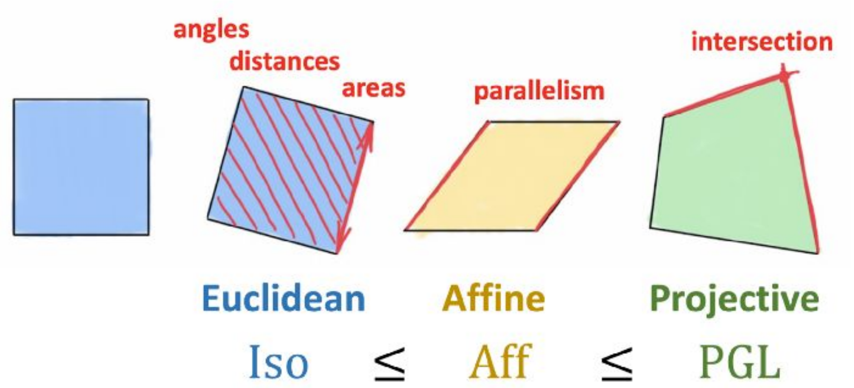
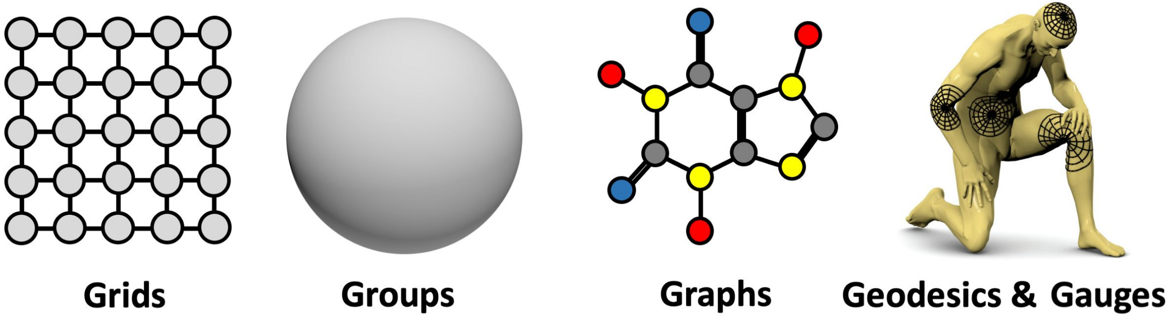
Geometrical machine learning



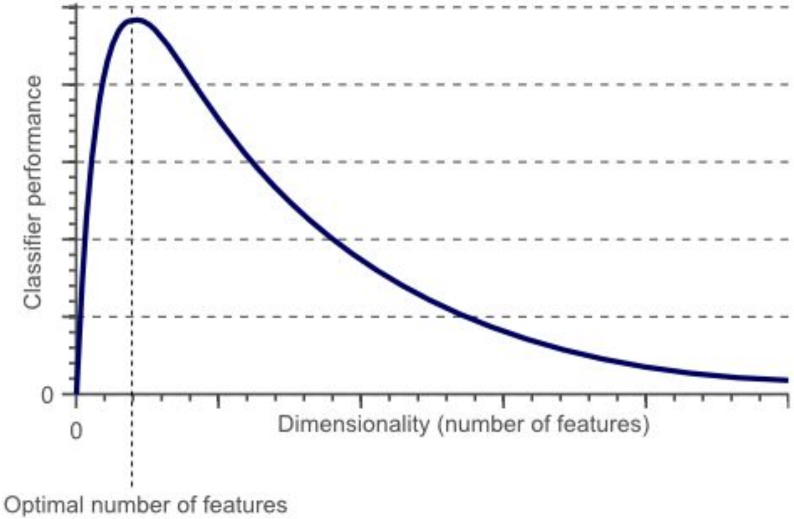
The breakthrough insight of Klein was to approach the definition of geometry as the **study of invariants**, or in other words, structures that are preserved under a certain type of transformations (symmetries)

Article introducing a book on Geometric Deep Learning

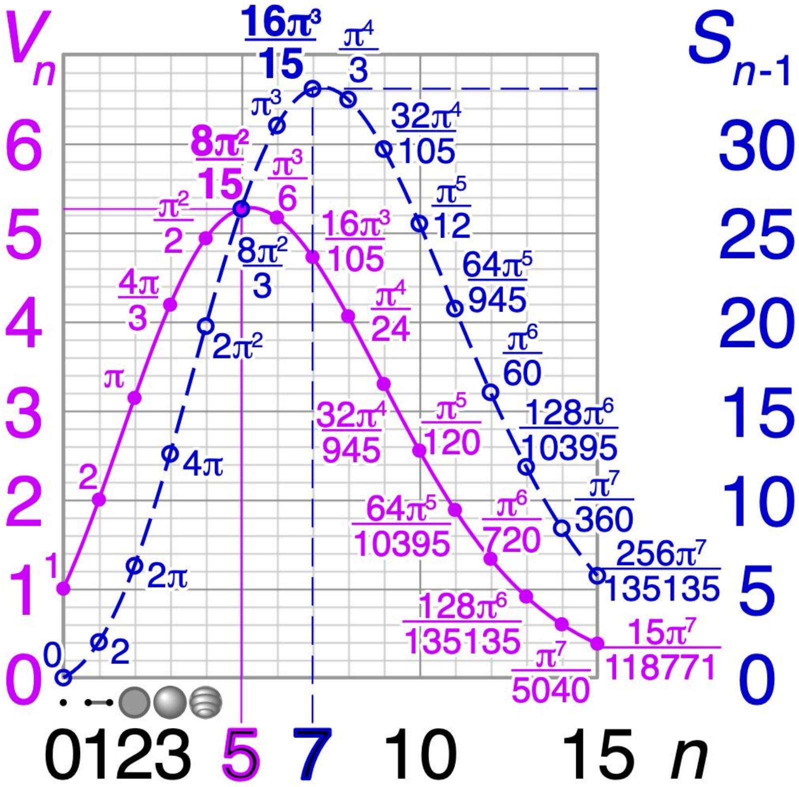


Dimensionality curse

Certain behaviours or effects that appear when analysing data in high dimensions, that do not occur in low-dimensional spaces



Sphere volume decrease



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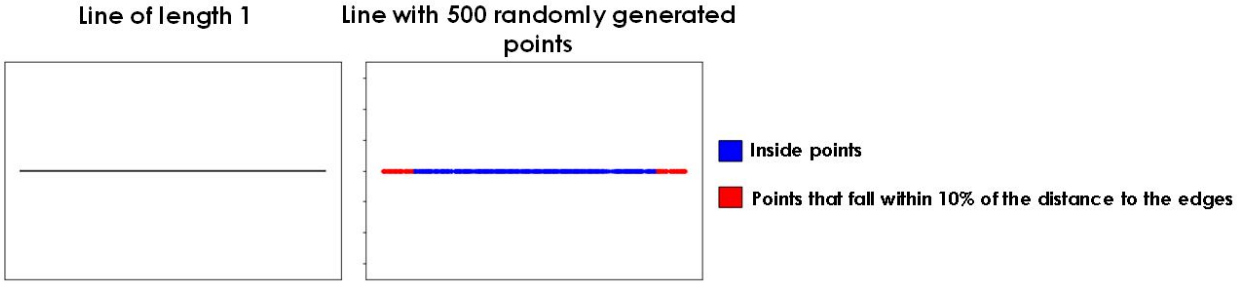
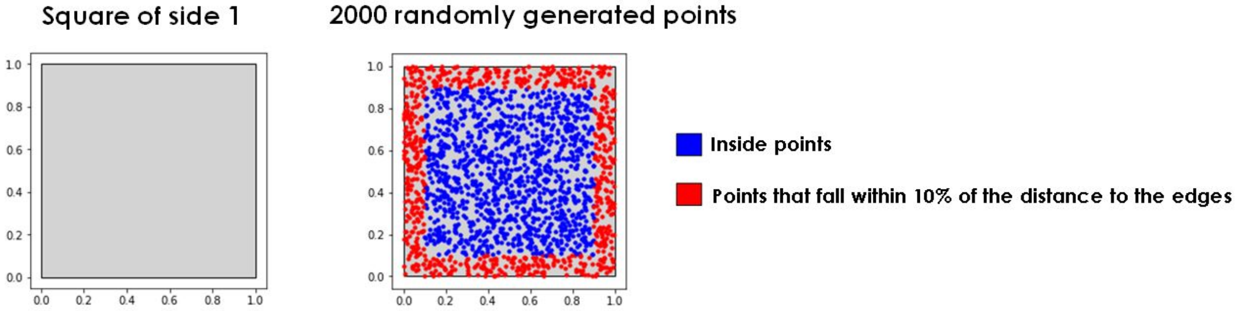
Distance in high dimensional space



Ratio of inside points to total points = 80%
Average Distance between 2 points = 0.34

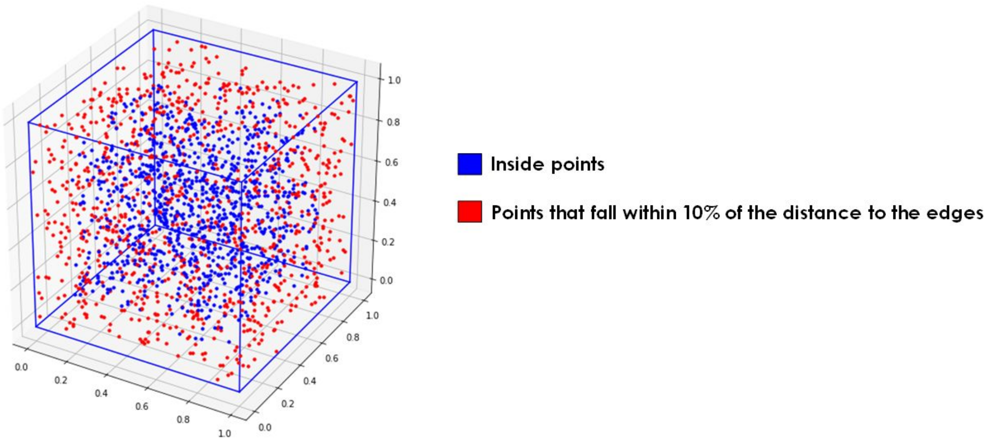


Ratio of inside points to total points = 63%
Average Distance between 2 points = 0.52

image source

Distance in high dimensional space

Cube of side 1

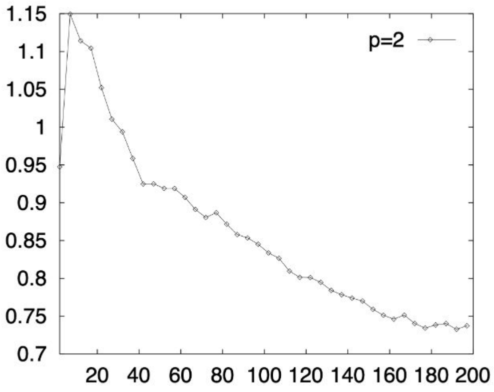


Ratio of inside points to total points = 51%
Average Distance between 2 points = 0.65

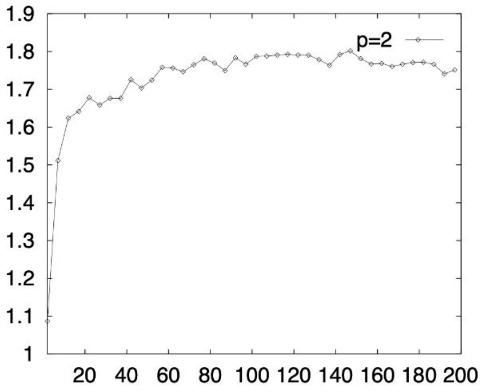
Nº of dimensions	% Outside Points	Average distance (A,B)
1	20%	0.34
2	37%	0.52
3	49%	0.65

Distance relative contrast

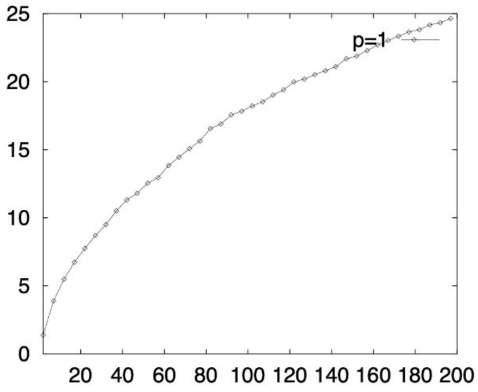
Take random points uniformly distributed in D dimensional cube and calculate distance to the farthest point and to the closest point. Plot their difference depending on D for different Minkowski metrics



L3



L2



L1

[On the Surprising Behavior of Distance Metric in High-Dimensional Space, Aggarwal et al., 2002]

Conclusions

- Distance loses its meaning - closest and farthest points are equally far
- Proximity concept becomes ill defined
- Lower powers of Minkowski metrics are more sustainable to dimensionality curse

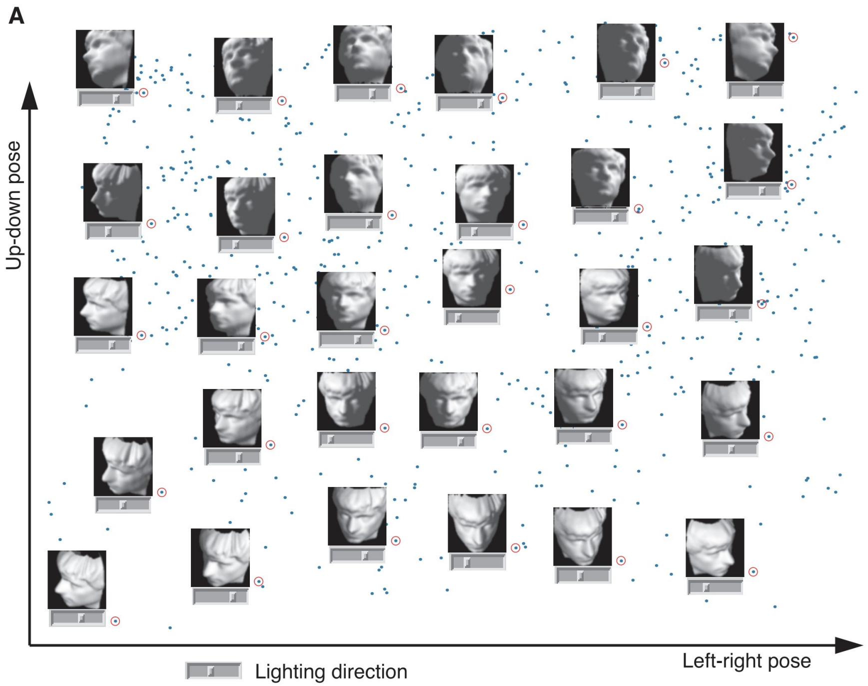
Nº of dimensions	% Outside Points	Average distance (A,B)
1	20%	0.34
2	37%	0.52
3	49%	0.65

Manifold assumption

The data lie approximately on a surface (called manifold) of usually much lower dimension than the input space

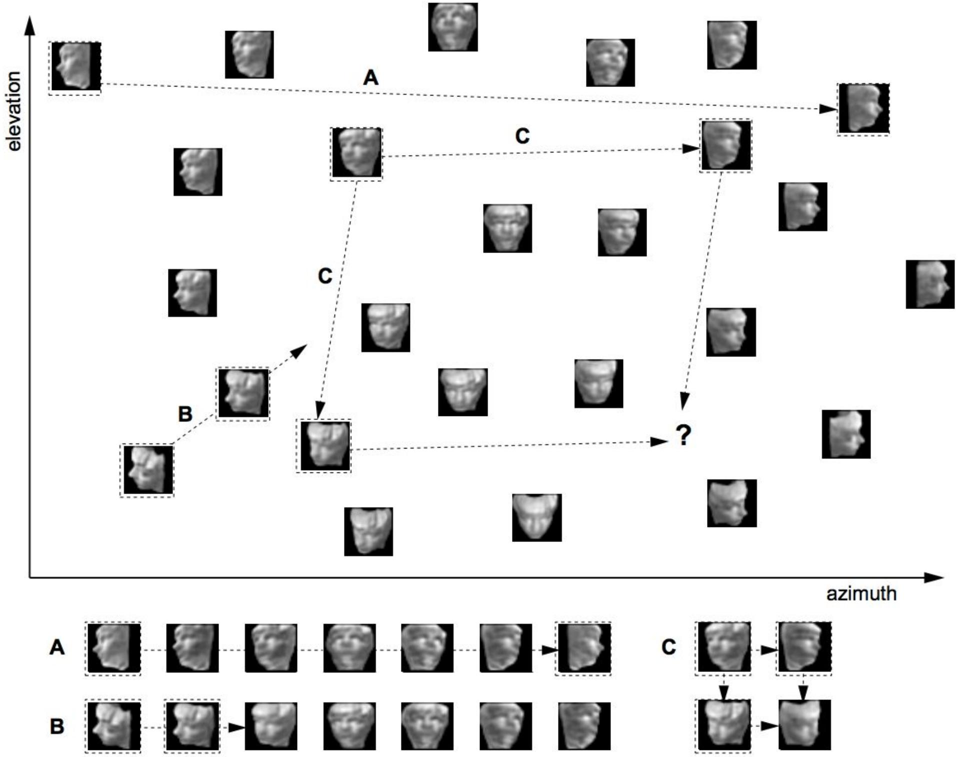
So problem dimensionality could be (non-)linearly reduced or other tasks solved

Sometimes dimensionality of manifold is referred as intrinsic dimension (see this article)



Tenenbaum, de Silva, Langford
A Global Geometric Framework for Nonlinear Dimensionality Reduction

Latent space



Latent (embedding) space describes data in coordinates more relevant to humans' reason and often allows useful linear operations:

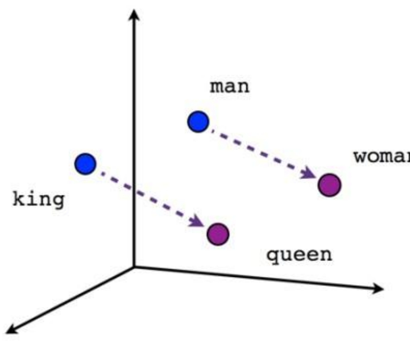
- Interpolation (A)
- Extrapolation (B)
- Analogy (C)

This process is also called embedding space 'walking'

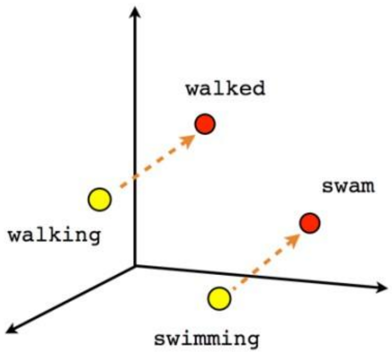
Latent space example

Word2vec is a method to embed words from text corpus into linear space

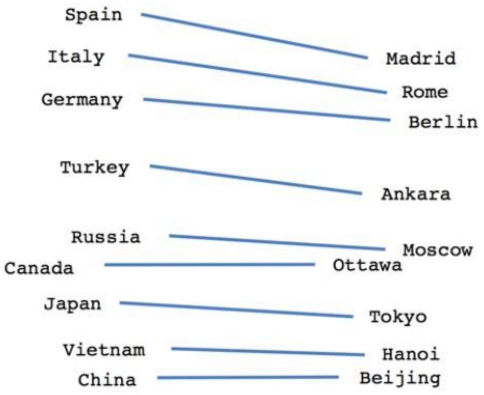
Read more: manifold assumption, assessing assumption



Male-Female



Verb tense



Country-Capital

Dimensionality reduction

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02

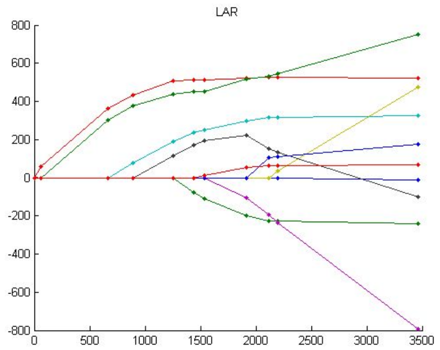
Feature selection

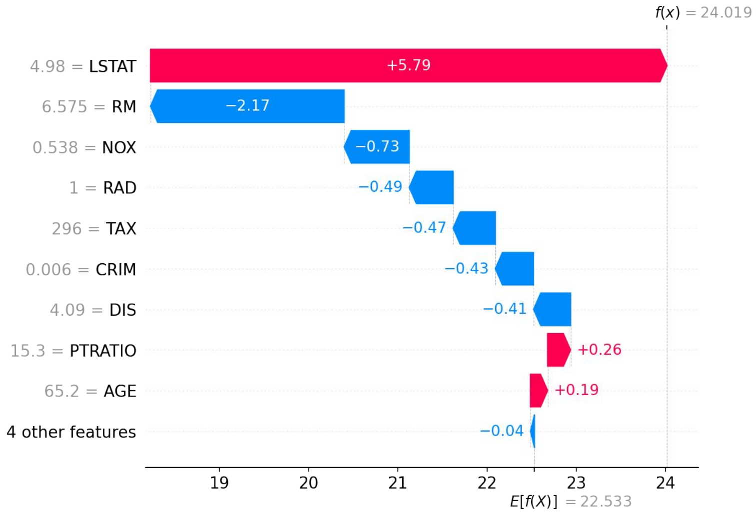
Select subset of existing features to use in further modelling

Usually is based on some supervised method

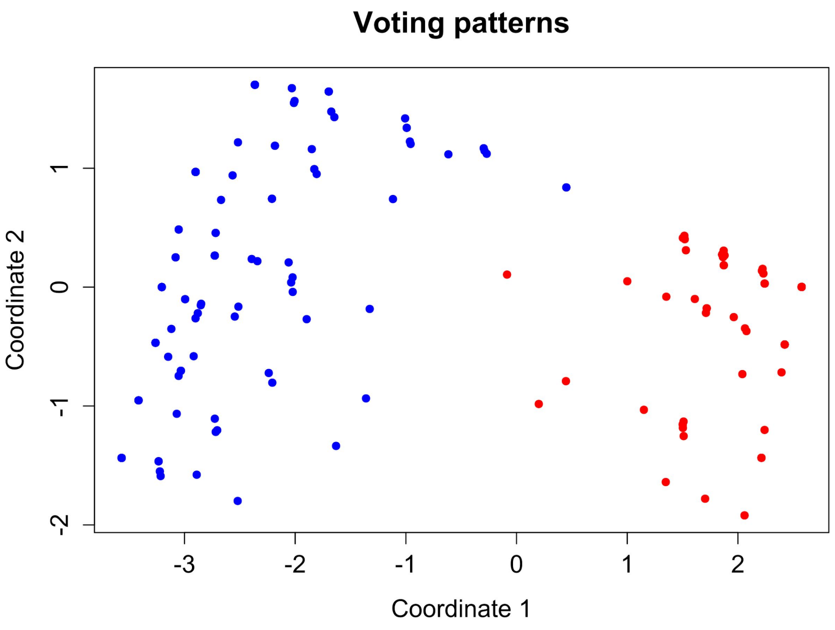
Examples:

- stepwise regression
- LARS
- SHAP values
- etc...





Multidimensional Scaling (MDS)



[Voting patterns in the United States House of Representatives]

Goal:

Linearly embed to given lower space

Solution:

PCA

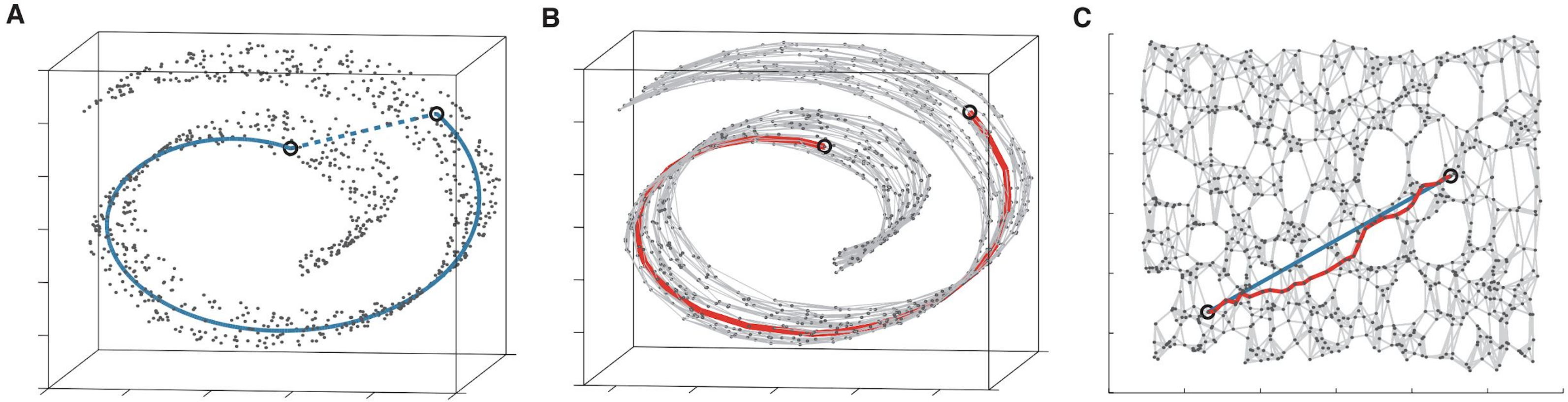
$$L = ||D_x - D_y||_2 \rightarrow \min_{y=Ax}$$

$$y = \Lambda^{1/2} V^T$$

Params: p - target dimensionality

Also could be non-linear

Isomap



Now make distancies geodesic!
And measure distances on the produced graph

[A Global Geometric Framework for Nonlinear Dimensionality Reduction, Tenenbaum et al., Science, 2002.]

Params:
n - number of neighbours to connect
p - dimensionality of manifold

Isomap algorithm

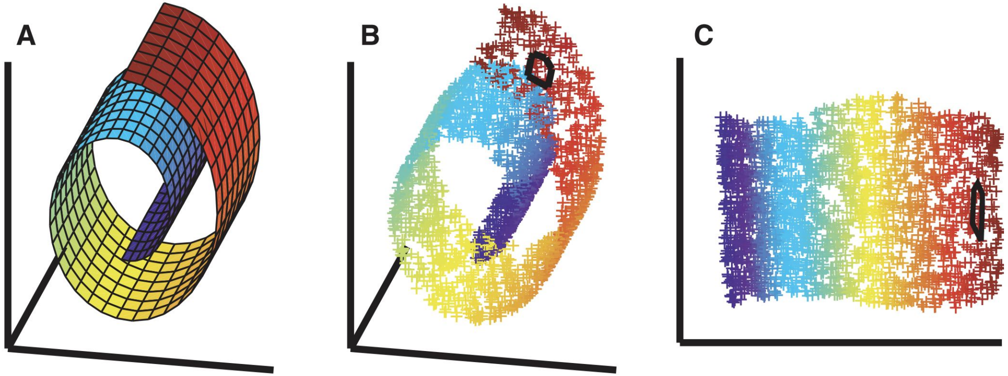
Step		
1	Construct neighborhood graph	Define the graph G over all data points by connecting points i and j if [as measured by $d_X(i,j)$] they are closer than ϵ (ϵ-Isomap), or if i is one of the K nearest neighbors of j (K-Isomap). Set edge lengths equal to $d_X(i,j)$.
2	Compute shortest paths	Initialize $d_G(i,j) = d_X(i,j)$ if i,j are linked by an edge; $d_G(i,j) = \infty$ otherwise. Then for each value of $k = 1, 2, \ldots, N$ in turn, replace all entries $d_G(i,j)$ by $\min\{d_G(i,j), d_G(i,k) + d_G(k,j)\}$. The matrix of final values $D_G = \{d_G(i,j)\}$ will contain the shortest path distances between all pairs of points in G (*16*, *19*).
3	Construct d-dimensional embedding	Let λ_p be the p-th eigenvalue (in decreasing order) of the matrix $\tau(D_G)$ (*17*), and v_p^i be the i-th component of the p-th eigenvector. Then set the p-th component of the d-dimensional coordinate vector $\mathbf{y}_i$ equal to $\sqrt{\lambda_p} v_p^i$.

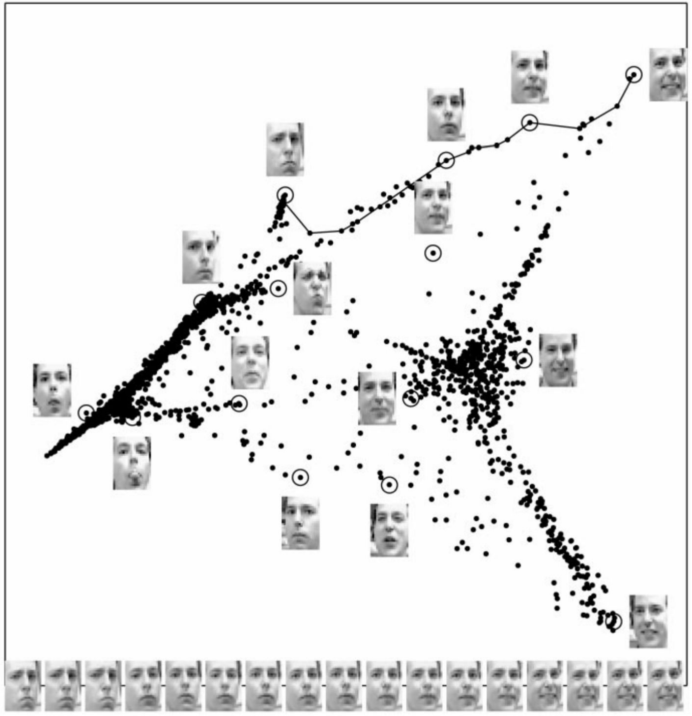
17. The operator τ is defined by $\tau(D) = -HSH/2$, where S is the matrix of squared distances $\{S_{ij} = D_{ij}^2\}$, and H is the "centering matrix" $\{H_{ij} = \delta_{ij} - 1/N\}$ (*13*).

Locally linear embedding (LLE)

Smooth manifold locally approximated with hyperplane. Linear pieces are stitched together.

[Nonlinear Dimensionality Reduction by Locally Linear Embedding, Roweis et al., Science, 2000]





LLE algorithm

1. estimate point by its K neighbours

$$\varepsilon(W) = \sum_{i=1}^{n} ||x_i - \sum_{j=1}^{K} W_{ij} x_j||^2$$

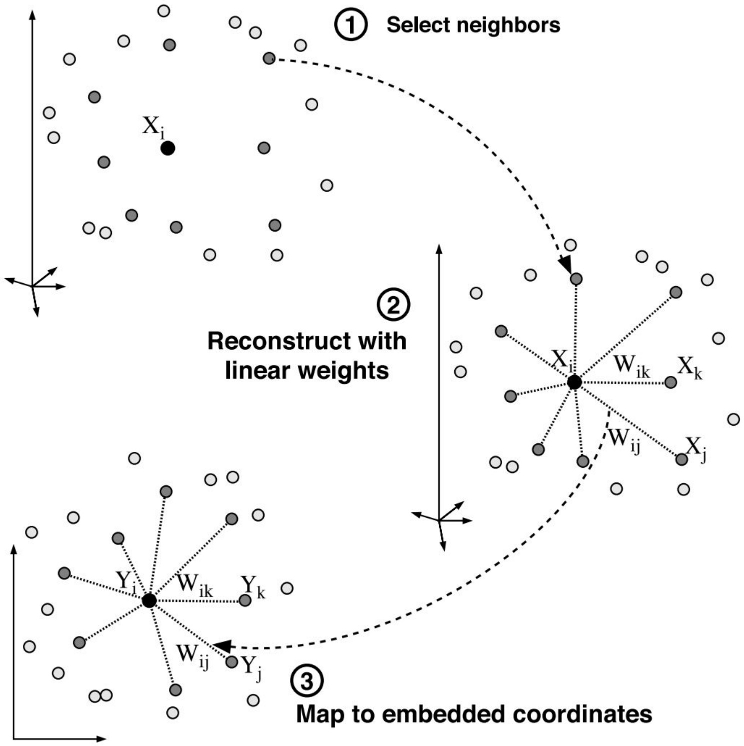
2. Estimate new points based on known relations

$$\Phi(Y) = \sum_{i=1}^{n} ||y_i - \sum_{j=1}^{n} W_{ij} y_j||^2$$

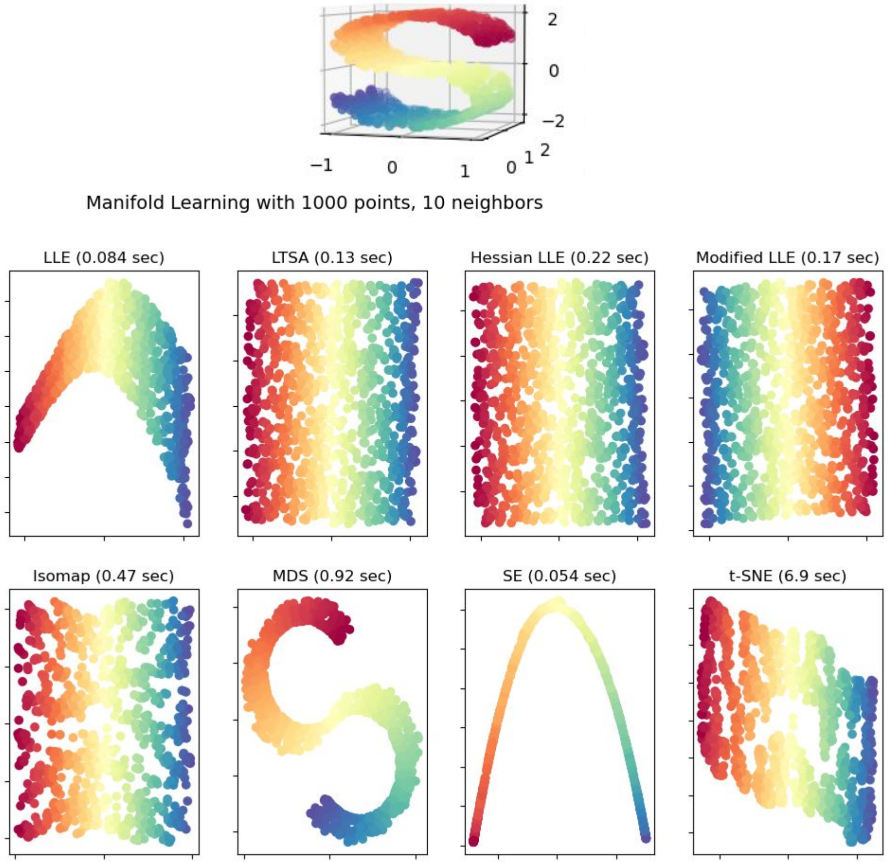
Params:

n - number of neighbours to connec

p - dimensionality of manifold



Many more



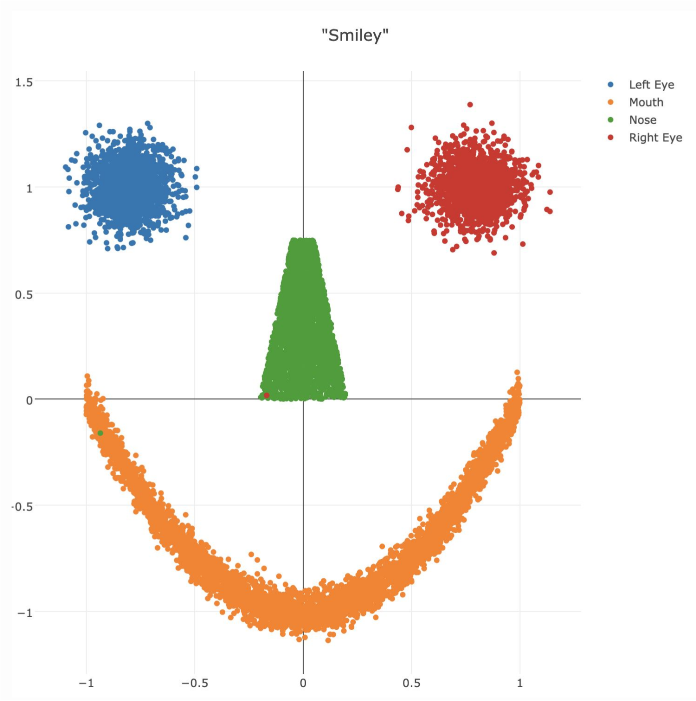
- Hessian Eigenmapping
- Spectral Embedding
- Local Tangent Space Alignment
- Riemannian Geometry
- UMAP
- ……

Read more:

sklearn manifold methods

sklearn signals decomposition

Next level: Neural Networks



[UMAP vs Ivis embeddings]

t-SNE

t-distributed $\underbrace{\text{Stochastic Neighbor Embedding}}_{\text{SNE}}$

[Stochastic Neighbor Embedding, Hinton et al., NIPS, 2002]

Stochastic Neighbor Embedding

Convert pairwise distances to probabilities, preserve probabilities through the spaces

$$p_{j|i} = \frac{\exp(-\frac{||x_i - x_j||^2}{2\sigma_i^2})}{\sum_{k \neq i} \exp(-\frac{||x_i - x_k||^2}{2\sigma_i^2})}$$

asymmetric probability
of object i chooses j as its neighbour

$$q_{j|i} = \frac{\exp(-||y_i - y_j||^2)}{\sum_{k \neq i} \exp(-||y_i - y_k||^2)}$$

the same in target space

Let's construct embedding s.t. this distributions are close.

What are close distributions?

Kullback–Leibler divergence

$$D_{KL}(P \,||\, Q) = \sum_{i,j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

Suspiciously similar to Shannon entropy

Learn more

SNE problem

$$p_{j|i} = \frac{\exp(-\frac{||x_i - x_j||^2}{2\sigma_i^2})}{\sum_{k \neq i} \exp(-\frac{||x_i - x_k||^2}{2\sigma_i^2})}$$

$$q_{j|i} = \frac{\exp(-||y_i - y_j||^2)}{\sum_{k \neq i} \exp(-||y_i - y_k||^2)}$$

$$D_{KL}(P \,||\, Q) \rightarrow \min_{Y}$$

t-distributed SNE

Patches over SNE:

1. choose common variance
2. make distributions symmetric

$$p_{ij} = \frac{\exp\left(-\|x_i - x_j\|^2 / 2\sigma^2\right)}{\sum_{k \neq l} \exp\left(-\|x_k - x_l\|^2 / 2\sigma^2\right)}$$

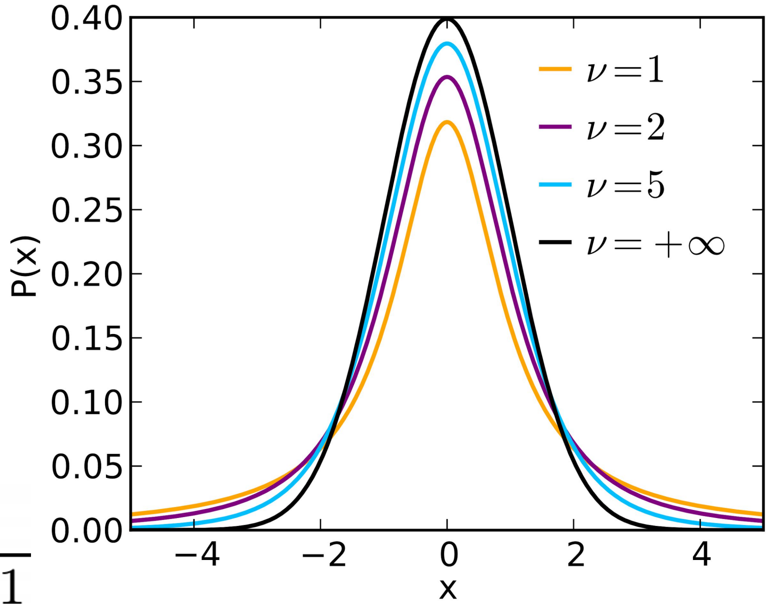
$$p^s_{ij} = \frac{p_{ij} + p_{ji}}{2N}$$

[Visualizing Data using t-SNE, Maaten, Hinton, 2008, JMLR]()

t-distributed SNE

Patches over SNE:

1. choose common variance
2. make distributions symmetric
3. make it decrease faster than Gaussian (use Student's t-distribution)



$$q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_{k \neq l} (1 + ||y_k - y_l||^2)^{-1}}$$

t-SNE problem

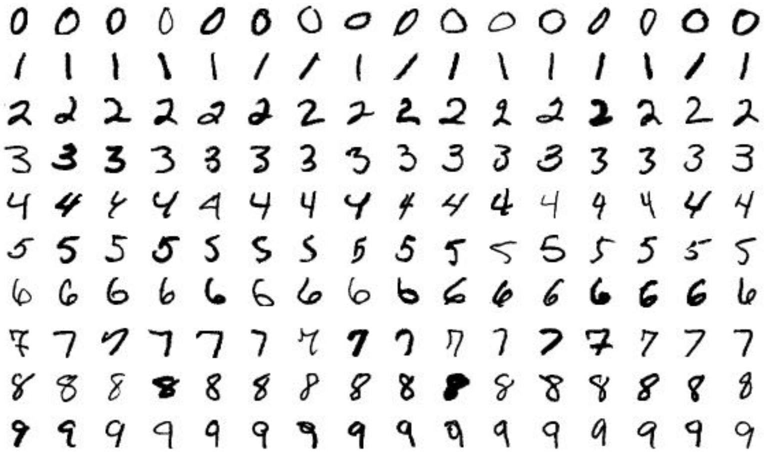
$$p_{ij} = \frac{\exp\left(-\|x_i - x_j\|^2 / 2\sigma^2\right)}{\sum_{k \neq l} \exp\left(-\|x_k - x_l\|^2 / 2\sigma^2\right)} \qquad p^s_{ij} = \frac{p_{ij} + p_{ji}}{2N}$$

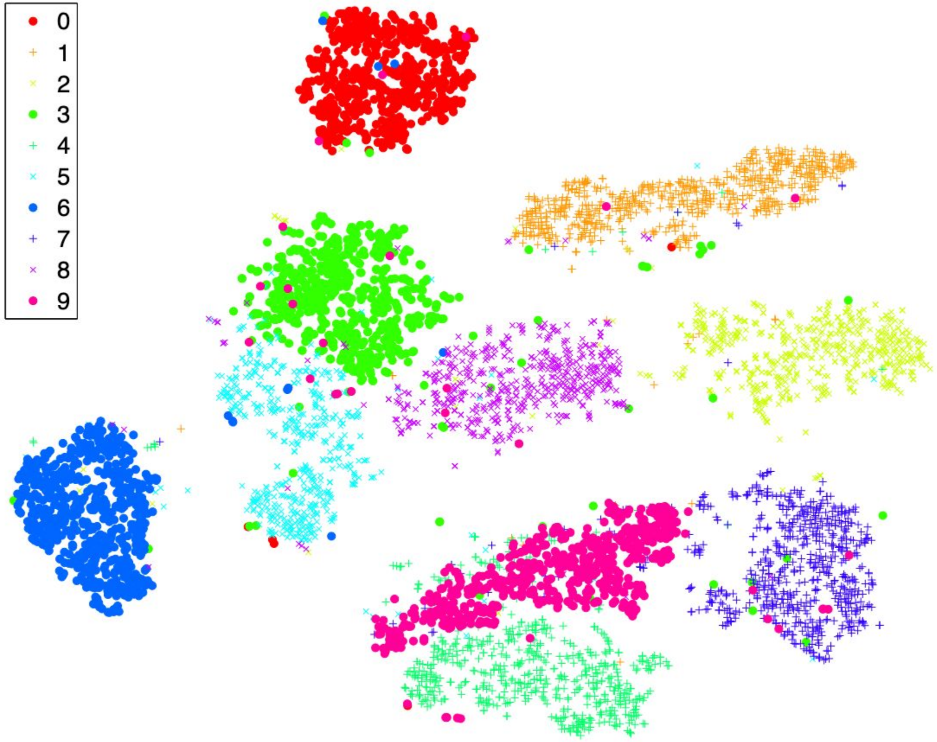
$$q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_{k \neq l} (1 + ||y_k - y_l||^2)^{-1}}$$

$$D_{KL}(P \,||\, Q) \to \min_{Y}$$

Result: nice and light visualizations

t-SNE on [MNIST dataset]()





Comparison

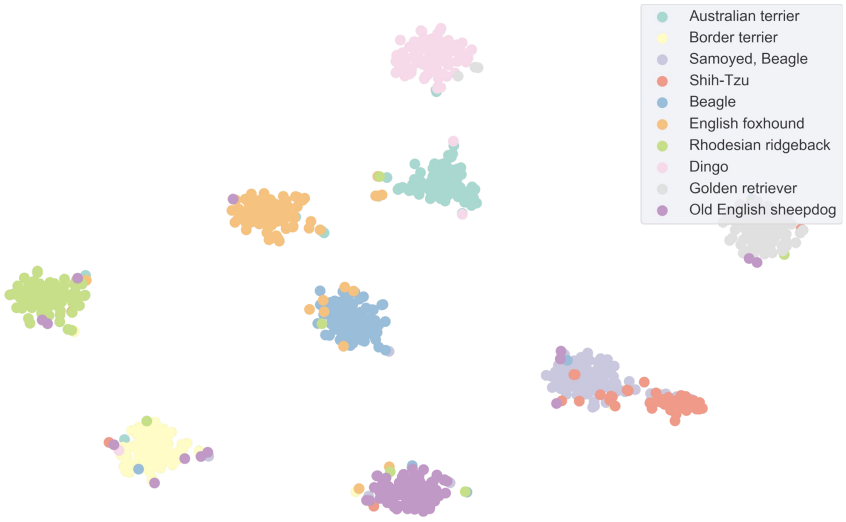
t-SNE Isomap LLE

Real life example

MDS (PCA) on faces embeddings

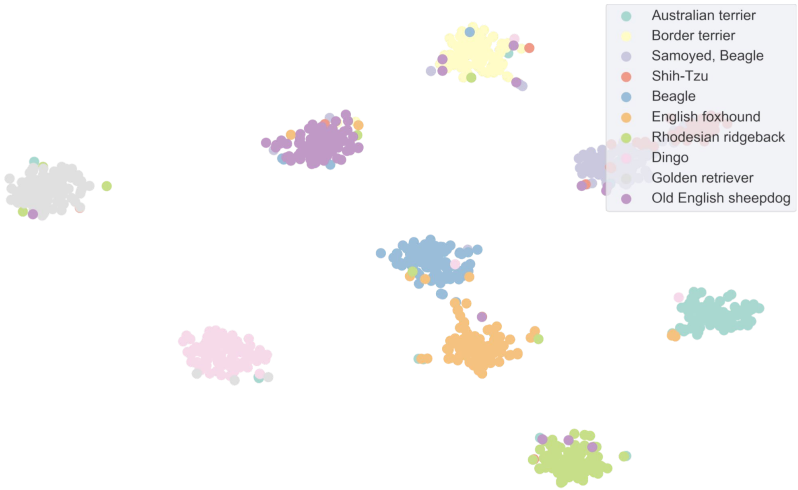
image source

Real life example



t-SNE on ArcFace

t-SNE on CosFace



Clustering

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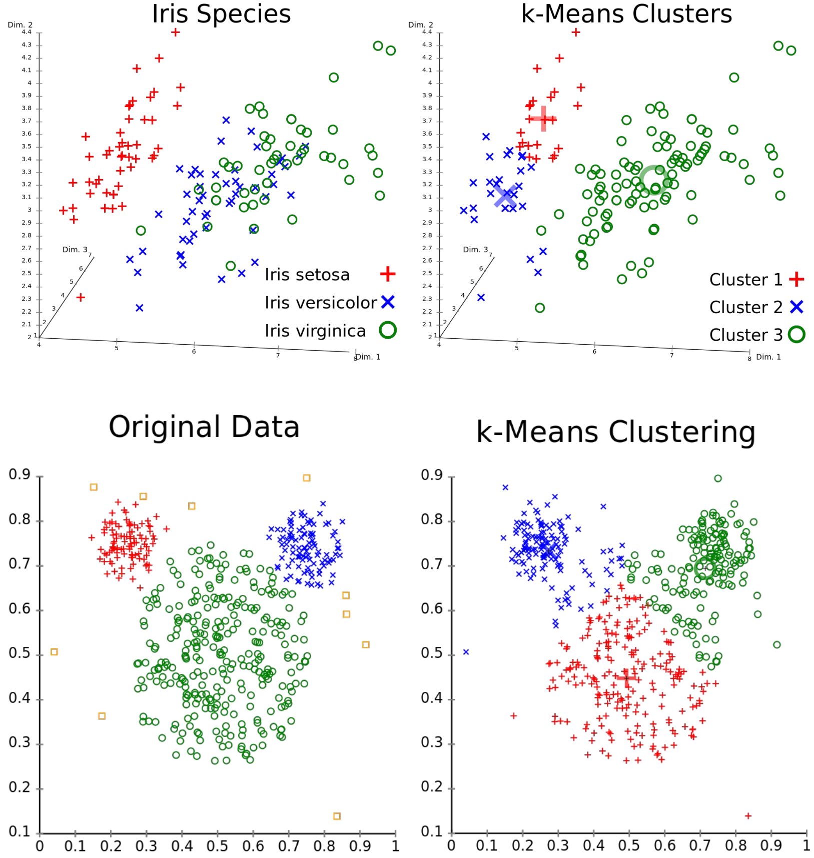
03

k-means



Based on K nearest neighbours algorithm

1. Init clusters centers randomly
2. Define current cluster of an object as a nearest center
3. Calculate new cluster center as a mean of all objects in cluster
4. Repeat from p. 2 until convergence

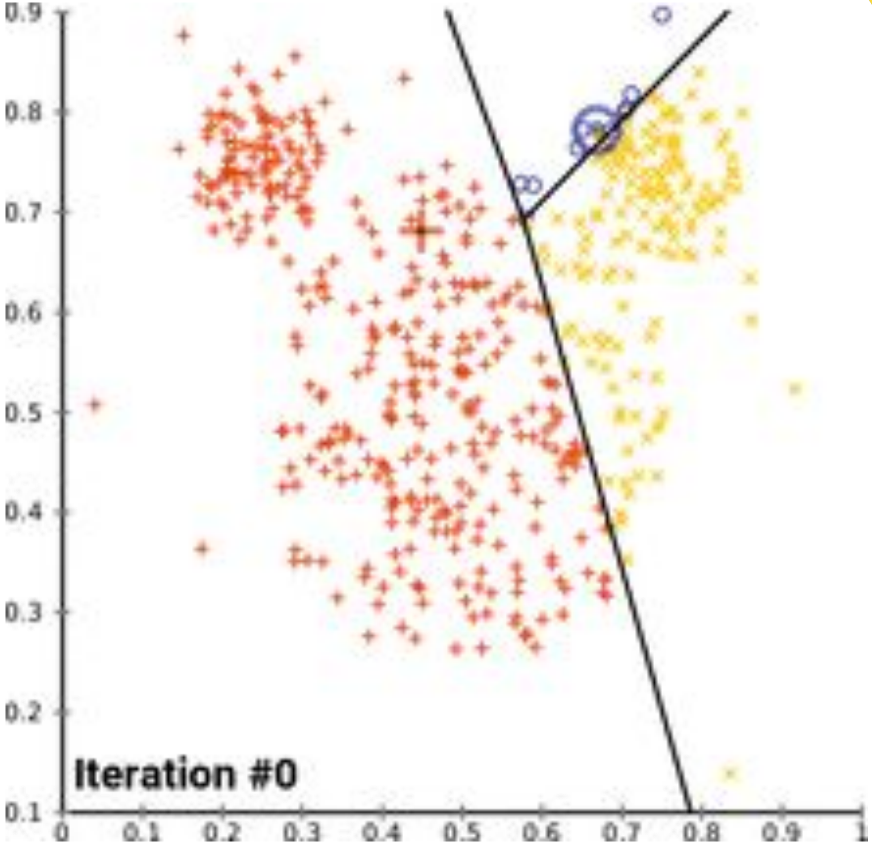
k-means

Params:

k - number of clusters

Advanced version: k-means++

[The Advantages of Careful Seeding, Arthur, Vassilvitskii, 2007, ACM-SIAM SODA]



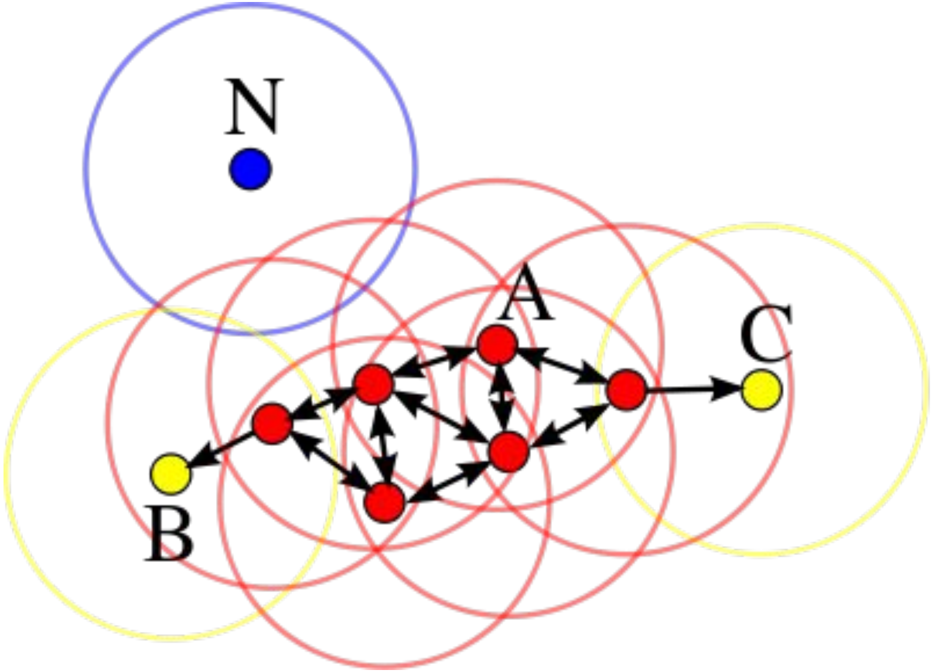
DBSCAN

Density-Based Spatial Clustering of Applications with Noise

Split all data points into 3 groups:

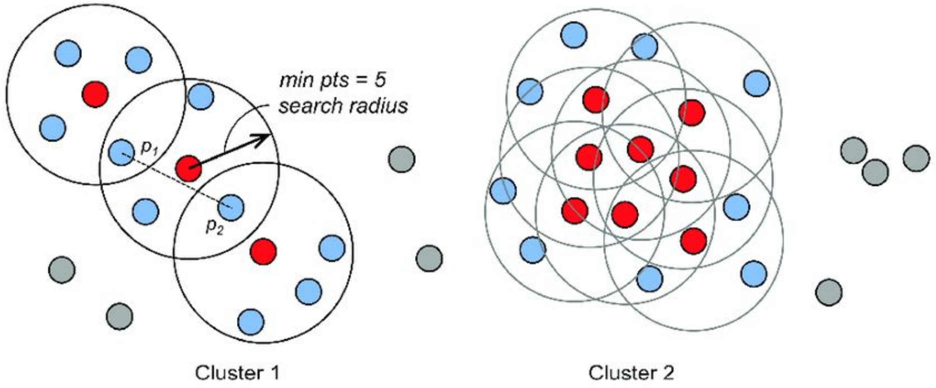
1. Core (red)
2. Border (yellow)
3. Noise (blue)

Core point has at least k other points in ε-neighbourhood



[A density-based algorithm for discovering clusters in large spatial databases with noise, Ester et al., 1996, KDD-96]

DBSCAN



Any two core or border points in ε-neighbourhood noted as connected points

Two points both connected to a common point also defined connected (transitivity)

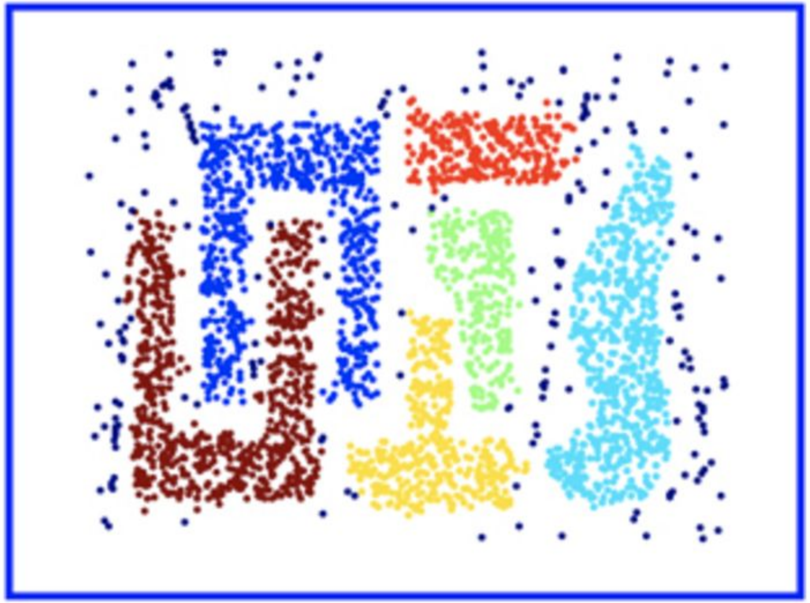
Cluster is defined as maximum connected set of points

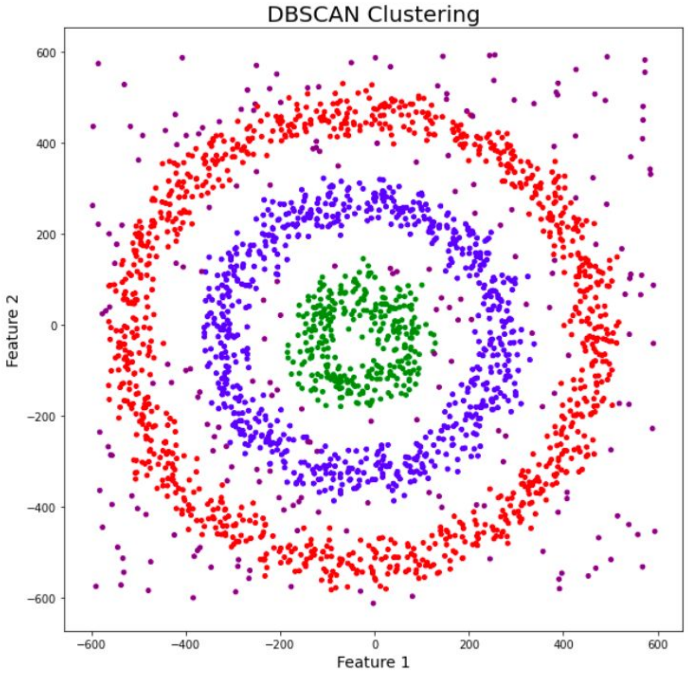
Params:

ε - radius of neighbourhood

k - minimal number of neighbours of core point

DBSCAN examples

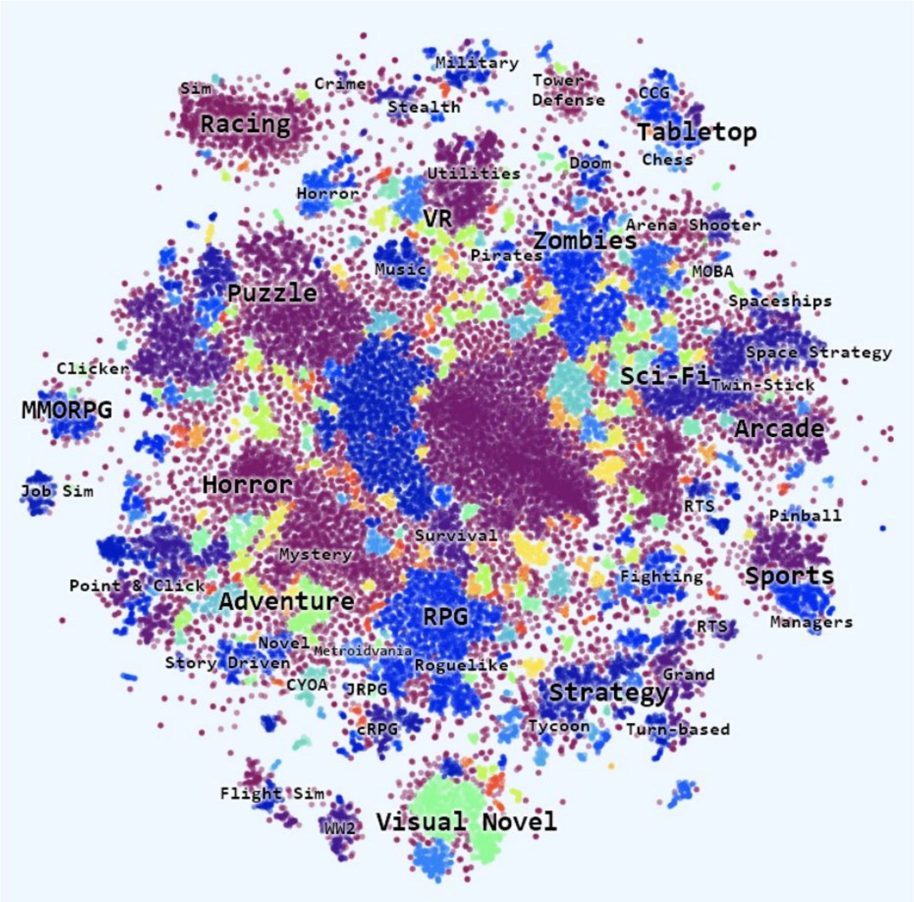




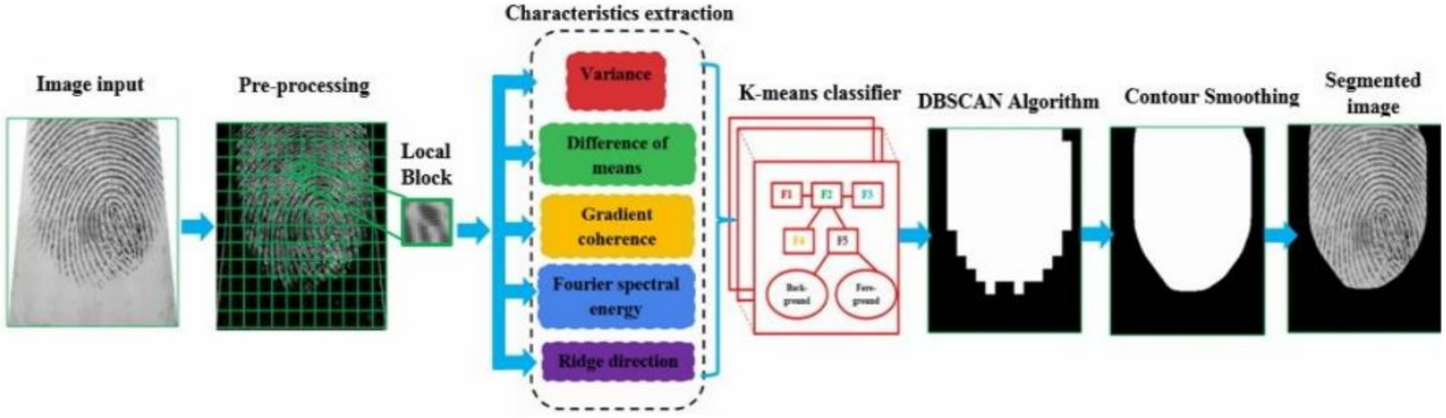
DBSCAN examples

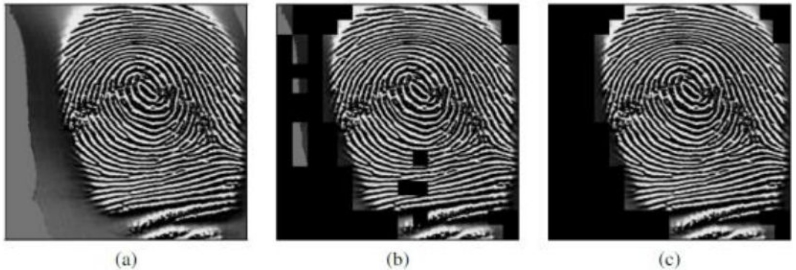
DBSCAN on t-SNE output
to analyze embeddings (Doc2vec)
of video games

image source



DBSCAN examples





a - original, b - k-means, c - DBSCAN

[Improving of Fingerprint Segmentation Images Based on K-MEANS and DBSCAN Clustering, Cherrat et al., 2019, IJECE]

Hierarchical clustering

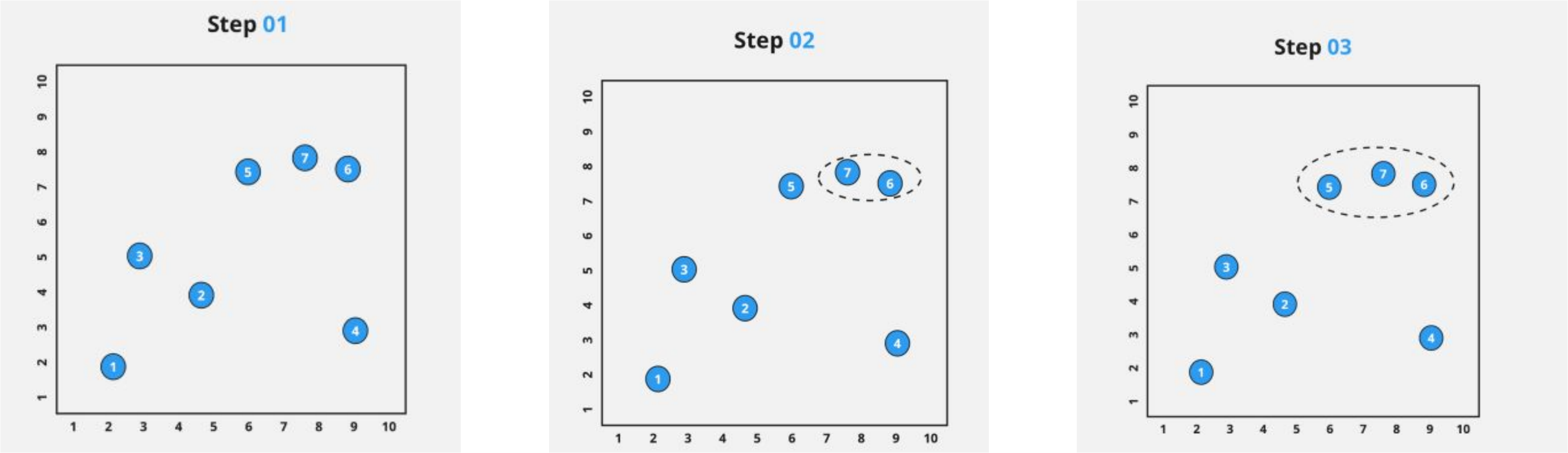
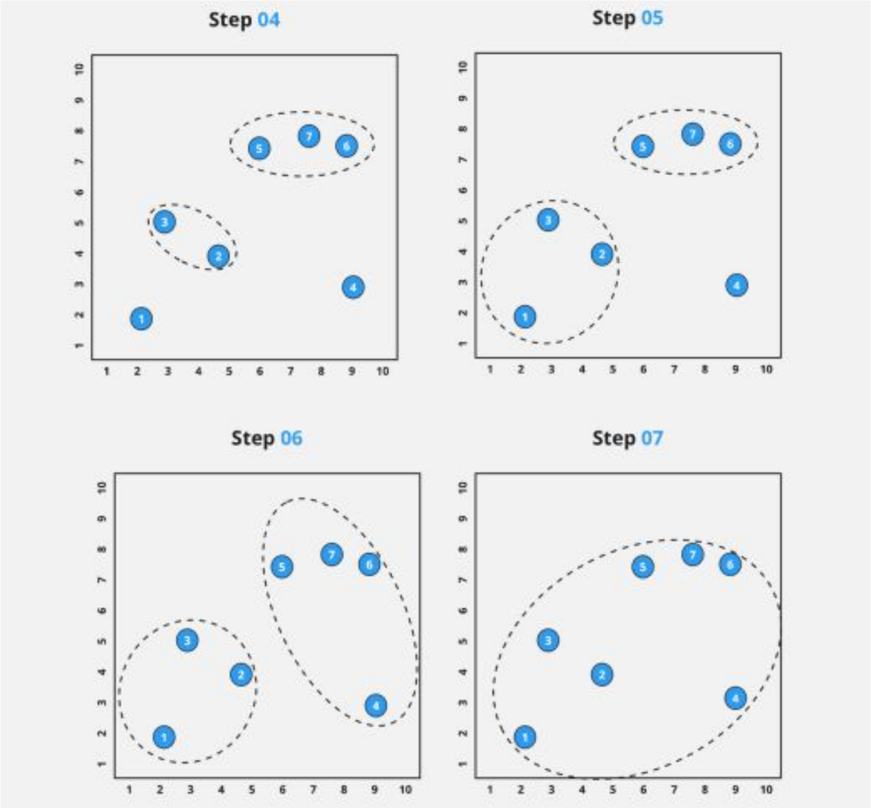
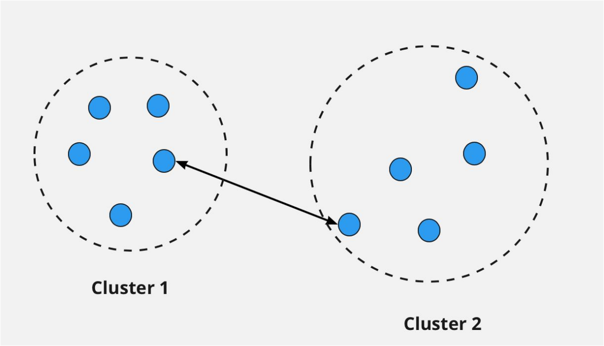


image source

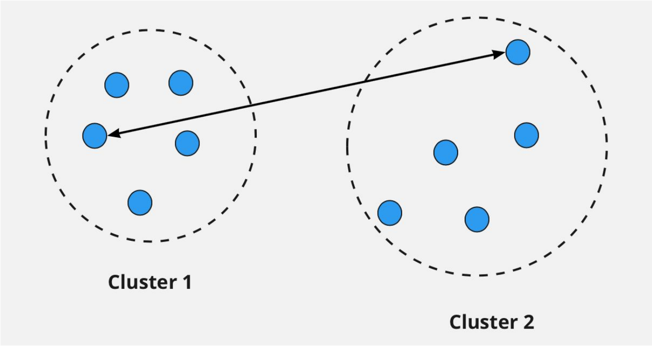
Hierarchical clustering



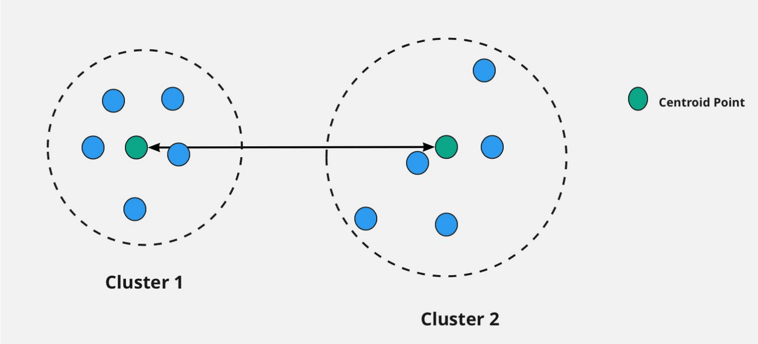
Distance between clusters



Closest point



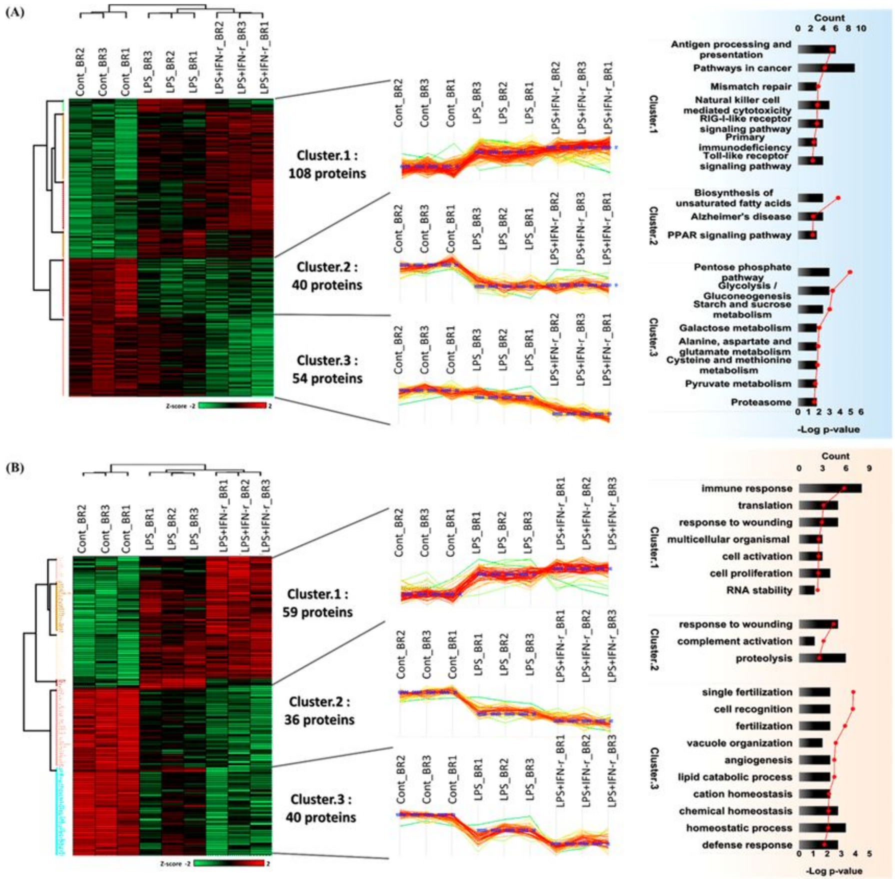
Farthest point



Centroid

Dendrogram

Dendrograms example

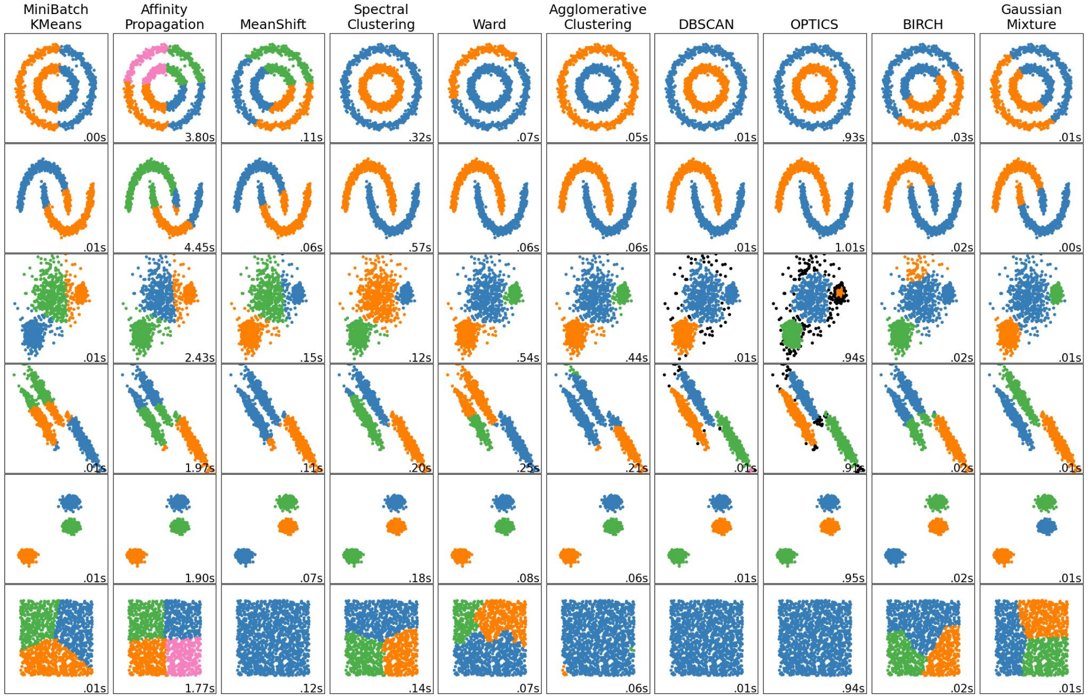


Hierarchical clustering and dendrograms often used in bioinformatics to visualize heatmaps of molecules interactions

[Image source]

Practical case: [seriation], [historical overview], [Python implementation for images]

Many more



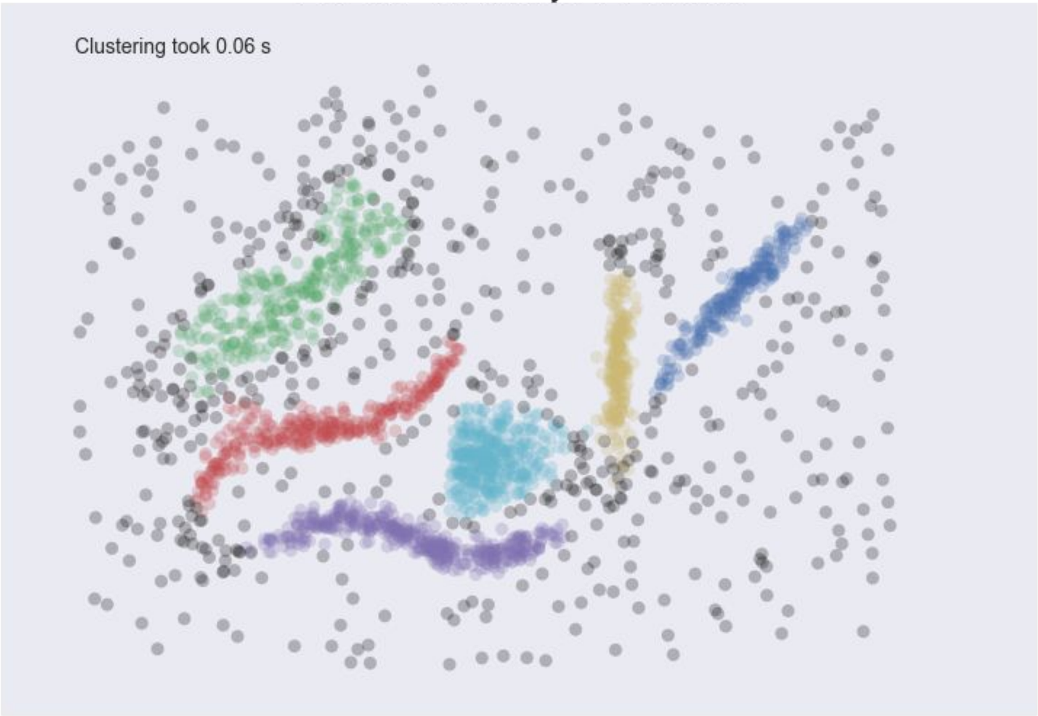
Read more:

[sklearn huge overview]
[HDBSCAN (hierarchy + DBSCAN)]
[timeseries clusterization] (ru)

Clustering metrics

- Label based
  - Rand index
  - Mutual Information
  - Homogeneity
  - Completeness
  - V-measure
  - …
- Label free
  - Silhouette Coefficient
  - Calinski-Harabasz Index
  - Davies-Bouldin Index
  - …

Clusters found by HDBSCAN



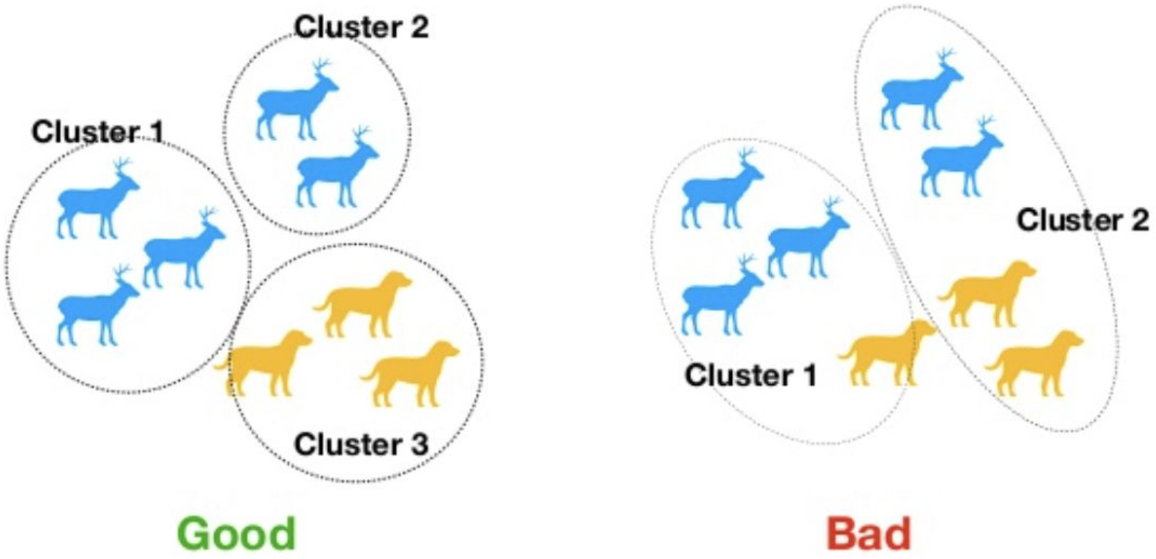
[Nice overview [ru]]

[Detailed explanations (sklearn docs)]

[image source]

Homogeneity

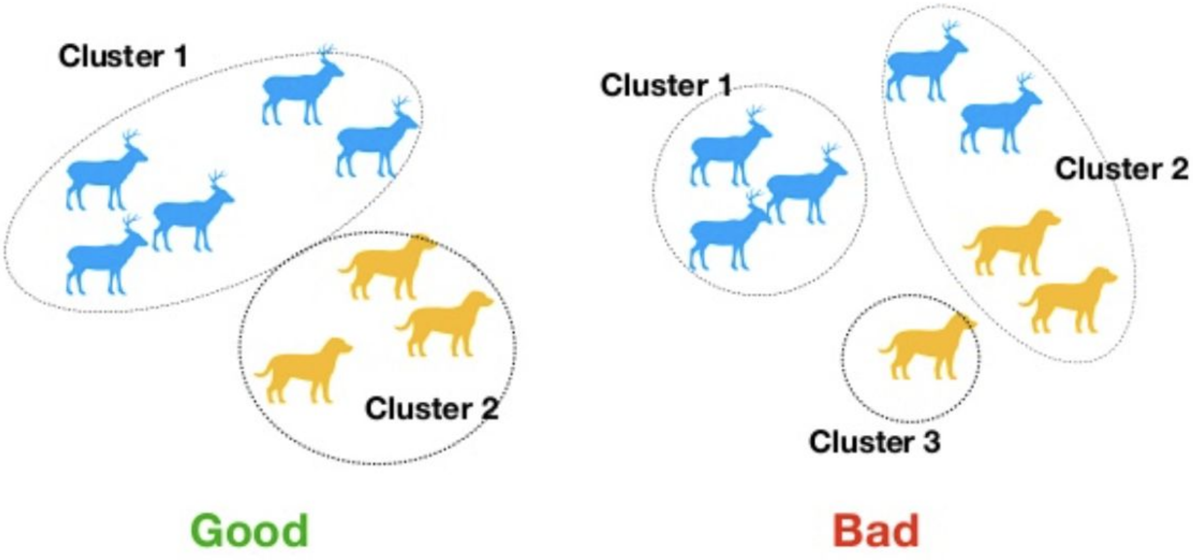
Each cluster contains only members of a single class



[image source](#)
and great slides on topic

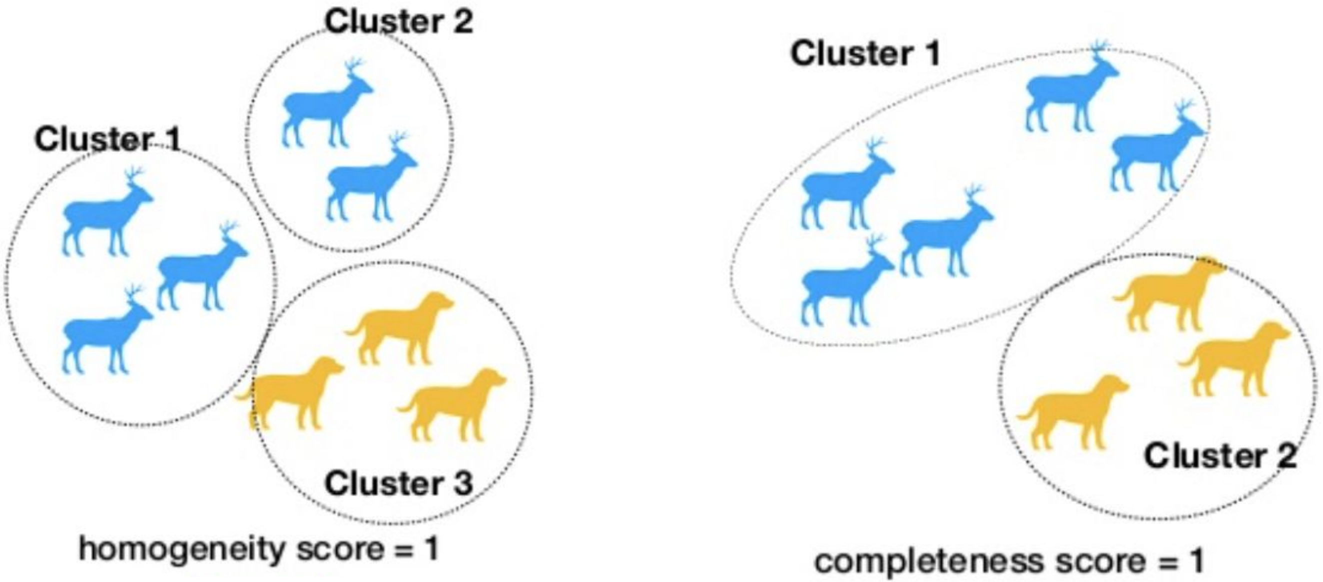
Completeness

all members of a given class are assigned to the same cluster



V-measure

geometric mean of Homogeneity and Completeness



Silhouette coefficient

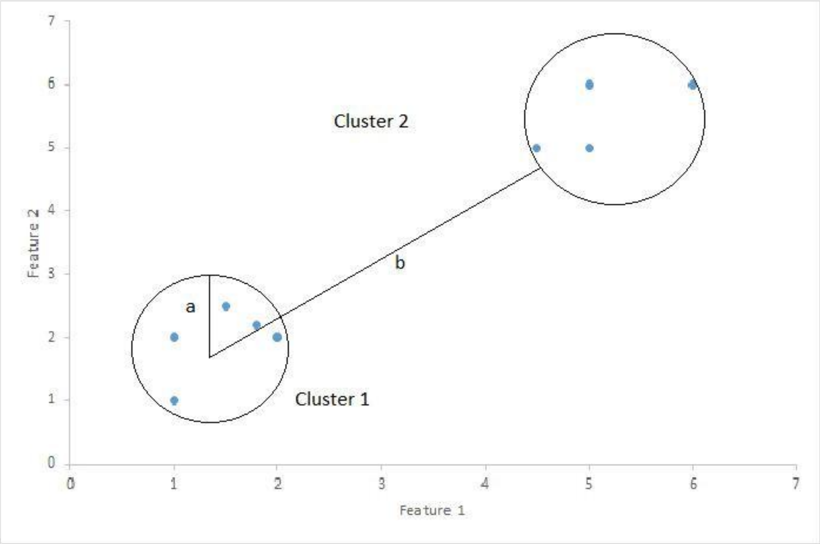


image source

a: mean distance to points in the *same cluster*

b: mean distance to points in the *next nearest cluster*

$$s_i = \frac{b_i - a_i}{max(a_i, b_i)}$$

Silhouette analysis

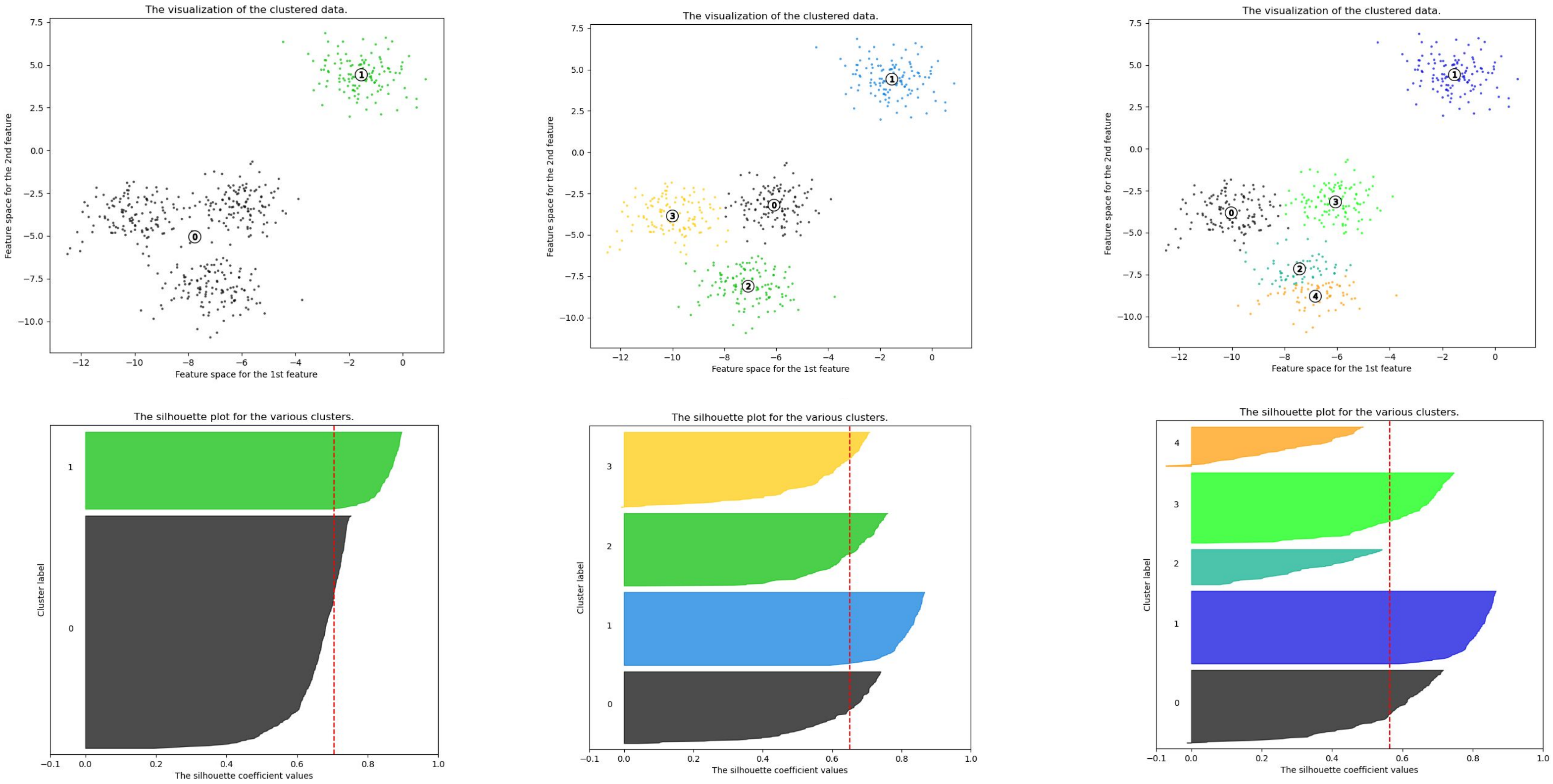


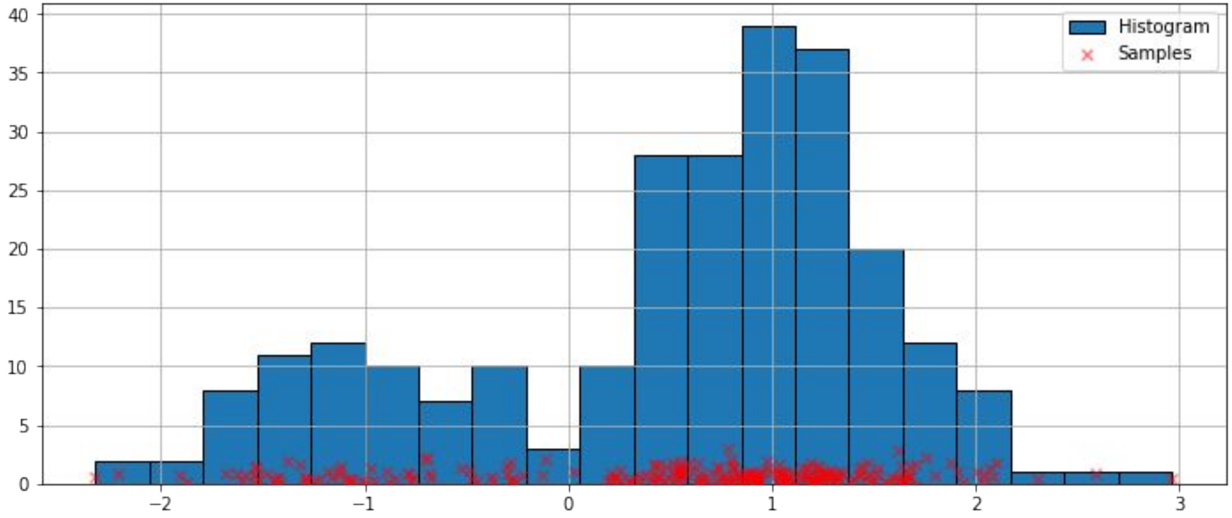
image source

Density estimation

girafe ai

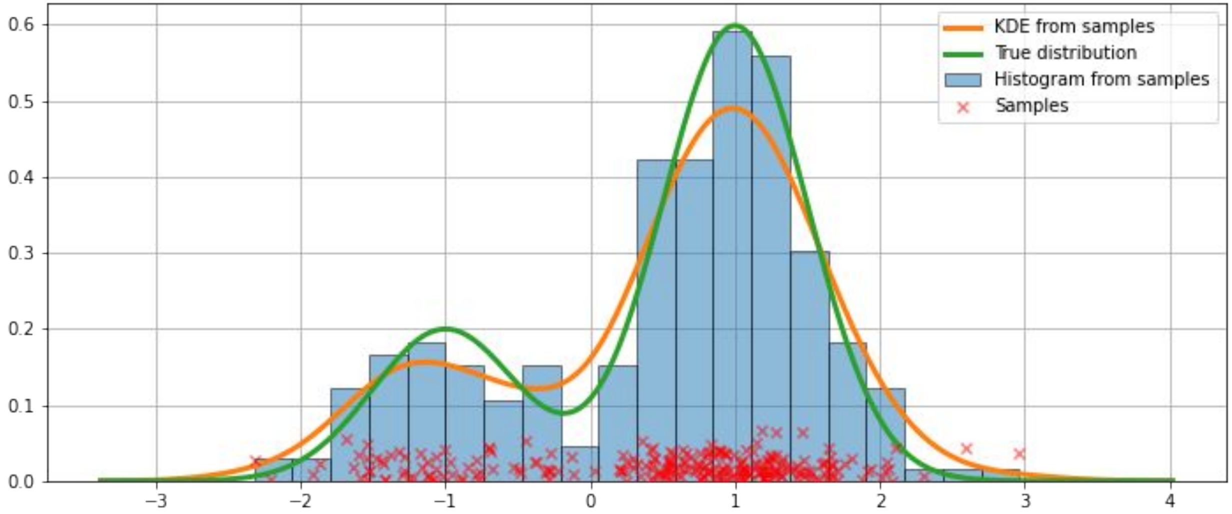
04

Kernel density estimation

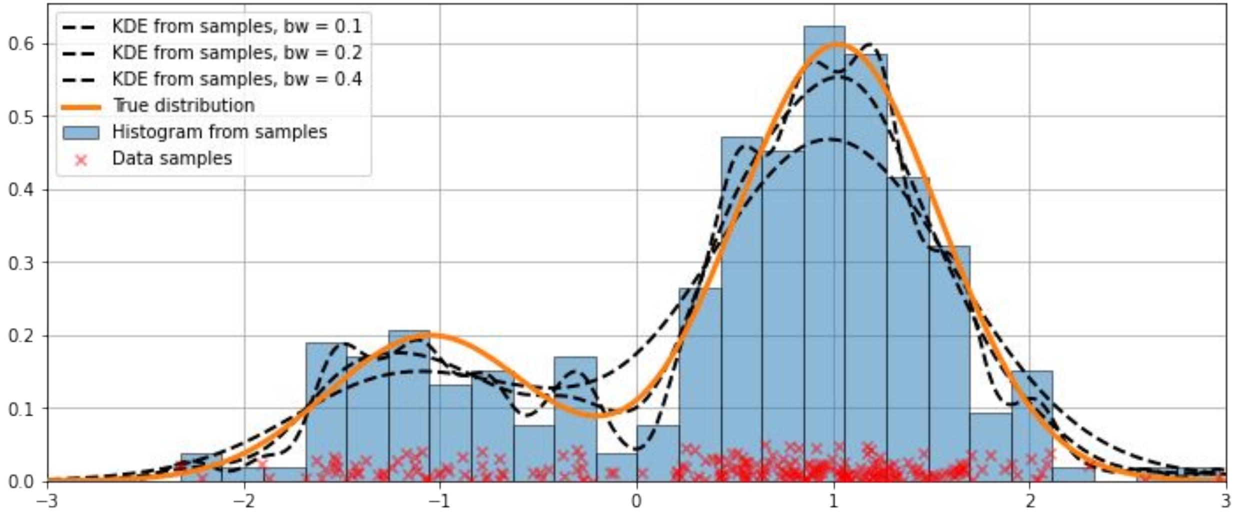


statsmodels documentation example

Kernel density estimation

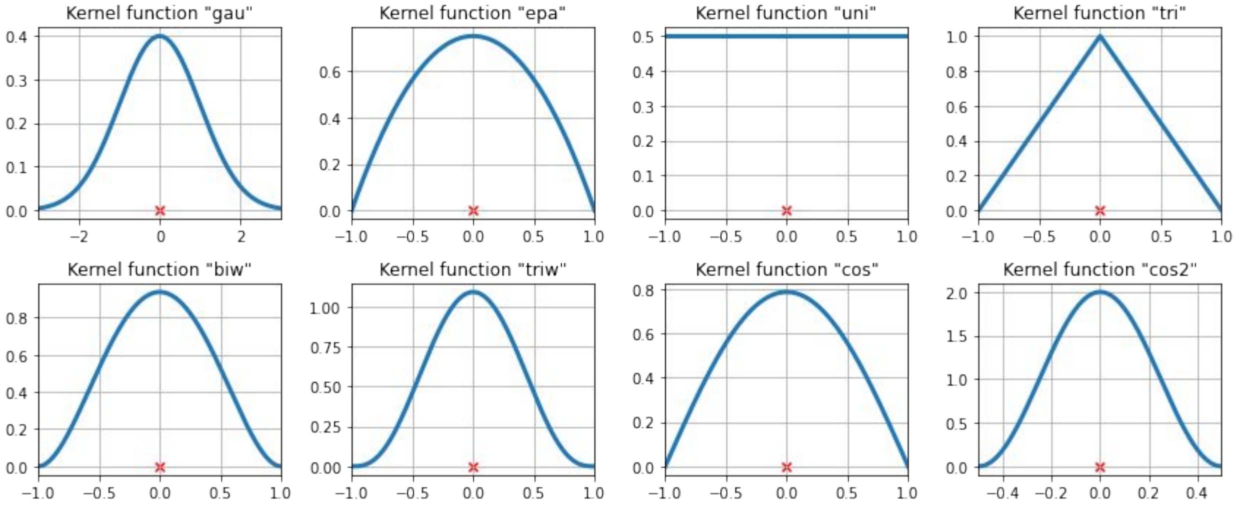


Window size



KDE from samples, bw = 0.1
KDE from samples, bw = 0.2
KDE from samples, bw = 0.4
True distribution
Histogram from samples
Data samples
0.0
0.1
0.2
0.3
0.4
0.5
0.6
−3
−2
−1
0
1
2
3

Kernel types



Revise

- Geometrical machine learning
  - Dimensionality curse
  - Manifold assumption
- Dimensionality reduction
  - Feature selection
  - Multidimensional Scaling (MDS)
  - Isomap
  - Locally linear embedding (LLE)
  - t-SNE
- Clustering
  - k-means
  - DBSCAN
  - Hierarchical clustering
  - metrics
- Density estimation
  - Kernel density estimation

Thanks for attention!

Questions?

girafe
ai

Notable links

1. Good lecture on MDS, Isomap, LLE
2. Lecture on t-SNE (this one is good too)
3. Slides about clusterization
4. Metrics in clusterization
5. Slides about ICA
6. More clustering methods (in Russian)