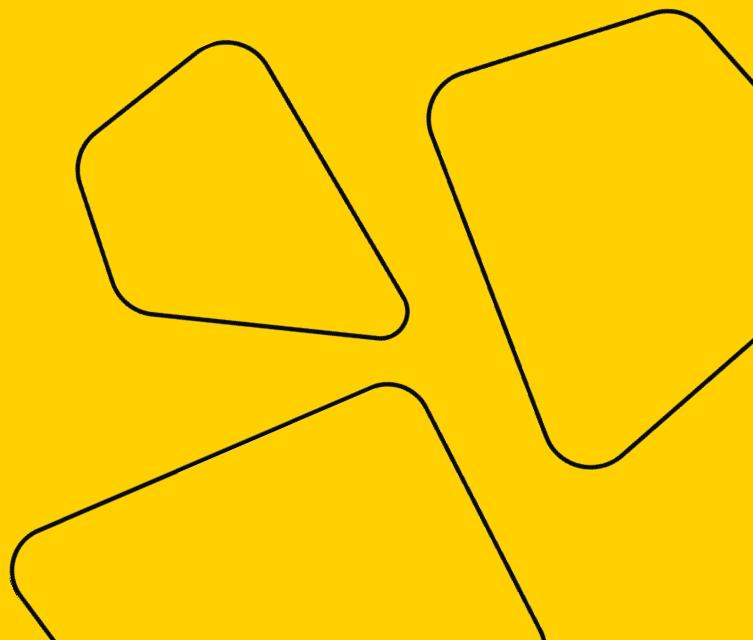


Unsupervised Learning

MIPT, 2021



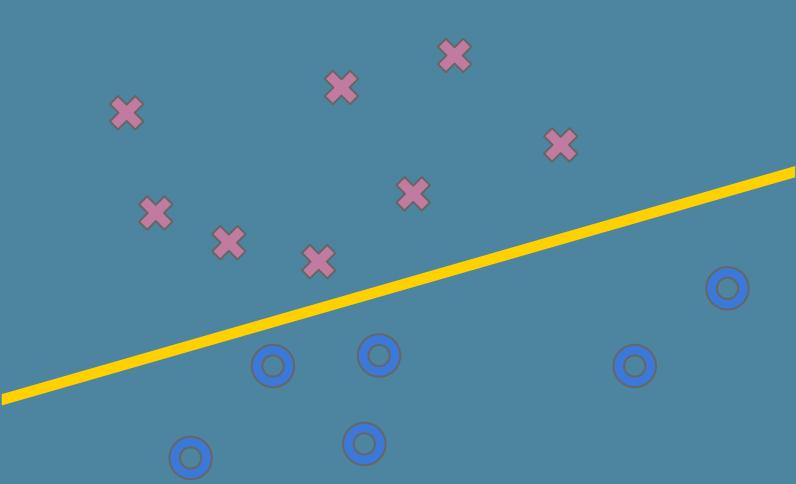
girafe
ai



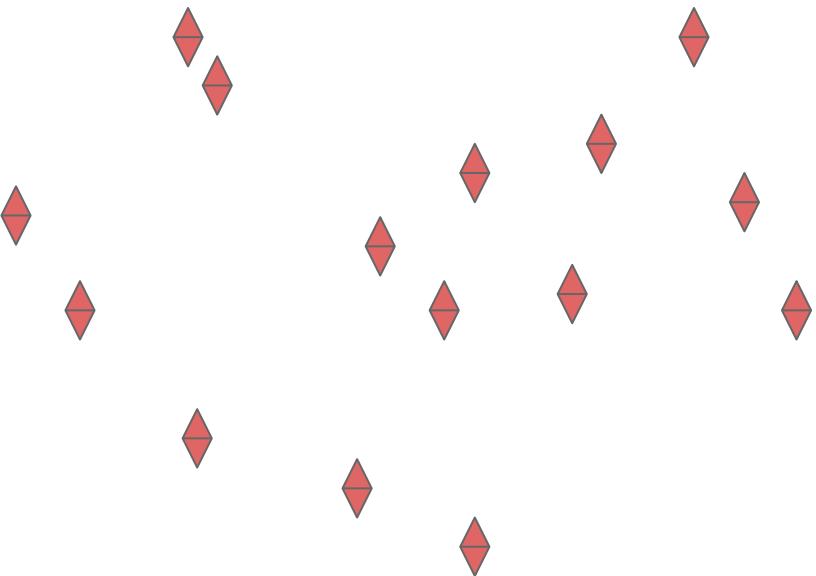
Outline

- 
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

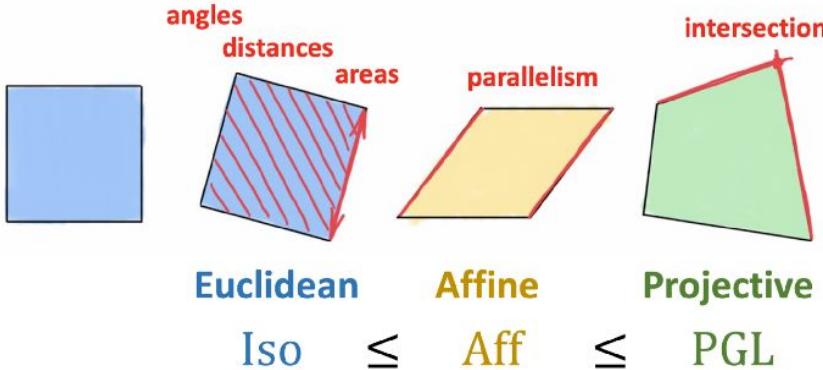


Geometrical machine learning

girafe
ai

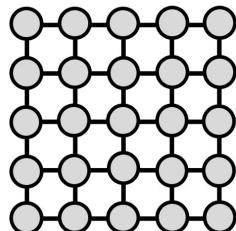
01

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)

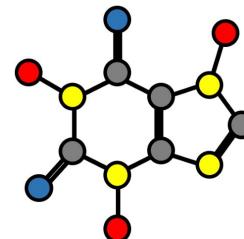
[Article introducing a book on Geometric Deep Learning](#)



Grids



Groups



Graphs

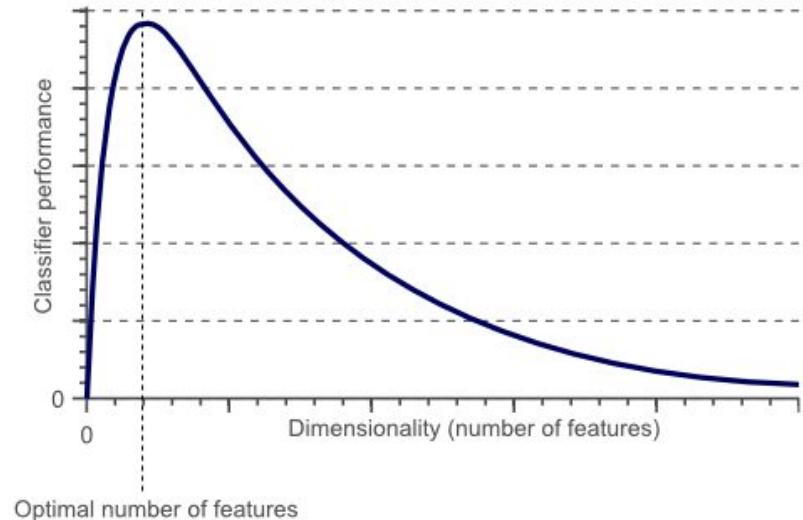


Geodesics & Gauges

Dimensionality curse

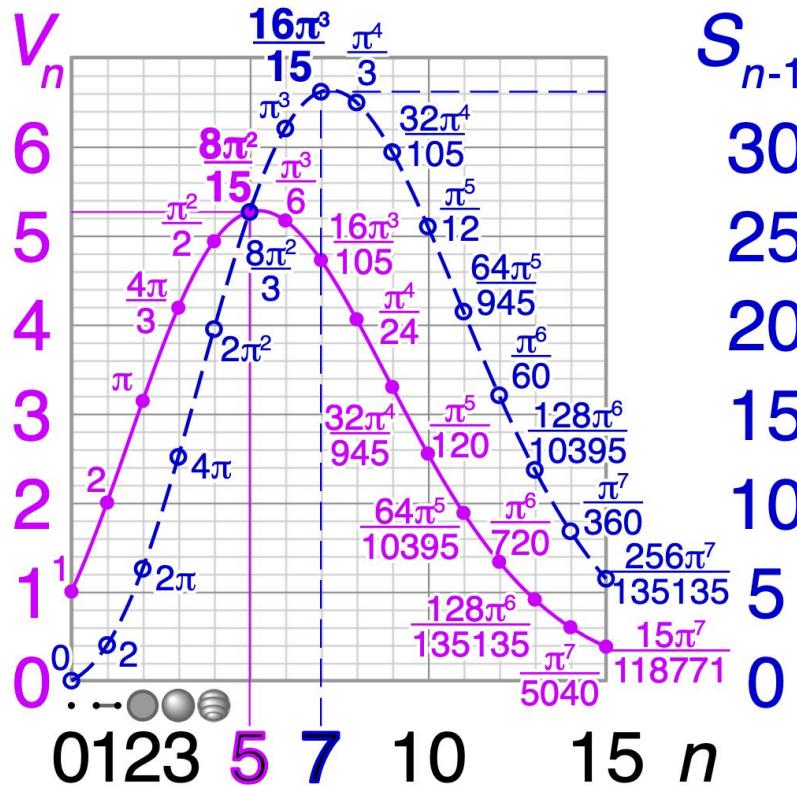


Certain behaviours or effects that appear when analysing data in high dimensions, that do not occur in low-dimensional spaces





Sphere volume decrease

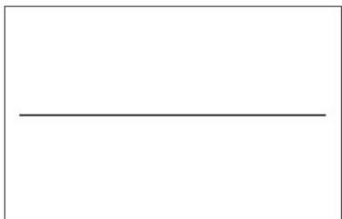


[image source](#)

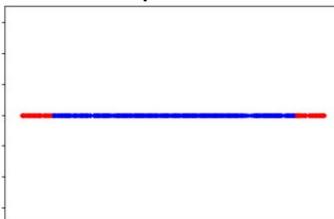
Distance in high dimensional space



Line of length 1



Line with 500 randomly generated points



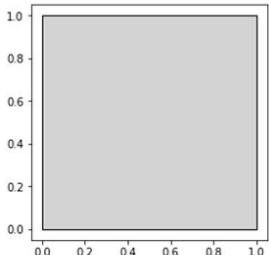
Inside points

Points that fall within 10% of the distance to the edges

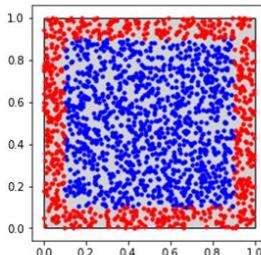
Ratio of inside points to total points = 80%

Average Distance between 2 points = 0.34

Square of side 1



2000 randomly generated points



Inside points

Points that fall within 10% of the distance to the edges

Ratio of inside points to total points = 63%

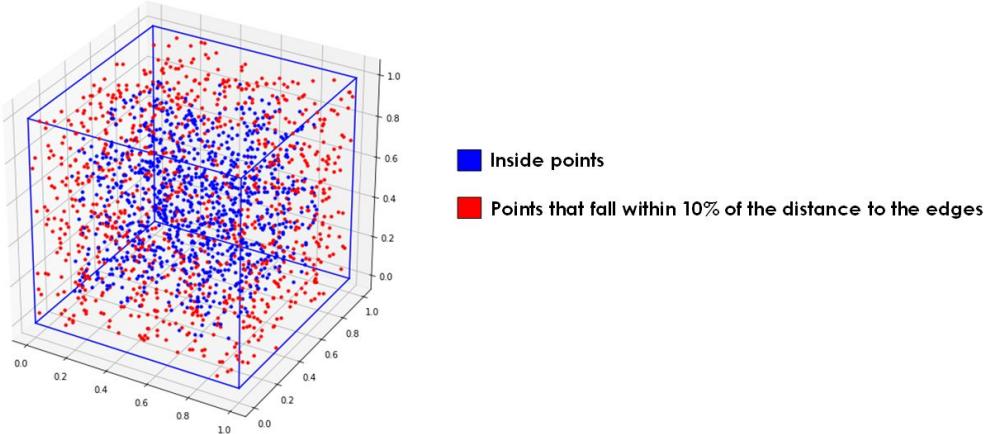
Average Distance between 2 points = 0.52

[image source](#)

Distance in high dimensional space



Cube of side 1



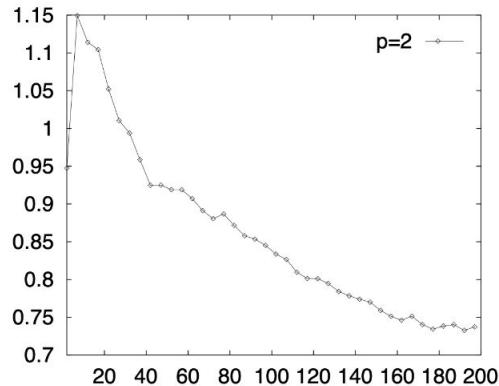
Ratio of inside points to total points = 51%
Average Distance between 2 points = 0.65

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

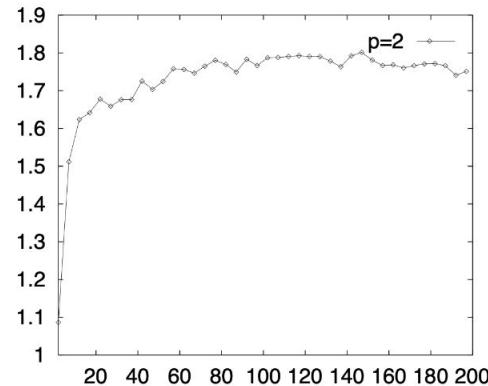
Distance relative contrast



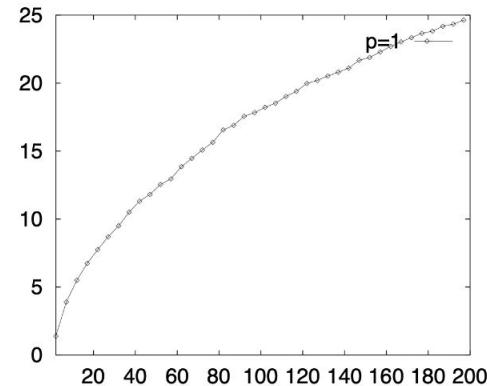
Take random points uniformly distributed in D dimensional cube and calculate distance to the farthest point and to the closest point. Plot their difference depending on D for different Minkowski metrics



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

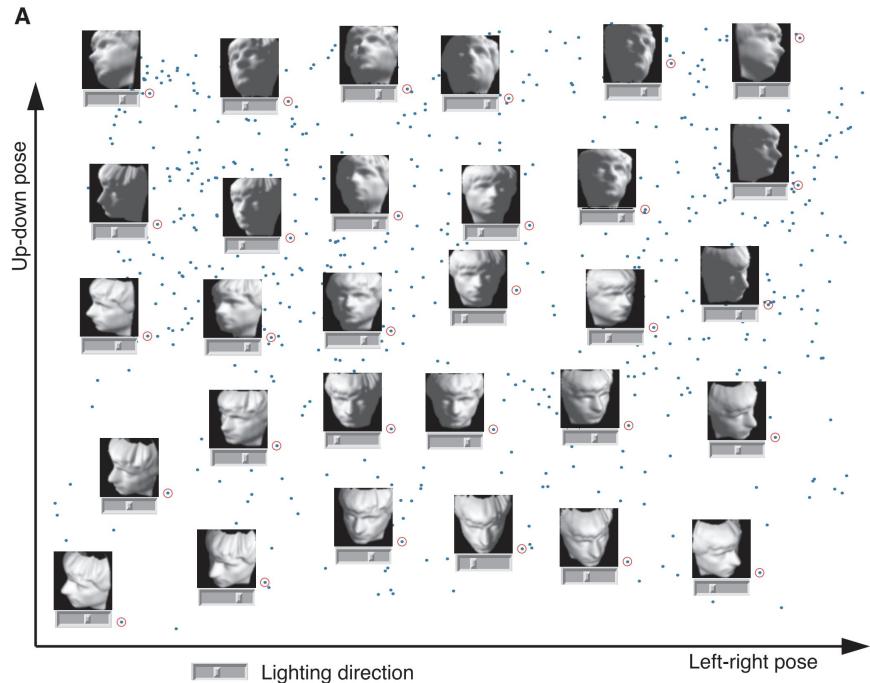
Manifold assumption



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

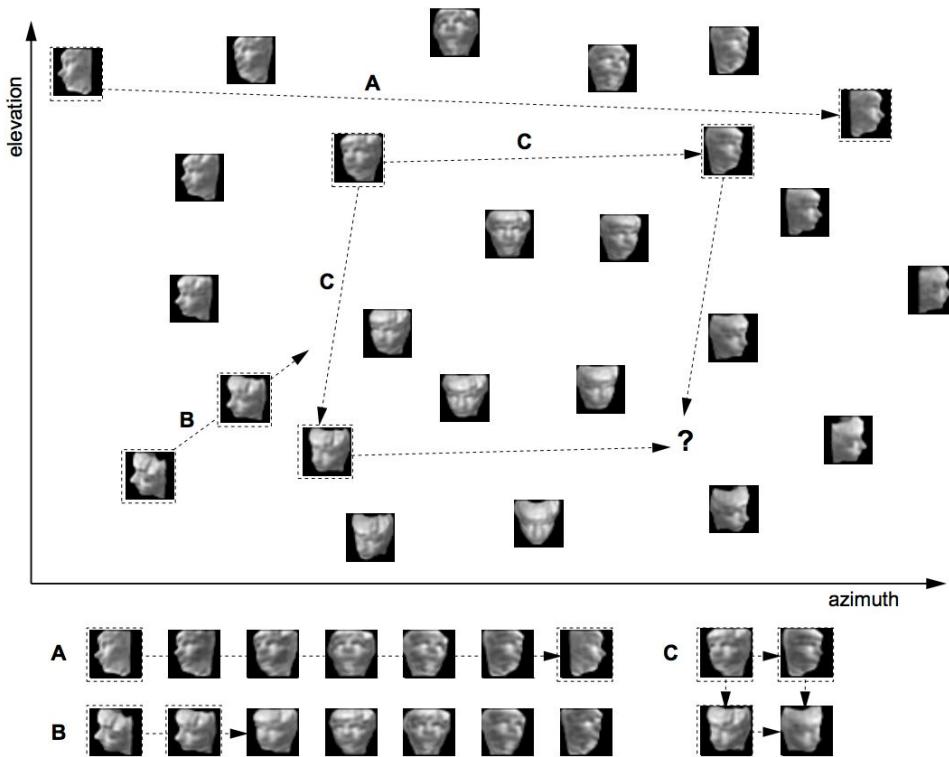
Sometimes dimensionality of manifold is referred as [intrinsic dimension](#) (see [this article](#))



[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)

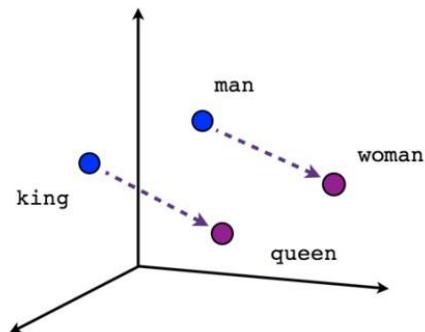
This process is also called embedding space 'walking'



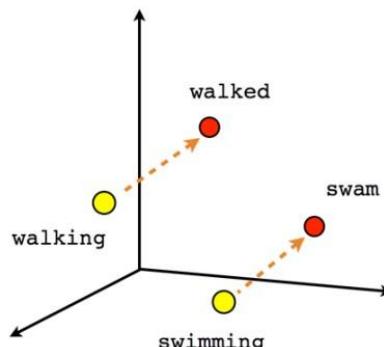
Latent space example

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

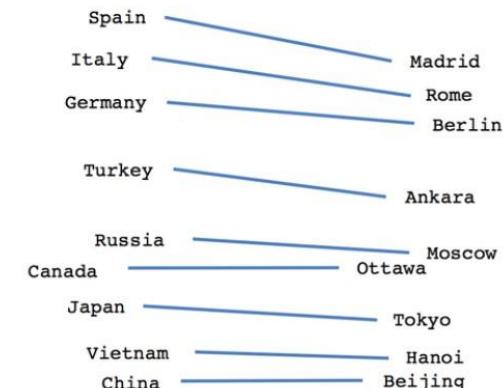
Read more: [manifold assumption](#), [assessing assumption](#)



Male-Female



Verb tense



Country-Capital

Dimensionality reduction

girafe
ai

02

Поставить задачу!



Feature selection

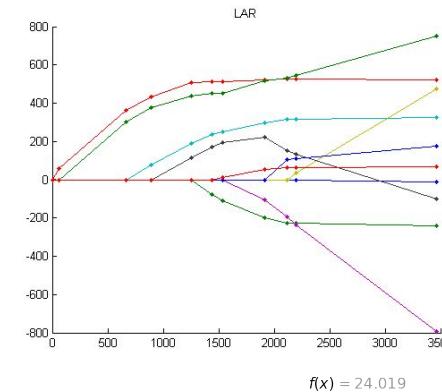


Select subset of existing features to use in further modelling

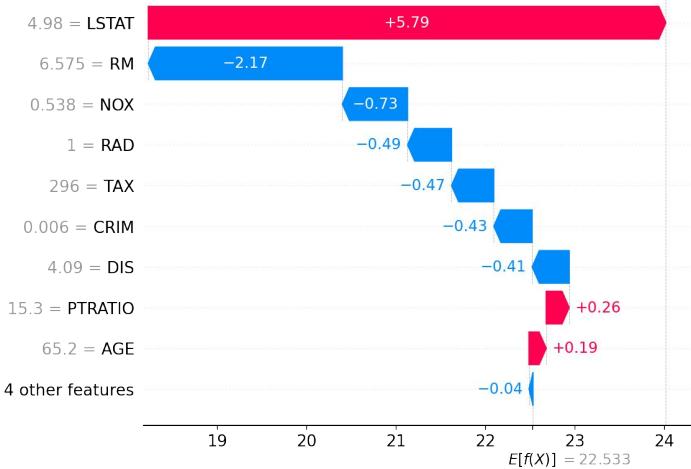
Usually is based on some supervised method

Examples:

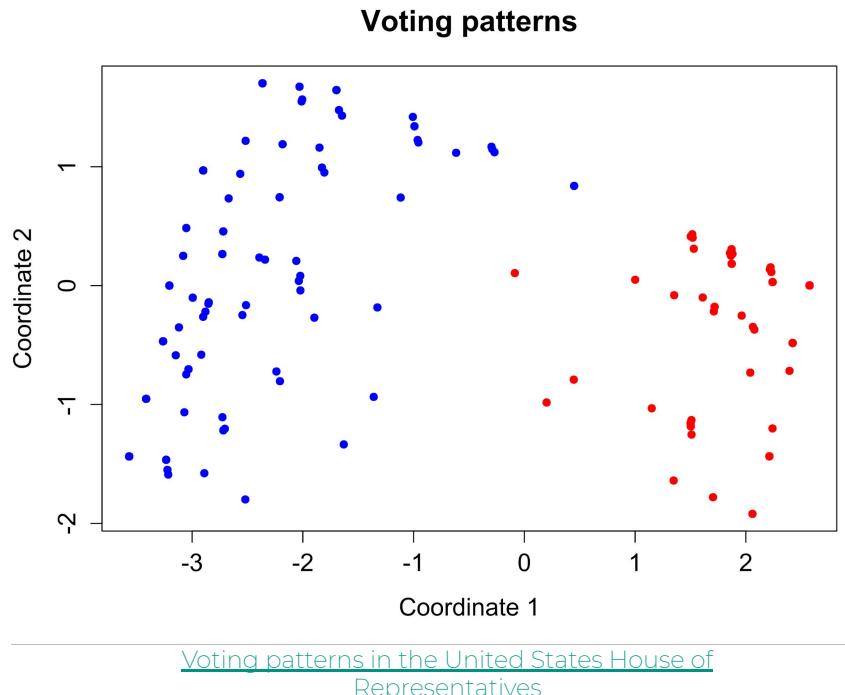
- stepwise regression
- LARS
- SHAP values
- etc...



$$f(x) = 24.019$$



Multidimensional Scaling (MDS)



Goal:

Linearly embed to given lower space

Solution:

PCA

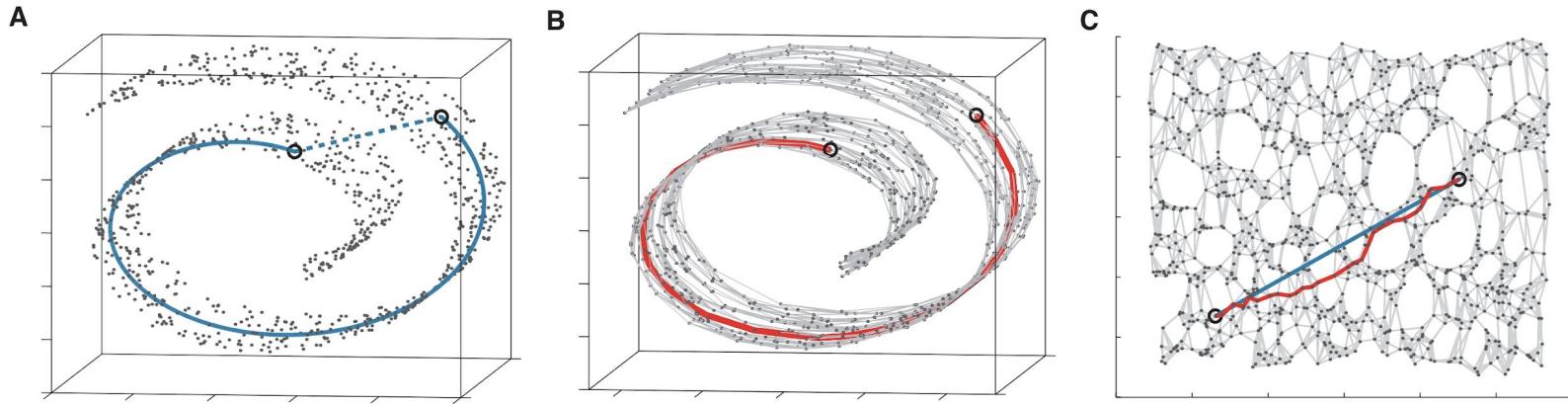
$$L = ||D_x - D_y||_2 \rightarrow \min_{y = Ax}$$

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

Params: p - target dimensionality

Also could be non-linear

Isomap



Now make distancies geodesic!

And measure distances on the produced
graph

Params:

n - number of neighbours to connect

p - dimensionality of manifold

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



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 $k = 1, 2, \dots, N$ 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 $\sqrt{\lambda_p} v_p^i$.

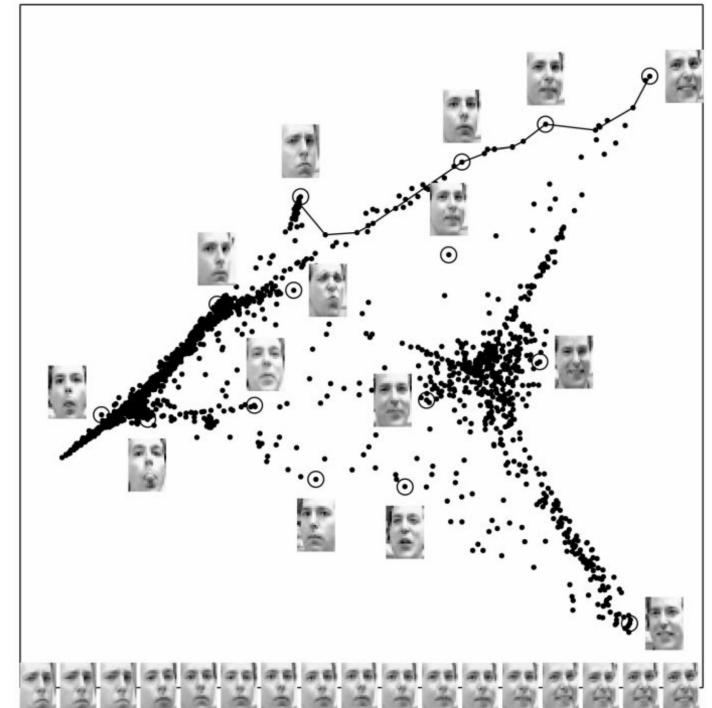
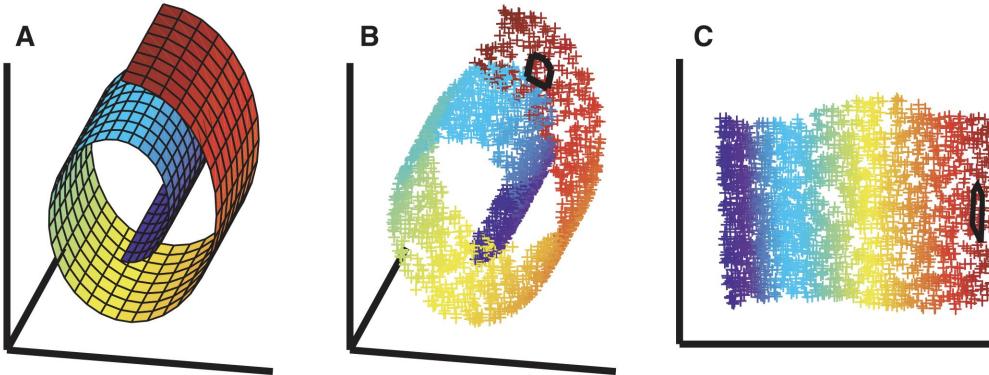
17. The operator τ is defined by $\tau(D) = -HSH/2$, where S is the matrix of squared distances $\{S_{ij} = D_{ij}^2\}$, and H is the "centering matrix" $\{H_{ij} = \delta_{ij} - 1/N\}$ (13).

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

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

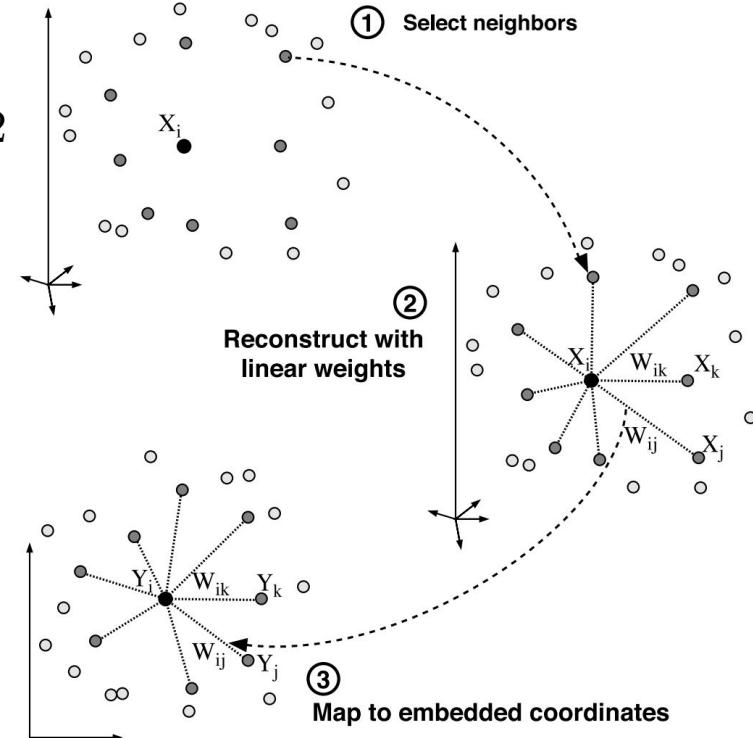
2. Estimate new points based on known relations

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

Params:

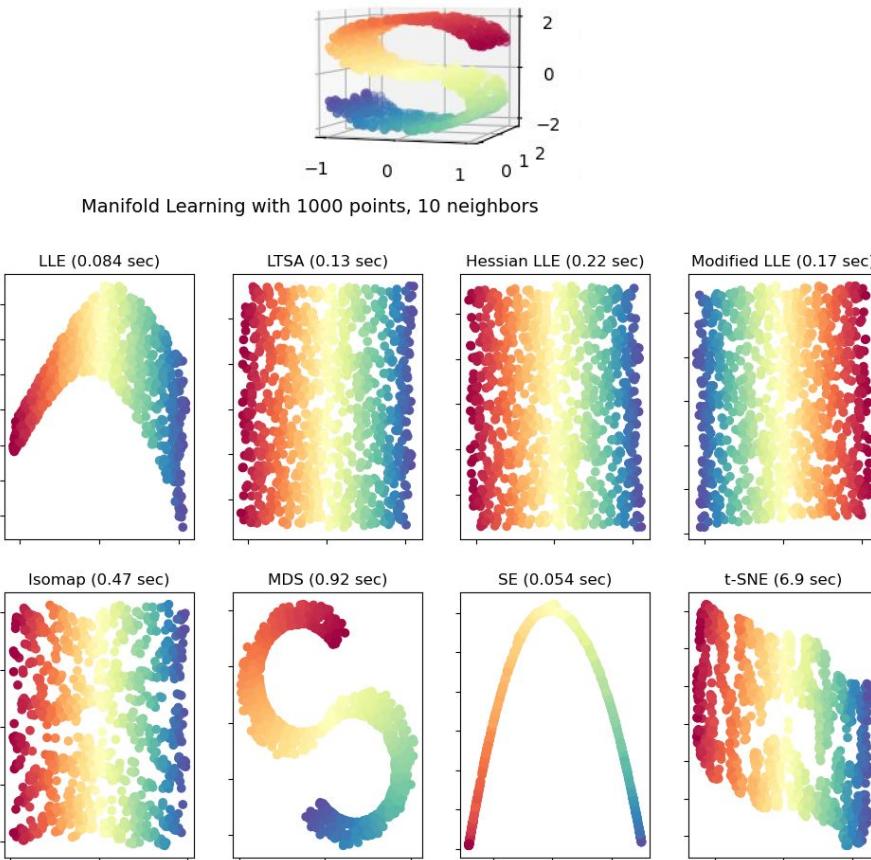
n - number of neighbours to connect

p - dimensionality of manifold





Many more

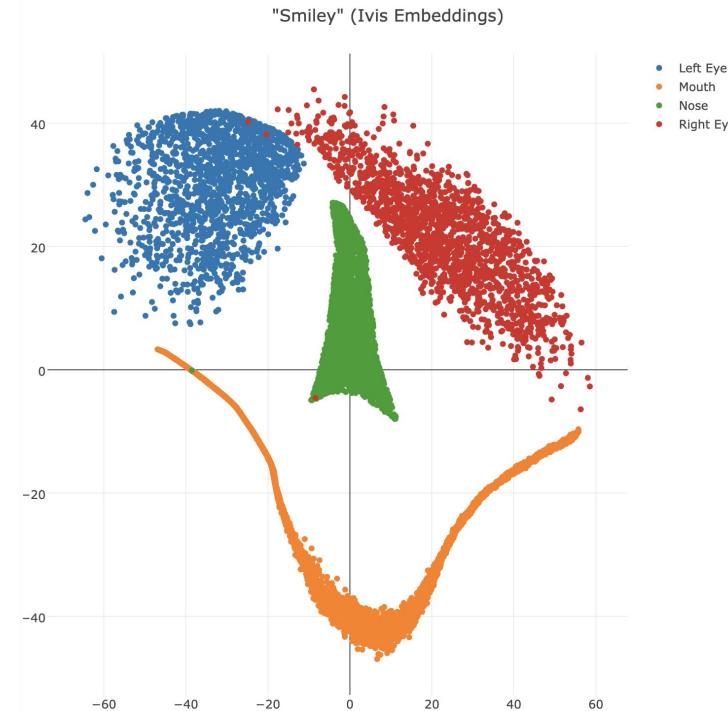
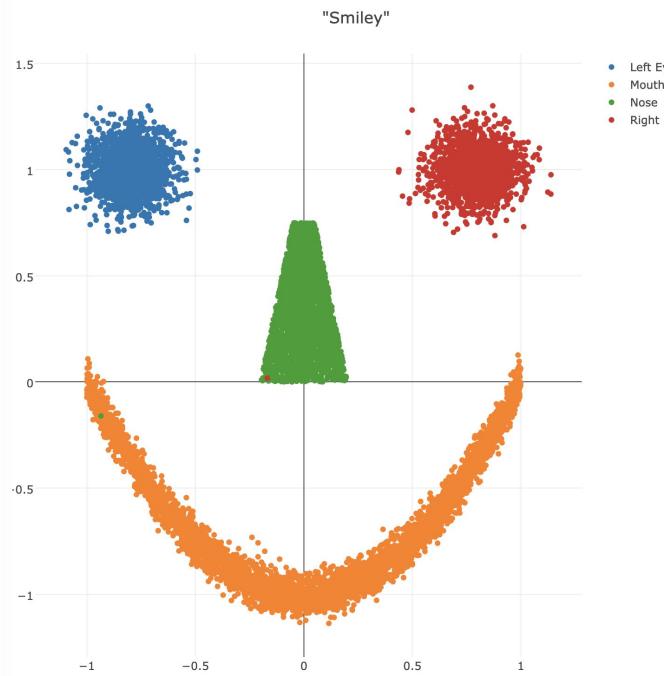


- Hessian Eigenmapping
- Spectral Embedding
- Local Tangent Space Alignment
- Riemannian Geometry
- UMAP
-

Read more:

[sklearn manifold methods](#)
[sklearn signals decomposition](#)

Next level: Neural Networks



UMAP vs Ivis embeddings

t-SNE



t-distributed Stochastic Neighbor Embedding

SNE

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

Stochastic Neighbor Embedding



Convert pairwise distances to probabilities, preserve probabilities through the spaces

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

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. these distributions are close.

What are close distributions?

Kullback–Leibler divergence



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



Suspiciously similar to Shannon entropy

[Learn more](#)



SNE problem

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

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

$$D_{KL}(P \parallel Q) \rightarrow \min_Y$$



t-distributed SNE

Patches over SNE:

1. choose common variance
2. make distributions symmetric

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

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

Visualizing Data using t-SNE,
Maaten, Hinton, 2008, JMLR

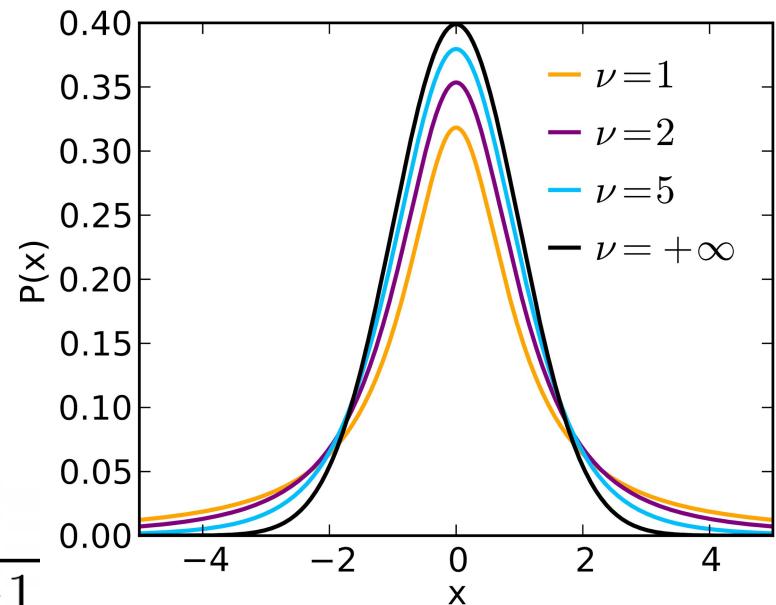
t-distributed SNE



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

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

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

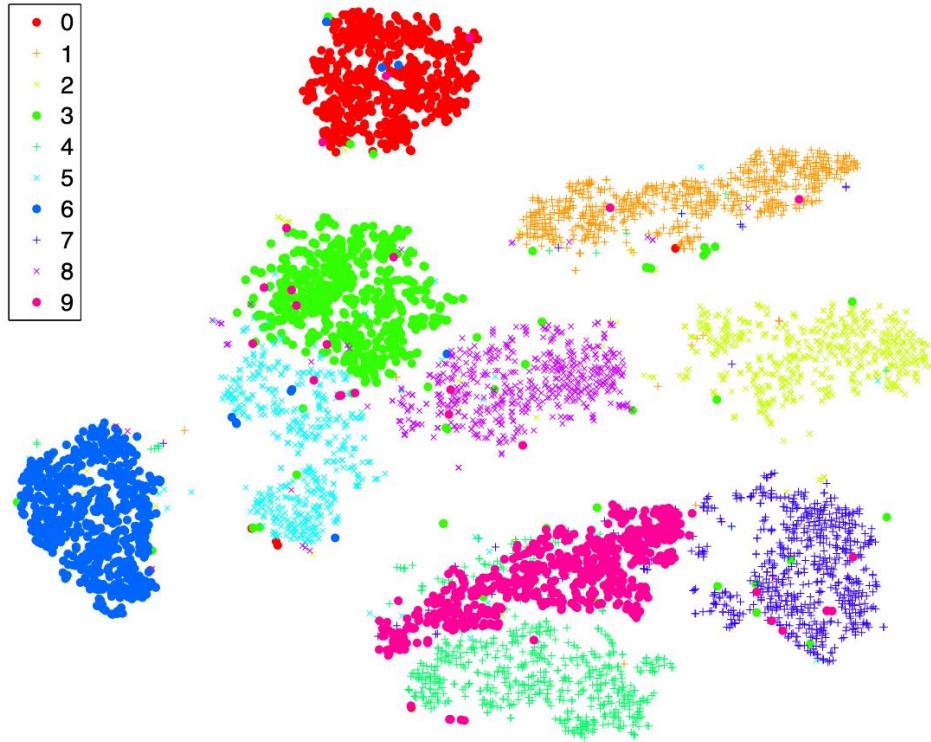
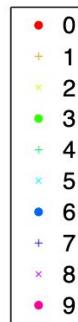
$$D_{KL}(P \parallel Q) \rightarrow \min_Y$$

Result: nice and light visualizations



t-SNE on [MNIST dataset](#)

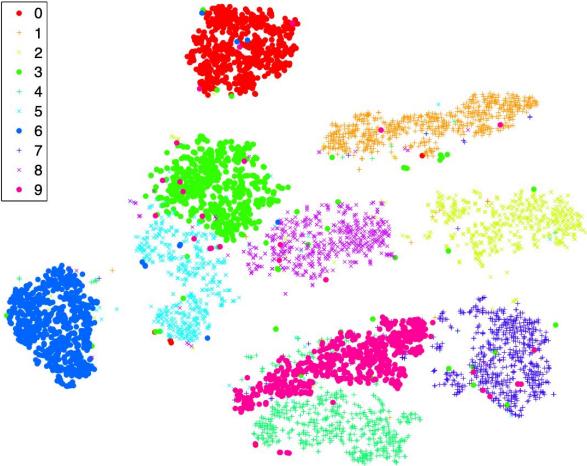
0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1
2 2 2 2 2 2 2 2 2 2 2 2 2 2
3 3 3 3 3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5 5 5 5 5
6 6 6 6 6 6 6 6 6 6 6 6 6 6
7 7 7 7 7 7 7 7 7 7 7 7 7 7
8 8 8 8 8 8 8 8 8 8 8 8 8 8
9 9 9 9 9 9 9 9 9 9 9 9 9 9



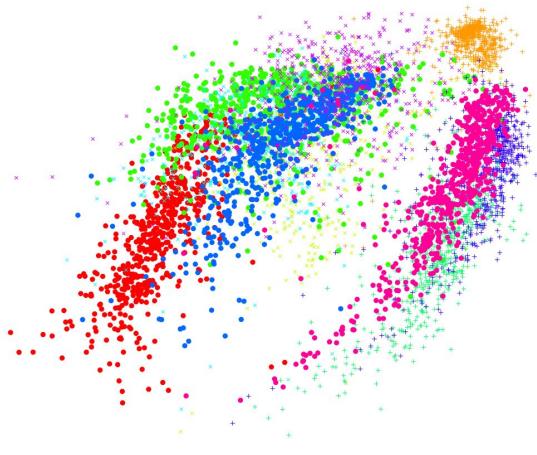
Comparison



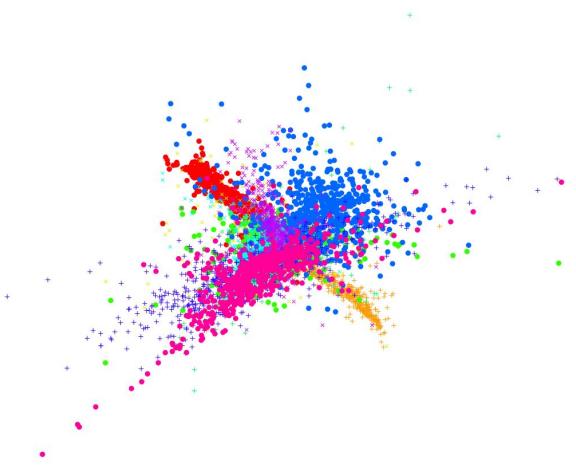
- 0
- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- 9



t-SNE



Isomap



LLE

Real life example

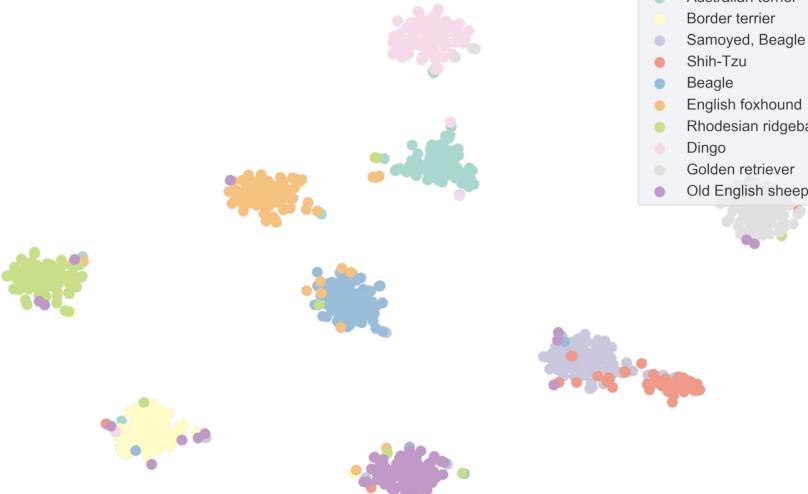


MDS (PCA) on faces
embeddings



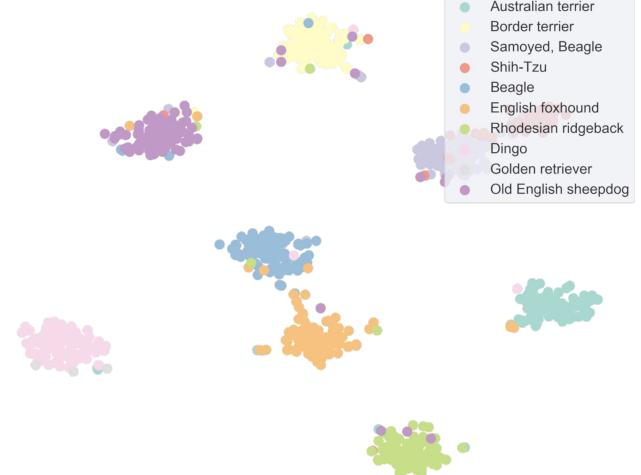
[image source](#)

Real life example



t-SNE on ArcFace

t-SNE on CosFace



Clustering

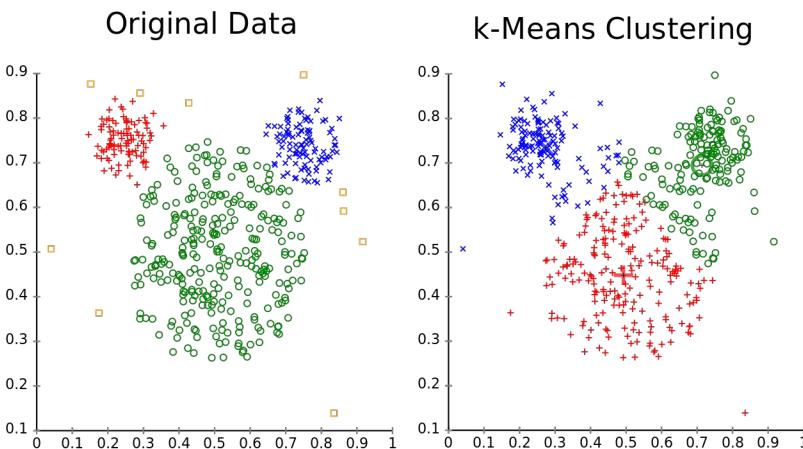
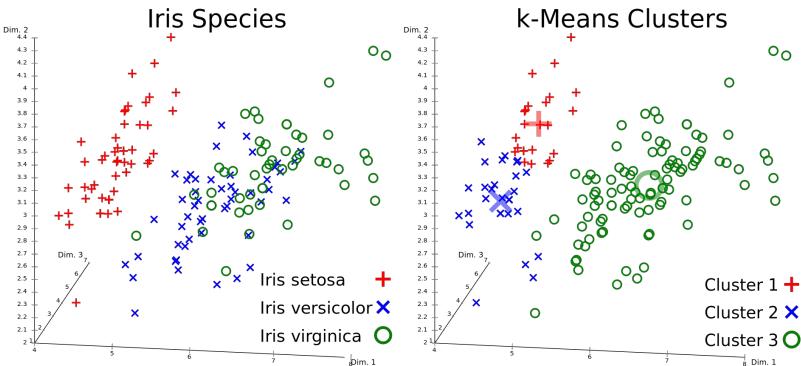
girafe
ai

03

Поставить задачу!



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

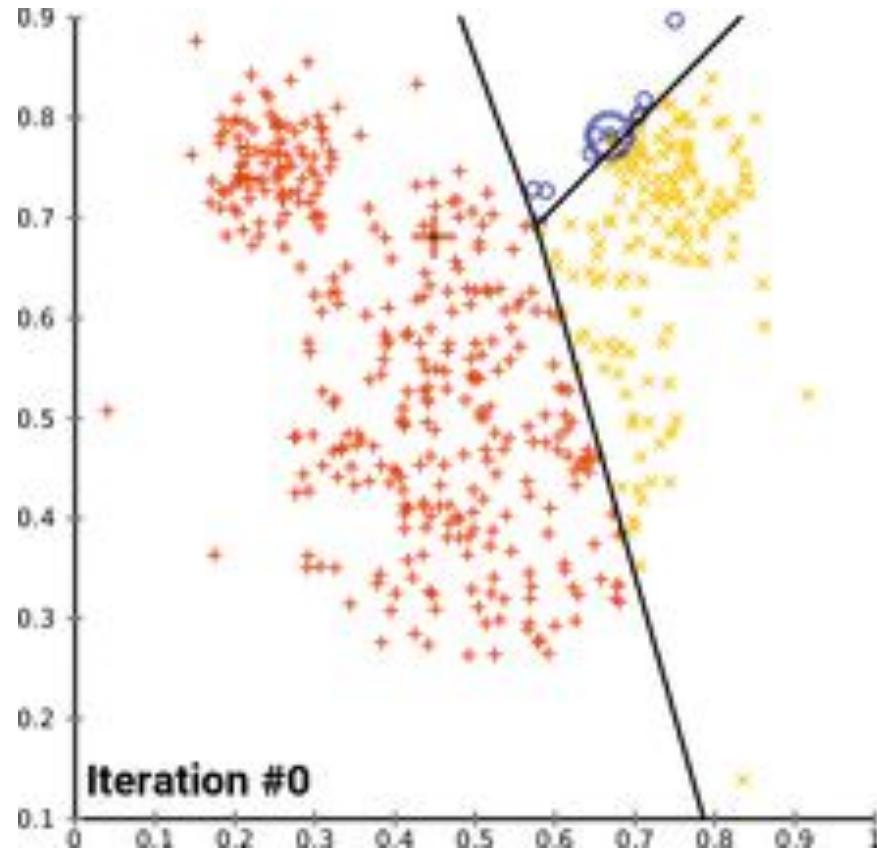


Params:

k - number of clusters

Advanced version: k-means++

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



DBSCAN

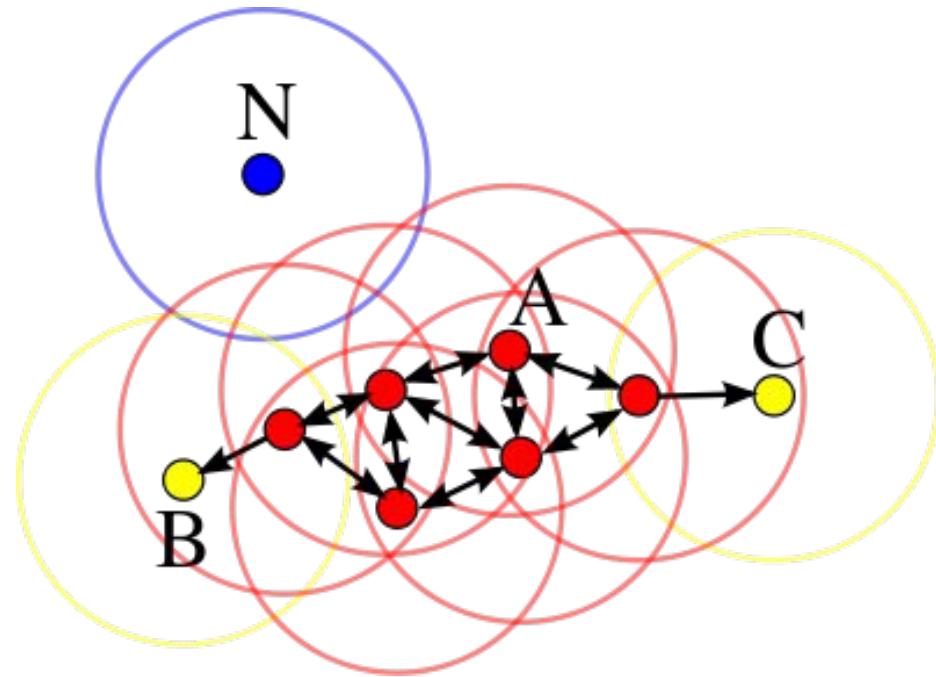


Density-Based Spatial Clustering of Applications with Noise

Split all data points into 3 groups:

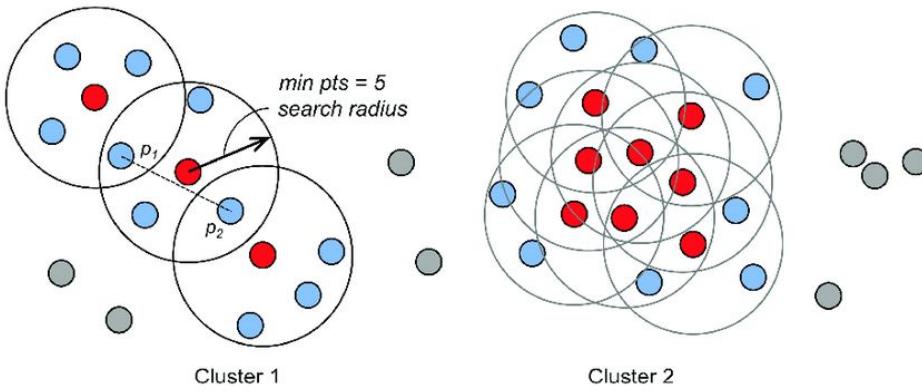
1. Core (red)
2. Border (yellow)
3. Noise (blue)

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)

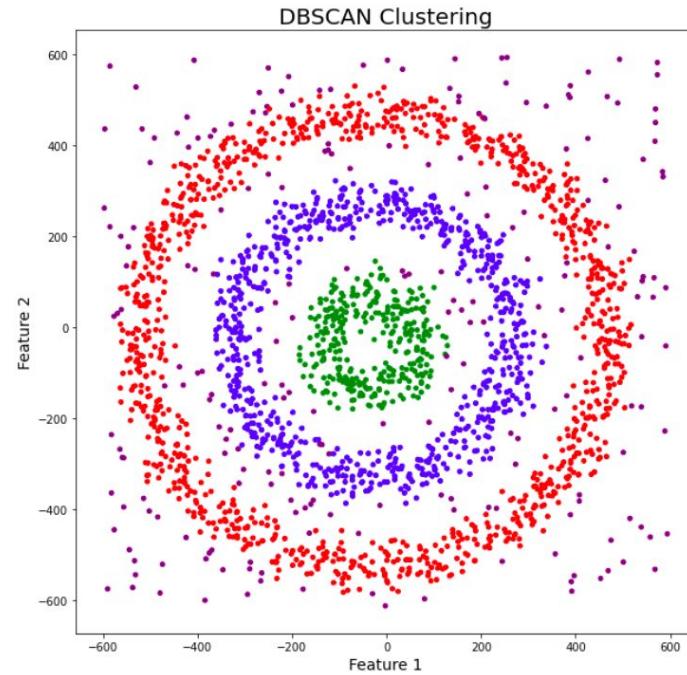
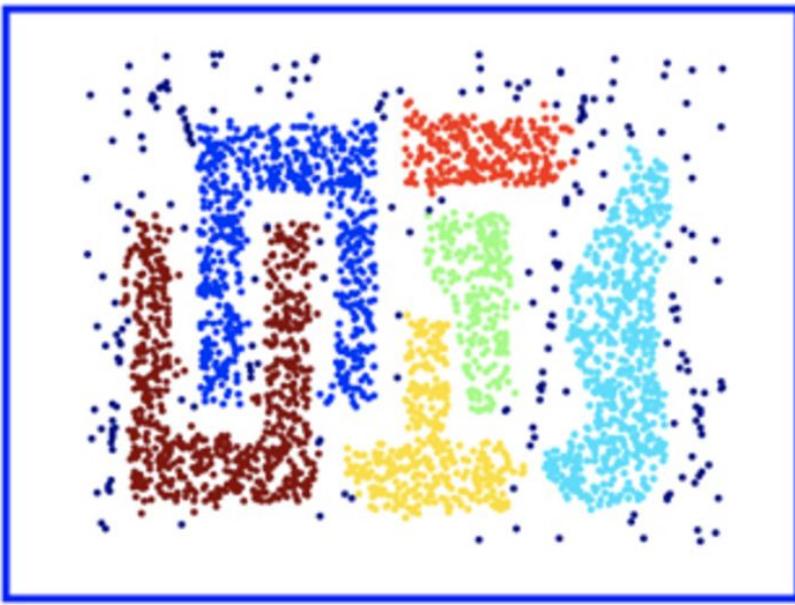
Cluster is defined as maximum connected set of points

Params:

ϵ - radius of neighbourhood

k - minimal number of neighbours of core point

DBSCAN examples

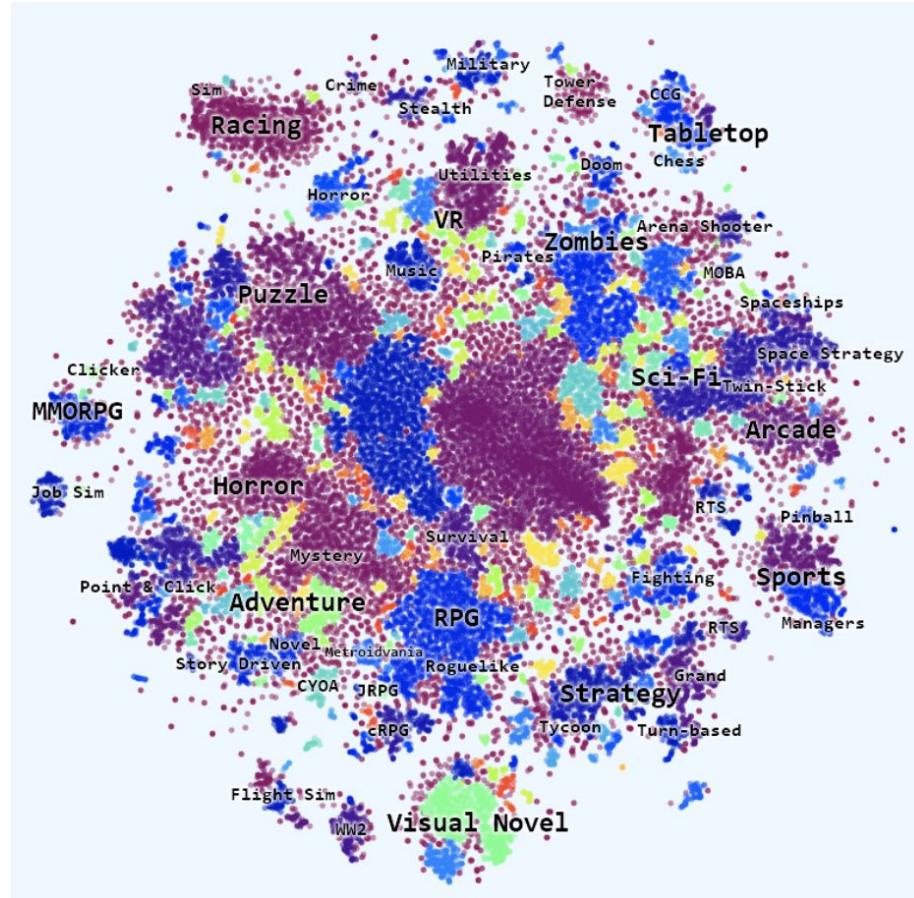


DBSCAN examples

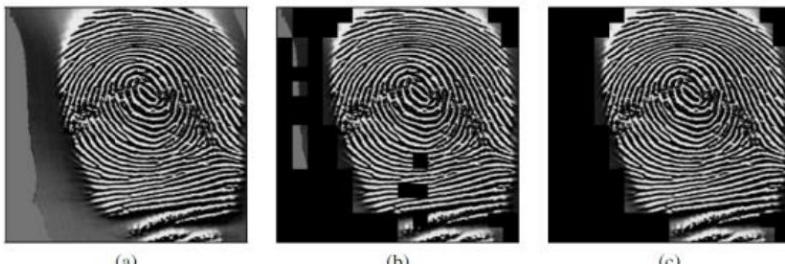
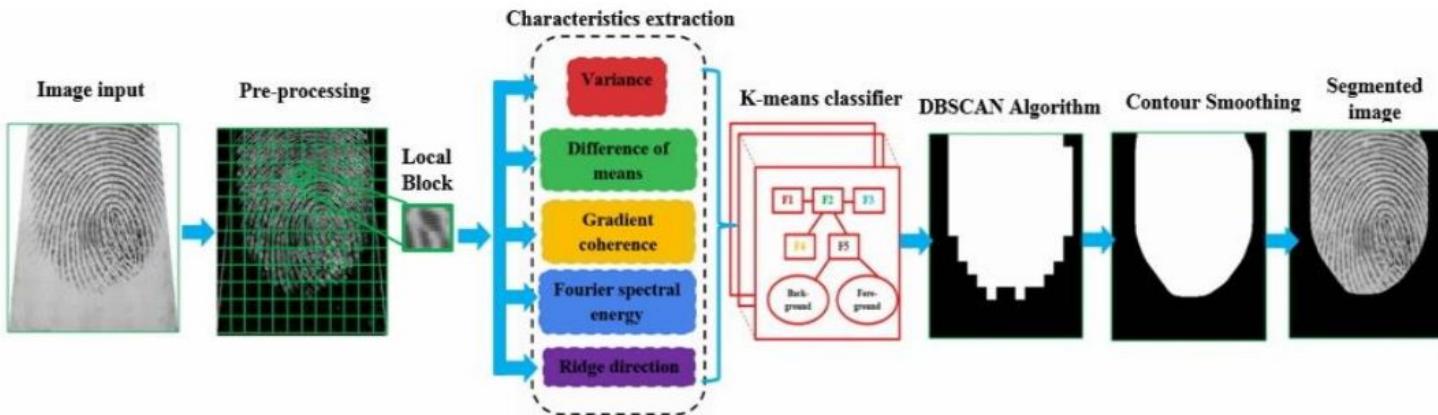


DBSCAN on t-SNE output
to analyze embeddings (Doc2vec)
of video games

[image source](#)



DBSCAN examples



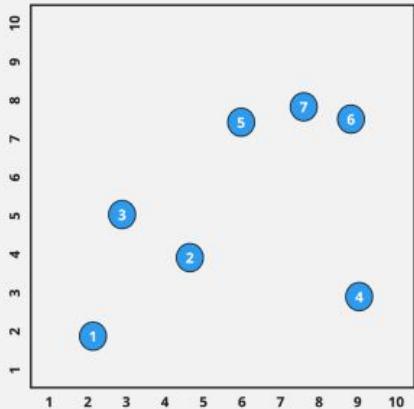
a - original, b - k-means, c - DBSCAN

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

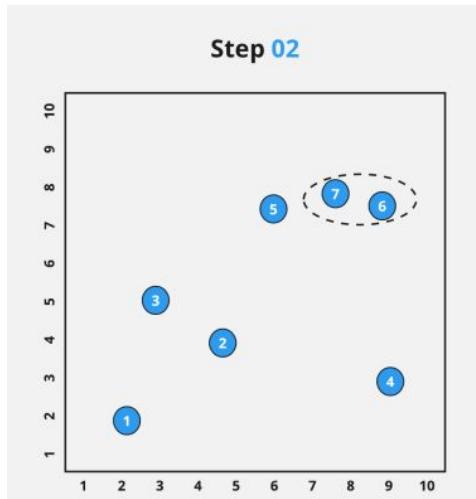
Hierarchical clustering



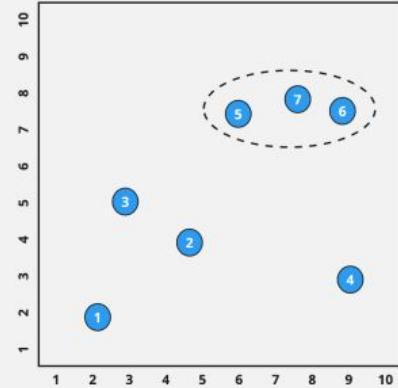
Step 01



Step 02



Step 03

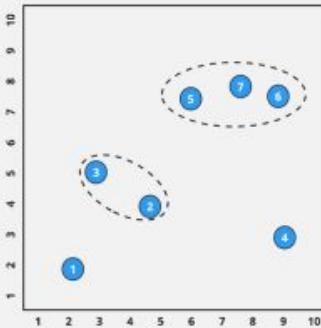


[image source](#)

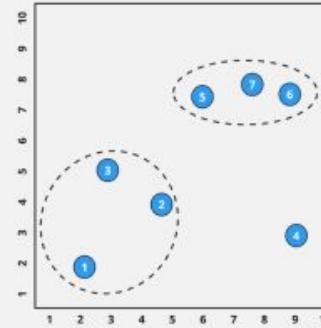
Hierarchical clustering



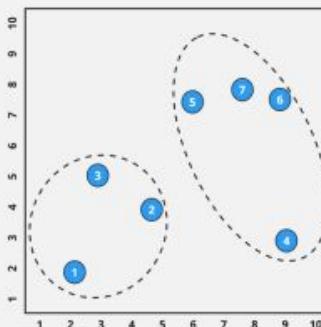
Step 04



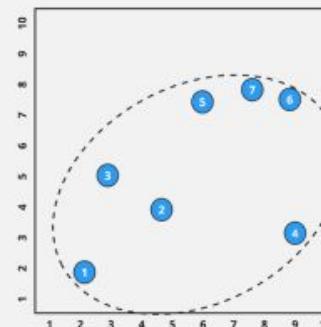
Step 05



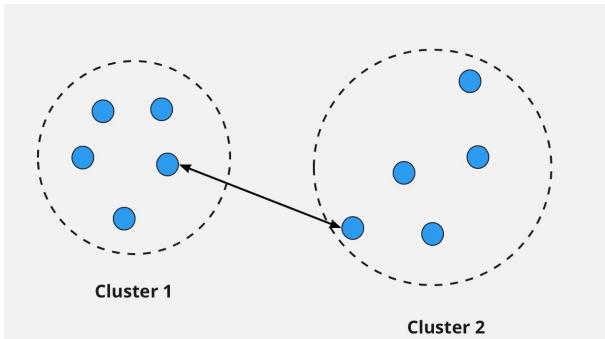
Step 06



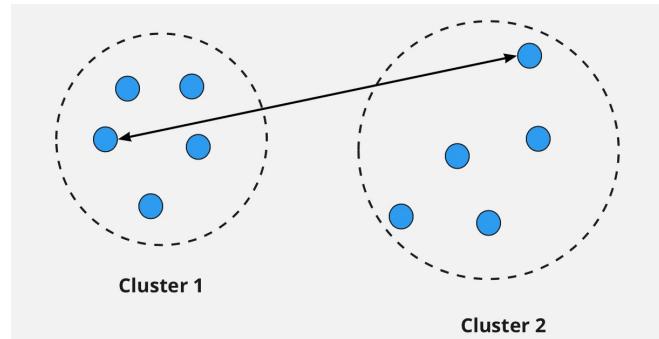
Step 07



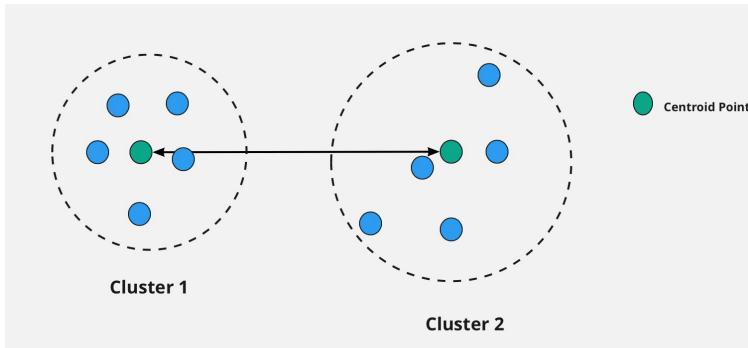
Distance between clusters



Closest point

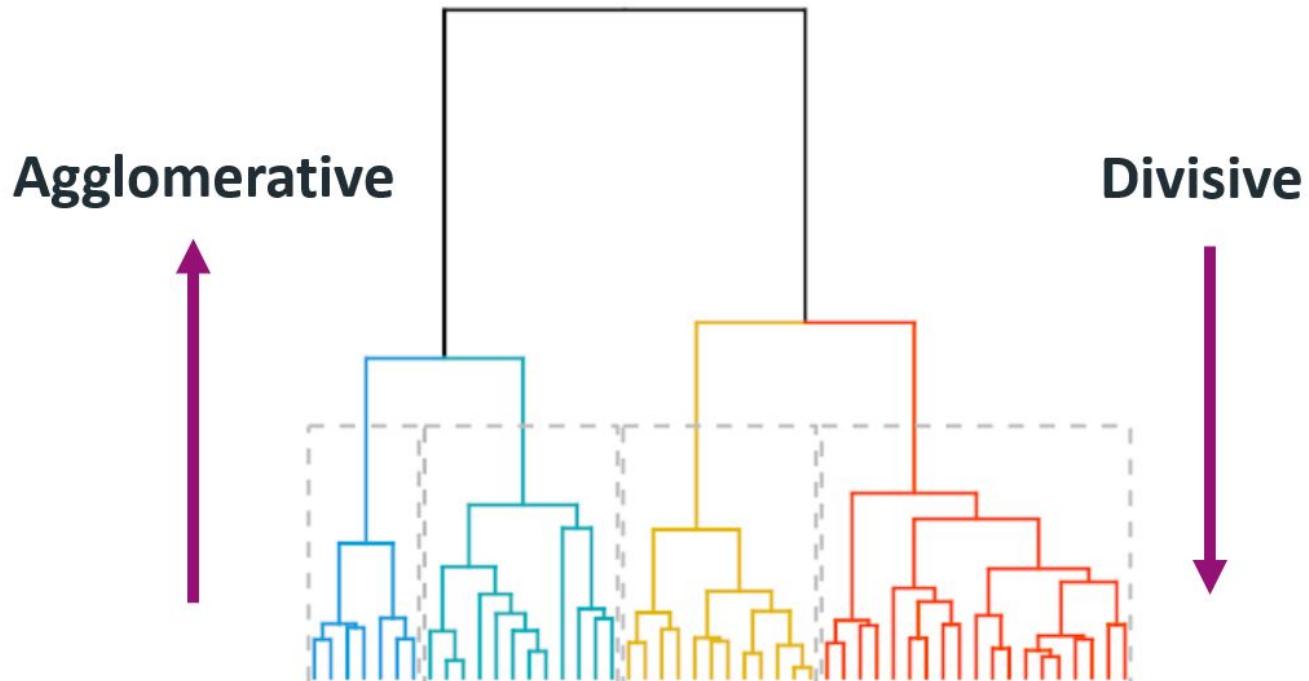


Farthest point

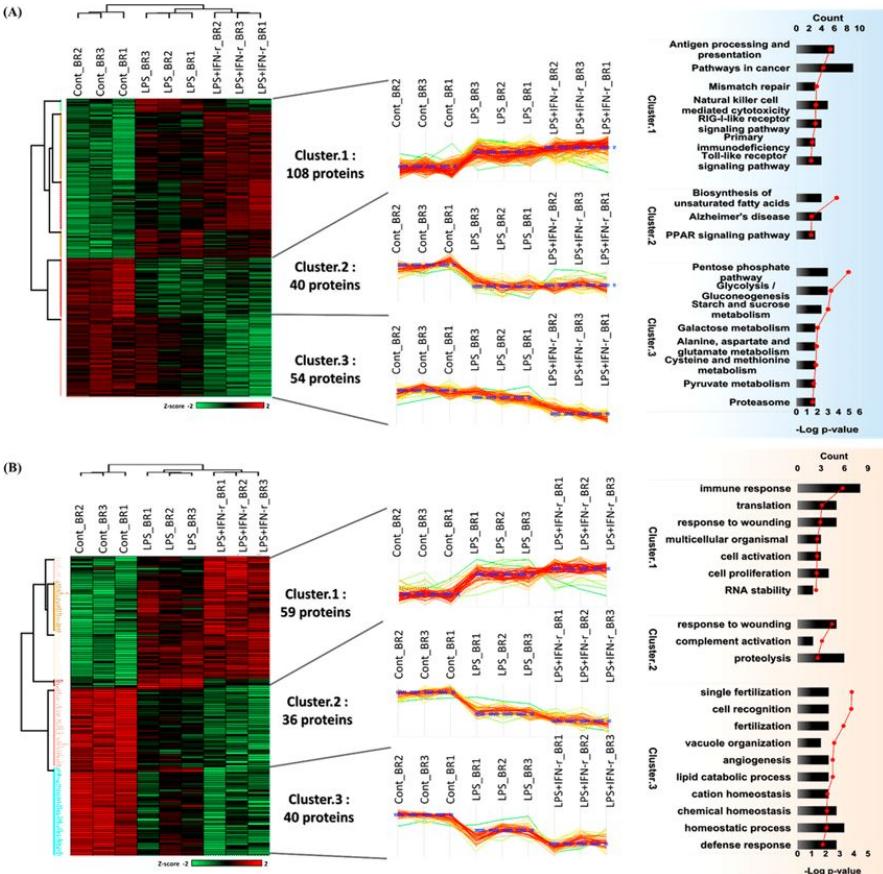


Centroid

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

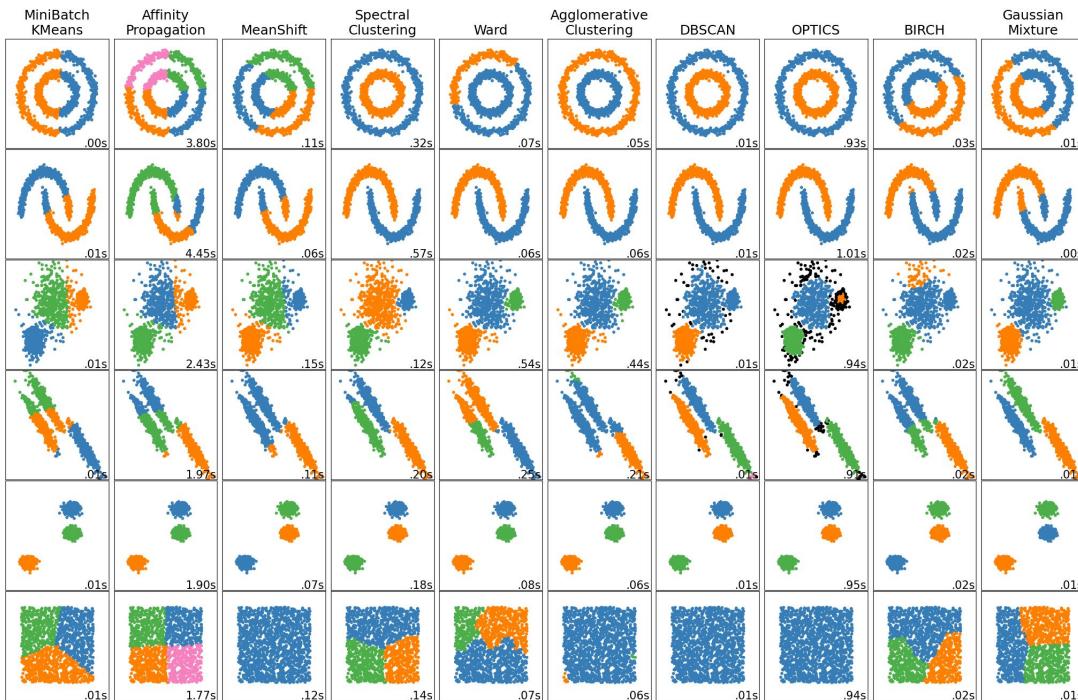
TODO



- spectral clustering
- business cases
 - see Viktor Kantor blog
 - call center - перенаправить пользователей в приложение (для этого сначала выделить группы, с которыми работать)
 - найти по кукам определённую группу пользователей (молодые мамочки и проч.)



Many more



Read more:

[sklearn huge overview](#)

[HDBSCAN \(hierarchy + DBSCAN\)](#)

[timeseries clusterization \(ru\)](#)

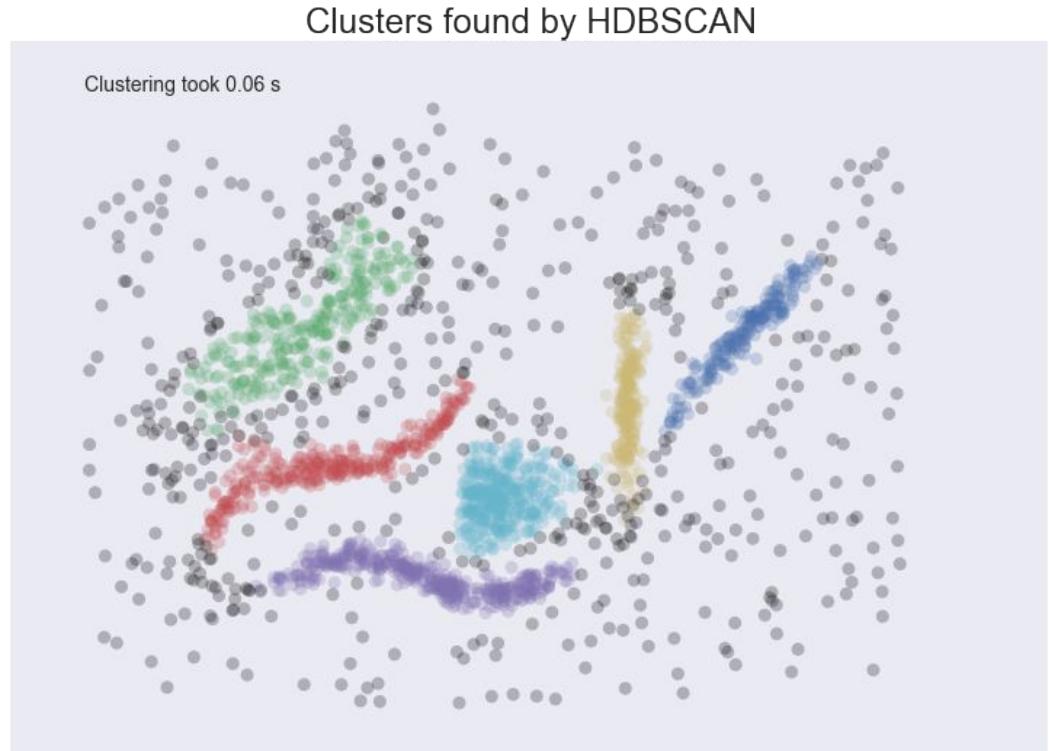
Clustering metrics



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

[Nice overview \[ru\]](#)

[Detailed explanations \(sklearn docs\)](#)

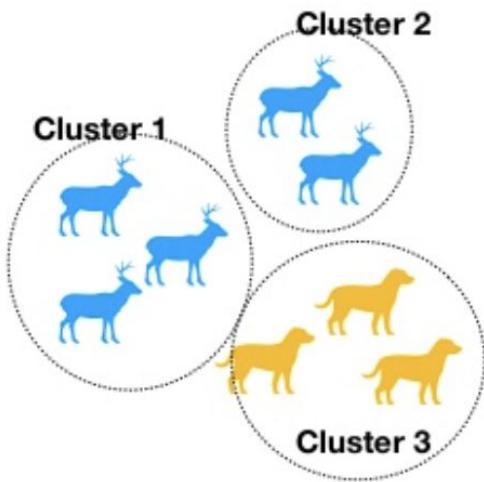


[image source](#)

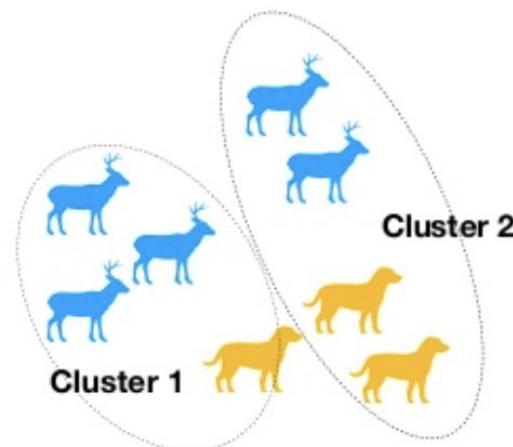


Homogeneity

Each cluster contains only members of a single class



Good



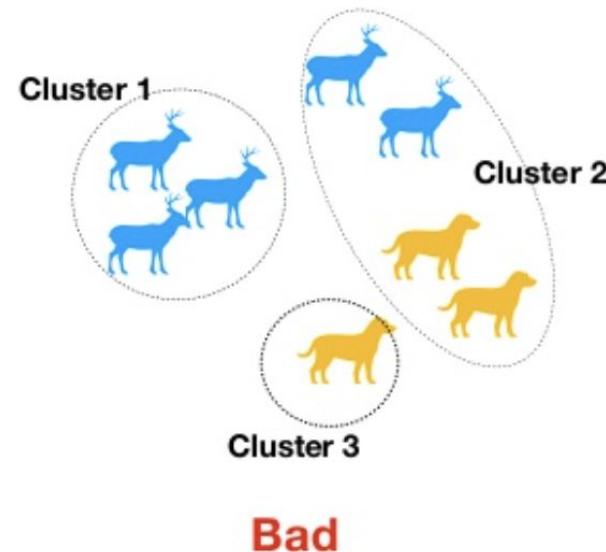
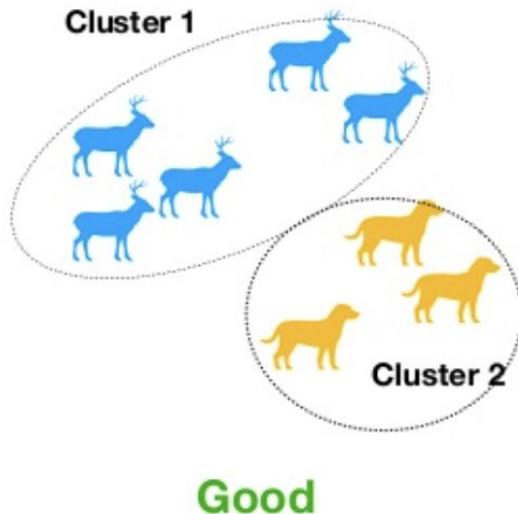
Bad

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

Completeness



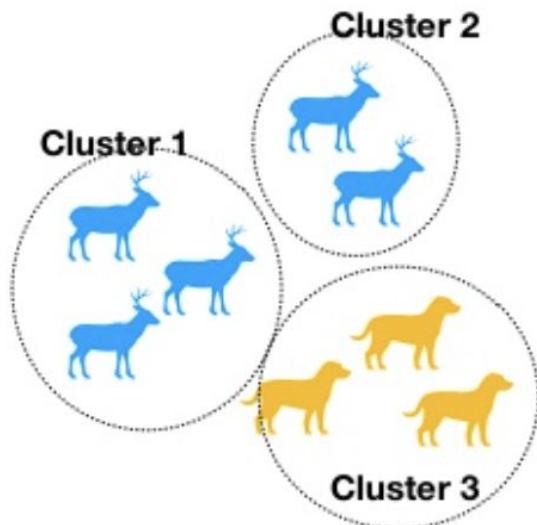
all members of a given class are assigned to the same cluster



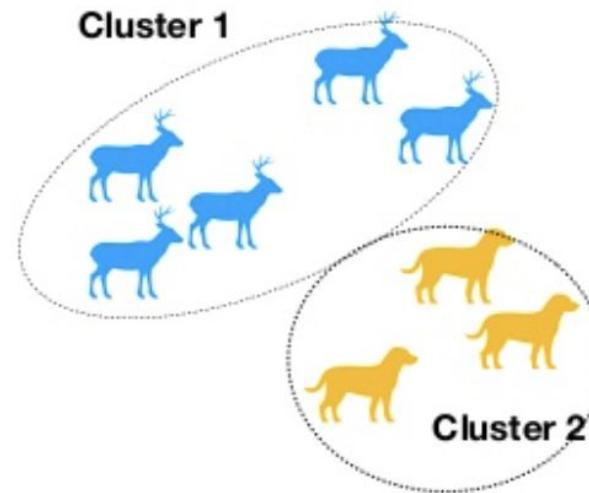
V-measure



geometric mean of Homogeneity and Completeness



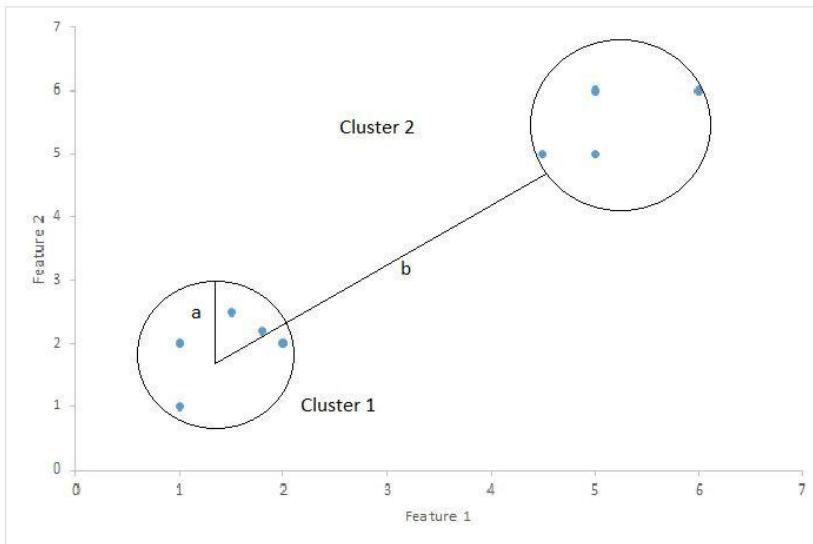
homogeneity score = 1



completeness score = 1



Silhouette coefficient



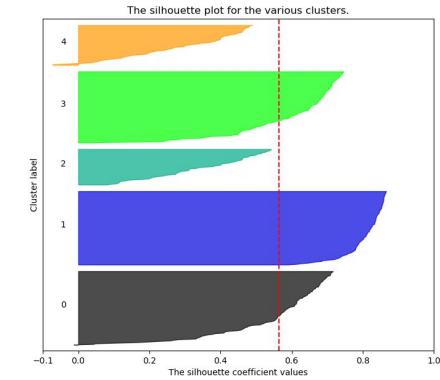
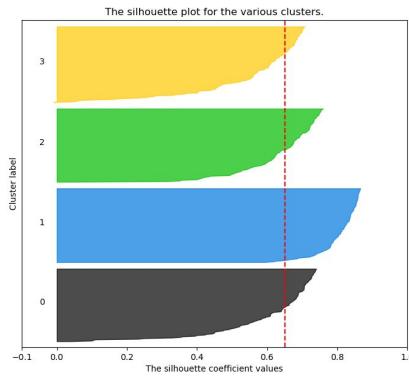
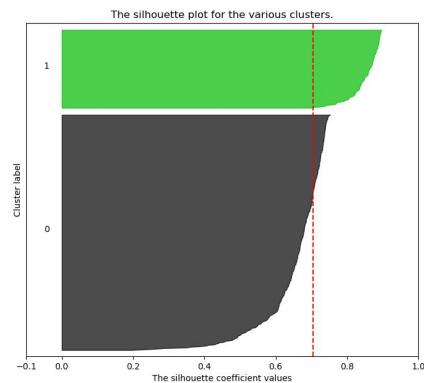
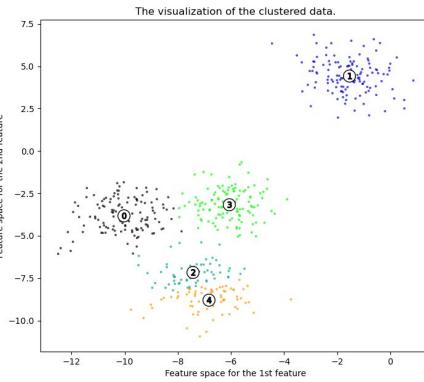
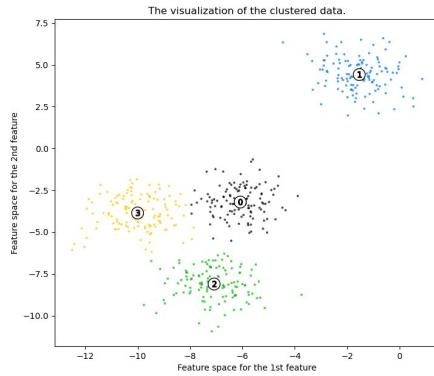
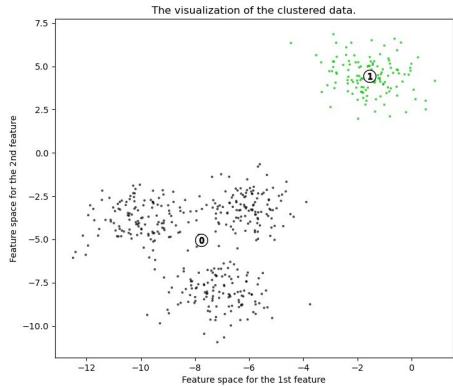
a: mean distance to points
in the *same* class

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

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

[image source](#)

Silhouette analysis



[image source](#)

Density estimation

girafe
ai

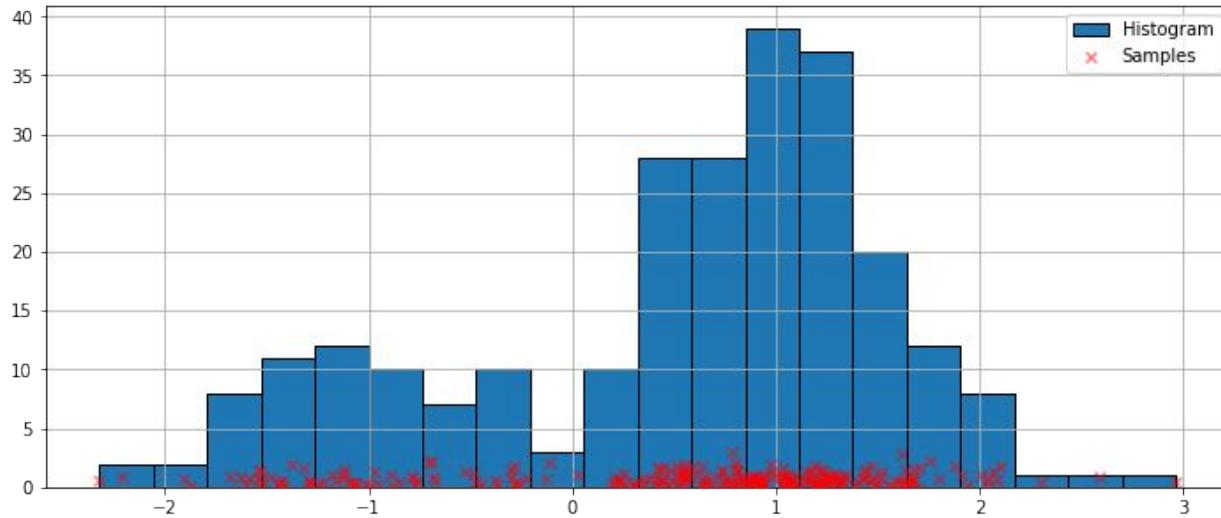
04

Поставить задачу!



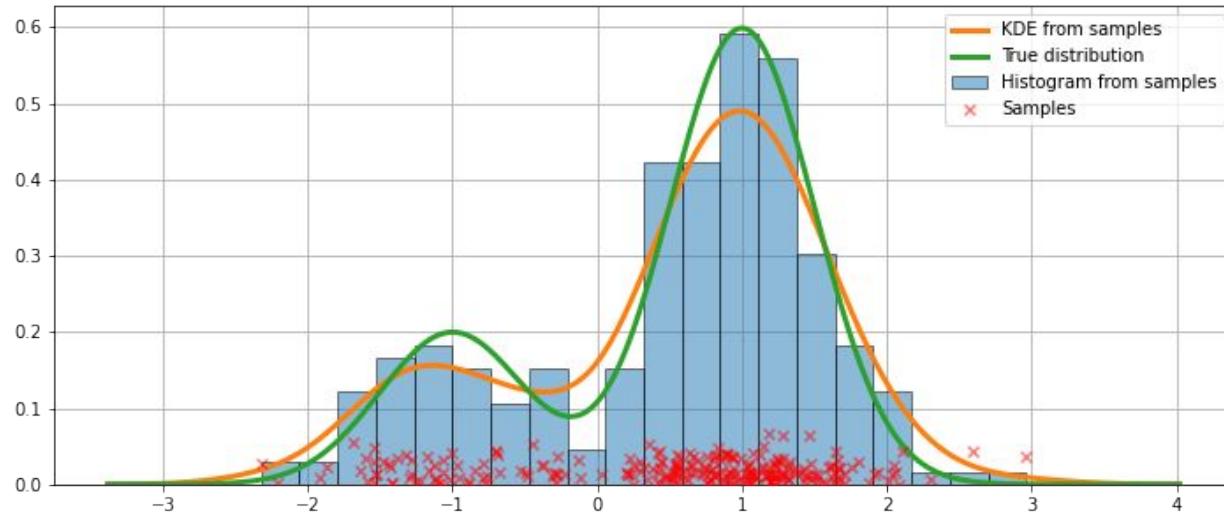


Kernel density estimation



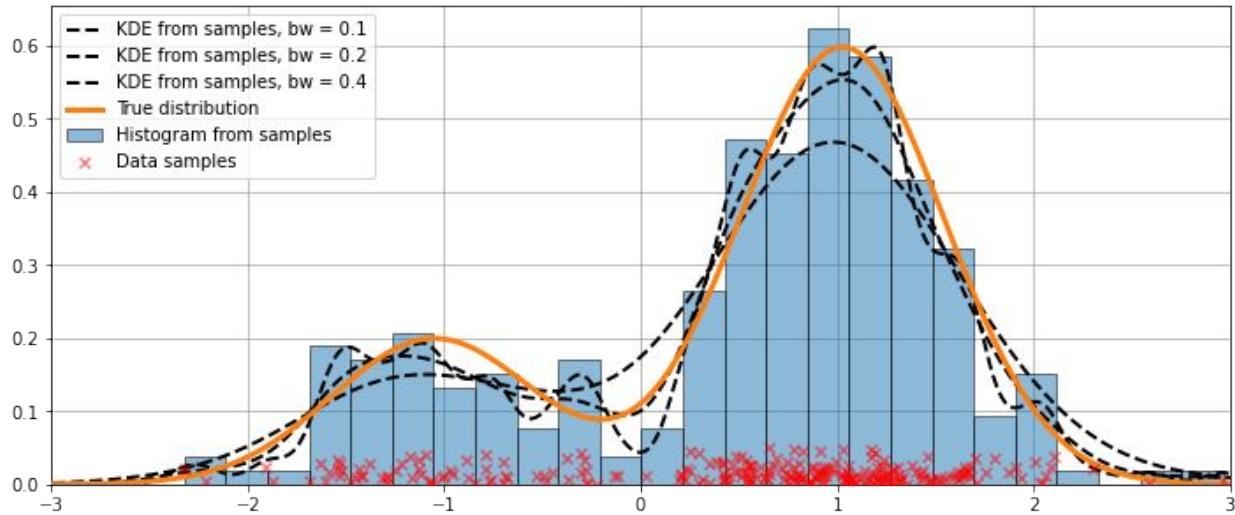
[statsmodels documentation example](#)

Kernel density estimation

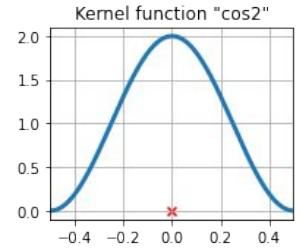
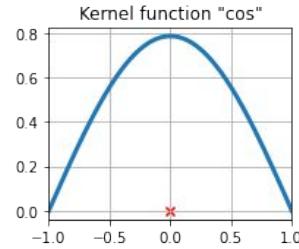
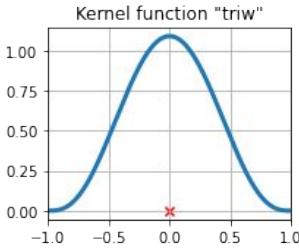
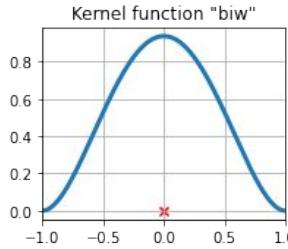
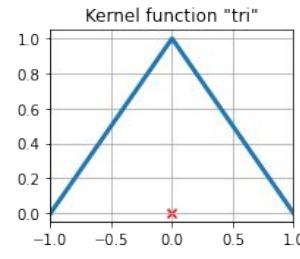
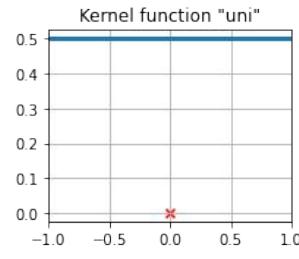
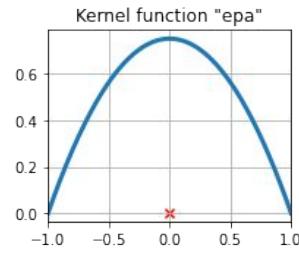
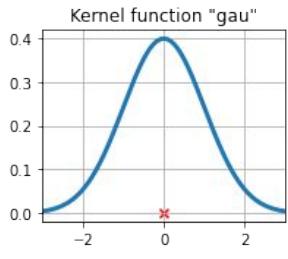




Window size



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)