Statistical Problems of Manifold Learning in Predictive Modeling

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ADASE group

- 30 researchers
- DL for
  - 3D Computer Vision
  - Predictive Analytics

~ 100 **papers** in major venues, incl. NIPS, ICML, CVPR, etc.

Moscow government prize for Scientific Achievements, 2018

Ilya Segalovich prize for Scientific Achievements, 2020

with the **President of Russian Academy of Science**
State Kremlin palace, 2018

Industrial Expertise: since 2007

AIRBUS, LOUIS VUITTON, AIRBUS HELICOPTERS, IPSEN Innovation for patient care, ALTRAN, SAHARA Force India, PORSCHE, SBERBANK, HUAWEI, Alibaba Group 阿里巴巴集团, BOSCH

and many others...

Overview

- Intro
- Dimension Reduction Problem Statements
- PCA, MDS and Sammon Mapping, Autoencoders
- ISOMAP and LLE
- TDA for Time Series Analysis
- References

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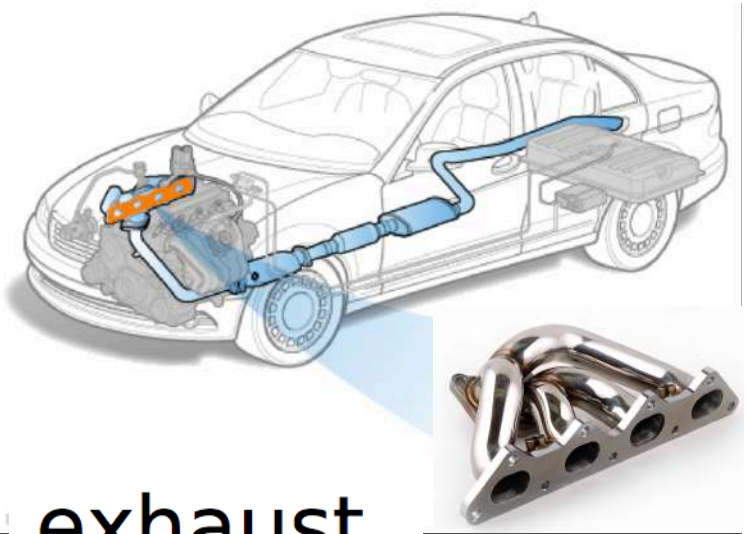
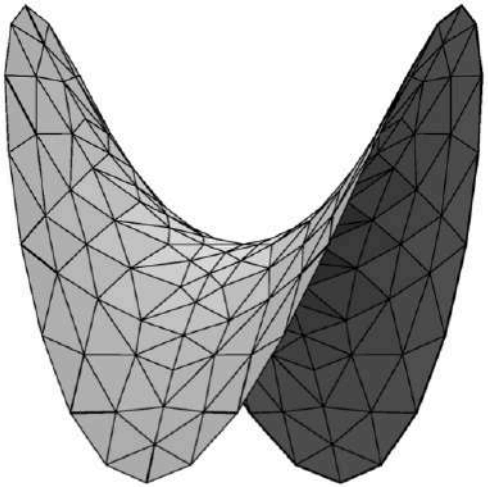
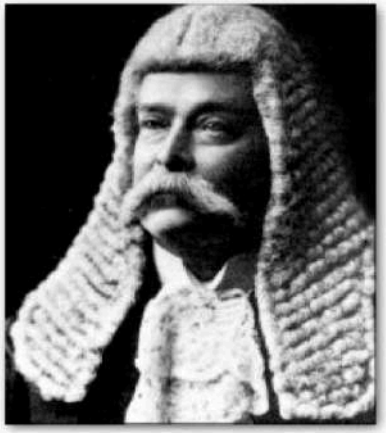
Types of manifold



- exhaust manifold

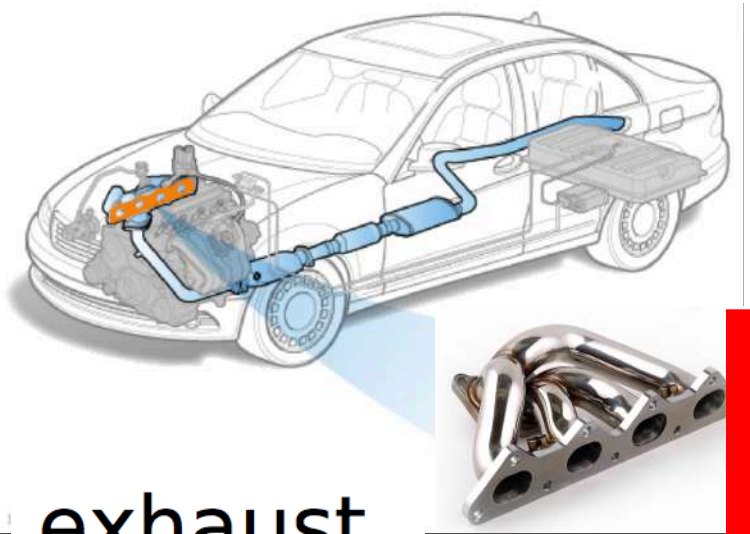


low-D surface embedded in high-D space



Sir Walter Synnot Manifold 1849-1928

Types of manifold



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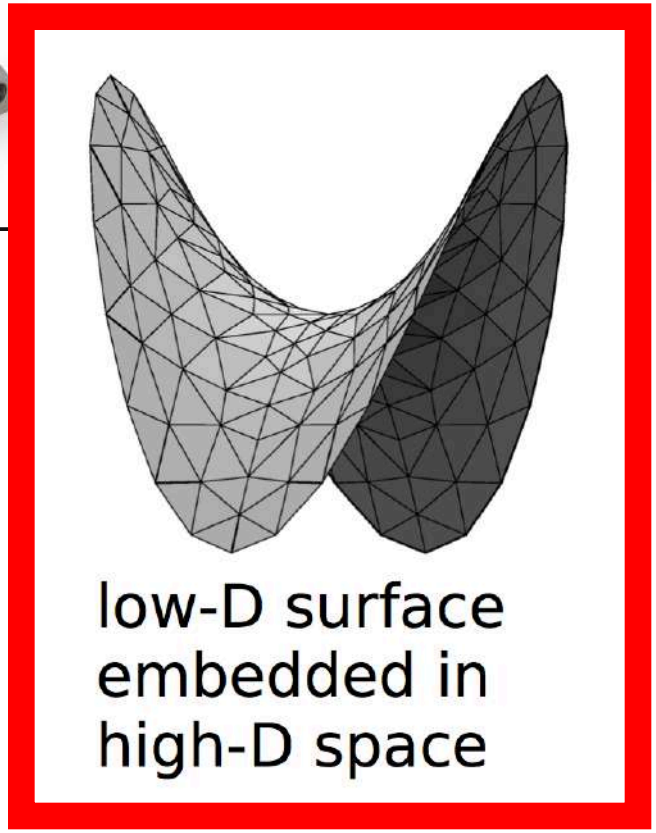
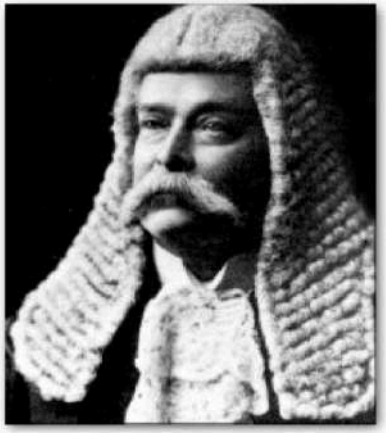




Sir Walter
Synnot Manifold
1849-1928

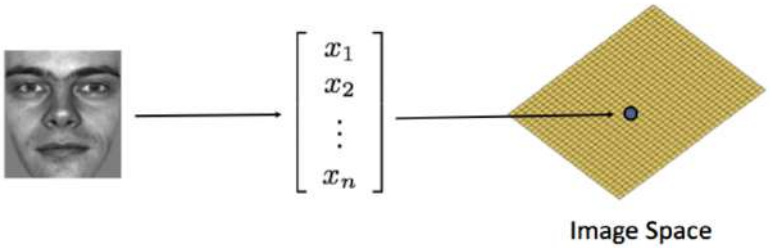
Manifold Learning

Manifold learning – Data Analysis technology based on **geometrical model** about high-dimensional data [1]

A. **The world is multidimensional**
B. **Multidimensional data are difficult to use**
C. **Real-world data have low-dimensional structure**
D. **The world is not flat (nonlinear)**

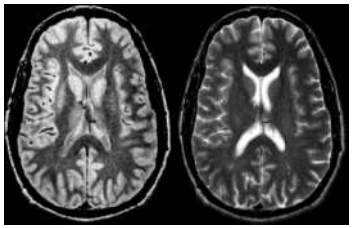
A. The world is multidimensional

Real-world data



1024×1024: $d \approx 10^6$

64×256: d = 16 384



fMRI: $d \approx 1.4 \times 10^6$/sec

B. Multidimensional data is difficult to analyze

1) **Regression:** (Ibragimov, Khasminskii (1979); Stone (1982); etc.)

If $\mathbf{F} = \{\psi : [0,1]^d \to \mathbb{R}^1,\ \psi \text{ is Lipschitz}\}$

then for any estimator $\hat{\psi}$ of any kind from n known measurements $\{(x_i, \psi(x_i))\}$:

$$\sup_{\psi \in \mathbf{F}} \mathbb{E}\left(\psi(x) - \hat{\psi}(x)\right)^2 \geq \text{Const} \times n^{-2/(2+d)}$$

The lower bound is nonasymptotic!

2) MSE in case of KDE ~ $O(n^{-4/(d+4)})$

Multidimensional data are difficult to analyze (cont.)

Data Analysis works for real multidimensional data – when and why?

Which properties of real-world data help? How?

- concentration of measures
- sparse representation
- latent structure models
- low-dimensional structure of data support

Multidimensional data are difficult to analyze (cont.)

Data Analysis works for real multidimensional data – when and why?

Which properties of real-world data help? How?

- concentration of measures
- sparse representation
- **latent structure models**
- **low-dimensional structure of data support**

C. Low-dimensional structure of real-world data

- Data from '**natural**' sources occupy usually a **small part** $\mathbf{X}$ in the 'observation space' $\mathbb{R}^d$
- $\mathbf{X}$ has **small 'intrinsic dimension'** $s < d$
- Data can be described by a small number s of parameters (features)

$d \approx 10^6$

$s = 84$

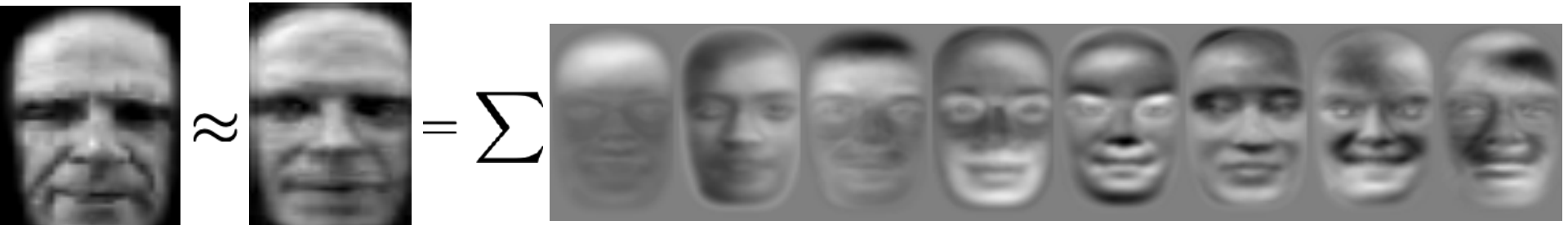
$s = 40$

Low-dimensional structure of real-world data

- **to find a low-dimensional structure of Data space**
  - ✓ to estimate an Intrinsic dimension s of $\mathbf{X} \subset \mathbb{R}^d$
  - ✓ to construct a s-dimensional features $z = h(x)$ describing $x \in \mathbf{X}$
- **to use extracted low-dimensional structure** to solve **specific Data analysis tasks**

Principal Component Analysis

Face-vector $x \in \mathbb{R}^{2061}$



$\approx \quad = \sum$

$(z_1 \times \mathbf{e}_1)+(z_2 \times \mathbf{e}_2)+(z_3 \times \mathbf{e}_3)+(z_4 \times \mathbf{e}_4)+(z_5 \times \mathbf{e}_5)+(z_6 \times \mathbf{e}_6)+(z_7 \times \mathbf{e}_7)+(z_8 \times \mathbf{e}_8)$

x_{PCA}= projection on L_{PCA} defined by features $z = (z_1, z_2, \ldots, z_s)$

$$x(face) \leftrightarrow z = (z_1, z_2, \ldots, z_s) \in \mathbf{R}^s$$

$$L_{PCA,s}(faces) = \{mean\ face + \sum_{i=1}^{s} EigenFace_i \times z_i\}$$

Principal Component Analysis (cont.)

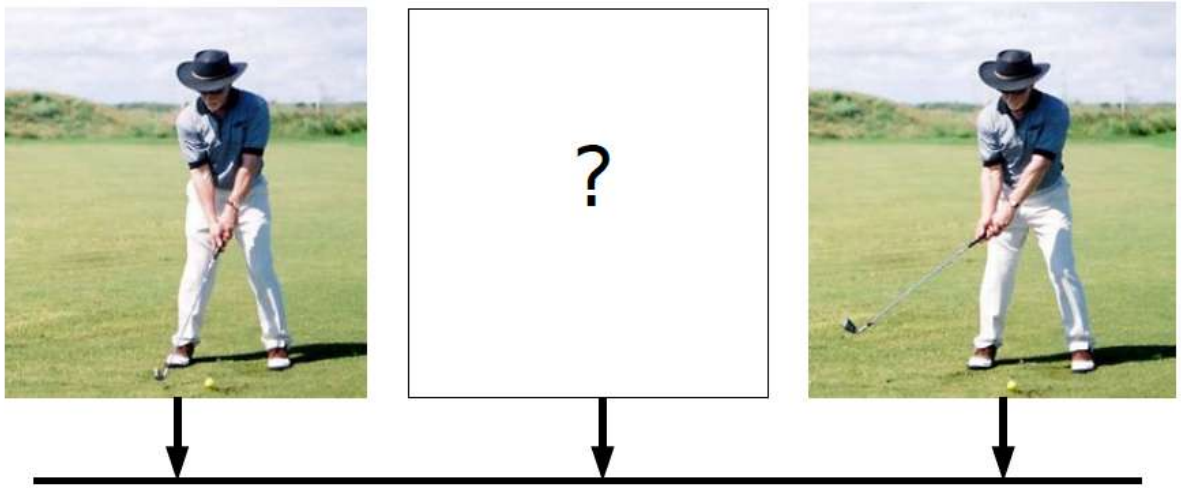
Original face described by 10^6-dimensional vector

Left to right: the same face described by ***s*** reduced features

s = 84 ***s*** = 40 ***s*** = 20 ***s*** = 3 ***s*** = 2 ***s*** = 1

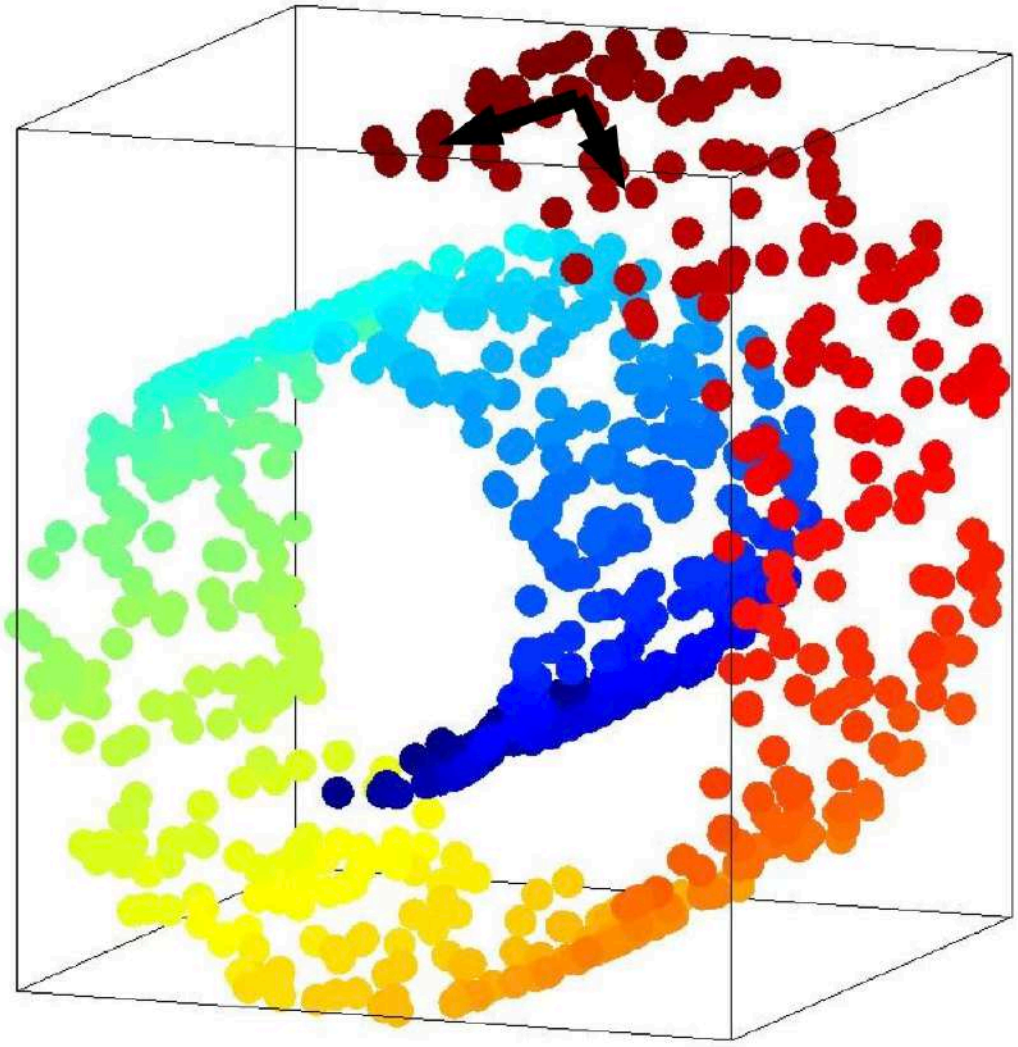
D. The world is not flat

Video stream



Frame rate conversion based on inter-frame interpolation

What is “Reasonable distance metrics”?



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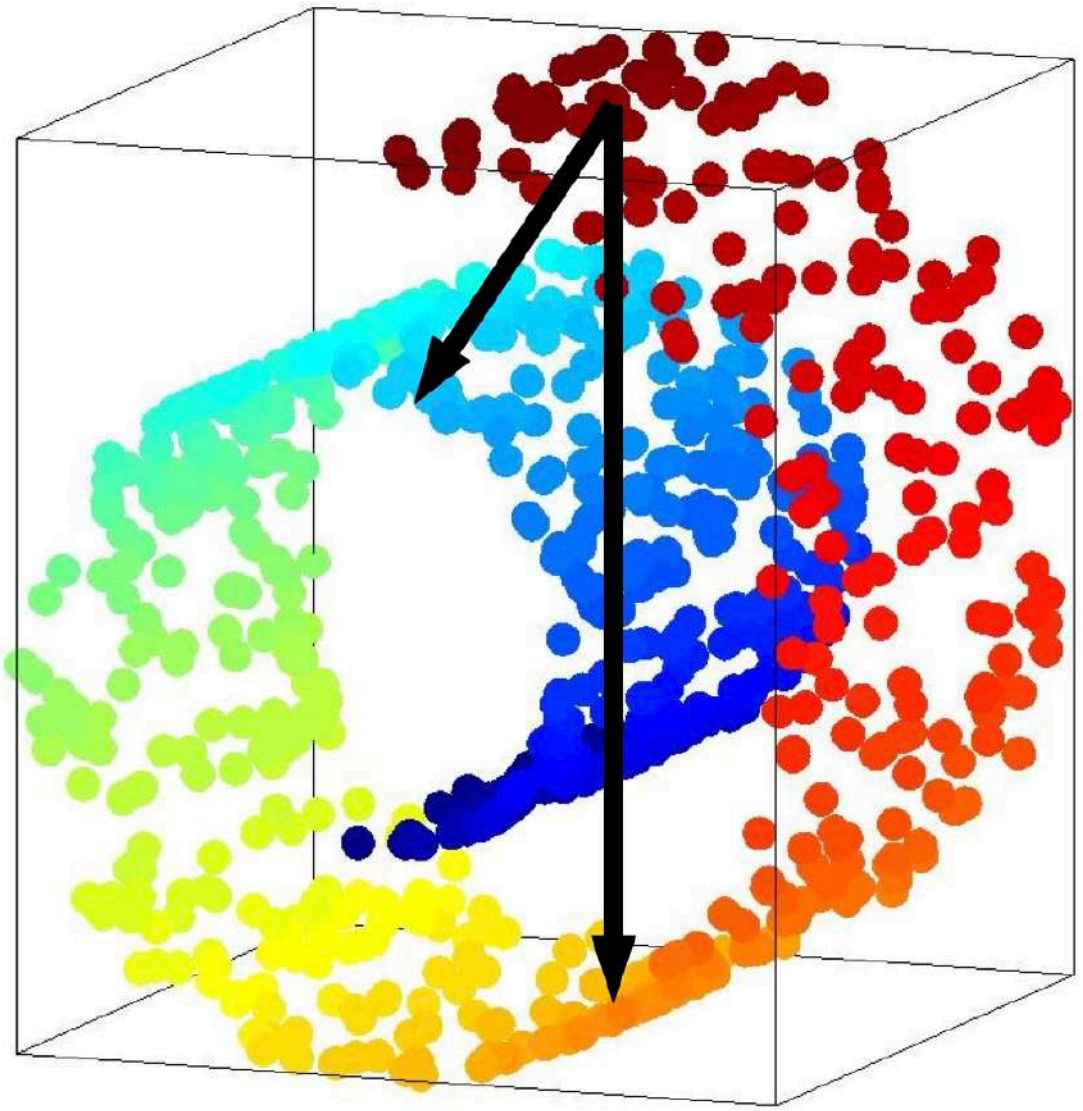
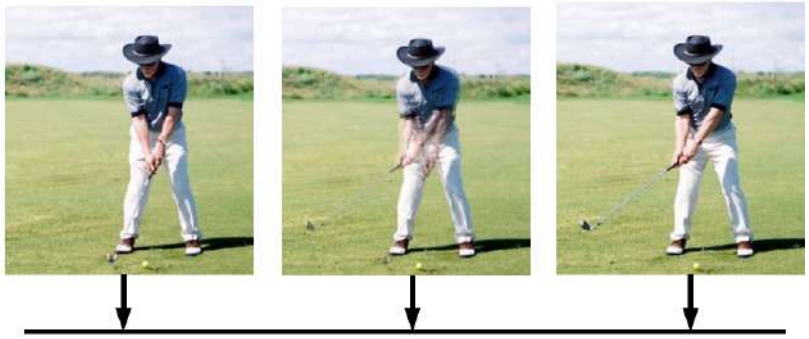


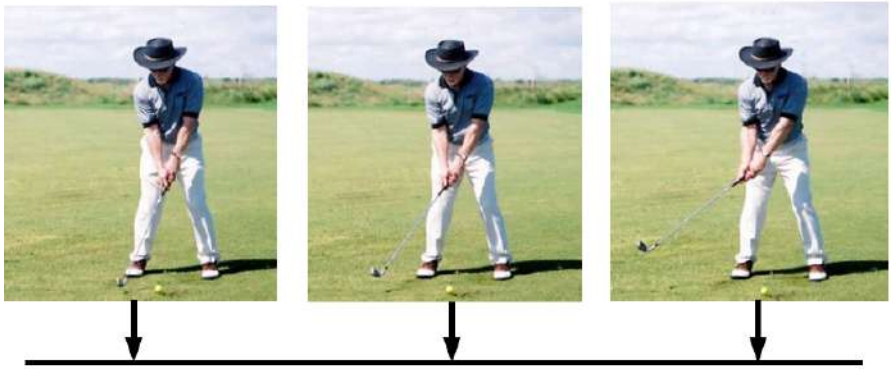
The world is not flat (cont)

‘Linear’ inter-frame interpolation

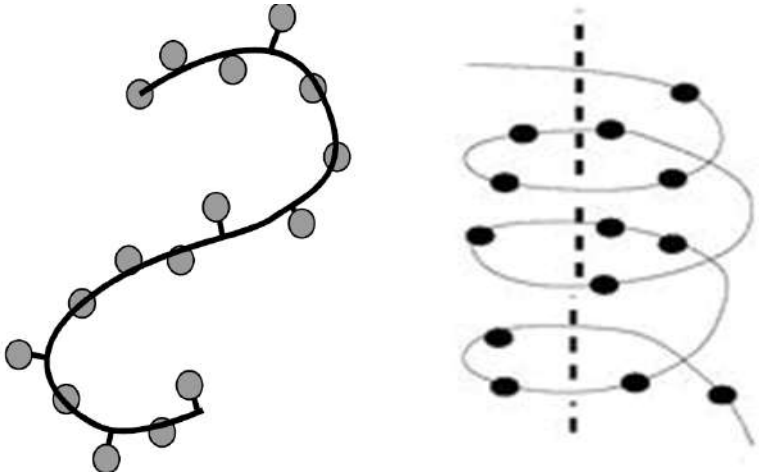


The world is not flat (cont.)

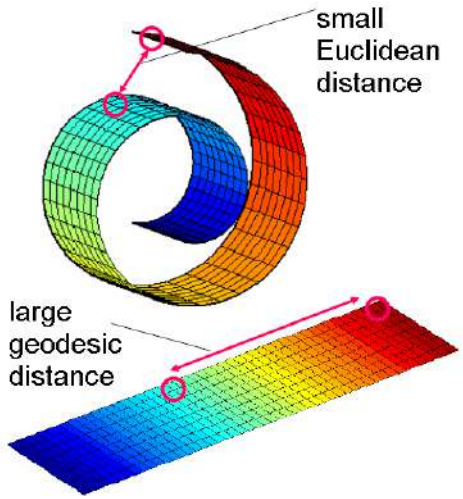
‘Nonlinear’ inter-frame interpolation



Data analysis for nonlinear data



- **Linear methods like PCA do not work**



- **Math: Multivariate Statistical analysis consider mainly ‘linear methods’**

Manifold learning

- **Electricity price curve modeling** and forecasting by **manifold learning** (2008)
- On the **manifold structure** of the space of **brain images** (2009)
- **Manifold Modeling** for **Brain Population Analysis** (2010)
- Simultaneous Learning of **Nonlinear Manifold** and **Dynamical Models** for **High-dimensional Time Series** (2007)
- A kernel entropy **manifold learning** approach for **financial data analysis** (2014)
- **Manifold learning** algorithms for localization in **wireless sensor networks** (2004)
- **Manifold Learning** for **Object Tracking with Multiple Motion Dynamics** (2010),
- **Manifold Learning** and Representations for **Image Analysis and Visualization** (2006)
- **Learning an Image Manifold** for **Retrieval** (2004)
- **Manifold Learning** for **medical image registration segmentation and classification** (2012),
- The **Manifold Tangent Classifier** (2011),
- **Inferring 3D body pose** from silhouettes using activity **manifold learning** (2004)
- Nonlinear **manifold learning** for **visual speech recognition** (2005)
- **Separating style and content** on a **nonlinear manifold** (2004)
- **Learning Nonlinear Manifolds** from **Time Series** (2006)
- A New **Manifold Learning** Technique for **Face Recognition** (2012)
- Regional **Manifold Learning** for **Deformable Registration of Brain MR Images** (2012)
- Regional **Manifold Learning** for **Disease Classification** (2014)
- Overview of **Manifold Learning** and Its **Application in Medical Data set** (2014)
- **Sparse pose manifolds** (2014)

Manifold model: mobile robot navigation [2]

64×256 pixels: d = 16384

Robot localization θ = **(2D Coordinates, Orientation)** $\in \mathbb{R}^3$

$x = \varphi(\theta) \in \mathbb{R}^d$ - captured image at Robot localization θ

Appearance space $\mathbf{M} = \{x = \varphi(\theta),\, \theta \in \Theta\}$
consisting of images which may be captured

under **all possible localizations** $\theta \in \Theta \subset \mathbb{R}^3$ is 3D-surface (**Appearance manifold**) in $\mathbb{R}^d$

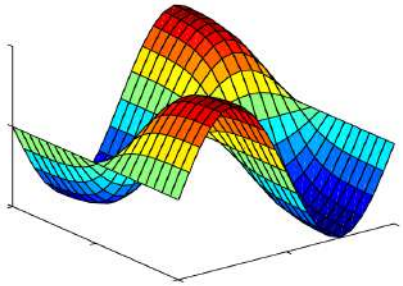
Manifold covered by single chart (surface in $\mathbb{R}^d$)

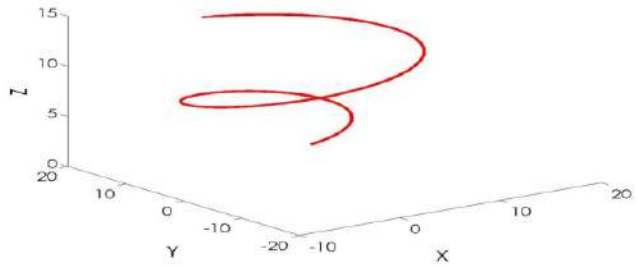
$$\mathbf{M} = \{x = g(z) \in \mathbb{R}^d : \; z \in \mathbf{Z} \subset \mathbb{R}^s\}$$

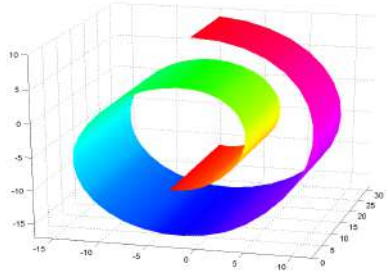
well-behaved **unknown** s -dimensional surface - **Data manifold**

covered by **single chart** g defined on **Coordinate space** $\mathbf{Z} \subset \mathbb{R}^s$

and embedded in ambient d-dimensional space, $s < d$

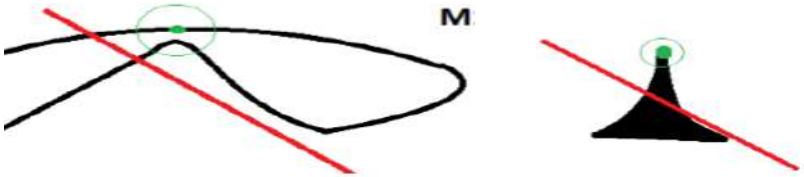






$h = g^{-1} : \mathbf{M} \to \mathbf{B}$ - inverse mapping – a parameterization

$z = h(x)$ on the Data manifold



Statistical analysis of manifold valued data

Let μ be some **unknown** probability measure on **unknown** s-dimensional manifold $\mathbf{M} = \mathrm{supp}(\mu)$ with **unknown** value of s

Based on given sample of independent observations

$$\mathcal{D}_n = \{x_1, x_2, \ldots, x_n\} \subset \mathbf{M}$$

solve various statistical problems such as:

- to estimate intrinsic dimension s
- to estimate low-dimensional parameterization h on the manifold $\mathbf{M}$
- to estimate the manifold $\mathbf{M}$
- to estimate tangent space $L(x)$ to the manifold $\mathbf{M}$ at point x
- to estimate a density $f(x) = \frac{d\mu}{dm}$, etc.

Manifold Learning in Data analysis

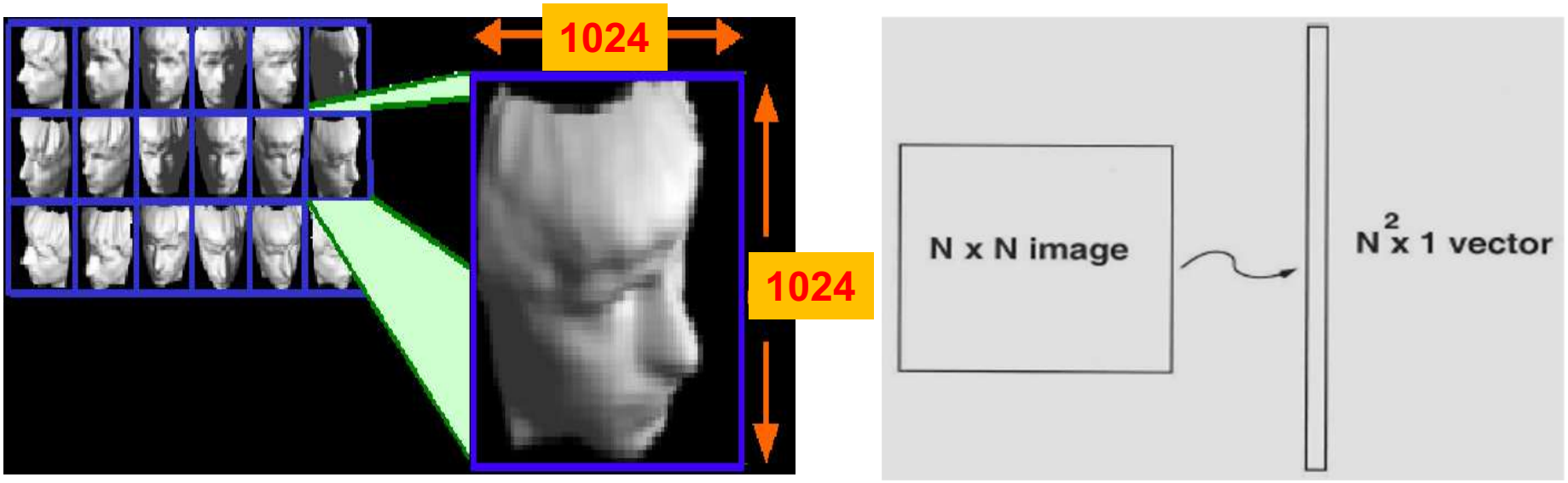
Data Analysis under Manifold Assumption

- Parameterization of the Data manifold
- Estimation of the Data manifold
- Denoising/Super-resolution/Impainting
- Classification
- Regression
- Anomaly Detection
- Other applications

Dimensionality Reduction Problem

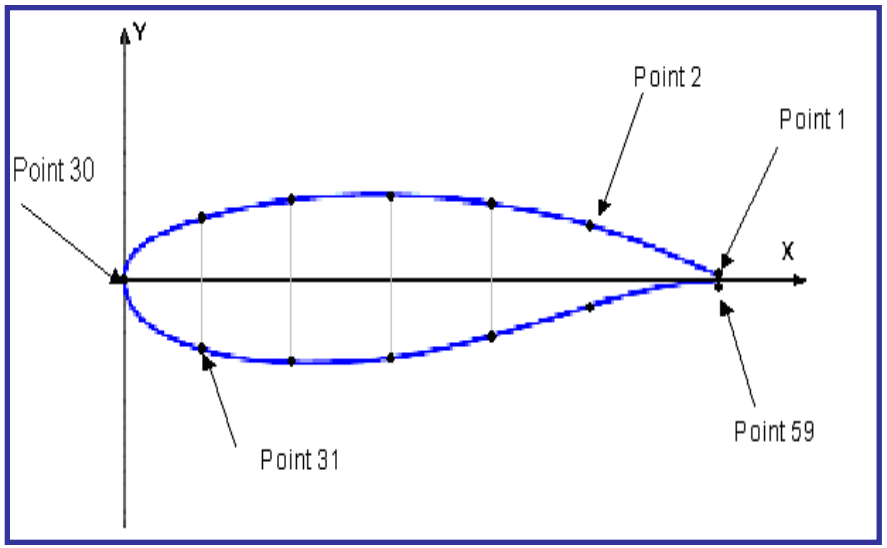
- object **O** is described by a **p**-dimensional vector **X(O)** $\in$ R^p. Components of **X(O)** are features of **O**

Example 1 (human face): grey-scale pixel-wise representation



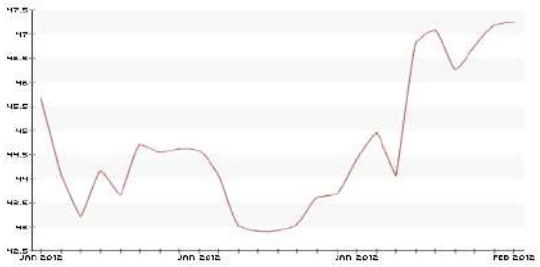
Face is represented by 1024×1024 pixels – dimension p = 10^{20} ~ 1 000 000

Example 2 (wing airfoil description).

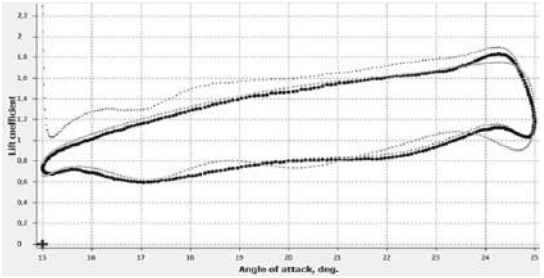


Airfoil **O** $\rightarrow$ **X(O)** = $(x_1, x_2, \dots, x_p)^T$ - ordinates of upper and lower contours, **p ~ 50 ÷ 200**

Example 3 (plots of dependences, multidimensional time-series)



Electricity price curve



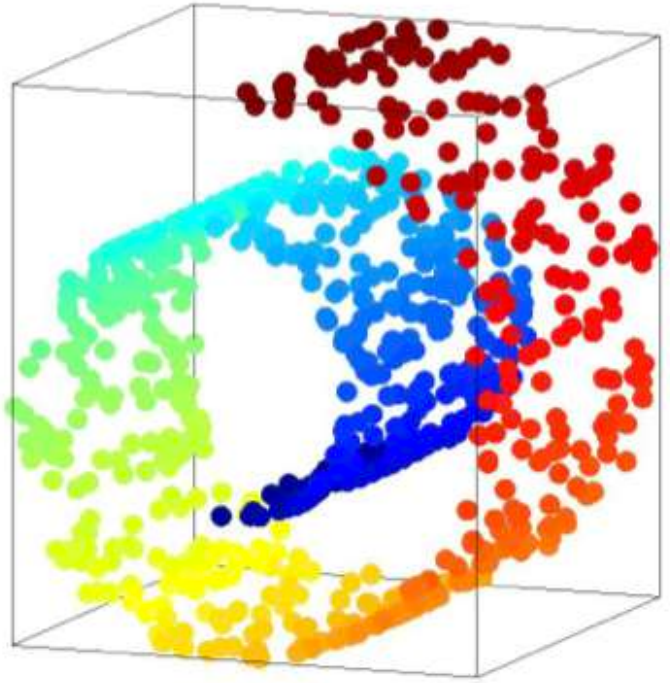
Lift force vs. AoA curve

Speech recognition

Curve f(x) is described by the vector $f = (f_1, f_2, \dots, f_p)^T \in R^p$, $f_j = f(t_j)$; time-series segment $(x_1, x_2, \dots, x_p)$ is considered as a **p-**dimensional vector

Example 4 (MNIST)

Example 5 Famous Toy Problem
"Swiss Roll"



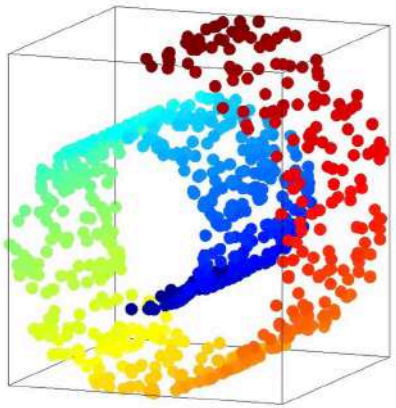
- High dimensionality **p** of **X(O)** is critical for efficient learning
- We can visualize only in 2D/3D

- Dimension Reduction = construct reduced dimension representation **$y(O) \in R^q$**, **$q << p$**, of **O** without "significant loss of information"

- DR for
  - ✓ Visualization
  - ✓ Data compression
  - ✓ "curse of dimensionality"
  - ✓ De-noising
  - ✓ Reasonable distance metrics

$X \rightarrow X'$ S.T.
$\dim(X') << \dim(X)$

uncovers the intrinsic dimensionality (invertible)



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Dimension Reduction as an Embedding Problem

Embedding Problem. Using a sample

$$\mathbf{X}_n = \{X_1, X_2, \ldots, X_n\} \subset R^p$$

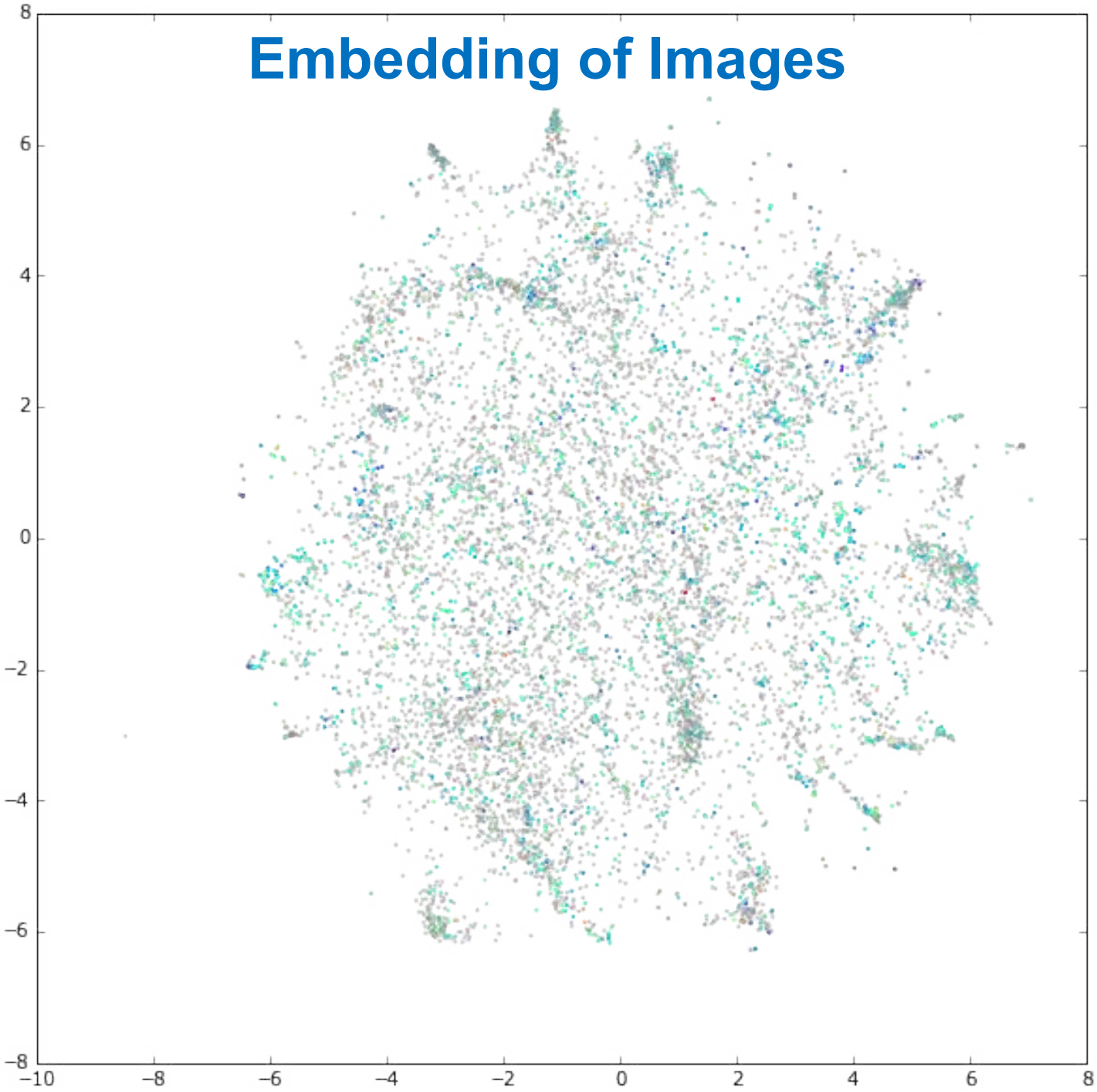
construct an embedding

$$h: \mathbf{X}_n \to \mathbf{Y}_n = h(\mathbf{X}_n) = \{y_1, y_2, \ldots, y_n\} \subset R^q$$

of sample points $\mathbf{X}_n$ в R^q, **q < p**, such that the set $\mathbf{Y}_n$ **«consistently represents»** the set $\mathbf{X}_n$

(e.g., the set $\mathbf{Y}_n$ should preserve some geometric structure of $\mathbf{X}_n$, etc.)

Embedding of Images



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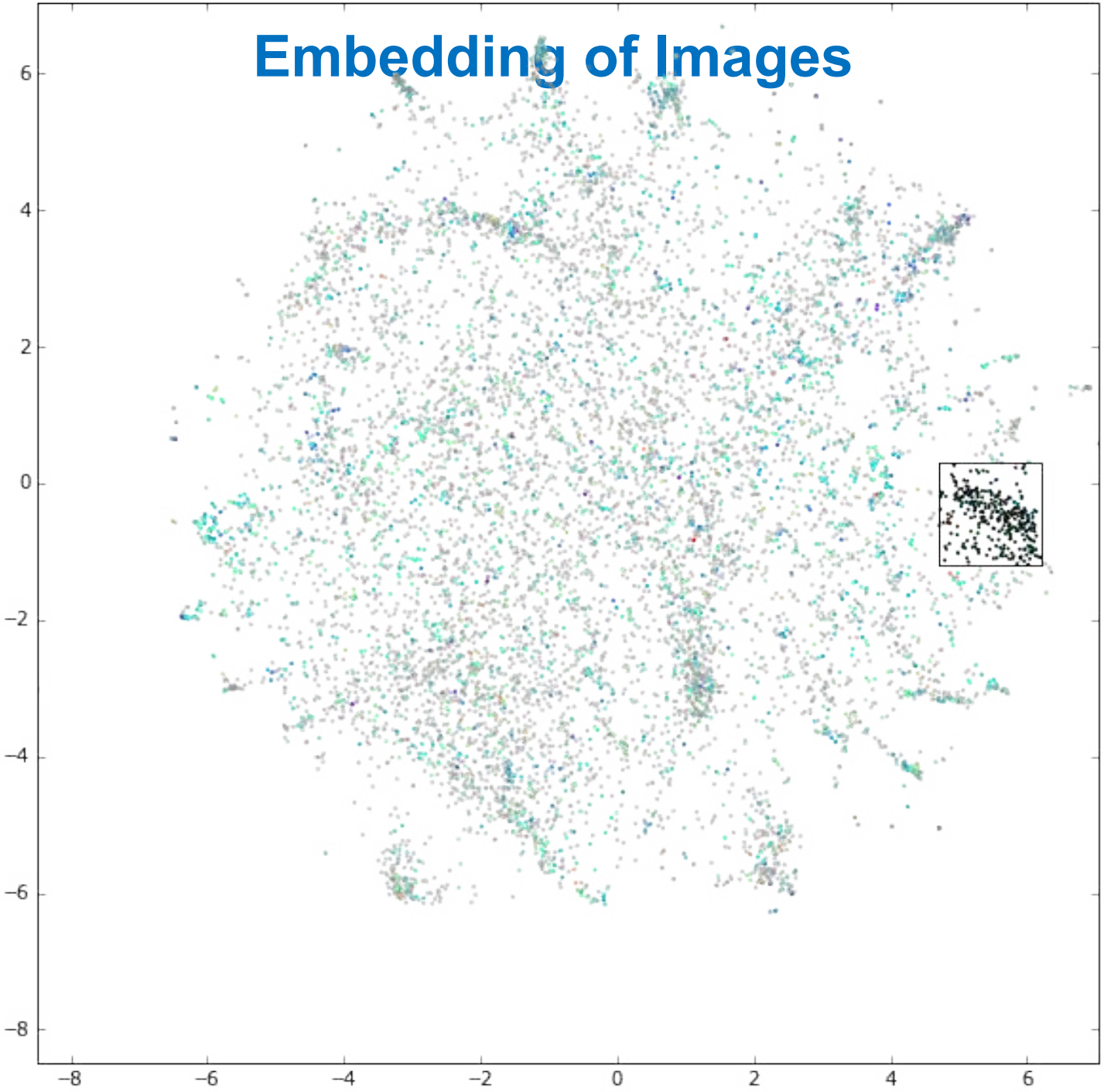





10 ДНЕЙ
ДО ЛЕТА













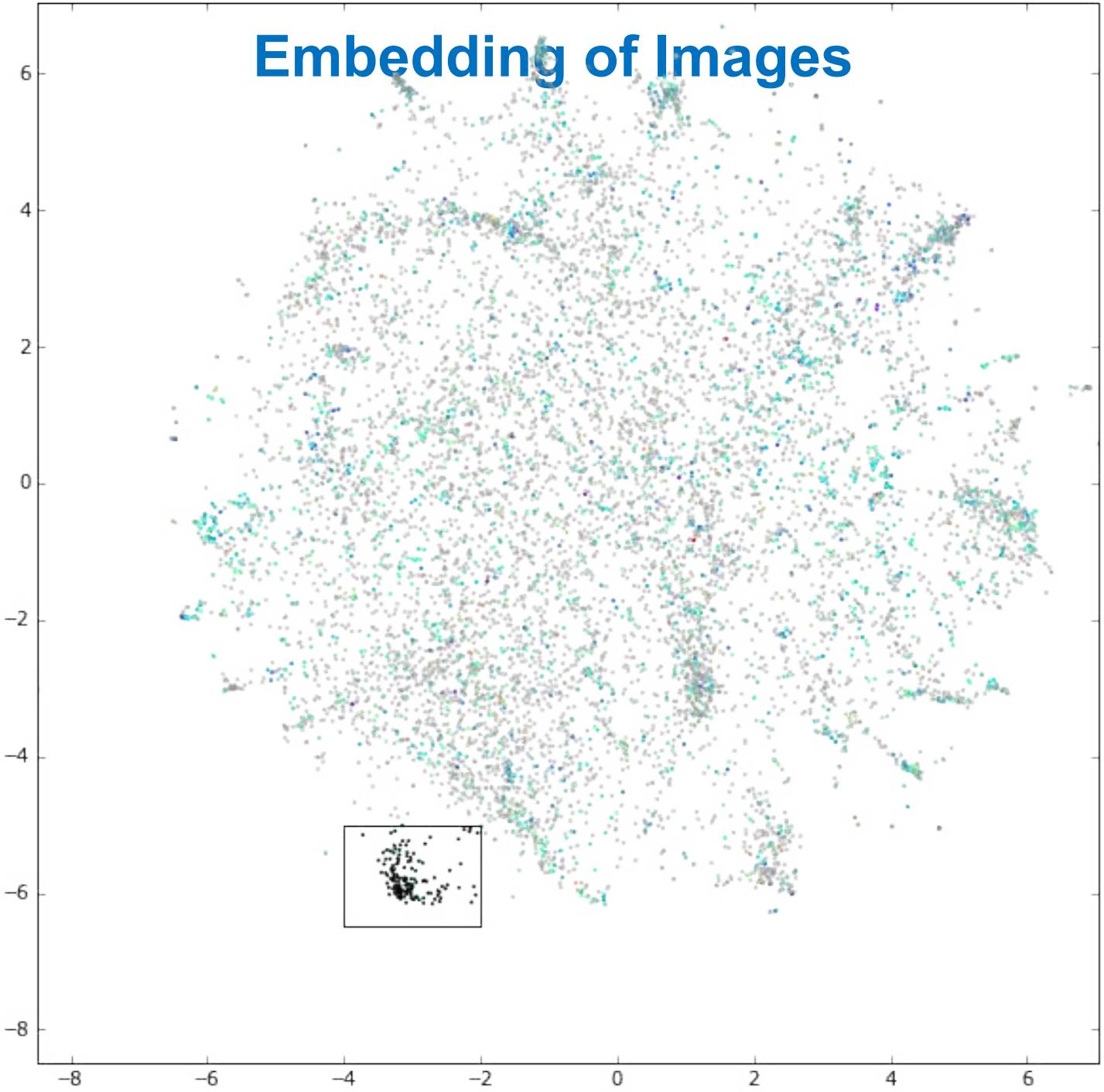


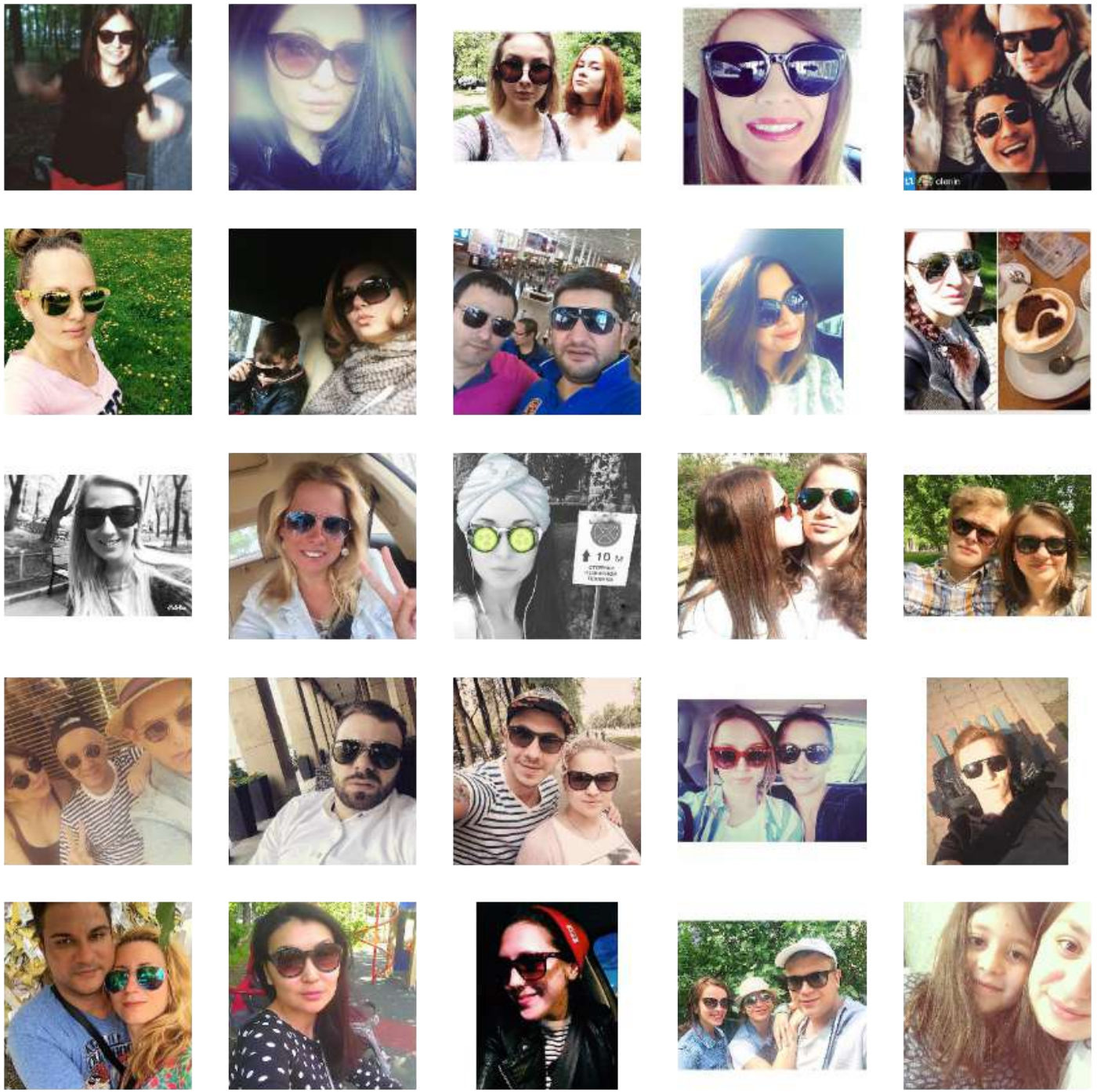






Embedding of Images





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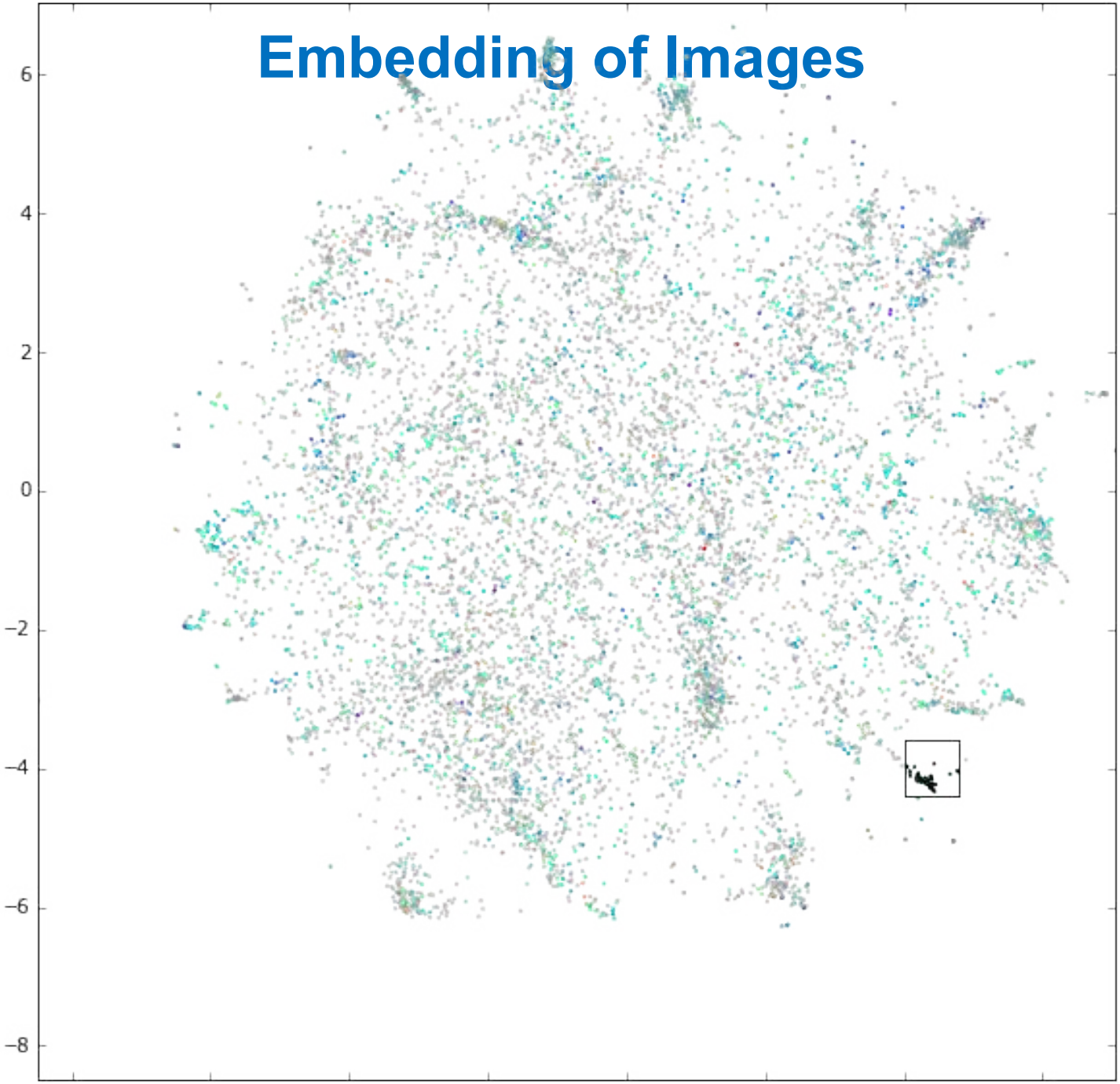



8 963 653 8888
8 963 653 8888
Беза-гель!!! С 01.06
по 07.06
Освободилось 1
место на курс!!!

Typical scheme:

• construct some cost function $L(y_1, y_2, \ldots, y_n)$. E.g. for Multi Dimensional Scaling, MDS

$$L(y_1, y_2, \ldots, y_n) = \sum_{i,j} \left(\rho(X_i, X_j) - \| y_i - y_j \| \right)^2$$

• optimize cost function

• visually analyze results (Swiss Roll, Spiral, …)

Popular methods to solve embedding problem:

- Pursuit Projection; Principal Component Analysis
- Locally Linear Embedding, LLE; Conformal Eigenmaps
- Laplacian Eigenmaps LE
- Hessian Eigenmaps, HE
- ISOmetric MAPing, ISOMAP; Landmark ISOMAP
- Kernel PCA, KPCA
- Local Tangent Space Alignment, LTSA

Extended Embedding Problem

Using a sample

$$\mathbf{X}_n = \{X_1, X_2, \ldots, X_n\} \subset R^p$$

construct an embedding transformation

$$h: \mathbf{X} \subset R^p \rightarrow \mathbf{Y} = h(\mathbf{X}) \subset R^q,$$

both for sample points $\mathbf{X}_n$, and for new (out-of-sample) points

$$X_{new} \in \mathbf{X} / \mathbf{X}_n$$

without solving embedding problem for $\mathbf{X}_n \cup \{X\}$ anew

Example – face recognition

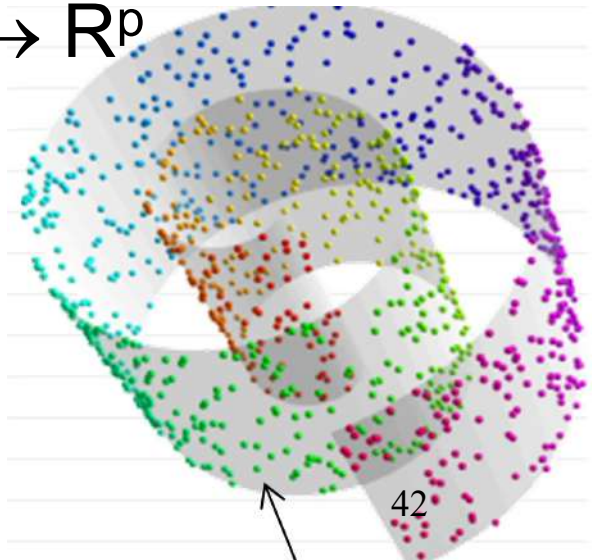
For extended embedding problem we need a Data Model **X:** description of **X**, and of a mechanism, which generates points $\mathbf{X}_n$ and new points X_{new} from **X**

Usually we assume that real data is well approximated by some manifold, i.e.

Manifold Data Model:

$$\mathbf{X} = \{X = f(b) \in R^p : b \in \mathbf{B} \subset R^q\} \subset R^p$$

- open set **B** (inner coordinate space)
- smooth bijective transformation $f: \mathbf{B} \to R^p$



Manifold Learning Problem!!!

Full Dimension Reduction problem

Using a sample

$$\mathbf{X}_n = \{X_1, X_2, \ldots, X_n\} \subset R^p$$

construct embedding transformation:

$$h: \mathbf{X} \subset R^p \rightarrow \mathbf{Y} = h(\mathbf{X}) \subset R^q$$

and **Reconstruction transformation**

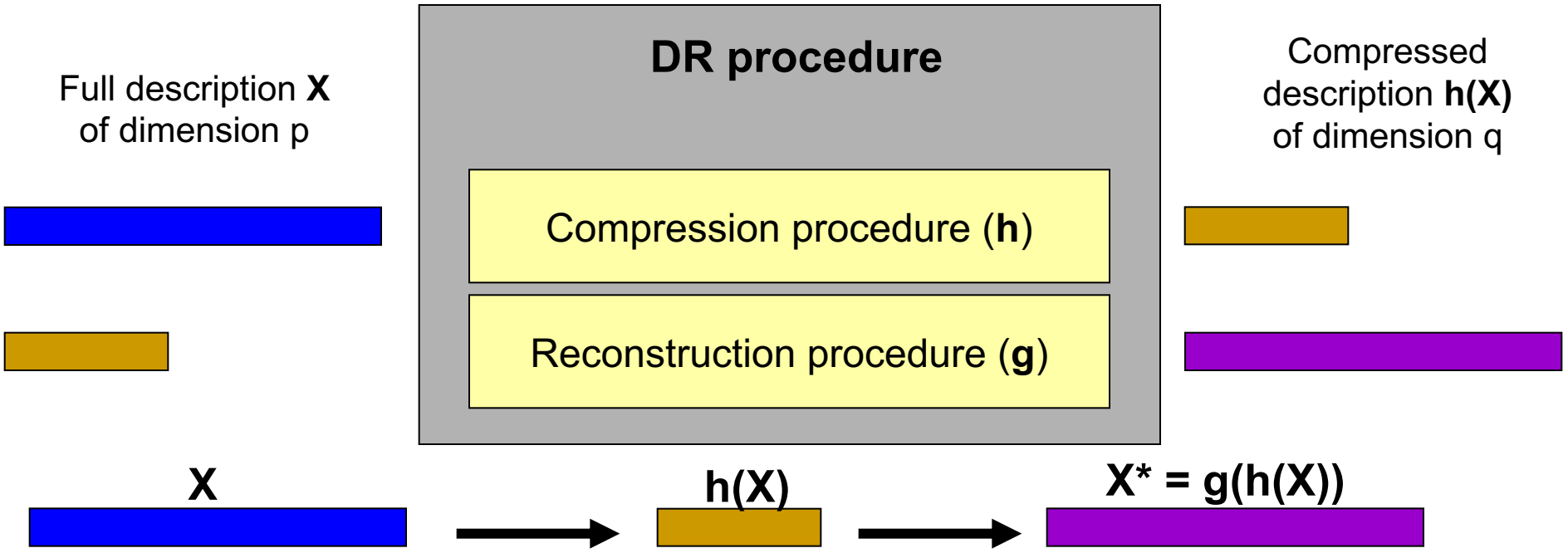
$$g: \mathbf{Y} \subset R^q \rightarrow \mathbf{X} \subset R^p$$

such that

$$g(h(X)) \approx X \quad \text{for } \mathbf{all}\ X \in \mathbf{X}$$

Example – dimension reduction of airfoils

Dimension Reduction



Requirements:

minimal dimension **q = Dim h(X)** of compressed description **h(X)**, providing required proximity between **X* = g(h(X))**) and **X**

or:

maximal proximity between **X** and **X* = g(h(X))** for a fixed dimension **q = Dim h(X)** of compressed description

Overview

- Intro
- Dimension Reduction Problem Statements
- **PCA, MDS and Sammon Mapping, Autoencoders**
- ISOMAP and LLE
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- References

Principal Component Analysis, PCA
(K. Pearson, 1899)

Problem: find in R^p an affine subspace

$$L(q) = \left\{ x \in R^p : x = x_0 + \sum_{j=1}^{q} y_j \times e_j,\ y_1, y_2, \ \ldots, y_q \in R^1 \right\}$$

of dimension q < p, **which best approximates the set of points**

$$\mathbf{X}_n = \{X_i,\ i = 1, 2, \ldots, n\} \subset R^p.$$

in PCA: "the best" = minimize w.r.t. $\mathbf{x_0}$, $\mathbf{\{e_1, e_2, \ldots, e_q\} \subset R^p}$

$$\frac{1}{n} \sum_{j=1}^{n} \left\| X_j - P_{L(q)} X_j \right\|^2$$

$$\Pr_{L(q)}(X) = x_0 + \sum_{j=1}^{q} y_j(X) \times e_j, \qquad y_j(X) = (X - x_0, e_j)$$

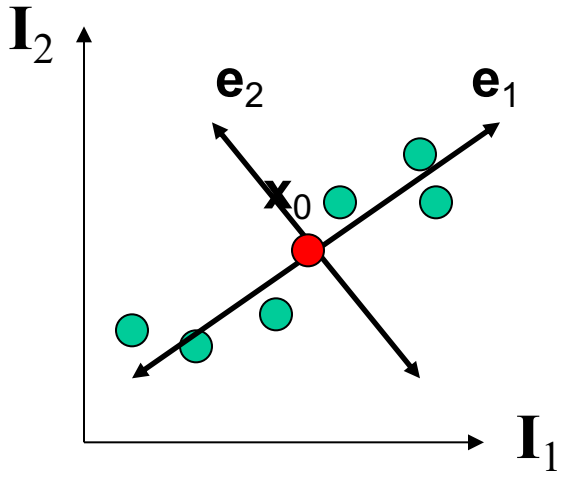
x_{mean} – empirical mean of $\{X_i, i = 1, 2, \dots, n\}$,

$\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_p\}$ – eigenvalues of an empirical covariance (p×p)-matrix

$$\Sigma = \frac{1}{n}\sum_{j=1}^{n}(X_j - x_{mean}) \times (X_j - x_{mean})^T$$

providing orthonormal basis in R^p

p = 2
q = 1



$L(1) = \{X \in R^2: X = x_0 + y \times \mathbf{e}_1, y \in R^1\}$

Solution: $x_0 = x_{mean}$, $L(q) = x_0 \oplus \text{Span}(\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_q)$,

where orthonormal eigenvectors $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_q\}$ of Σ

correspond to q highest eigenvalues of this matrix

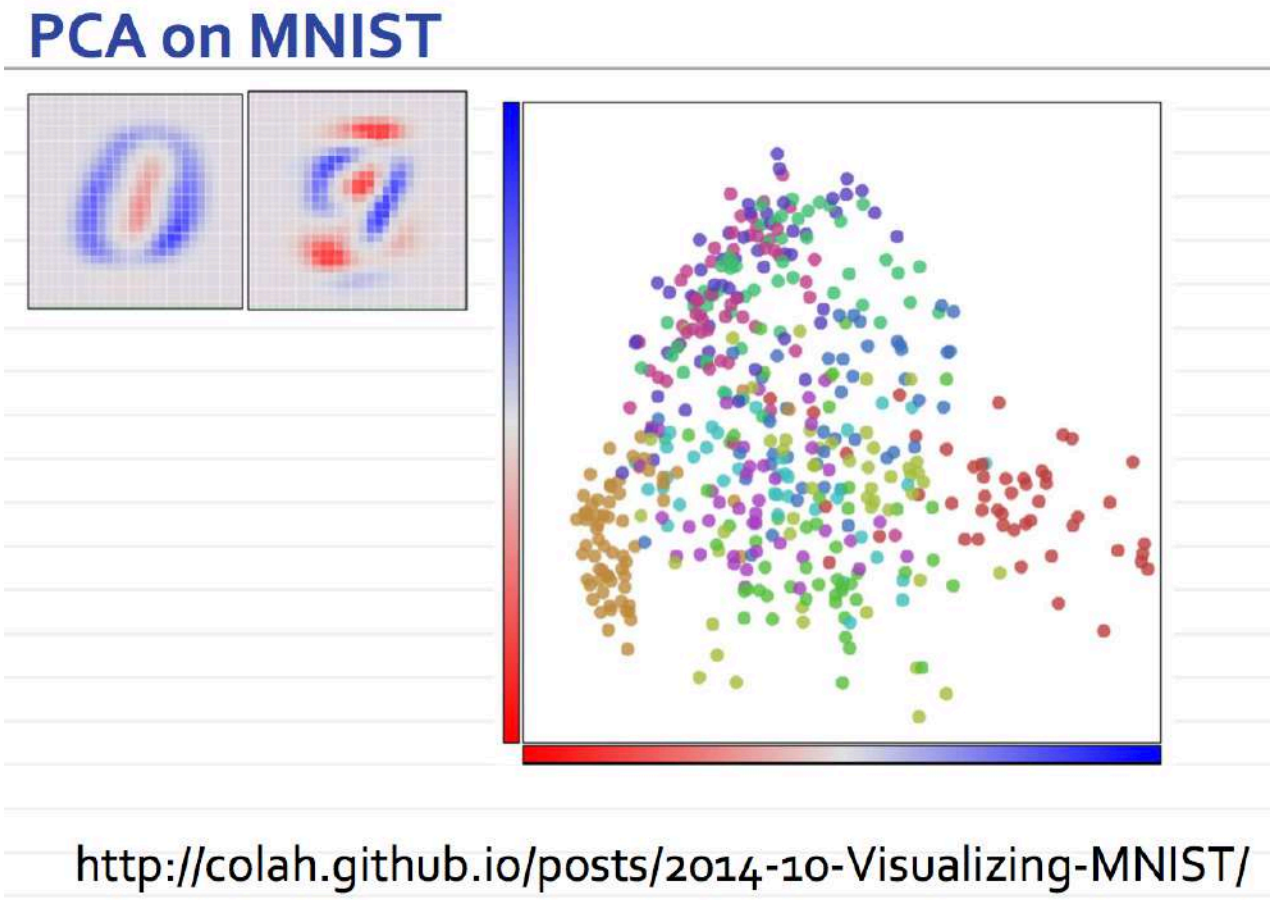
PCA solves E-Problem, EE-Problem and FULL DR problem:

embedding procedure:

$$X \in R^p \rightarrow h(X) = (y_1(X), y_2(X), \ldots, y_q(X))^T \in R^q$$

reconstruction procedure:

$$\mathbf{y} = (y_1, y_2, \ldots, y_q)^T \in R^q \rightarrow g(y) = x_0 + y_1 \times \mathbf{e}_1 + y_2 \times \mathbf{e}_2 + \ldots + y_q \times \mathbf{e}_q$$



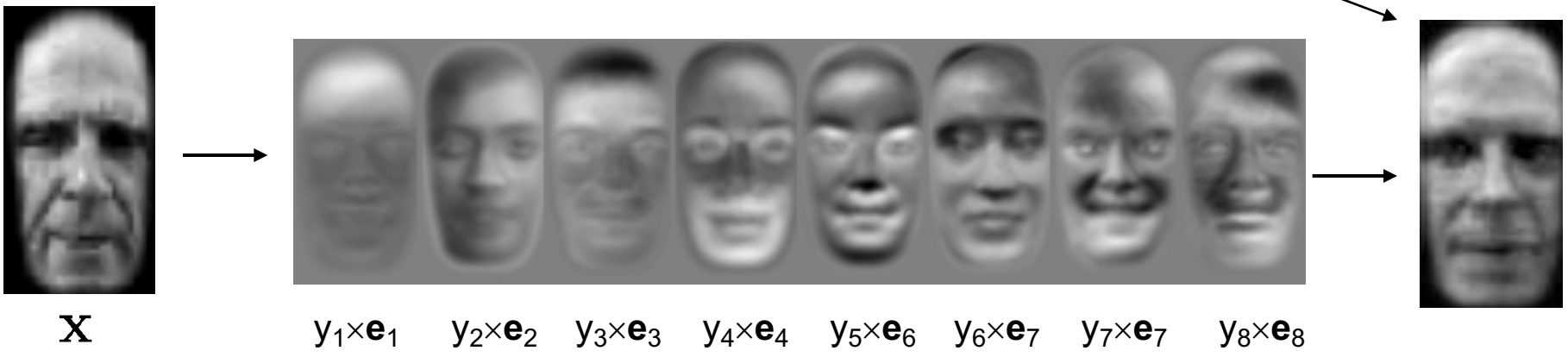
PCA for Face Recognition

- Eigenvectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_p \in R^p$ in a space of faces: $p \sim 10^6$

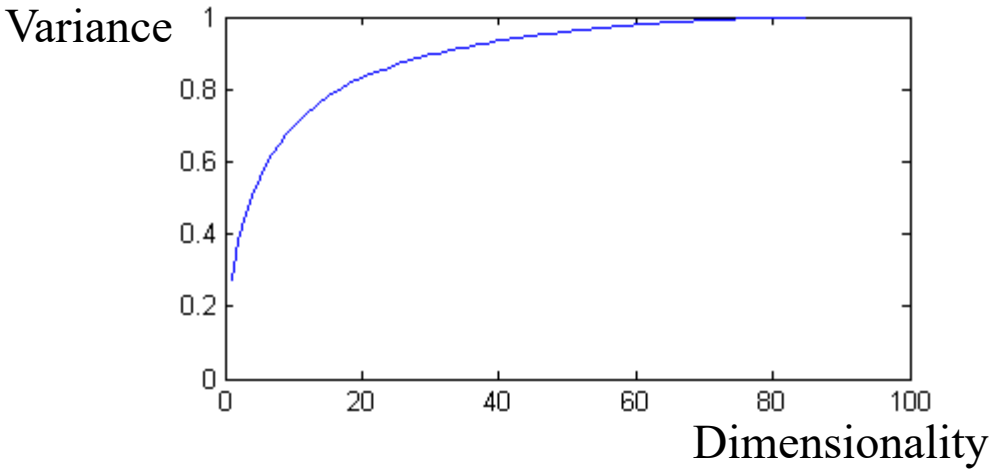
$$X \rightarrow (\underbrace{(X - x_0, \mathbf{e}_1)}_{y_1}, \underbrace{(X - x_0, \mathbf{e}_2)}_{y_2}, \ldots, \underbrace{(X - x_0, \mathbf{e}_p)}_{y_p})^T \in R^p$$

- We select first q, $q \sim 10^2$ eigenvectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_q \in R^q$

$$X^* \approx x_0 + y_1 \times \mathbf{e}_1 + y_2 \times \mathbf{e}_2 + \ldots + y_q \times \mathbf{e}_q$$



Left to right: original, reconstruction from 84, 40, 20, 3, 2, and 1 dimensions.



Pursuit Projection, PP: Similar to PCA, constructs **«the best» affine hyperplane** of smaller dimension

Multi Dimensional Scaling, MDS

Minimize quadratic form $\sum_{i,j}\left(\rho(O_i, O_j) - \|y_i - y_j\|\right)^2$

w.r.t. $y_1, y_2, \ldots, y_n \in R^q$, ρ is a some metrics in the object feature space

$y_1, y_2, \ldots, y_n \in R^q$ are defined **except for shift and rotation,** thus we use normalization, e.g.

$$\mathbf{Y}^T \times \mathbf{Y} = \mathbf{I_q} \quad \text{and} \quad \mathbf{Y}^T \times \mathbf{1} = \mathbf{0}$$

where $\mathbf{Y}^T = (y_1 : y_2 : \ldots : y_n)$ – (q×n)-matrix, $\mathbf{1} \in R^n$ – vectors of ones

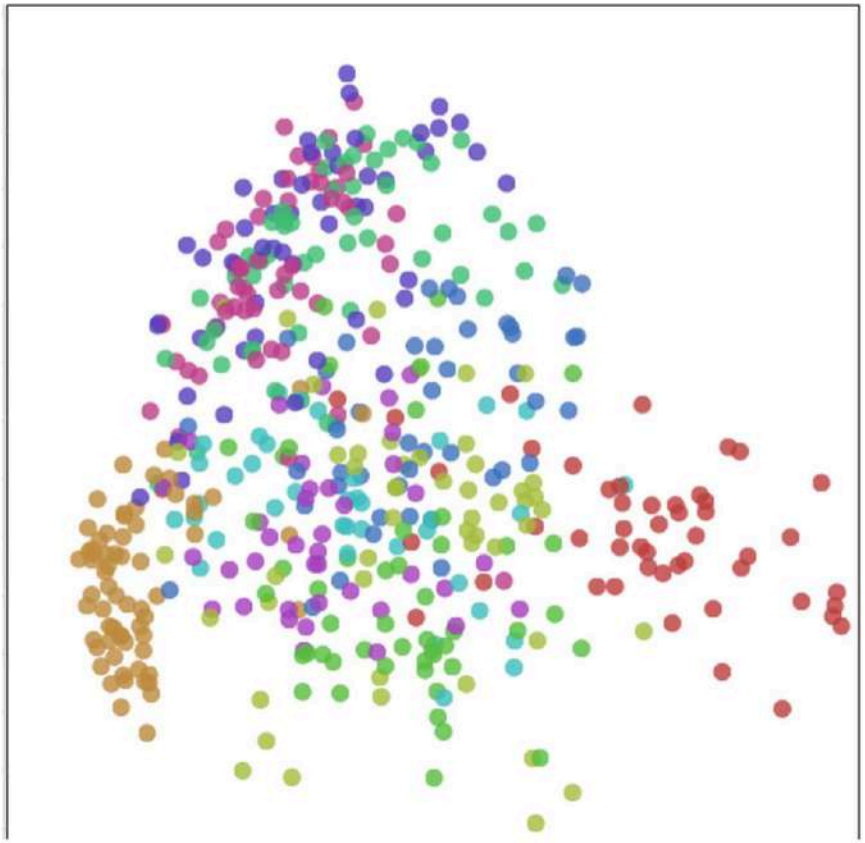
If $\rho(O_i, O_j) = \|X(O_i) - X(O_j)\|$, then MDS = PCA

Sammon mapping

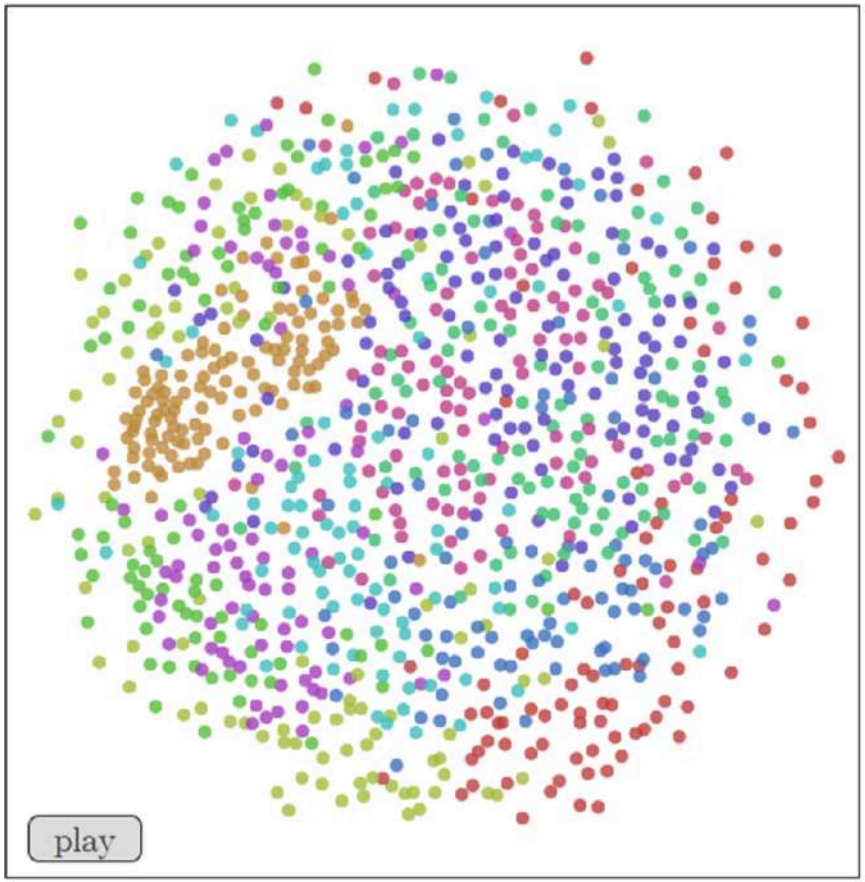
Common useful idea: local distances are often more important to preserve

$$\sum_{i,j} \frac{\left(\rho(O_i, O_j) - \left\| y_i - y_j \right\|\right)^2}{\left(\rho(O_i, O_j)\right)^2}$$

PCA vs. MDS

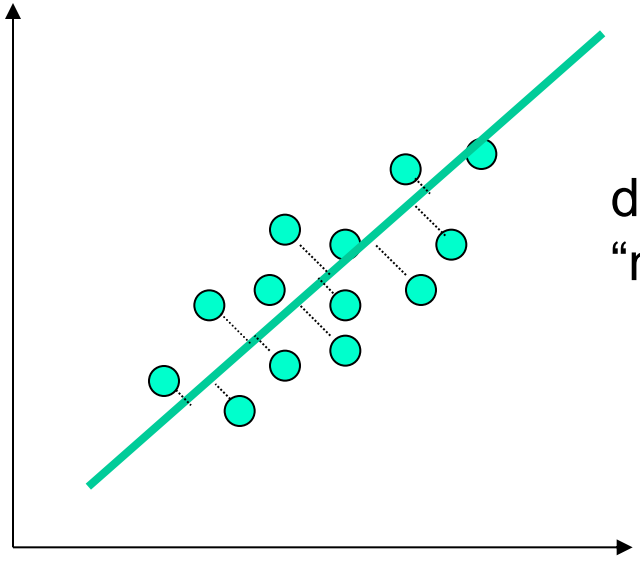


PCA



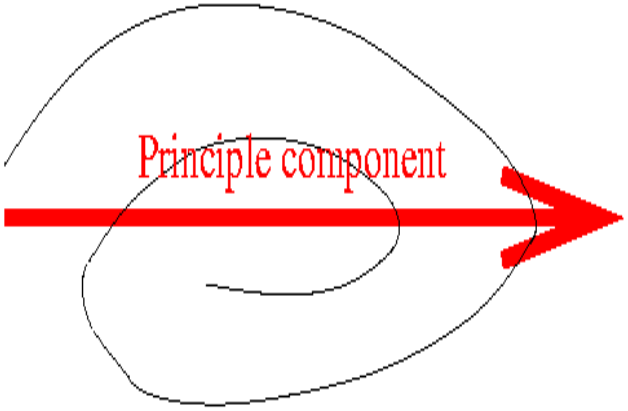
Sammon

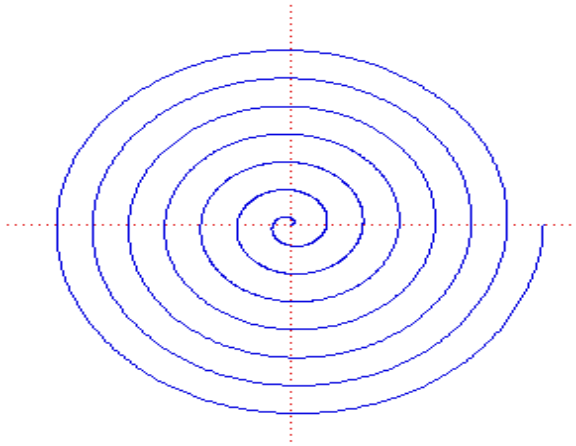
MDS, PCA, PP, MDS (for «Euclidean proximity») – linear methods,

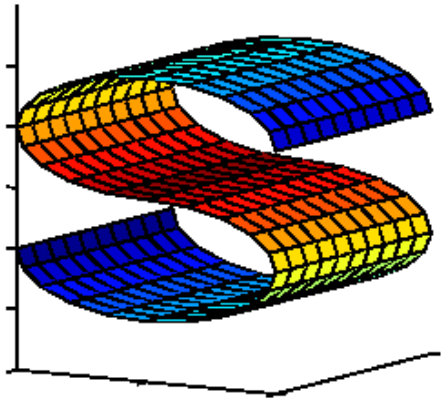


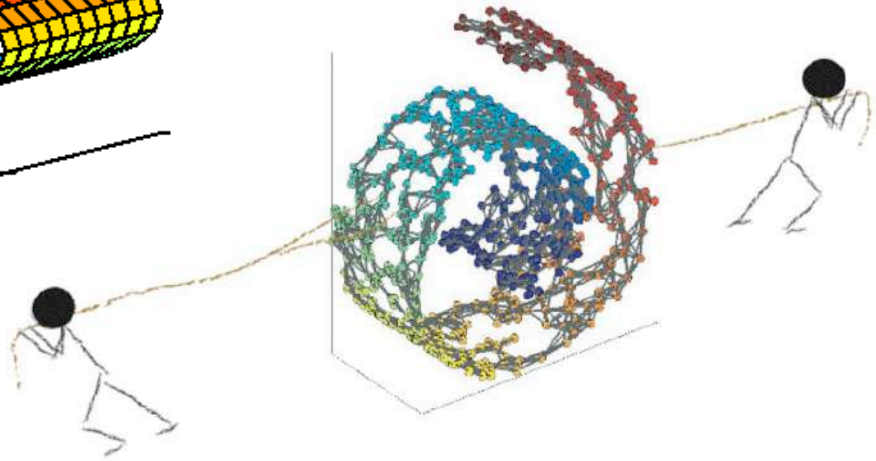
Spiral of Archimedes

do not work for
“nonlinear data”:

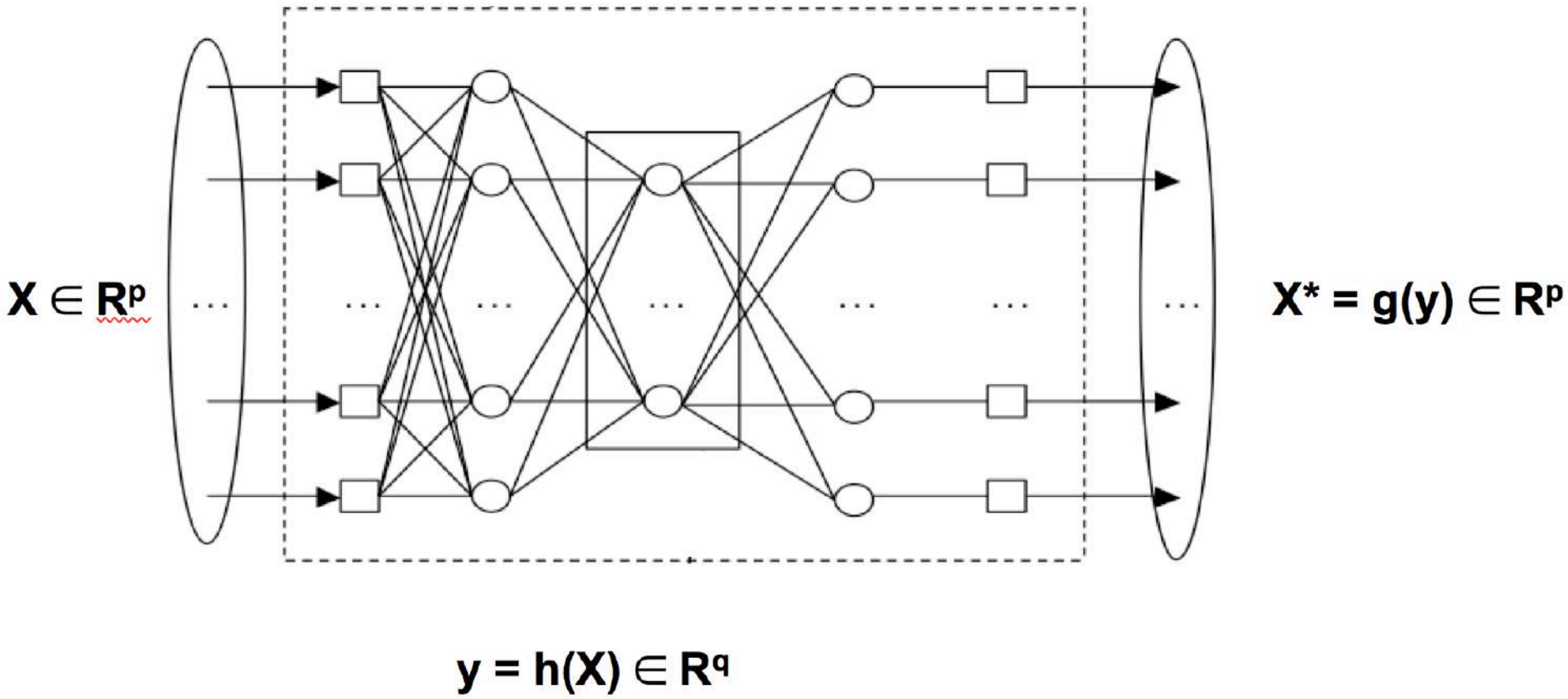




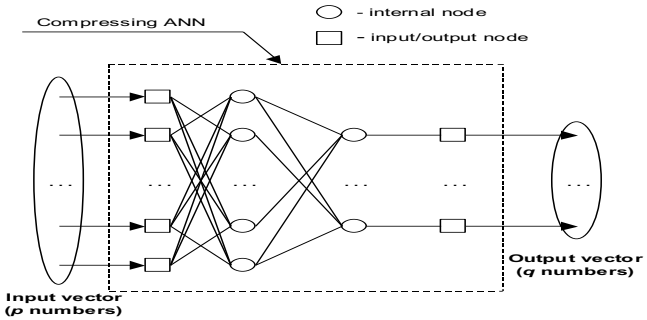


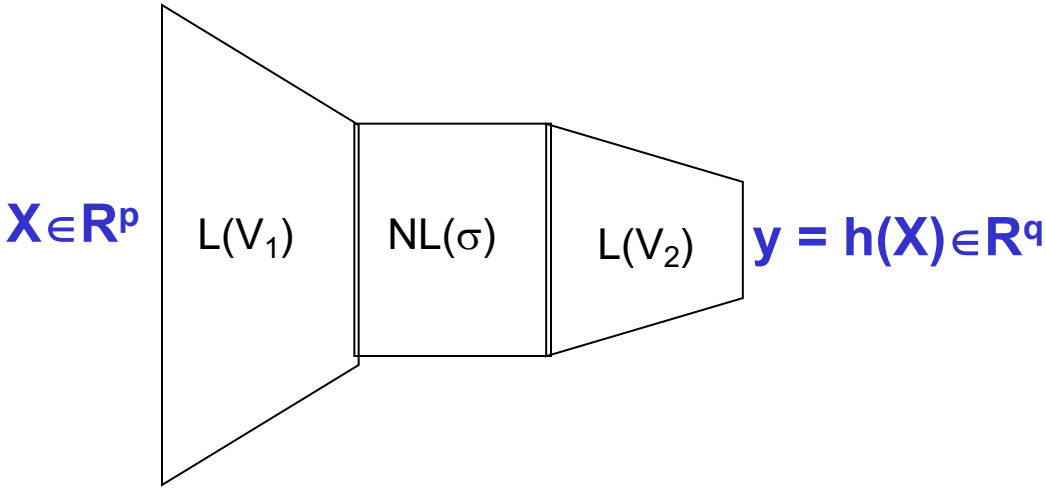


Replicative Neural Networks

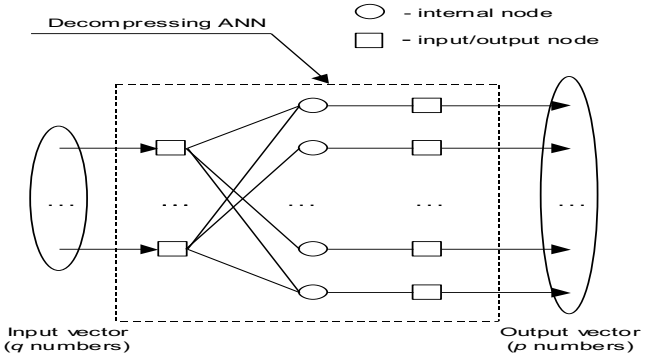


Compression transformation





Reconstruction transformation



$y \in R^q$ $\quad L(W_2) \quad NL(\sigma_R) \quad L(W_1)$ $\quad X^*=g(y) \in R^p$

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Nonlinear (local) DR methods

5) **Locally Linear Embedding, LLE**
6) **Laplacian Eigenmaps LE**
7) **Hessian Eigenmaps, HE**
8) **ISOmetric MAPing, ISOMAP**
9) Kernel PCA, KPCA - Spectral Embedding Algorithm, SEA
10) Riemannian Manifold Learning, RML
11) Local Tangent Space Alignment, LTSA, **…**

GRAPH: standard step for many “local” DR methods

Step 1. Construct neighborhoods (ε-Neighborhoods, k Nearest Neighbors)

$$U(X) = U(X|\rho, \varepsilon) = \{X_i \in \mathbf{X}_n: \rho(X, X_i) \le \varepsilon\}$$

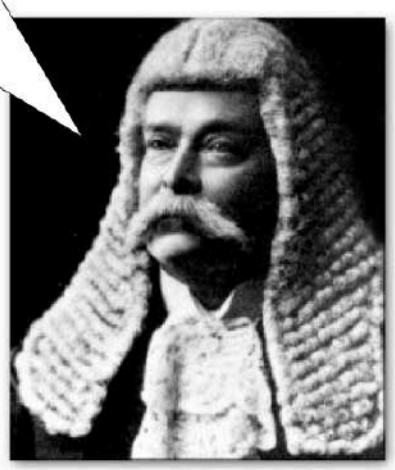
$\Rightarrow$ **Graph** $\Gamma(\mathbf{X}_n) = (\mathbf{X}_n, \mathbf{V})$: $(X_i, X_j) \in \mathbf{V} \Leftrightarrow X_j \in U(X_i)$ и $X_i \in U(X_j)$

Step 2. Construct weights $w_{ij} = w(X_i, X_j) = w(v)$, $v = (X_i, X_j) \in \mathbf{V}$

$w_{0,ij} = 1$ for all $(X_i, X_j) \in V$, $\quad w_{0,ij} = 0$ in other cases

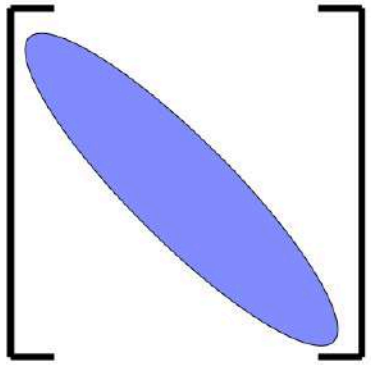
ISOMAP

Infer a distance matrix using distances along the manifold.

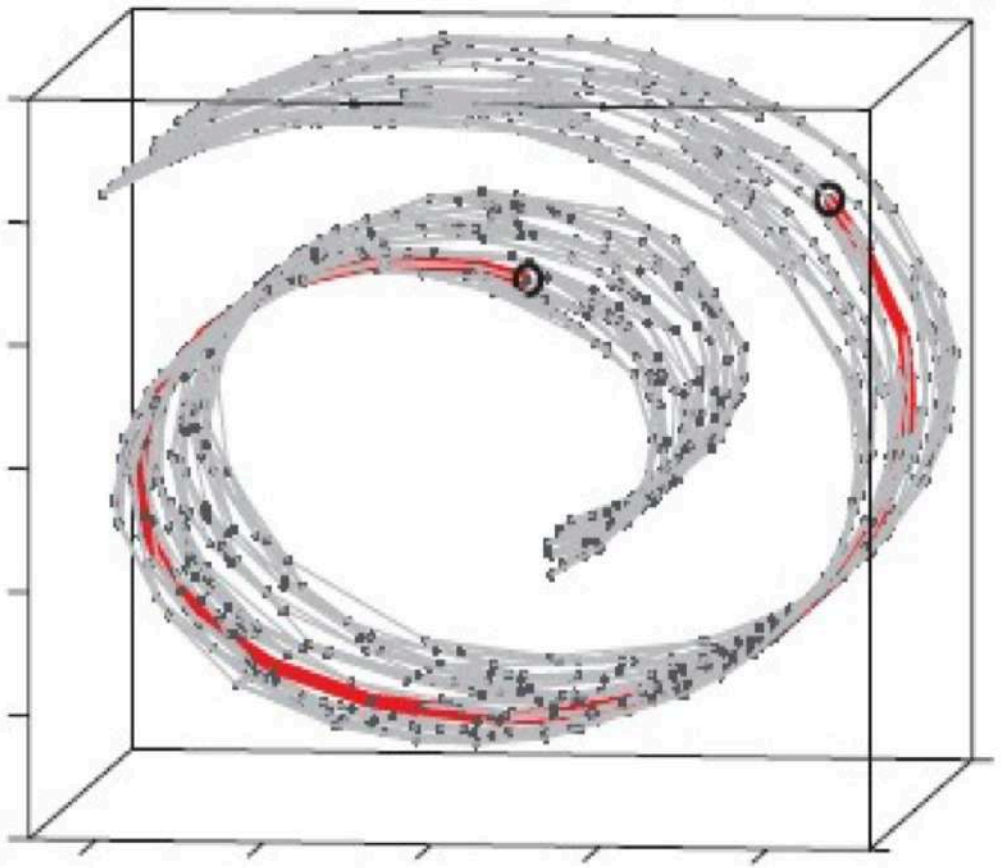


ISOMAP

1. Build a sparse graph with K-nearest neighbors

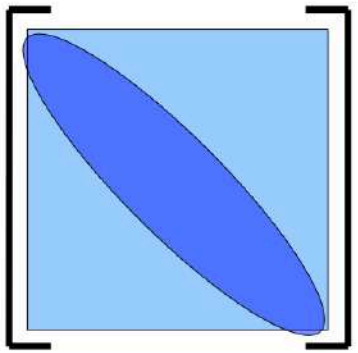
$D_g =$ 

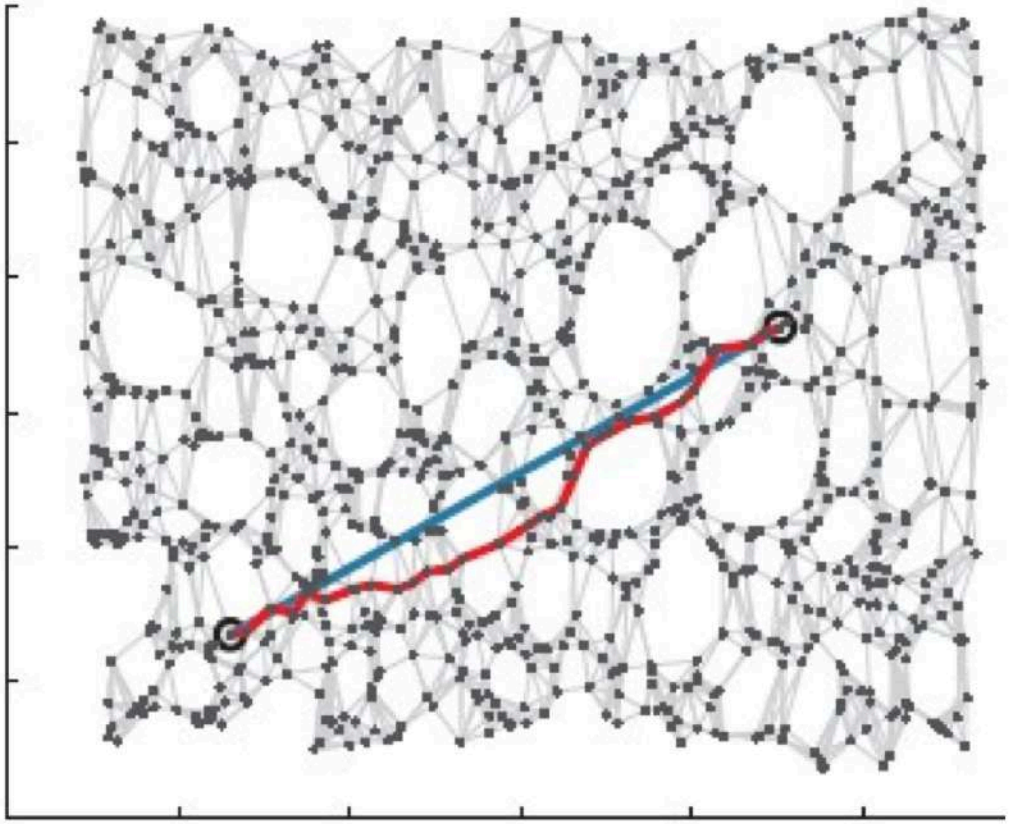
(distance matrix is sparse)



ISOMAP

2. Infer other interpoint distances by finding shortest paths on the graph (Dijkstra's algorithm).

$D_g =$ 



ISOMAP

Usual MDS

3. Build a low-D embedded space to best preserve the complete distance matrix.

Error function:

inner product distances in graph

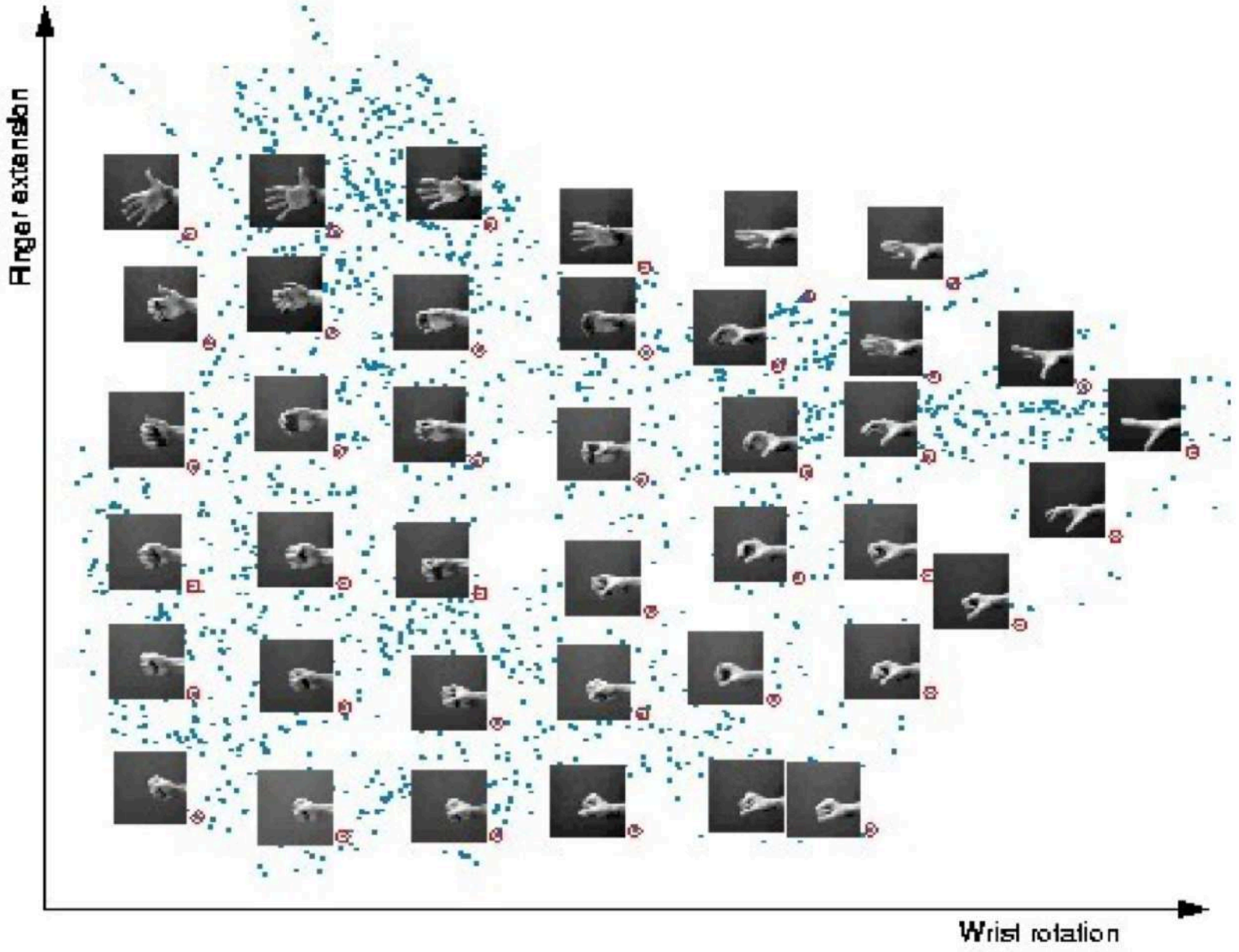
inner product distances in new coordinate system

L2 norm

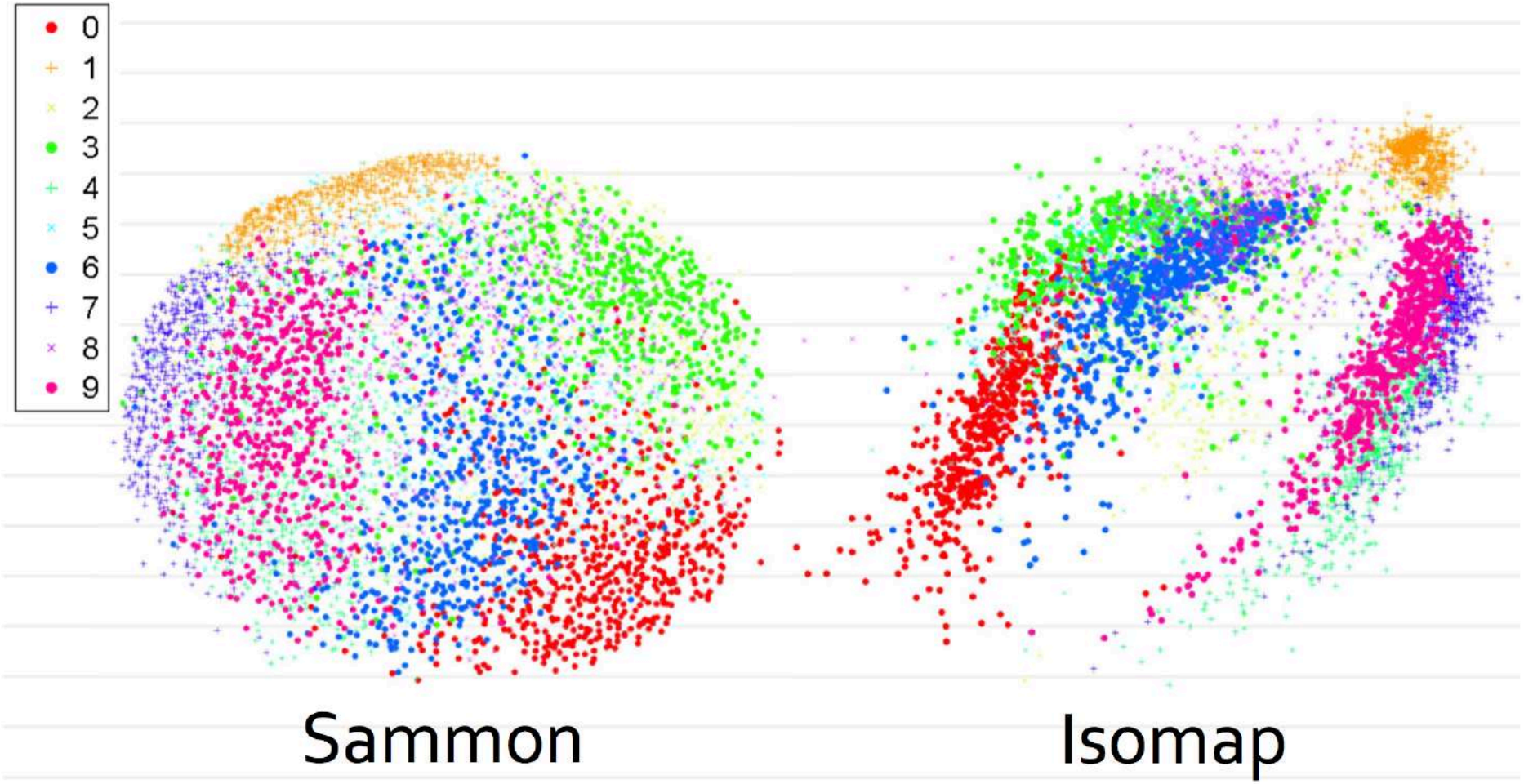
$$E = \|\tau(D_G) - \tau(D_Y)\|_{L^2}$$

Solution – set points Y to top eigenvectors of D_g

Isomap results: hands



MNIST: Sammon vs. ISOMAP



Isomap: pro and con

- preserves global structure

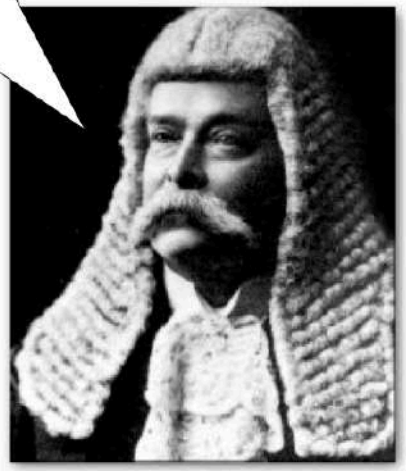
- few free parameters

- sensitive to noise, noise edges

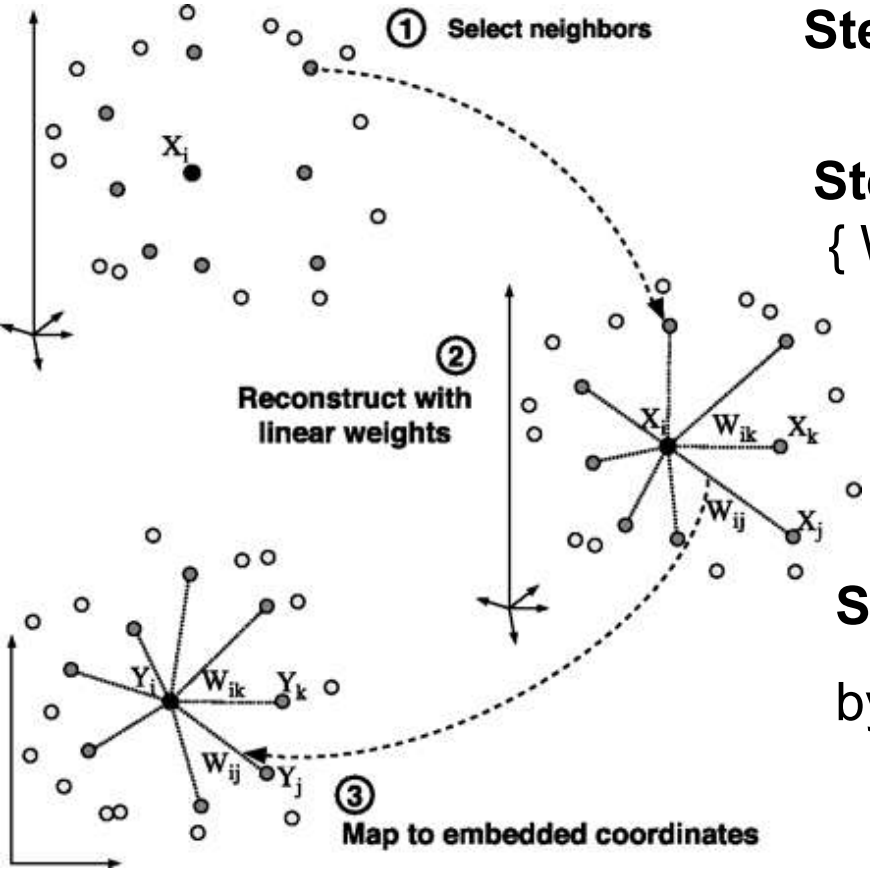
- computationally expensive (dense matrix eigen-reduction)

Locally Linear Embedding

Find a mapping to preserve local linear relationships between neighbors



Locally Linear Embedding, LLE (L.K. Saul, et al., 2000)



Step 1. K nearest neighbors

Step 2. Get "Baricentric" coordinates $\{ W_{ji}\}$ by minimizing

$$J_1(\mathbf{W}) = \sum_{i=1}^{n} \left\| \mathbf{x}_i - \sum_{j=1}^{K} W_{ji} \mathbf{x}_{j(i)} \right\|^2$$

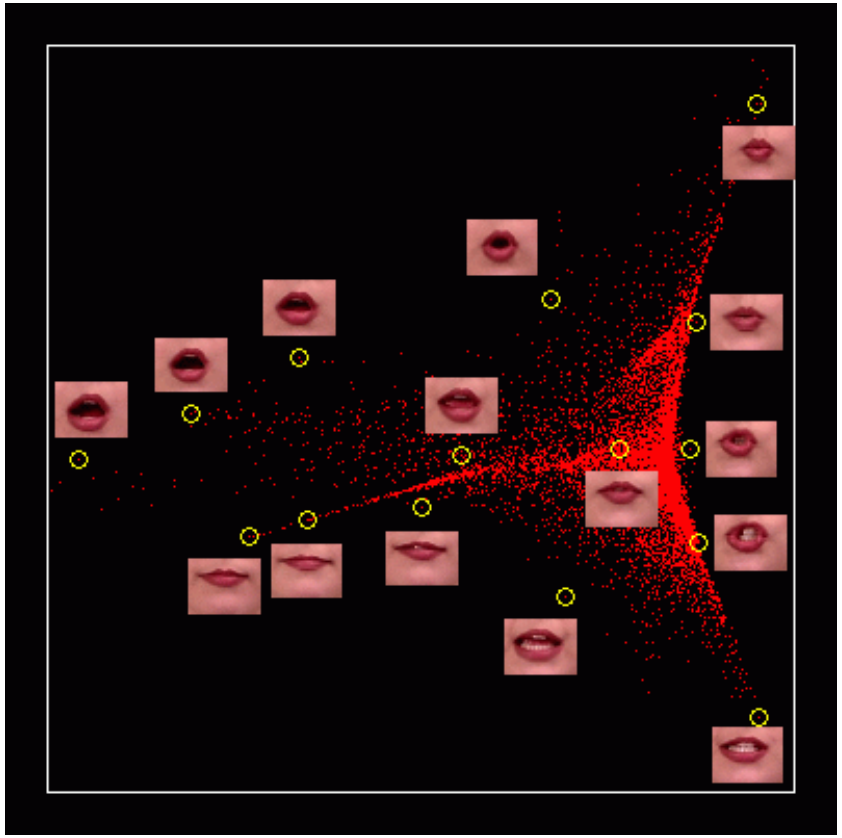
Step 3. Get $\{y_1, y_2, \ldots, y_n\} \in R^q$

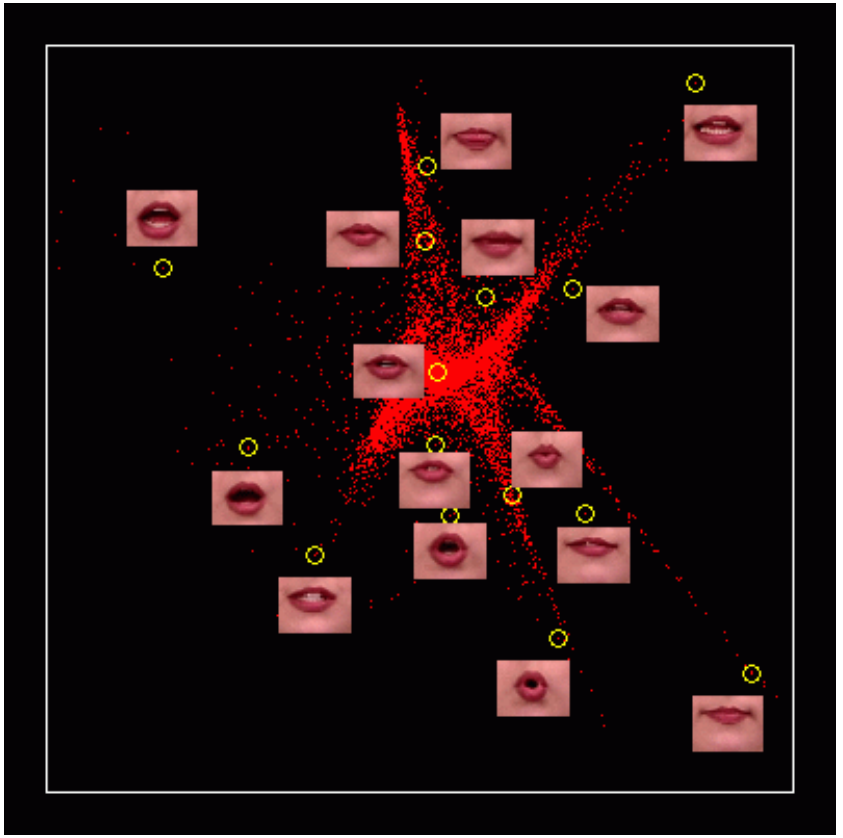
by minimizing

$$J_2(\mathbf{Y}) = \sum_{i=1}^{n} \left\| \mathbf{y}_i - \sum_{j=1}^{N} W_{ji} \mathbf{y}_{j(i)} \right\|^2$$

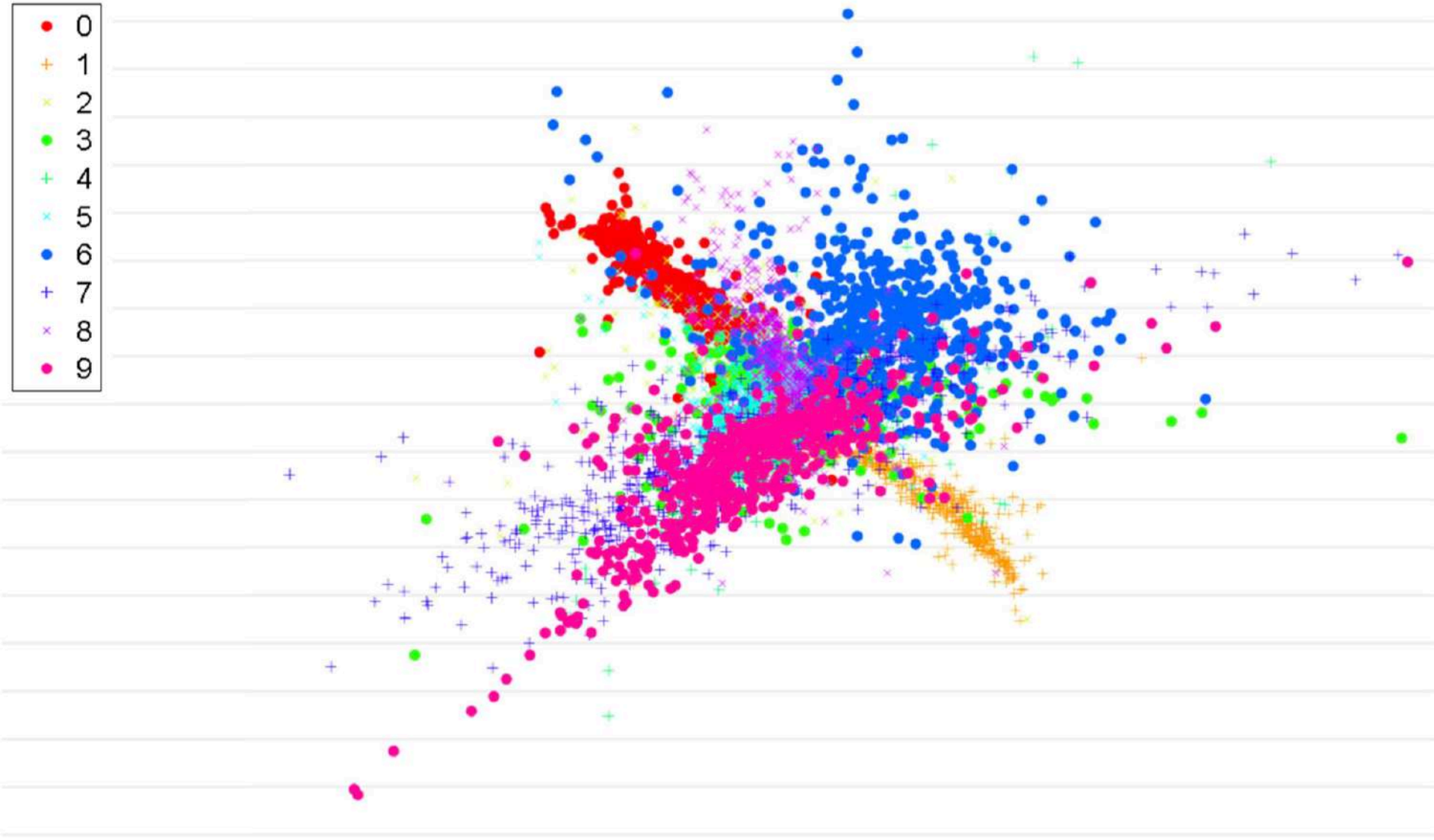
with standard normalizing conditions

LLE: Lips pictures





LLE: MNIST



LLE: pro and con

- no local minima, one free parameter

- incremental & fast

- simple linear algebra operations

- can distort global structure

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Demand Forecasting

Lots of customers

Limited resources

- Identifying **valuable customers** and **predicting demand**
- **Unified process** of marketing and demand forecasting

Use of the customer segmentation for demand forecasting

- **Millions** of time series to predict
- **Novelty** of the cloud computing, thus **historic data is limited**

This work proposes three different methods:

RFM, TS RFM and TDA RFM

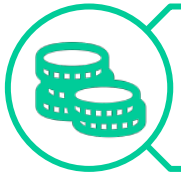
What is RFM?

Recency:

"**When** was the **last time** that a user was active?"

Frequency:

"**How frequently** has a user been active?"



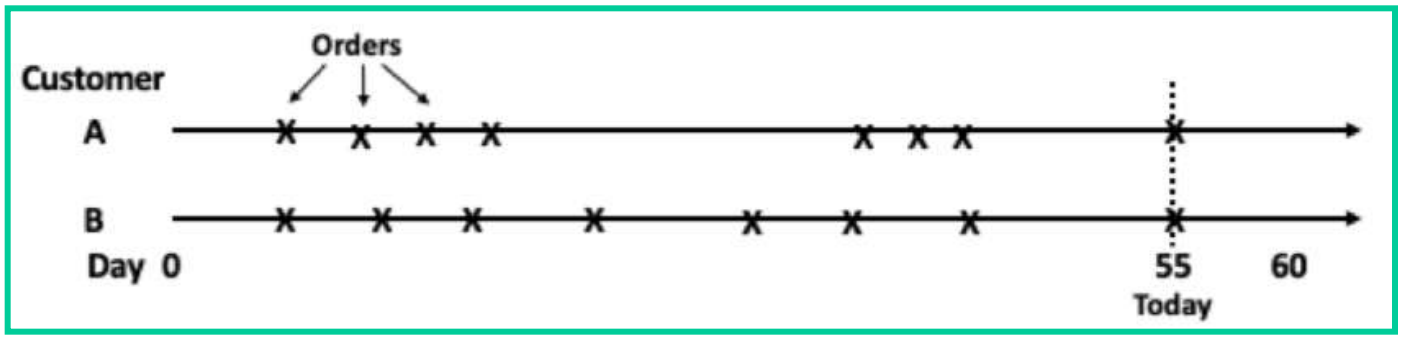
Monetary:

"**How much revenue** has this user generated?"

RFM score:

3 numbers

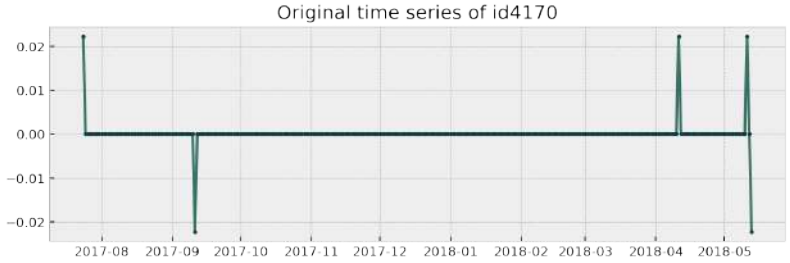
Why can it fail?

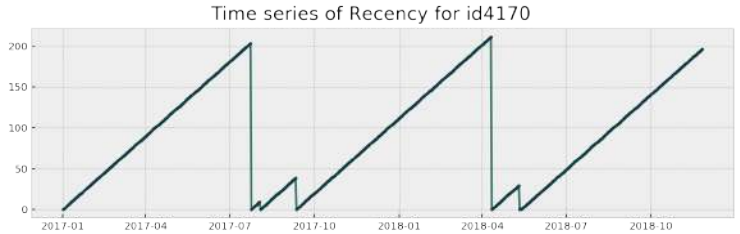


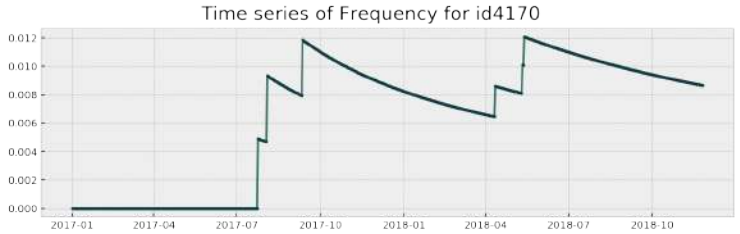
Two customers share the **same** RFM score

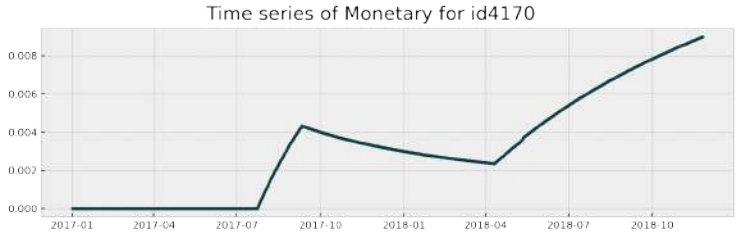
But **A** is likely to be **different** from **B**

How to improve it?







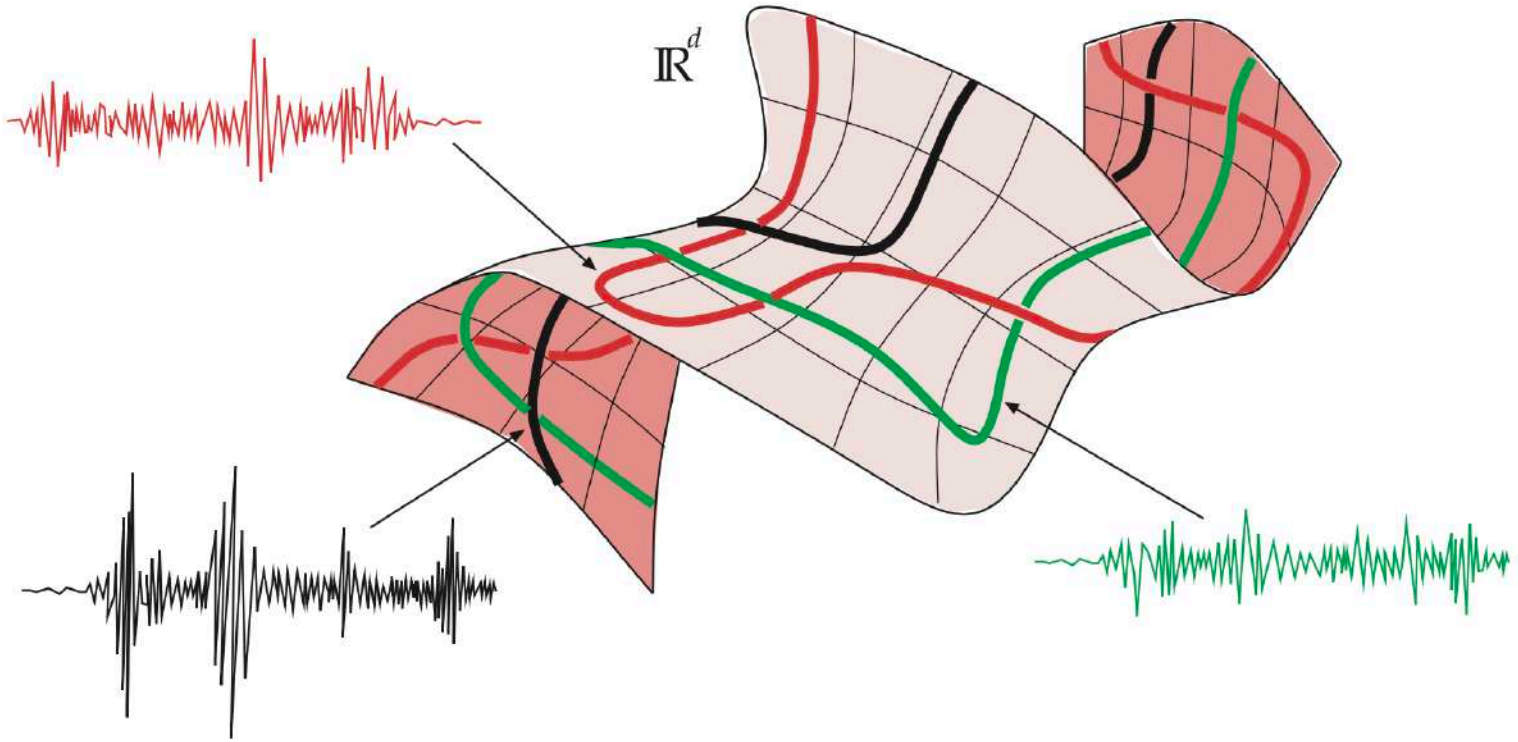


Point clouds representation

Sliding windows of size w are applied to each time series $X_j = \{x_1, x_2, \ldots, x_n\}$ in order to create point clouds Z_j of points in $\mathbb{R}^w$

$$Z_j = \begin{pmatrix} x_1, x_2, \ldots, x_w \\ \vdots \\ x_{n-w}, x_{n-w+1}, \ldots, x_n \end{pmatrix}$$

Trajectories from three different time-series lie along a smooth manifold

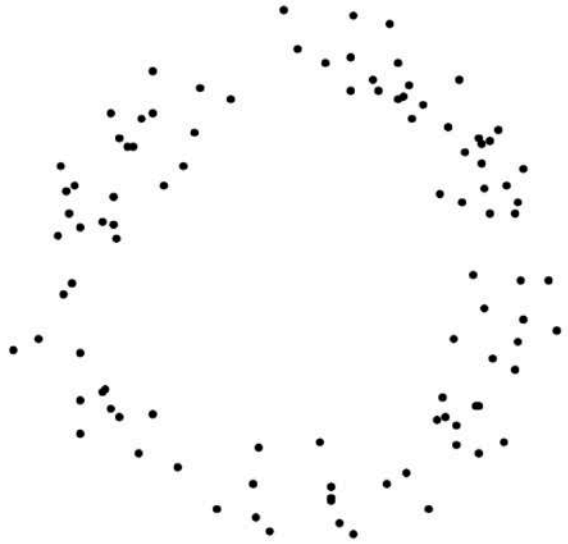


Picture credit to [Taylor et al. Geophys. J. Int. (2011) 185, 435–452]

Persistence homologies

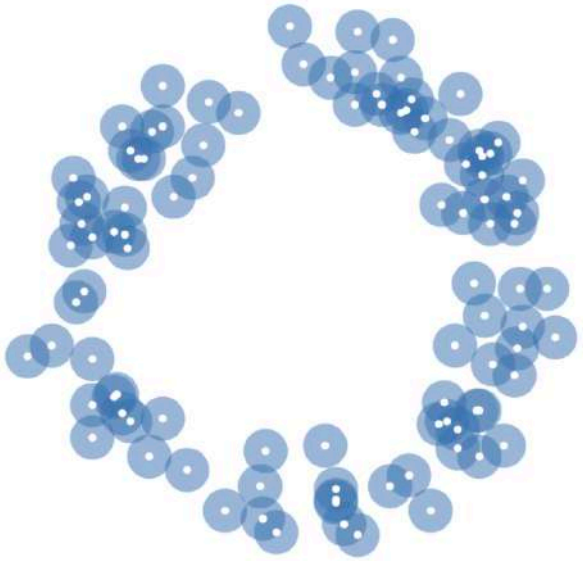
Picture credit to [Ulrich Bauer, MLSS 2019]

Persistence homologies



Picture credit to [Ulrich Bauer, MLSS 2019]

Persistence homologies



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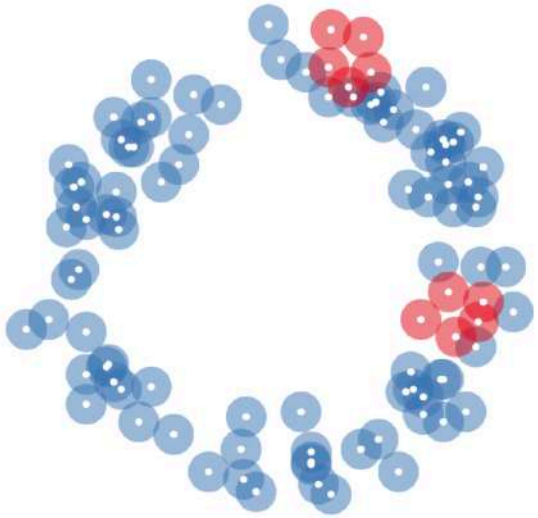
Persistence homologies



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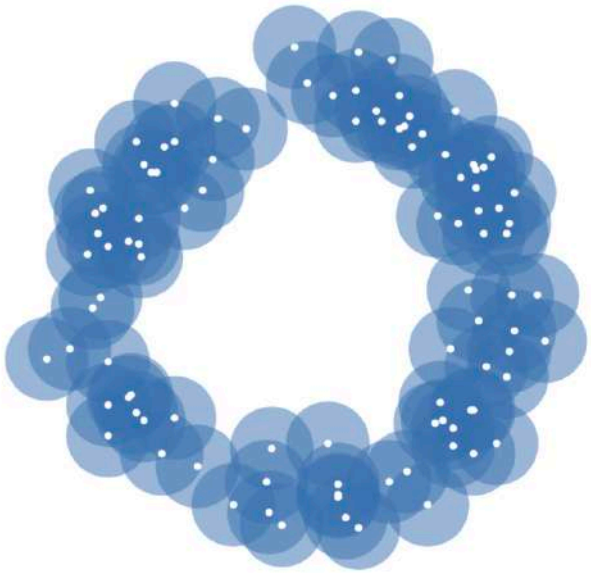

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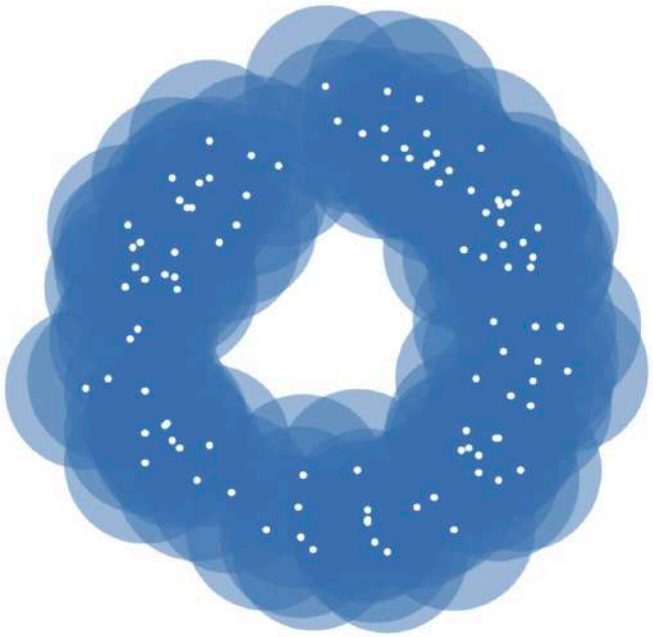
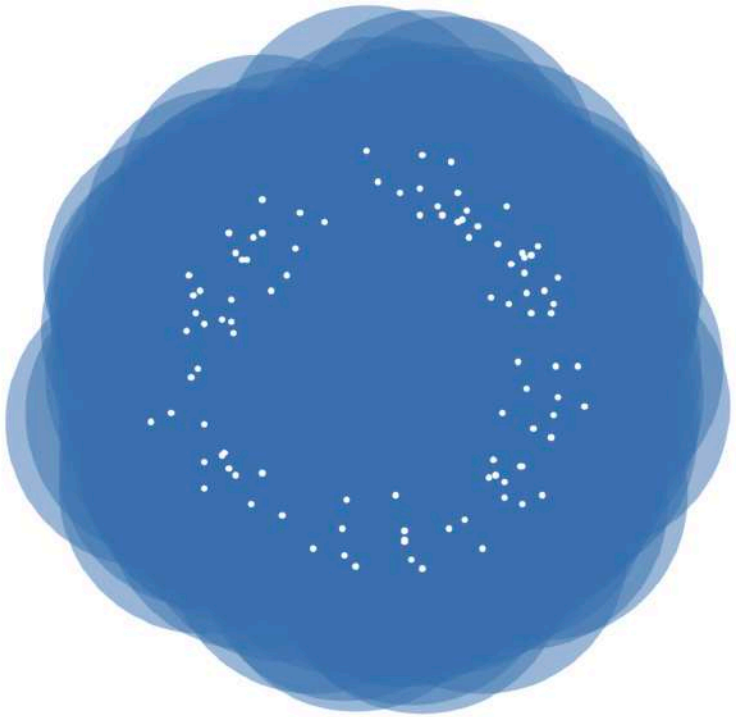
Persistence homologies



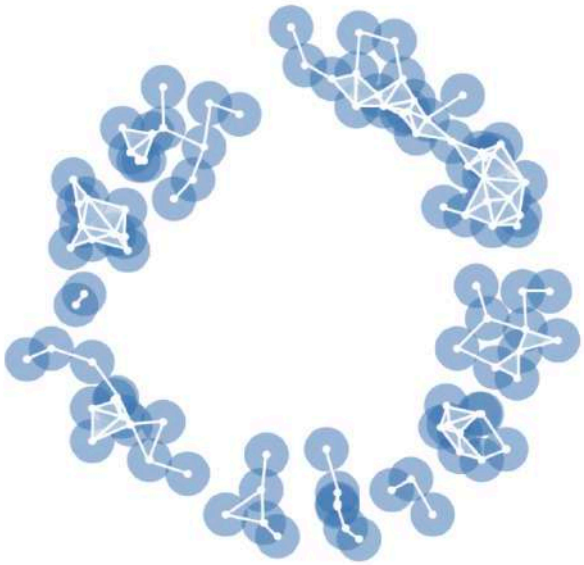
Picture credit to [Ulrich Bauer, MLSS 2019]

Persistence homologies



Picture credit to [Ulrich Bauer, MLSS 2019]

Persistence homologies



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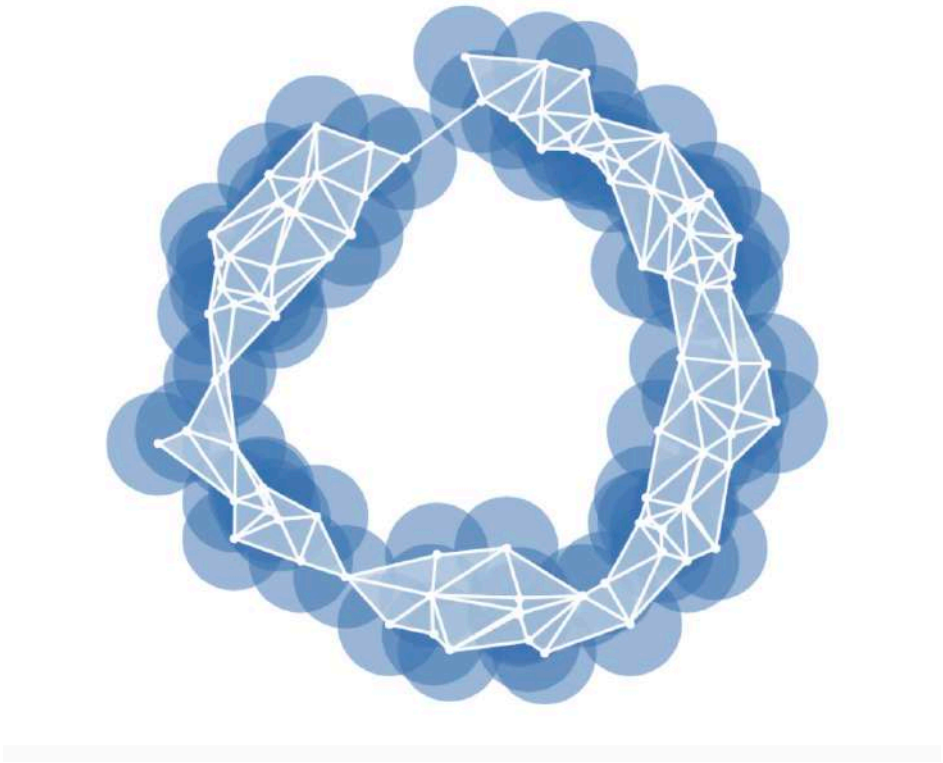
Persistence homologies



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Persistence homologies

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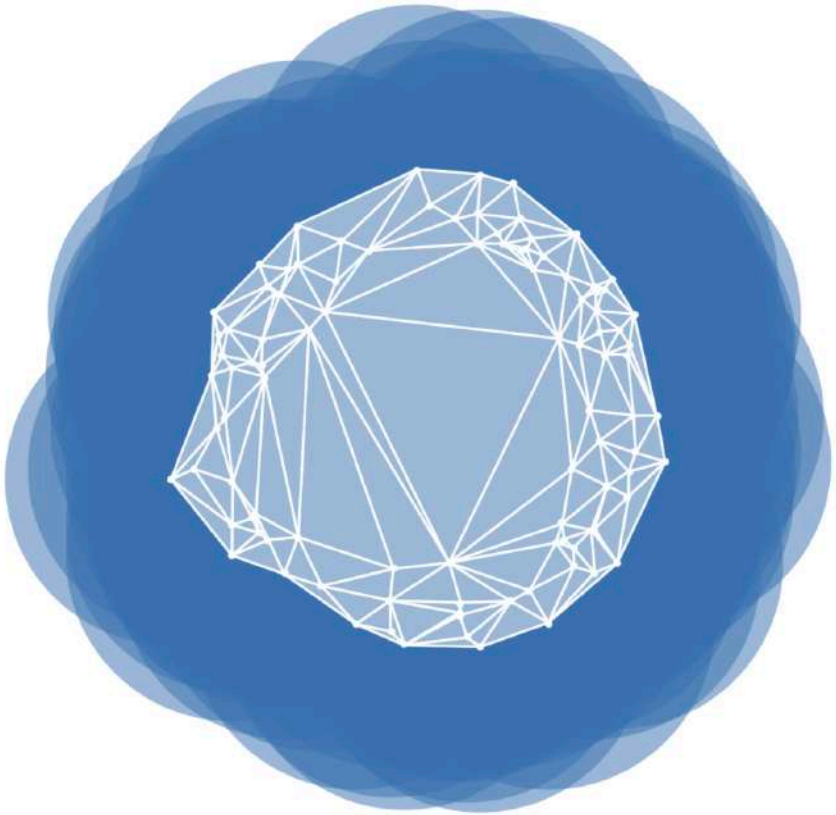
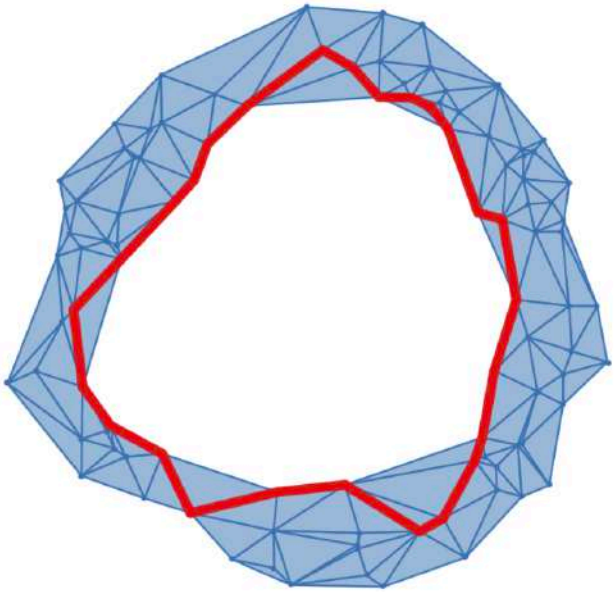
Persistence homologies



Picture credit to [Ulrich Bauer, MLSS 2019]

Persistence homologies



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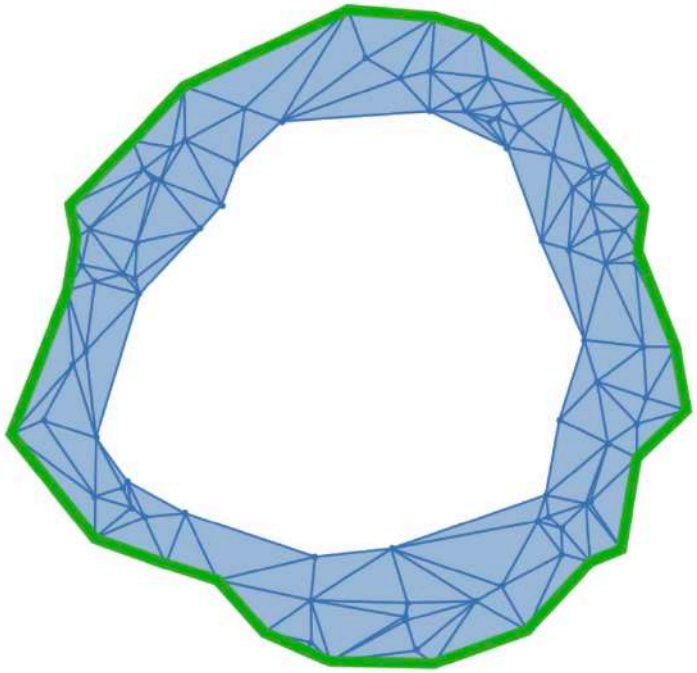

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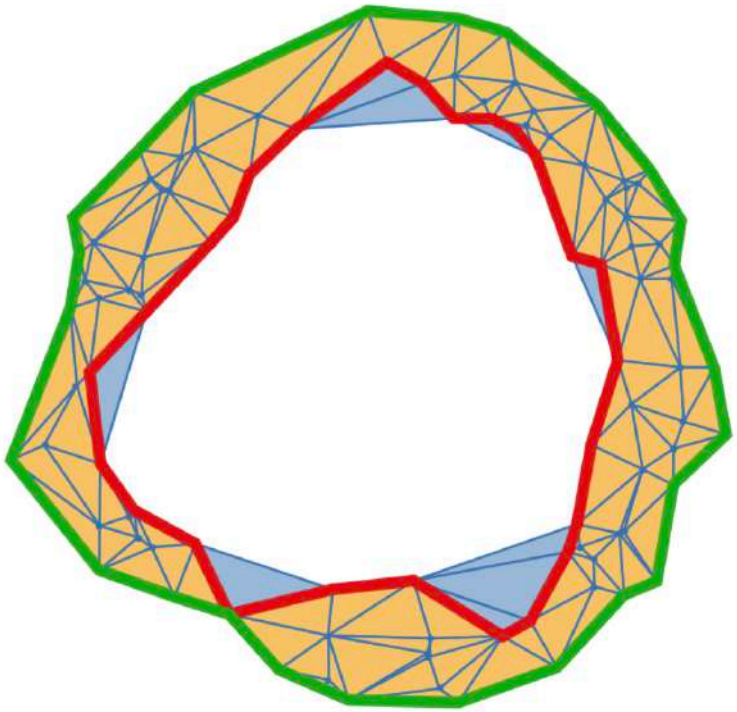

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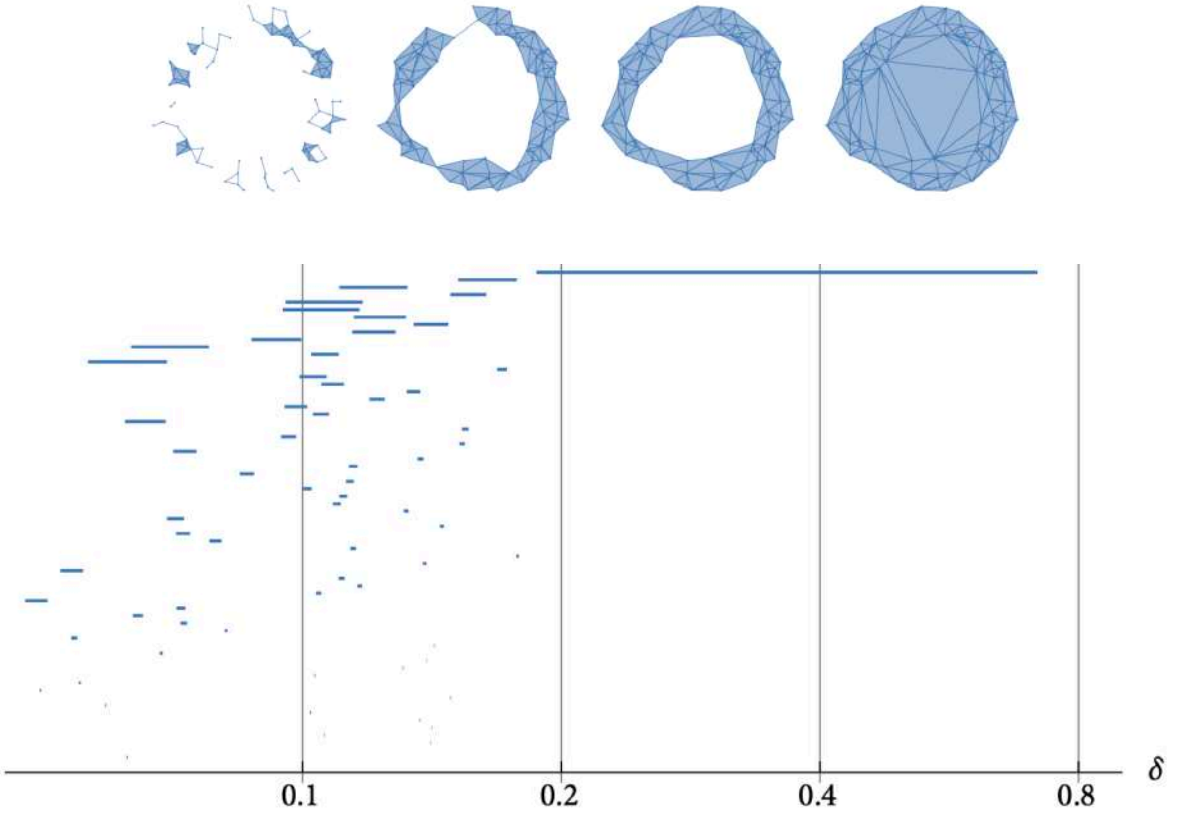

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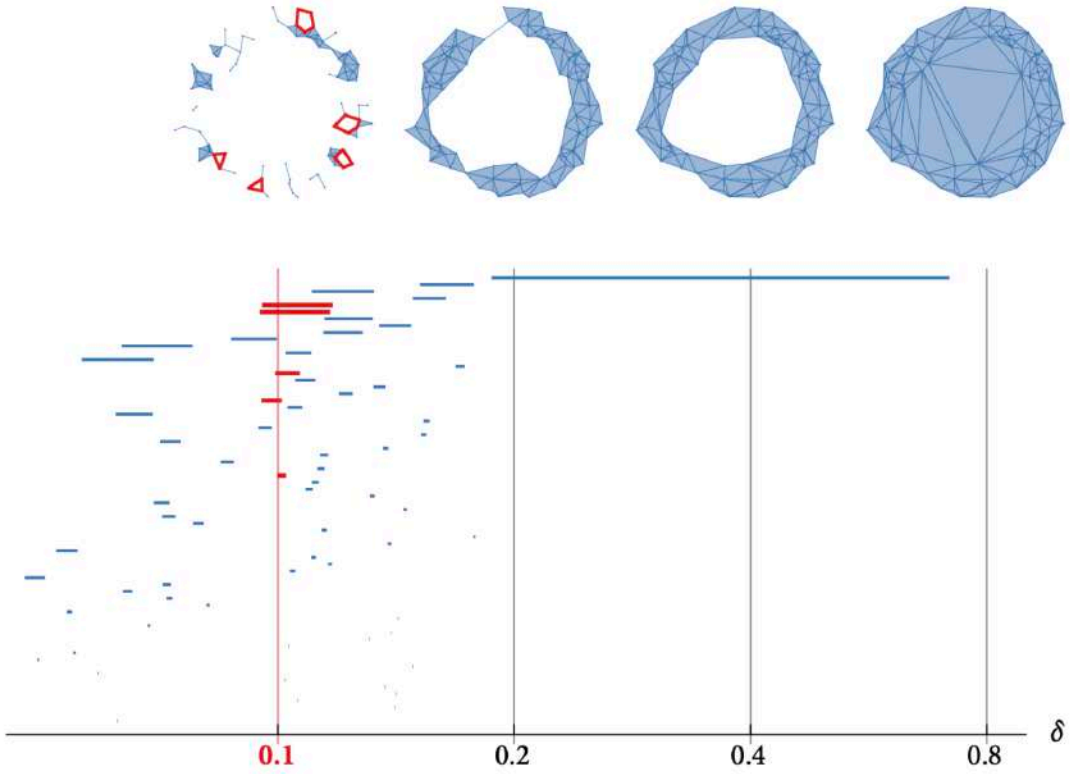
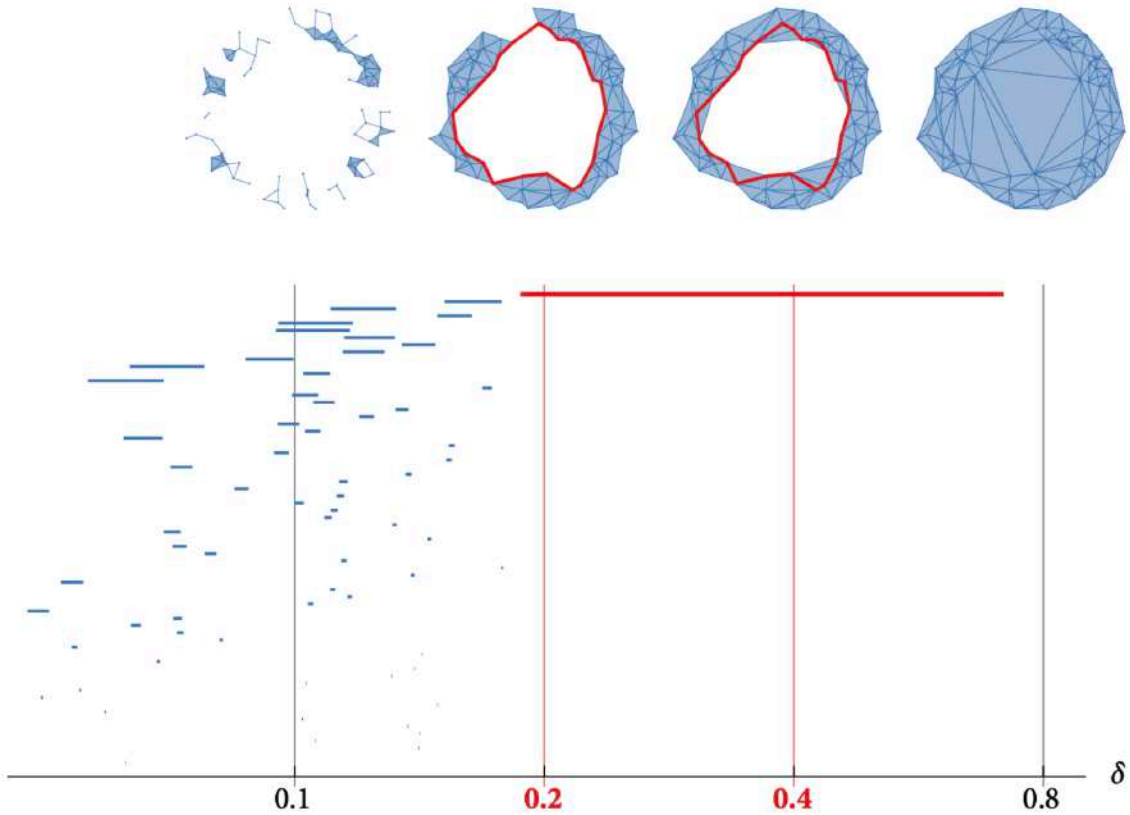
Persistence homologies



Picture credit to [Ulrich Bauer, MLSS 2019]

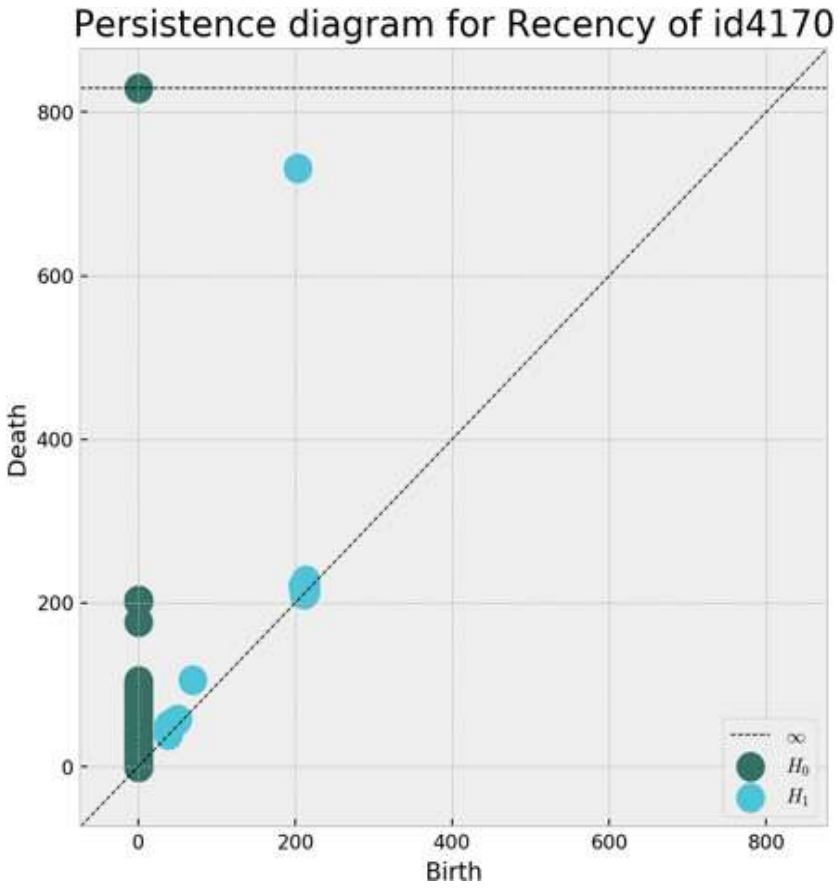
Persistence homologies



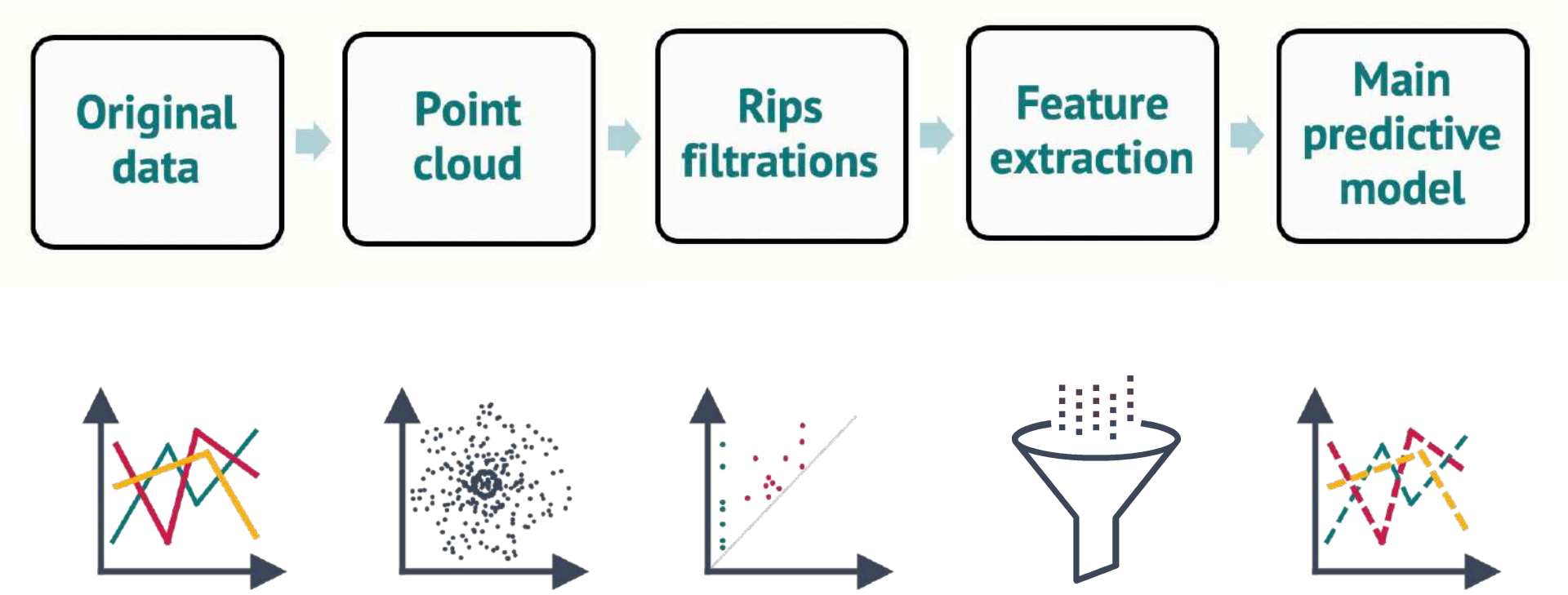
Picture credit to [Ulrich Bauer, MLSS 2019]

Persistence diagram

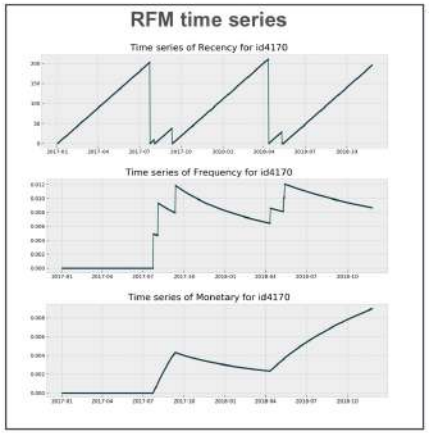
- Representation of **topological structure**
- Each point corresponds to a **homology**
- Each homology has **birth and death radius**
- Allows to extract **numerical features**

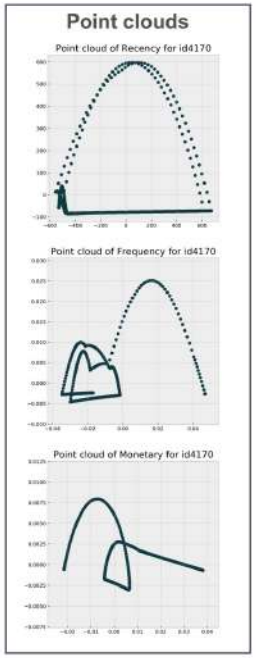


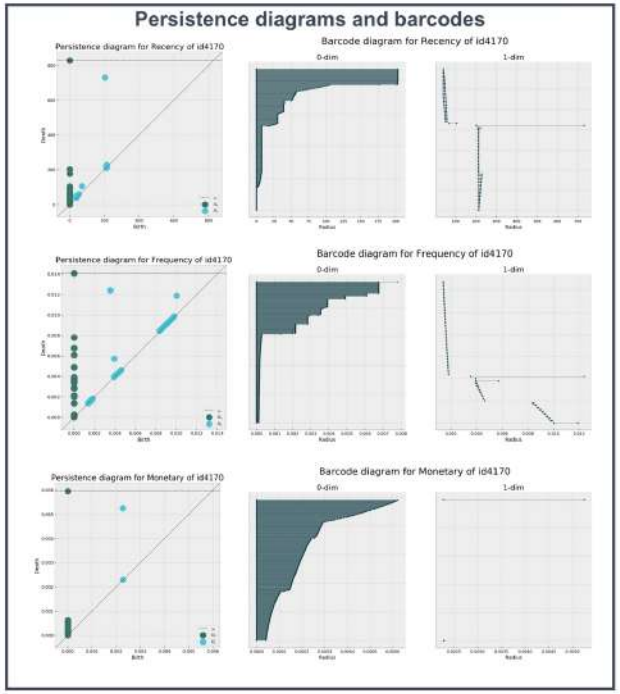
TDA pipeline

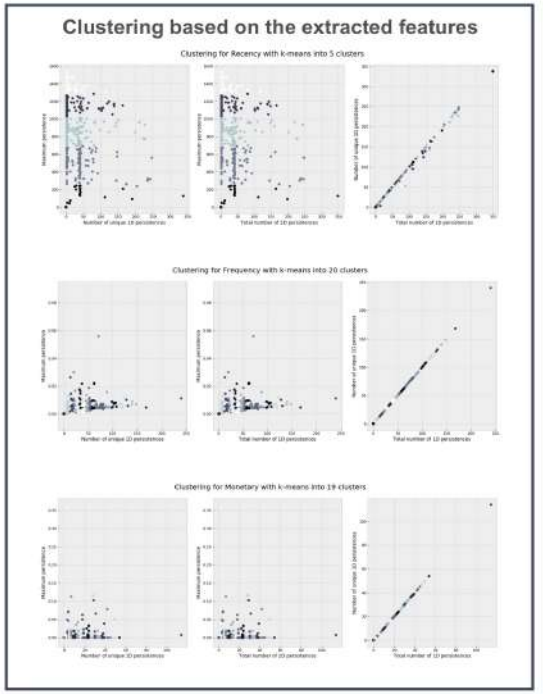


TDA RFM pipeline



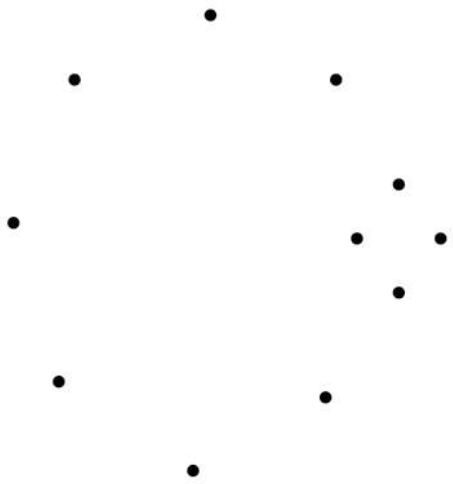






Why TDA?

- TDA has strong **mathematical foundation**
- Allows to **transform** time series into **features**, to use in common statistical tools
- **Unsupervised** learning with **no initial assumptions** on data
- TDA is **robust to noise** in data, which is especially useful for **financial data** and **client activities**



TS RFM pipeline

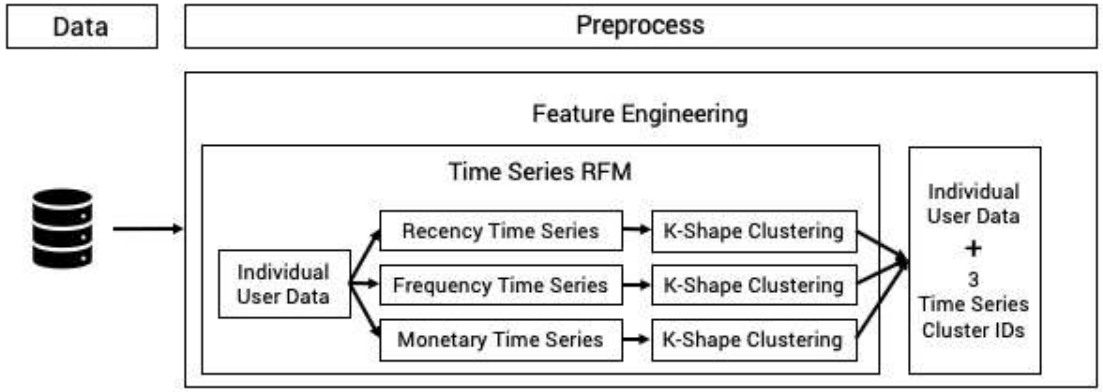
Obtain RFM time series

⇩

Apply k-shape clustering for each set of time series (RFM)

⇩

Use this clusters in further pipeline as features



Summary

RFM
(marketing person)

- Obtains RFM score as **3 numbers** for **each time series**
- Uses them in gradient boosting

TS RFM
(engineer)

- Creates **the time series of RFM scores**
- Uses **k-shape** clustering for each type of time series
- Uses this features in gradient boosting

TDA RFM

- Creates **the time series of RFM scores**
- **TDA pipeline** and feature extraction
- **k-means clustering** based on the features
- Gradient boosting on clusters

Datasets

CDnow — online store (public)

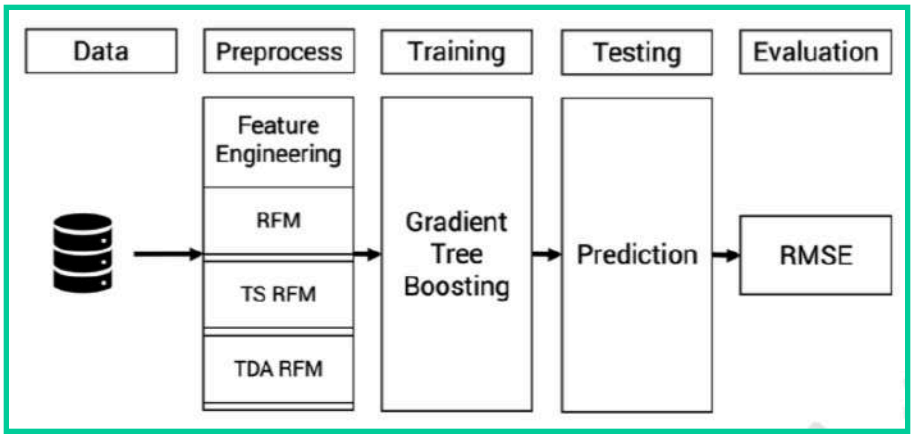
Bimbo — 2000 retail points of bakery (public)

Cloud — B2B cloud computing company (private)

Hospitality — B2B digital company in the goods procurement sector (private)

Experiments

- **Gradient boosting** to predict the value of the next activity
- $\boldsymbol{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(Predicted - Actual)^2}$



Results

- Pure **RFM** is **inferior** to all othe models
- Modified into **time series RFM** and **TDA RFM** are **superior** to others and **harshly decrease** the error
- Analysis of the **difference** between TDA and TS RFM is required

Dataset	Model	Error
CDNow	No RFM	13
	RFM	12,56
	TS RFM	**3**
	TDA RFM	18,87
Bimbo	No RFM	97
	RFM	172
	TS RFM	291
	TDA RFM	**18,97**
Cloud	No RFM	3,56
	RFM	3,98
	TS RFM	0,05
	TDA RFM	**0,03**
Hospitality	No RFM	219
	RFM	240
	TS RFM	**155**
	TDA RFM	275

Further steps

- **When** TDA is **better**
- **Too small** time series — how to **handle**
- Computational **intensity**
- **Other** statistics — which ones to use

- More applications
- Some other insights

Overview

- Intro
- Dimension Reduction Problem Statements
- PCA, MDS and Sammon Mapping, Autoencoders
- ISOMAP and LLE
- TDA for Time Series Analysis
- **References**

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