Dimension reduction for data visualization

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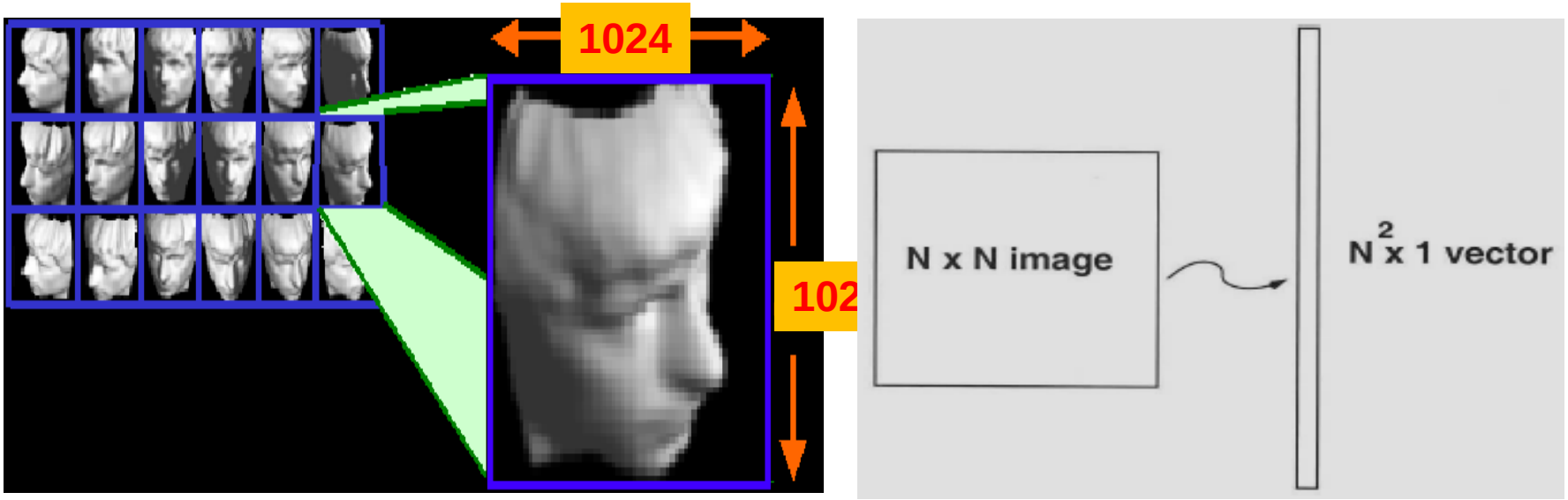
Some slides by Evgeny Burnaev are used
Also Ermek Kapushev helped during the preparation of these slides

Dimensionality Reduction Problem

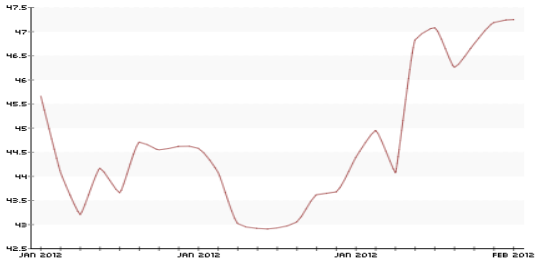
Object O ois described by p-мdimensional vector $X(O) \in \mathbb{R}^p$.
Components $X(O)$ are features O

Example 1 a face: pixel representation at a greyscale



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

Multidimensional time series



Electricity price

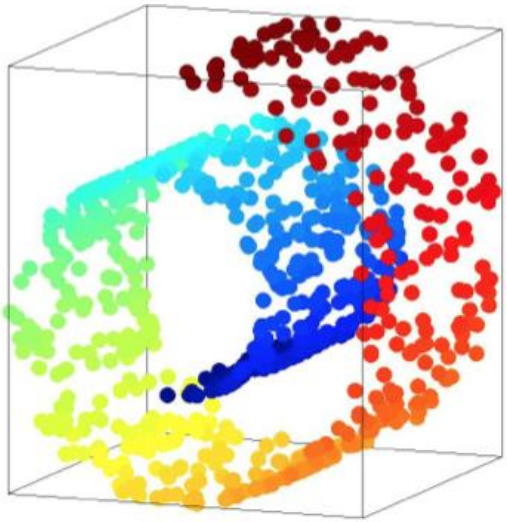
Speech recognition

- A curve f(x) is a vector

$$f = (f_1, \dots, f_p)^\top \in \mathbb{R}^p, f_j = f(t_j)$$

Example 2 (MNIST)

Example 3 Toy “Swiss Roll” Problem



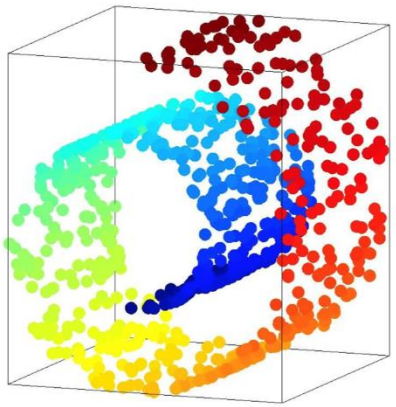
We need dimension reduction

- High dimensionality $\boldsymbol{p}$ of $X(\boldsymbol{O})$ is critical for efficient learning
- We can visualize only in 2D/3D

- Dimension Reduction = construct reduced dimension representation $y(\boldsymbol{O}) \in \mathbb{R}^q, q \ll p$, of $\boldsymbol{O}$ without "significant loss of information"

X → X' S.T.
dim(X') << dim(X)

uncovers the intrinsic dimensionality (invertible)



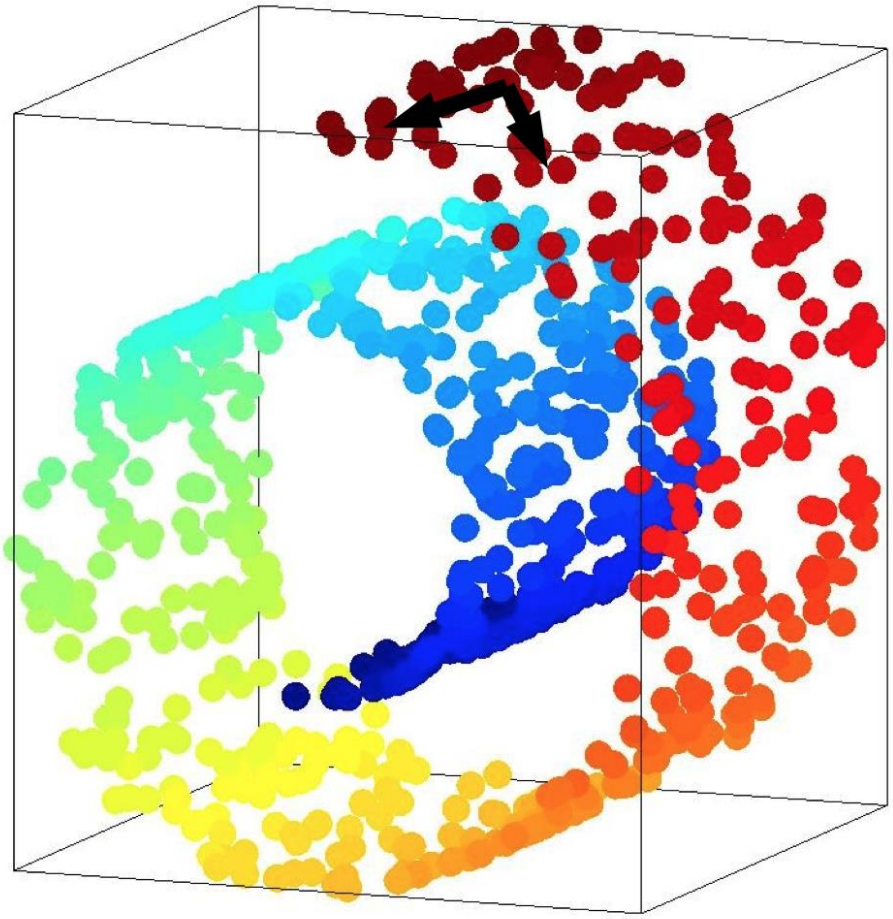
There are various purposes for usage of dimension reduction

- **Visualization**
- Data compression
- “curse of dimensionality”
- De-noising
- Reasonable distance metrics

What is “a smart distance”?

Деформация

What is “a smart distance”?



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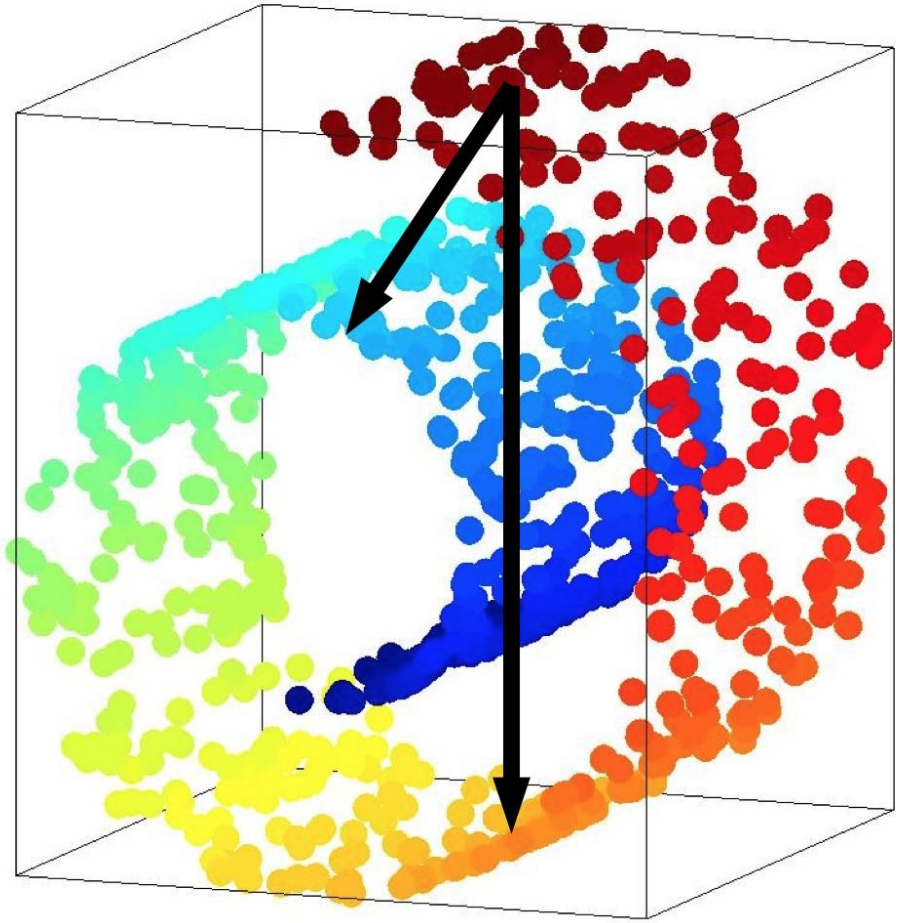
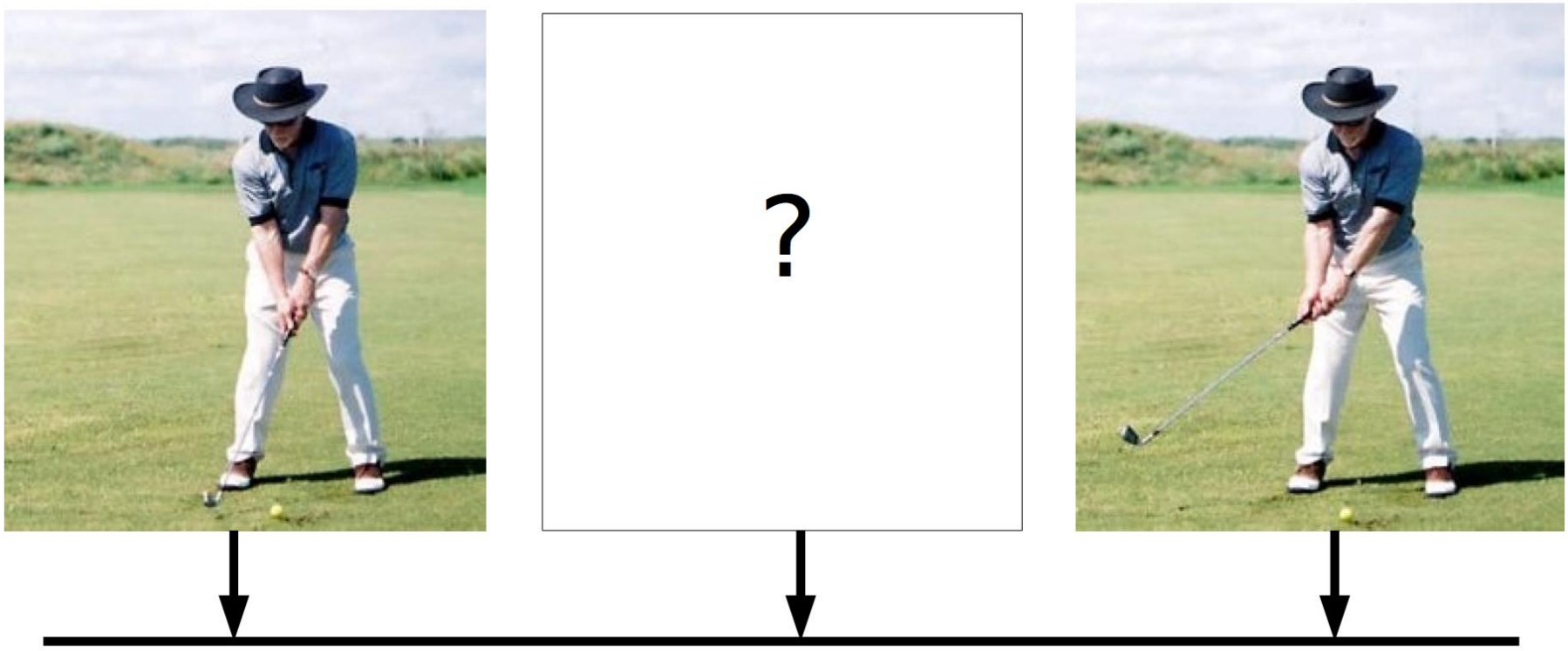
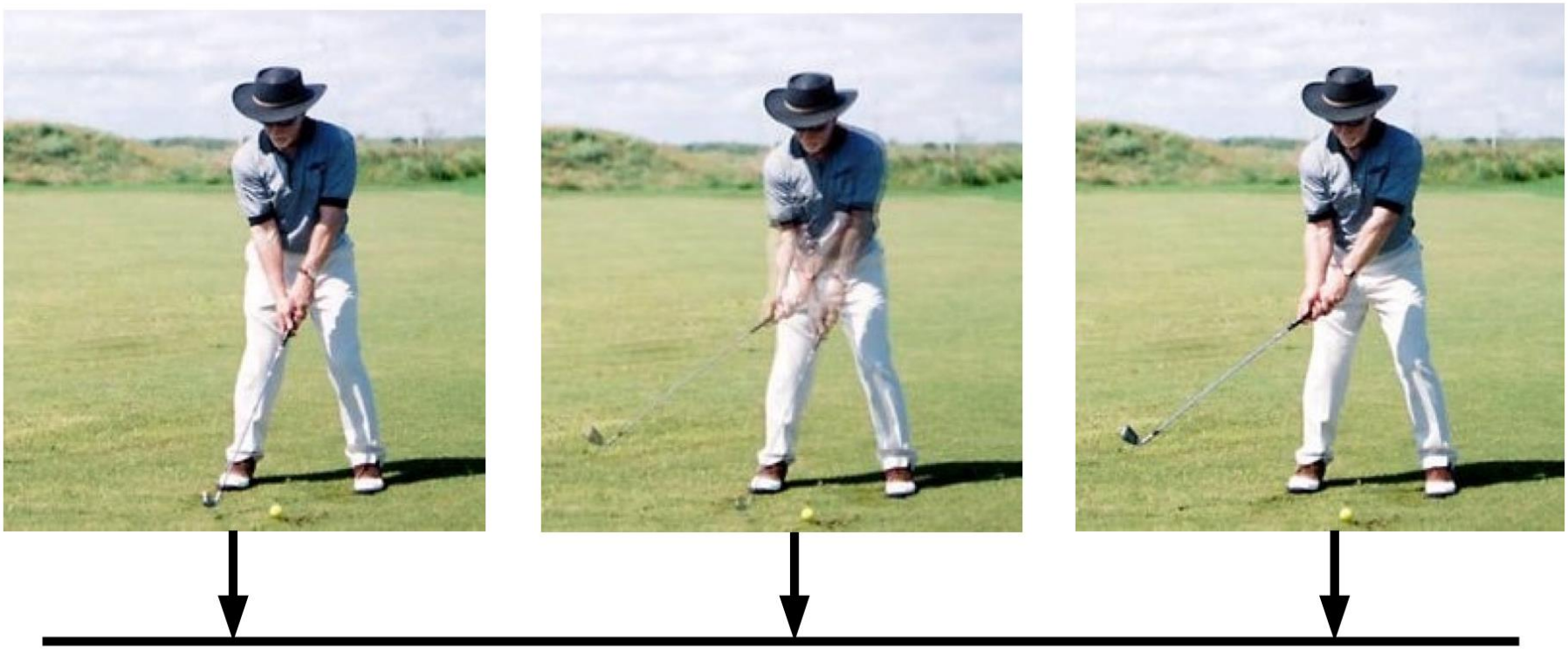
What is “a smart distance”?



Smart distance

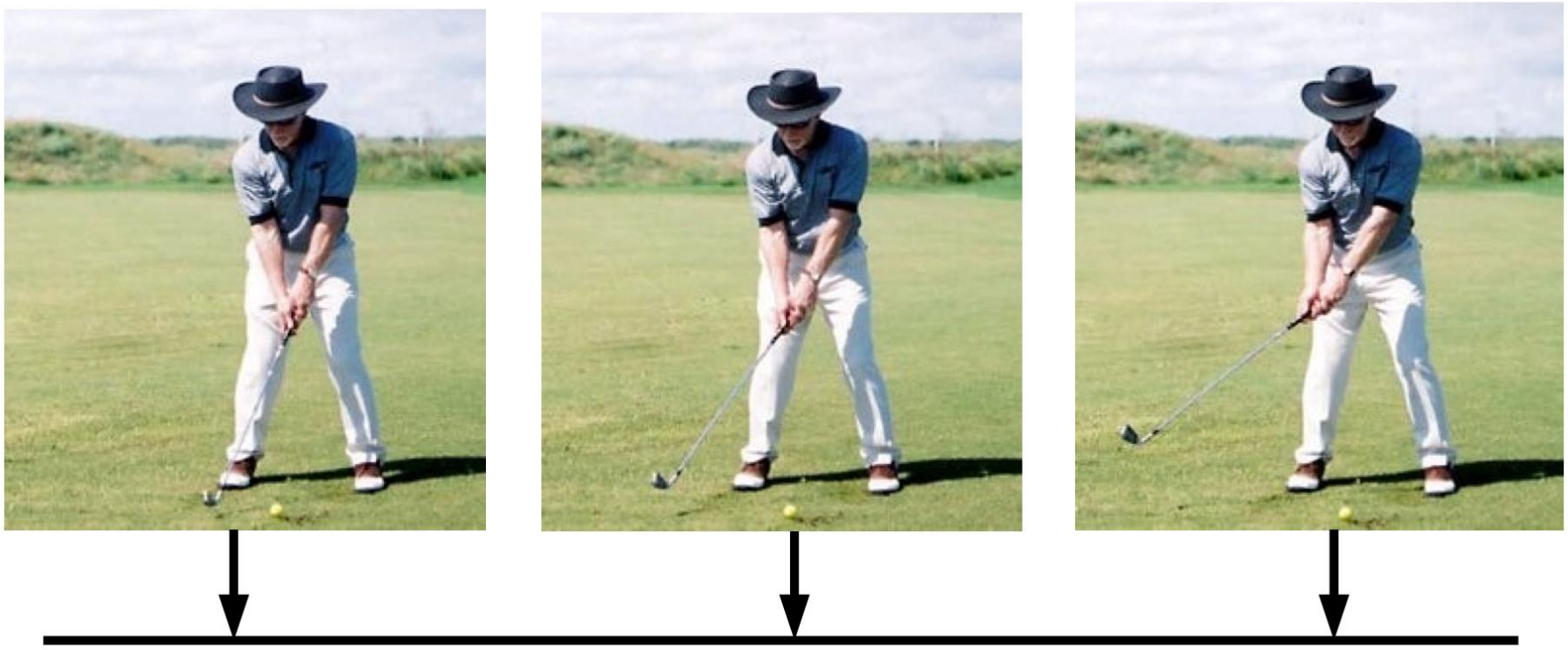


Smart distance



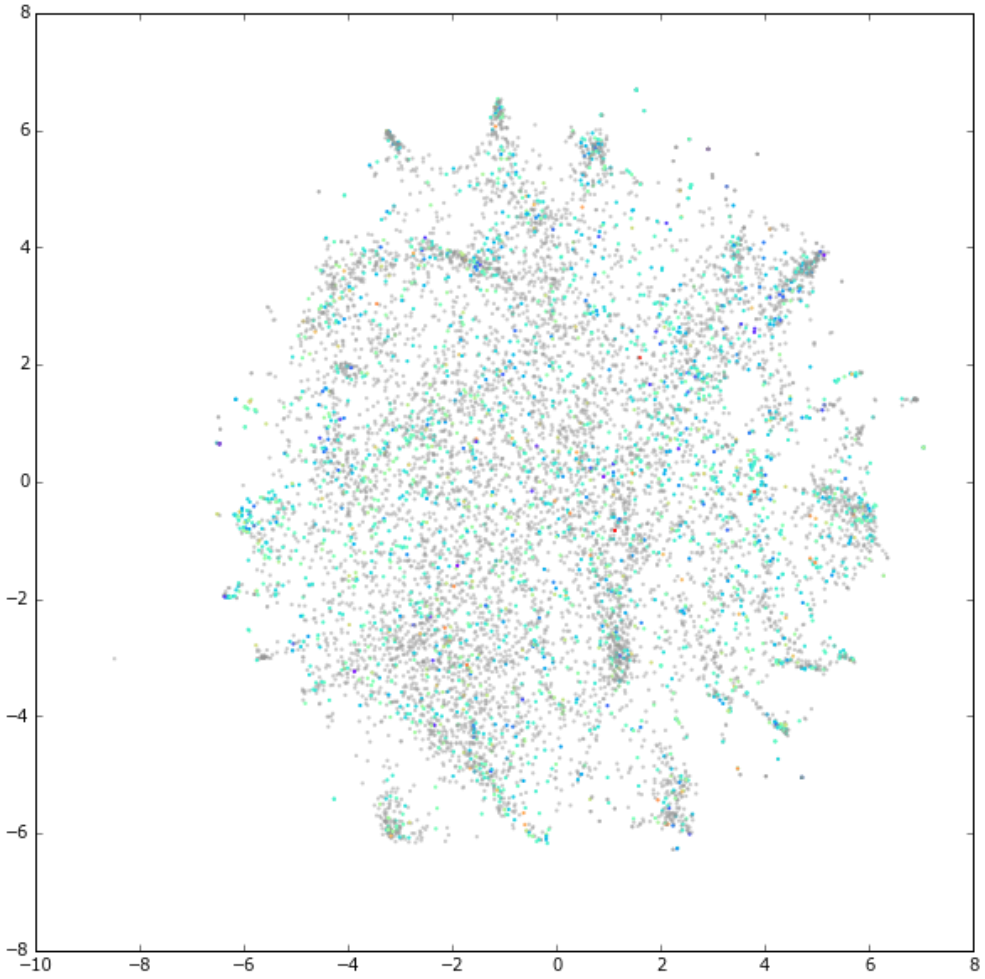
Linear interpolation

Smart distance



Manifold distance

Embedding of images



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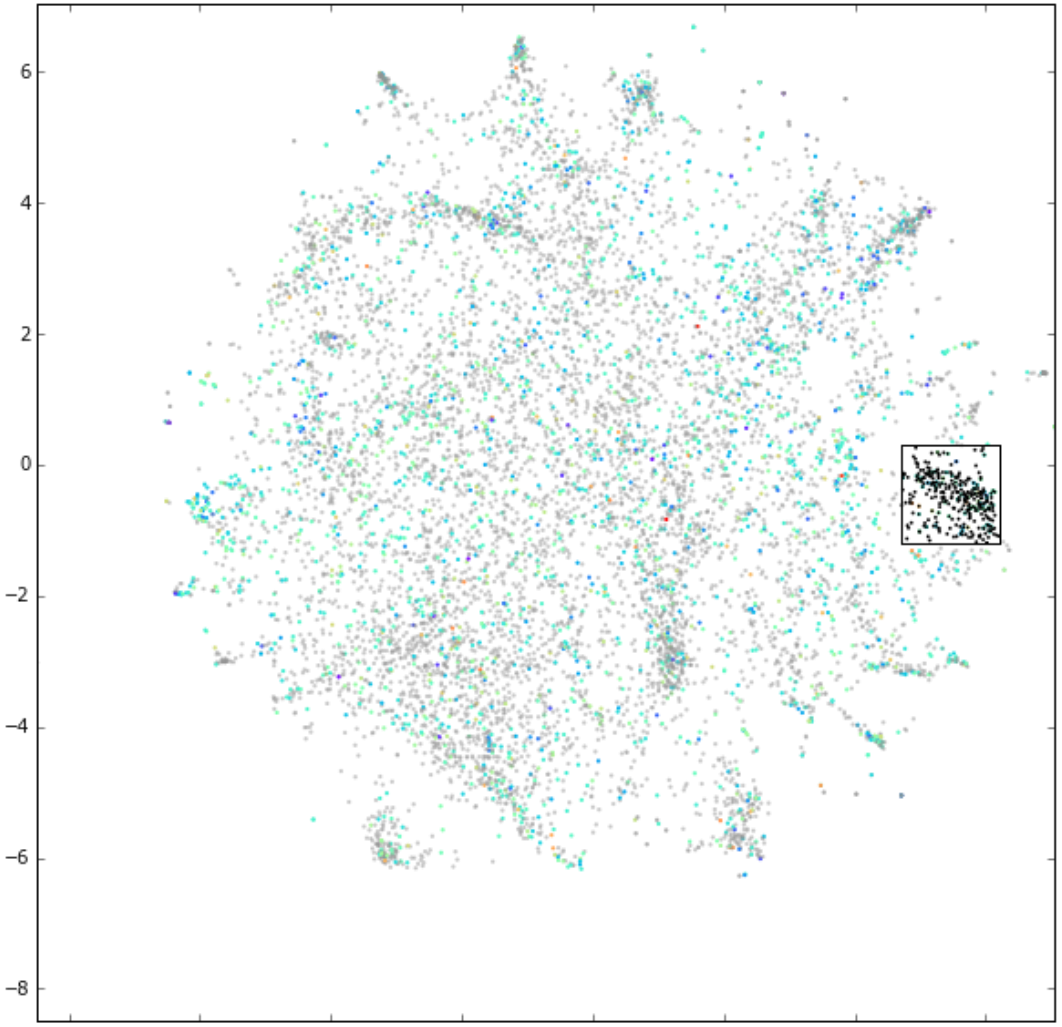

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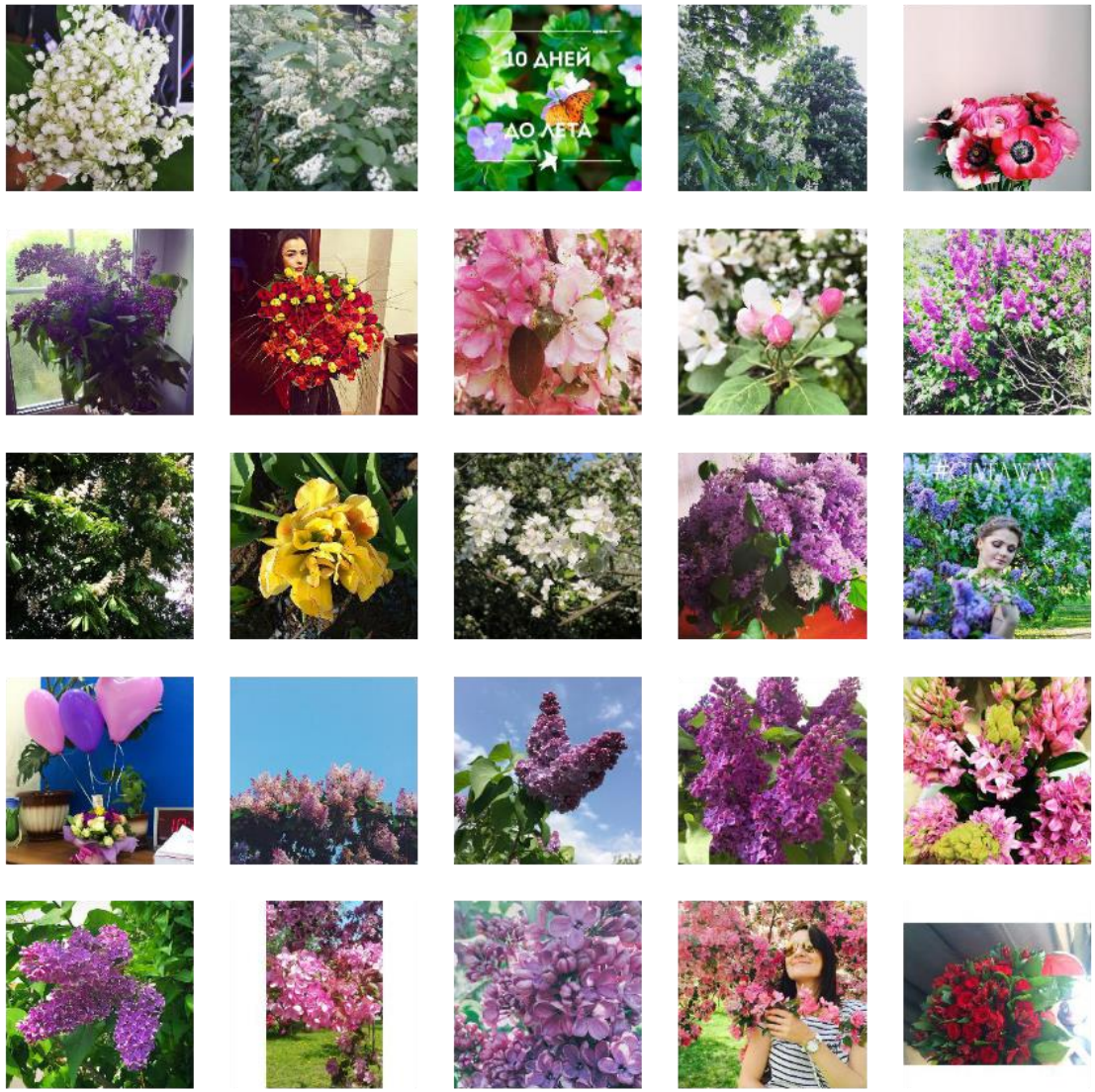

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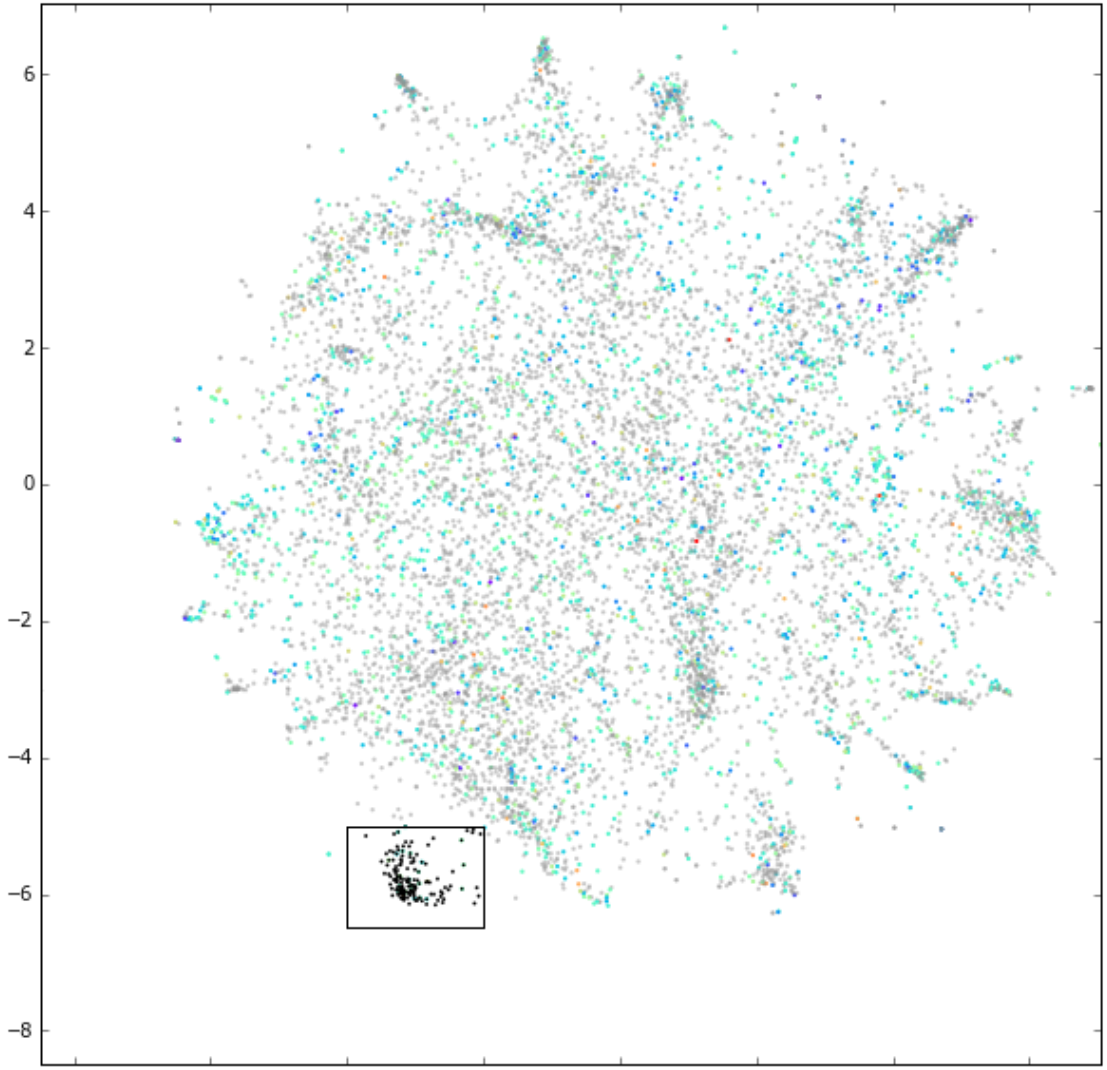

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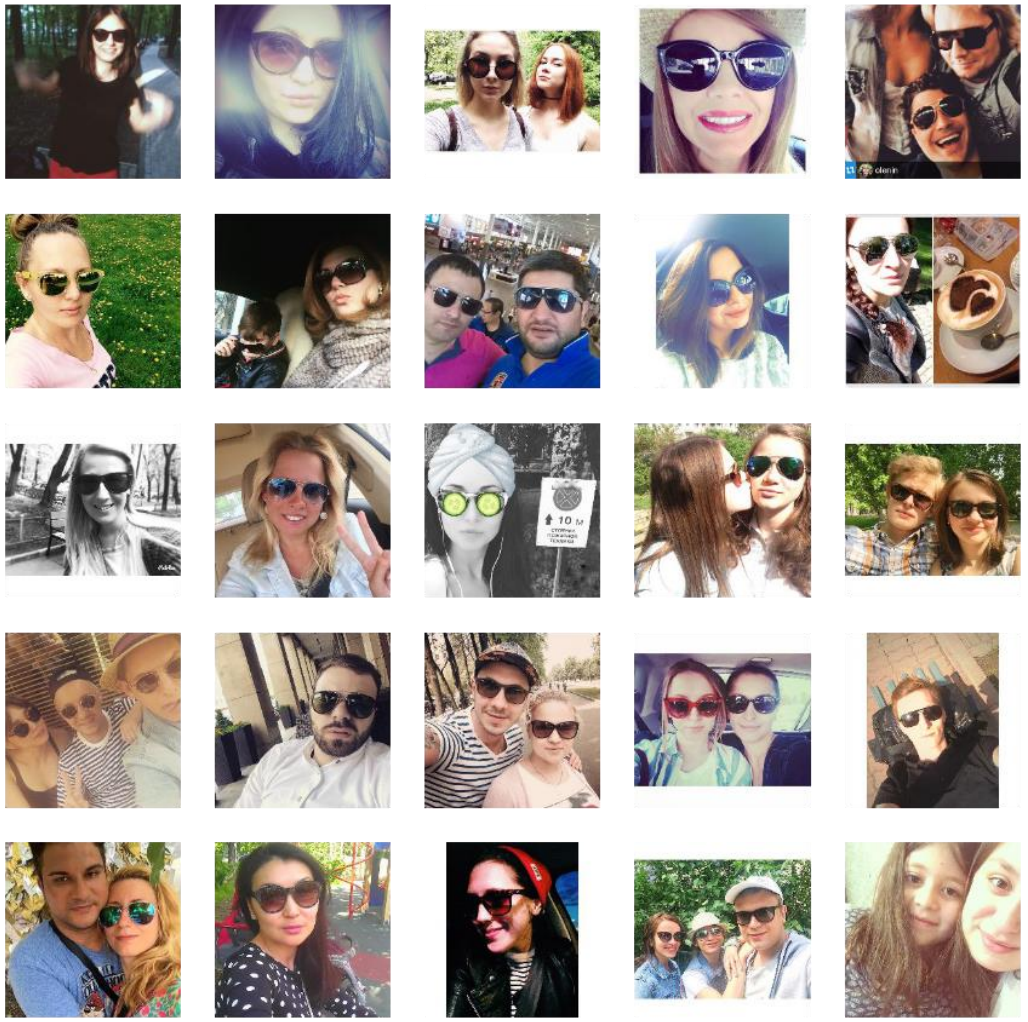

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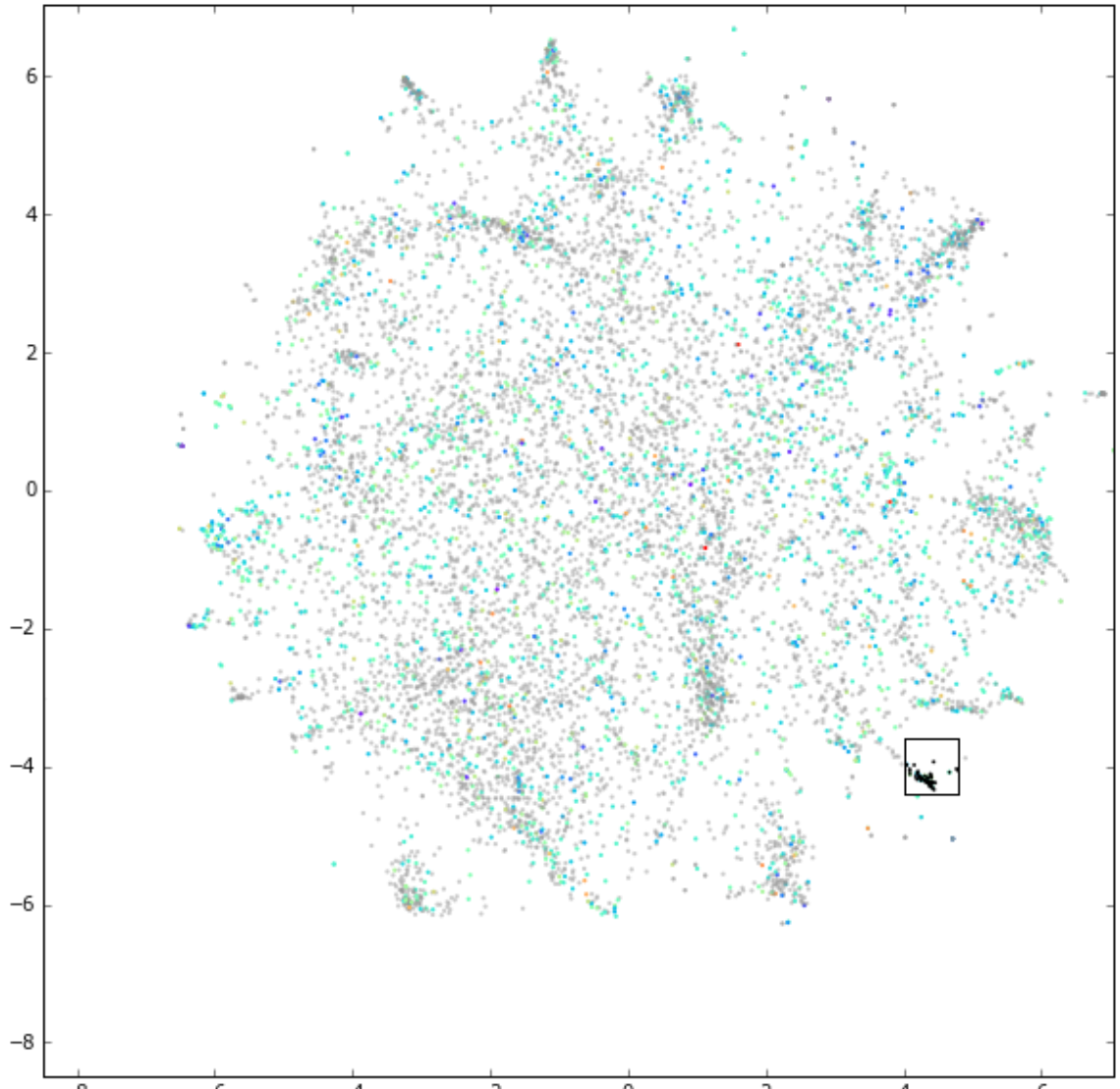
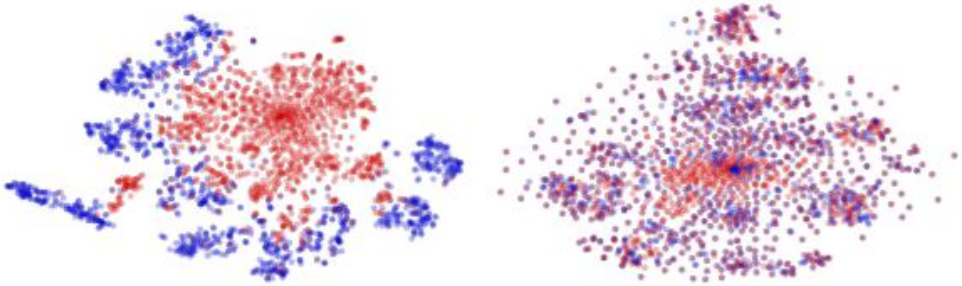


Embedding of images

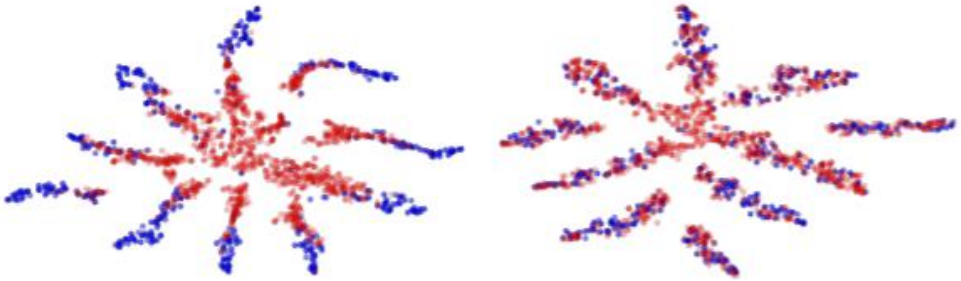
How and **how well** does our domain adaptation work?

MNIST → MNIST-M: top feature extractor layer



(a) Non-adapted (b) Adapted

SYN NUMBERS → SVHN: last hidden layer of the label predictor



(a) Non-adapted (b) Adapted

Ganin, Yaroslav, and Victor Lempitsky. "Unsupervised domain adaptation by backpropagation." *arXiv preprint arXiv:1409.7495* (2014).

MSCVS2011: V. Lempitsky, Skoltech - Writing a computer vision paper https://youtu.be/-Oq8AHIC92A

How to Write a Great Research Paper, S.P. Jones, Microsoft Research. https://youtu.be/WP-FkUaOcOM

Typical scheme for dimension reduction

1. Construct a loss function $L(y_1, \dots, y_n)$. E.g. for Multi Dimensional Scaling, MDS

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

2. Optimize loss function
3. Visually analyze results

Popular embedding methods:

- Principal Component Analysis (PCA)
- Kernel PCA, KPCA
- Locally Linear Embedding, LLE; Conformal Eigenmaps
- Laplacian Eigenmaps, Hessian Eigenmaps
- ISOmetric MAPing, ISOMAP
- Local Tangent Space Alignment, LTSA

Principal Component Analysis (PCA)

Problem: in $\mathbb{R}^p$ find an affine subspace

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

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

$$\boldsymbol{X}_n = \{X_i, i = 1, 2, \dots, n\} \subset \mathbb{R}^p.$$

В PCA: "best" = minimizes $\boldsymbol{x_0}, \{\boldsymbol{e_1}, \boldsymbol{e_2}, \dots, \boldsymbol{e_q}\} \subset \mathbb{R}^{\mathrm{p}}$

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

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

Principal Component Analysis (PCA)

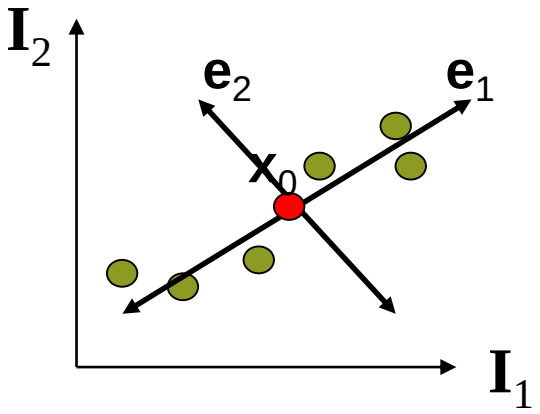
- x_{mean} – empirical mean $\{X_i, i = 1, 2, \dots, n\}$,
- $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \dots, \boldsymbol{e}_p\}$ – eigenvectors of $(p \times p)$-covariance matrix

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

They form an orthonormal basis in $\mathbb{R}^p$

Example: $p = 2, q = 1$

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



Solution:

- $x_0 = x_{mean}$,
- $L(q) = x_0 \oplus Span(\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_q)$, the eigenvectors $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_q\}$ of the matrix Σ correspond to q largest eigenvalues

PCA solves the full dimension reduction problem

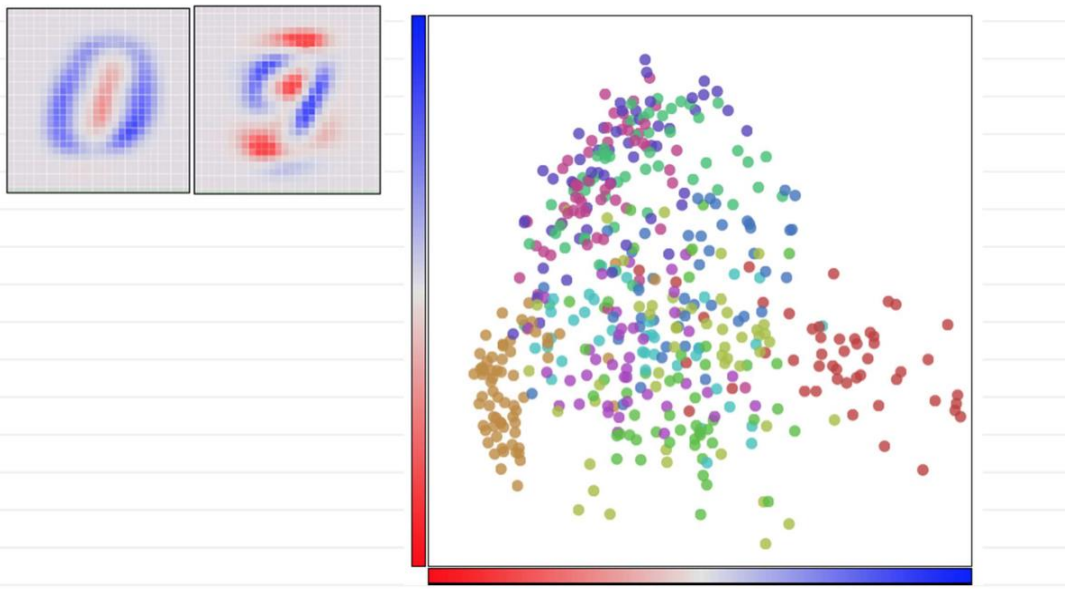
Dimension reduction:

$$X \in \mathbb{R}^p \to h(X) = \left(y_1(X_1), y_2(X_2), \ldots, y_q(X_q)\right)^T \in \mathbb{R}^q$$

Reconstruction:

$$\boldsymbol{y} = \left(y_1, y_2, \ldots, y_q\right)^T \in \mathbb{R}^q \to g(y) = x_0 + y_1 \times \boldsymbol{e}_1 + y_2 \times \boldsymbol{e}_2 + \ldots + y_q \times e_q$$

PCA for MNIST



http://colah.github.io/posts/2014-10-Visualizing-MNIST/

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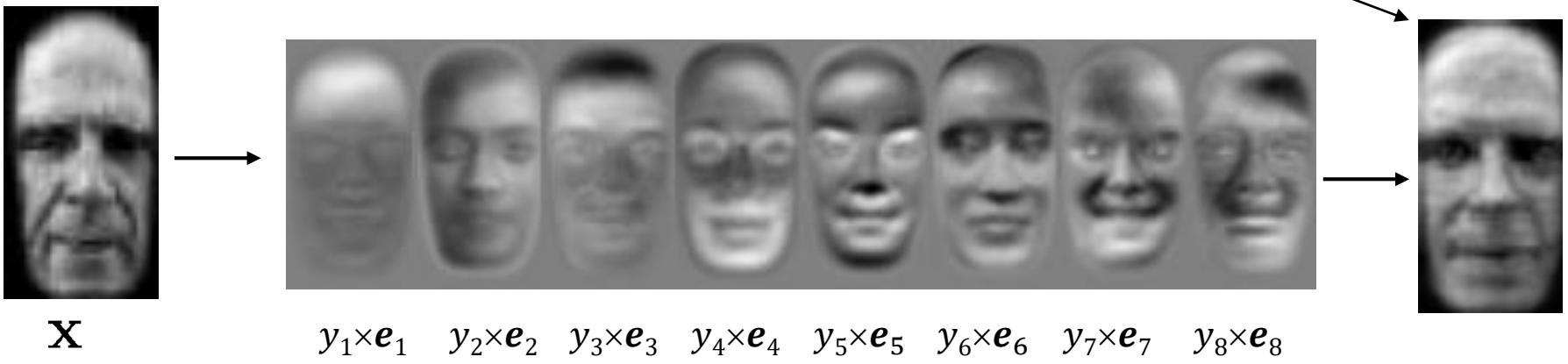
PCA for face recognition

- Eigenvectors $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_p \in \mathbb{R}^p$ for faces space: $p \sim 106$

$$X = \Big(\underbrace{(X - x_0, \boldsymbol{e}_1)}_{y_1}, \ldots, \underbrace{\big(X - x_0, \boldsymbol{e}_p\big)}_{y_p}\Big)^T \in \mathbb{R}^p$$

- Select $q \sim 102$ eigenvectors $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_q \in \mathbb{R}^p$

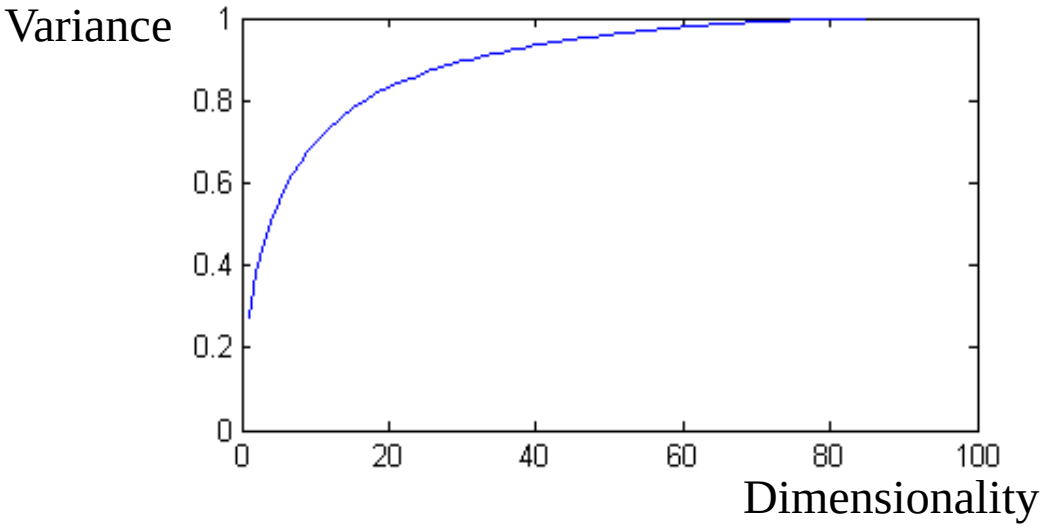
$$X^* \approx x_0 + y_1 \times \boldsymbol{e}_1 + y_2 \times \boldsymbol{e}_2 + \ldots + y_q \times \boldsymbol{e}_q$$



$\mathbf{X}$ $\quad y_1{\times}\boldsymbol{e}_1 \quad y_2{\times}\boldsymbol{e}_2 \quad y_3{\times}\boldsymbol{e}_3 \quad y_4{\times}\boldsymbol{e}_4 \quad y_5{\times}\boldsymbol{e}_5 \quad y_6{\times}\boldsymbol{e}_6 \quad y_7{\times}\boldsymbol{e}_7 \quad y_8{\times}\boldsymbol{e}_8$

PCA for face recognition

From the left to the right: reconstruction using 84, 40, 20, 3, 2, and 1 dimensions.



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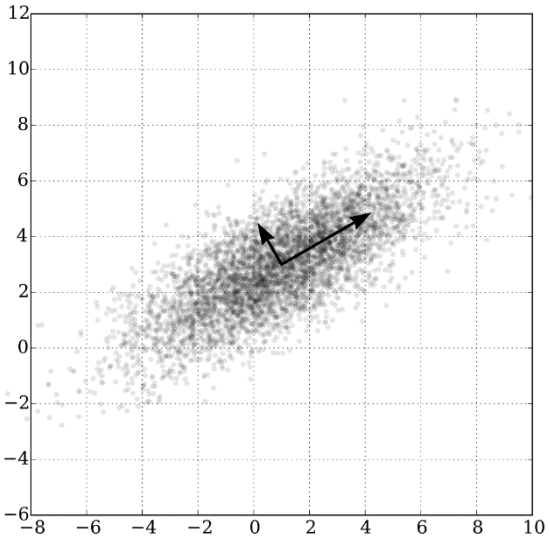
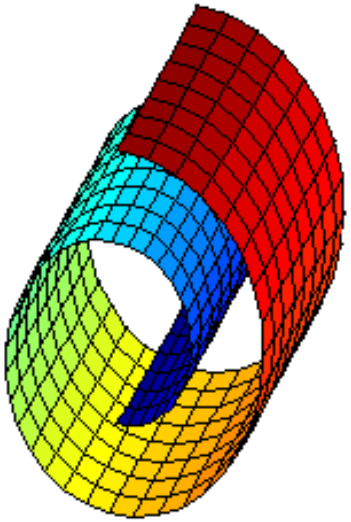
PCA for face recognition

- PCA is a linear approach to dimension reduction
- It was quite popular before 2000s
- The idea is to find the best projections

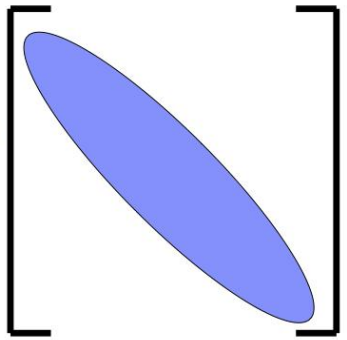


PCA fails in a nonlinear setting

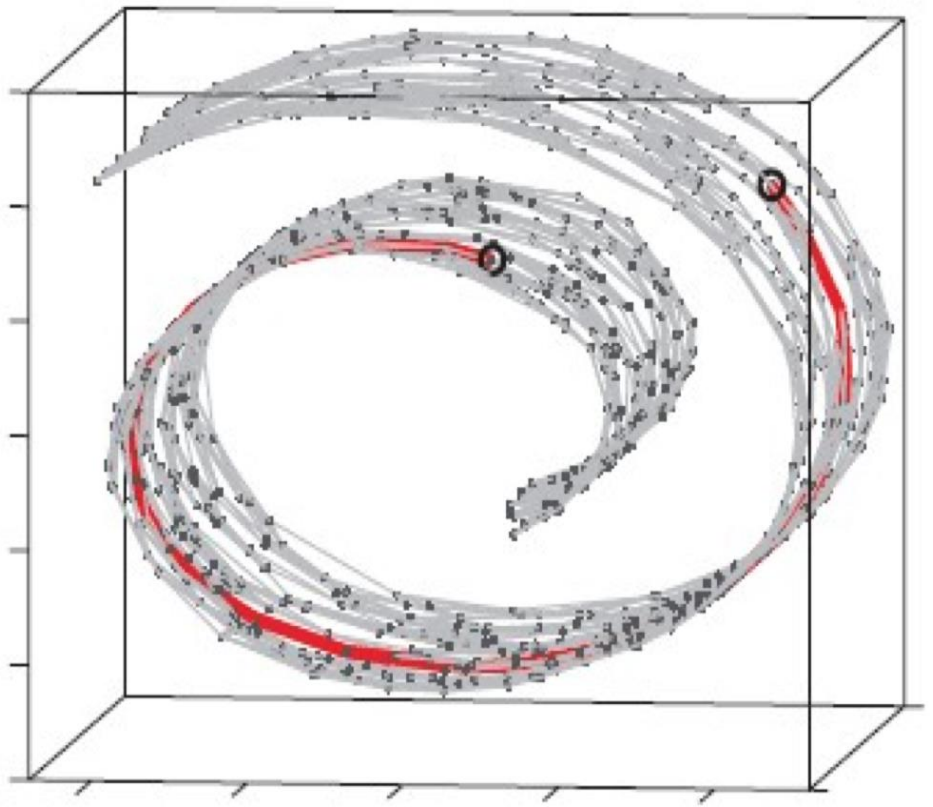


ISOMAP

1. Construct sparse k nearest neighbors graph

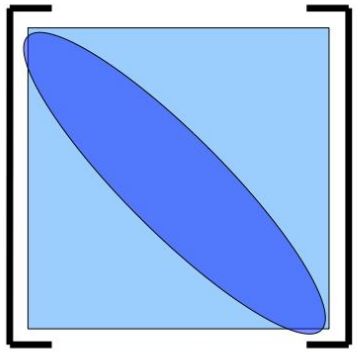
$D_g =$ 

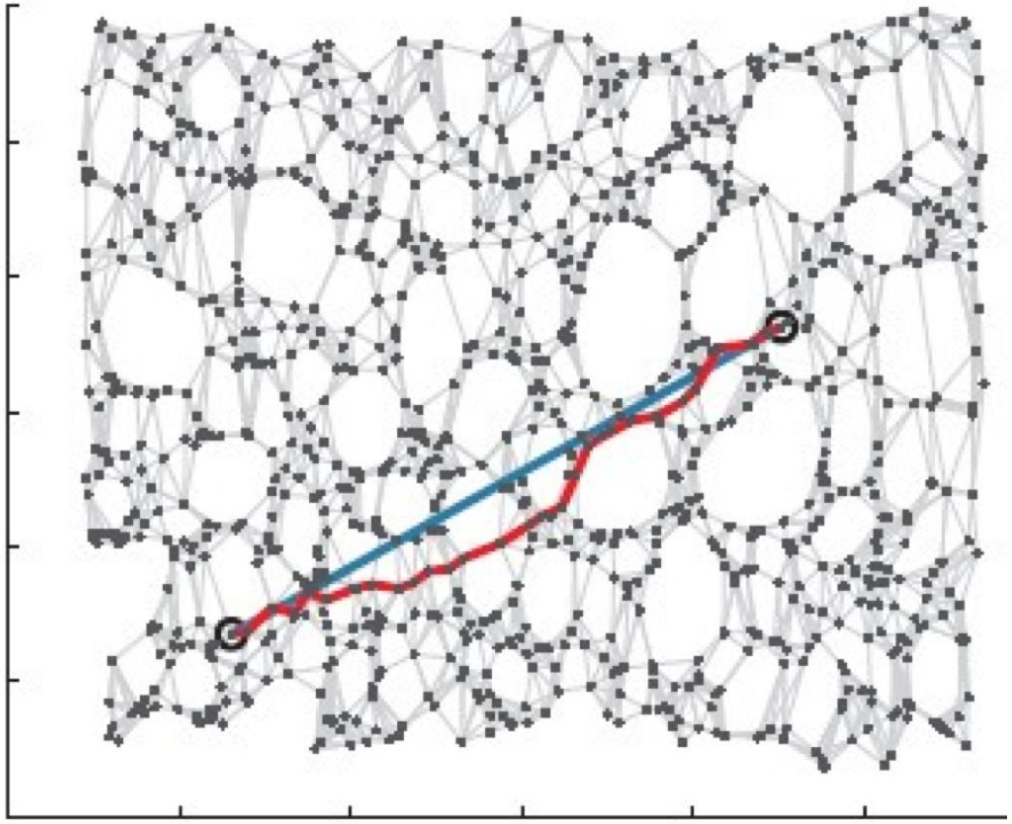
(distance matrix is sparse)



ISOMAP

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

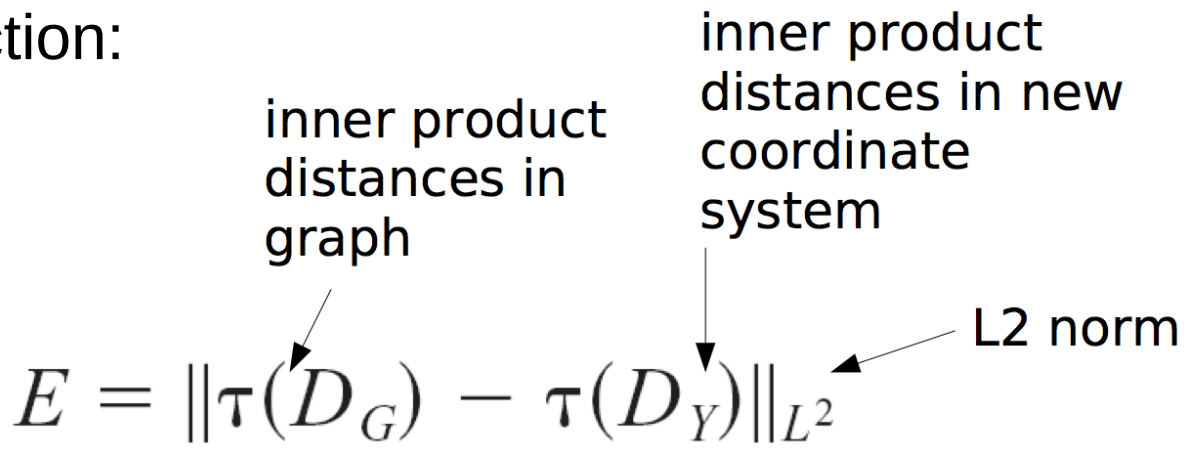
$D_g =$ 



ISOMAP

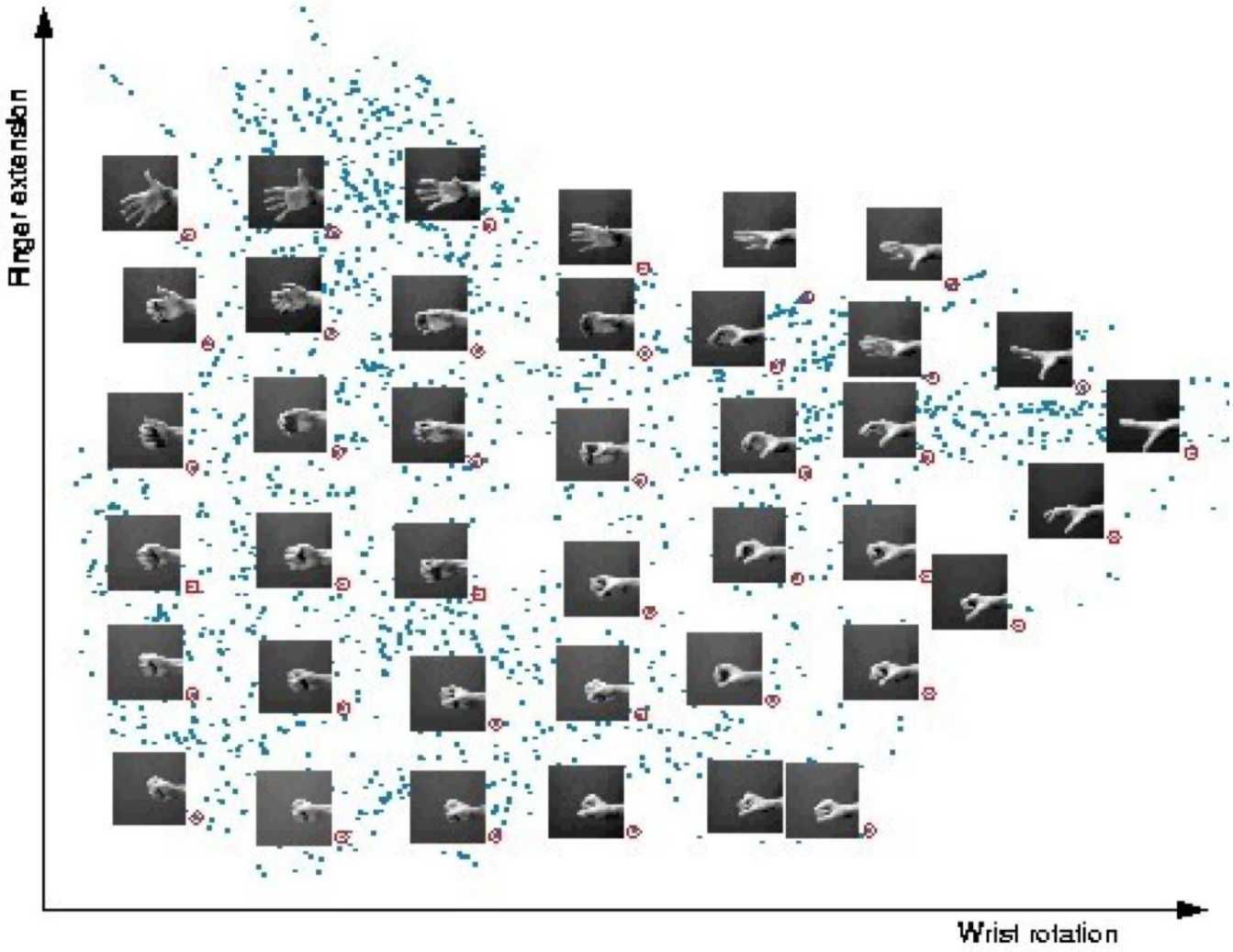
3. MDS: find low-dimensional embedding, that preserves distance matrix

Error function:

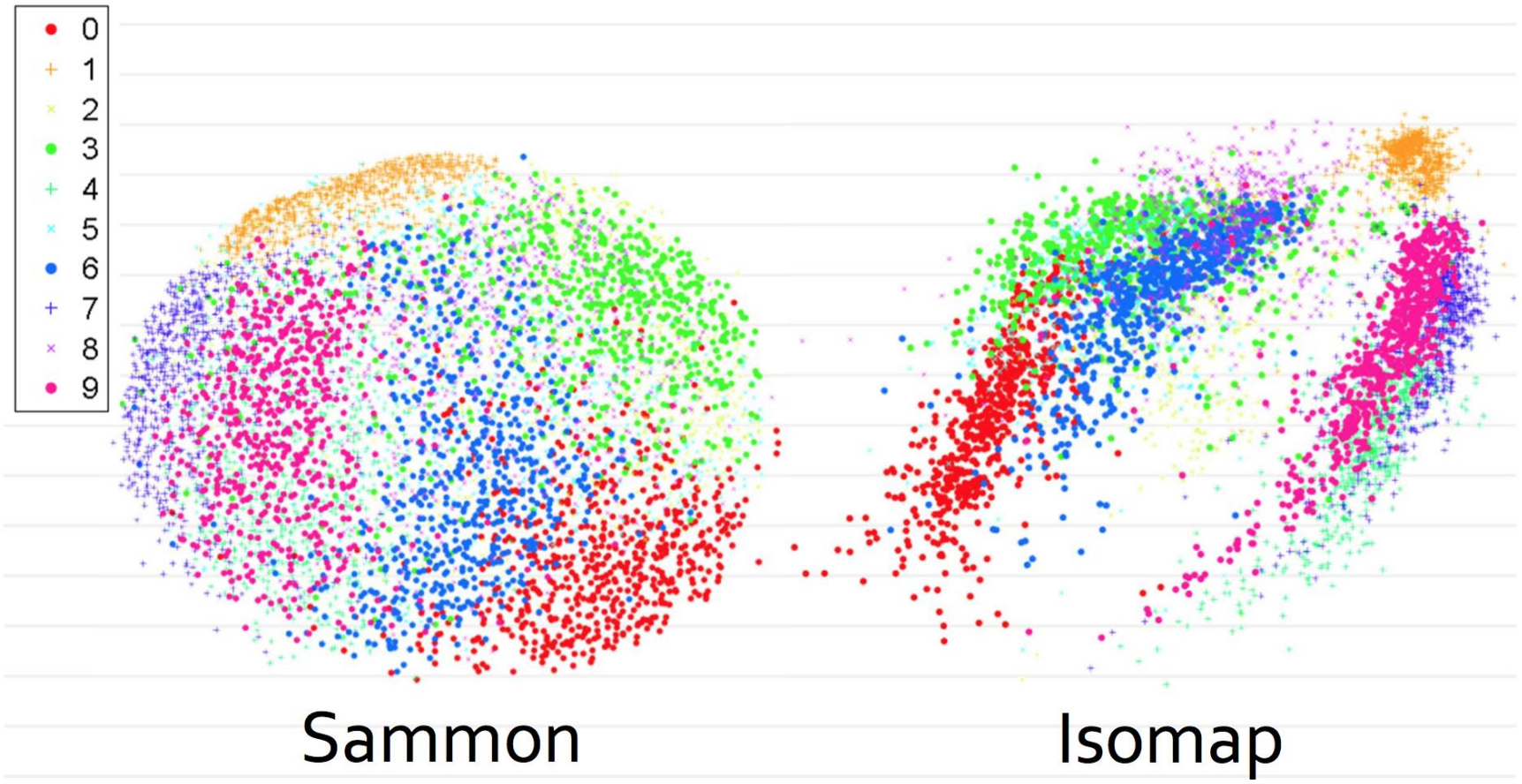


Solution – set points Y to top eigenvectors of D_g

ISOMAP results: hands embedding



MNIST: Linear approach vs. ISOMAP



Pros and cons of ISOMAP

- Preserves global structure
- Small number of parameters
- Sensitive to noise, noisy edges
- Computationally expensive: requires eigenvectors and eigenvalues of a dense matrix

Stochastic neighbours embedding (SNE)

"Stochastic" closeness in the initial space

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

Closeness in a new space

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

t-SNE

"Stochastic" closeness in the initial space

$$\frac{\partial Cost}{\partial y_i} = 2\sum_j \left(p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j}\right)\left(y_i - y_j\right)$$

To avoid local optimum:

- Initialize with Gaussian noise
- Add noise of decreasing variance at each step

t-SNE: define closeness on the base of $t(1)$ distribution

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

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t-SNE

t-sne: minimize KL between P and Q

$$Cost = KL(P||Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$$

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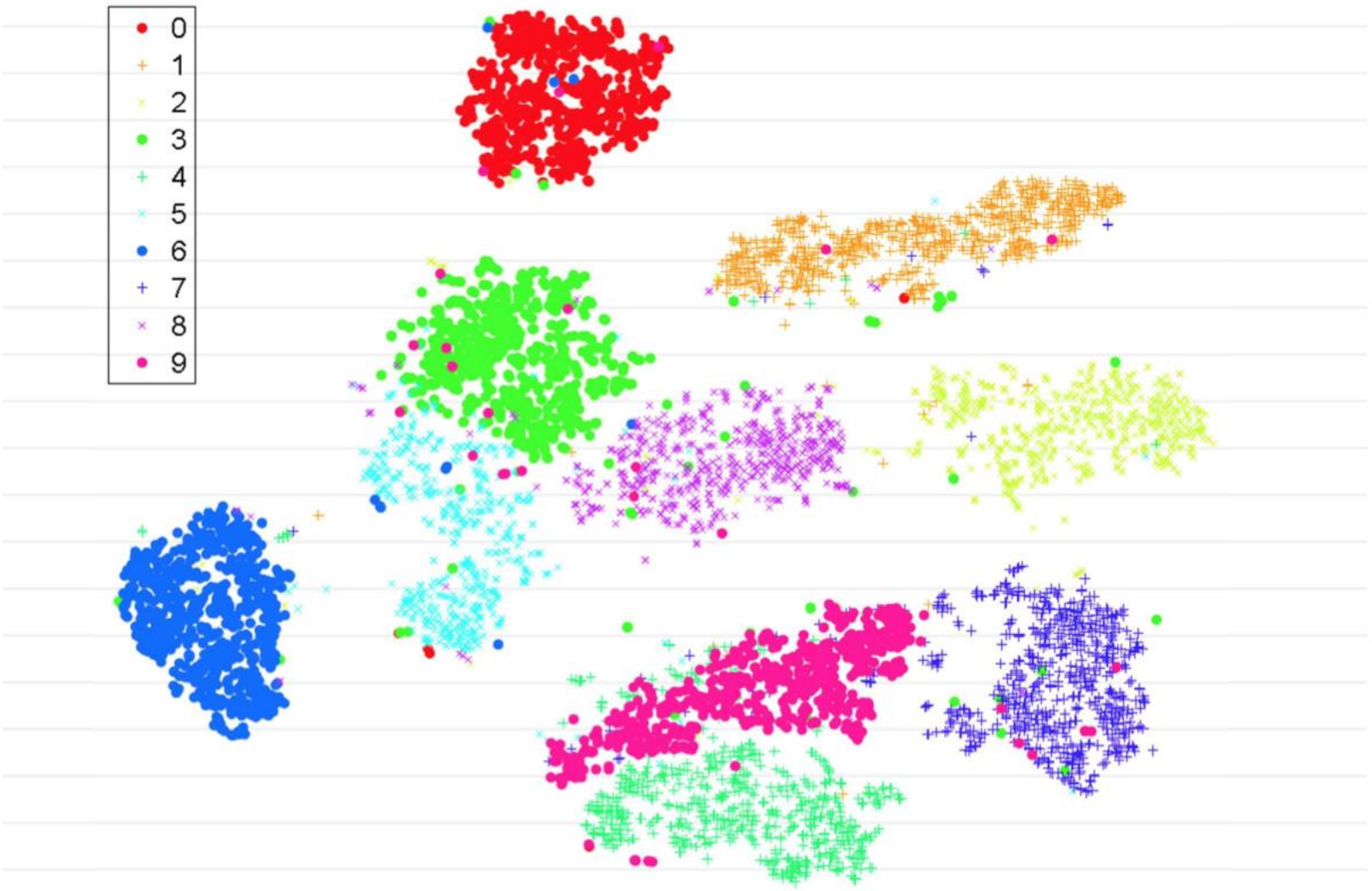
t-SNE for MNIST is good!



Pros and cons of tSNE

Pros:

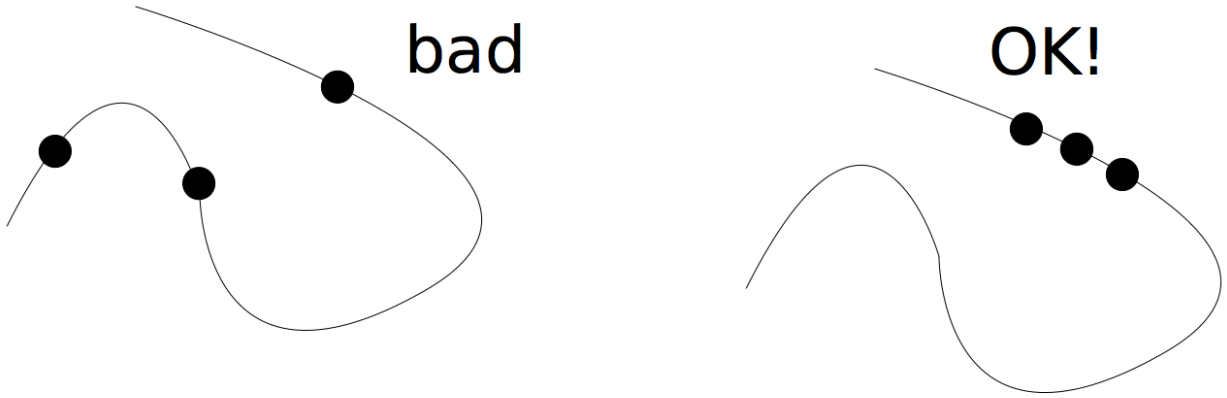
- works surprisingly well in 2D/3D visualization
- Provide nonlinear embedding

Cons:

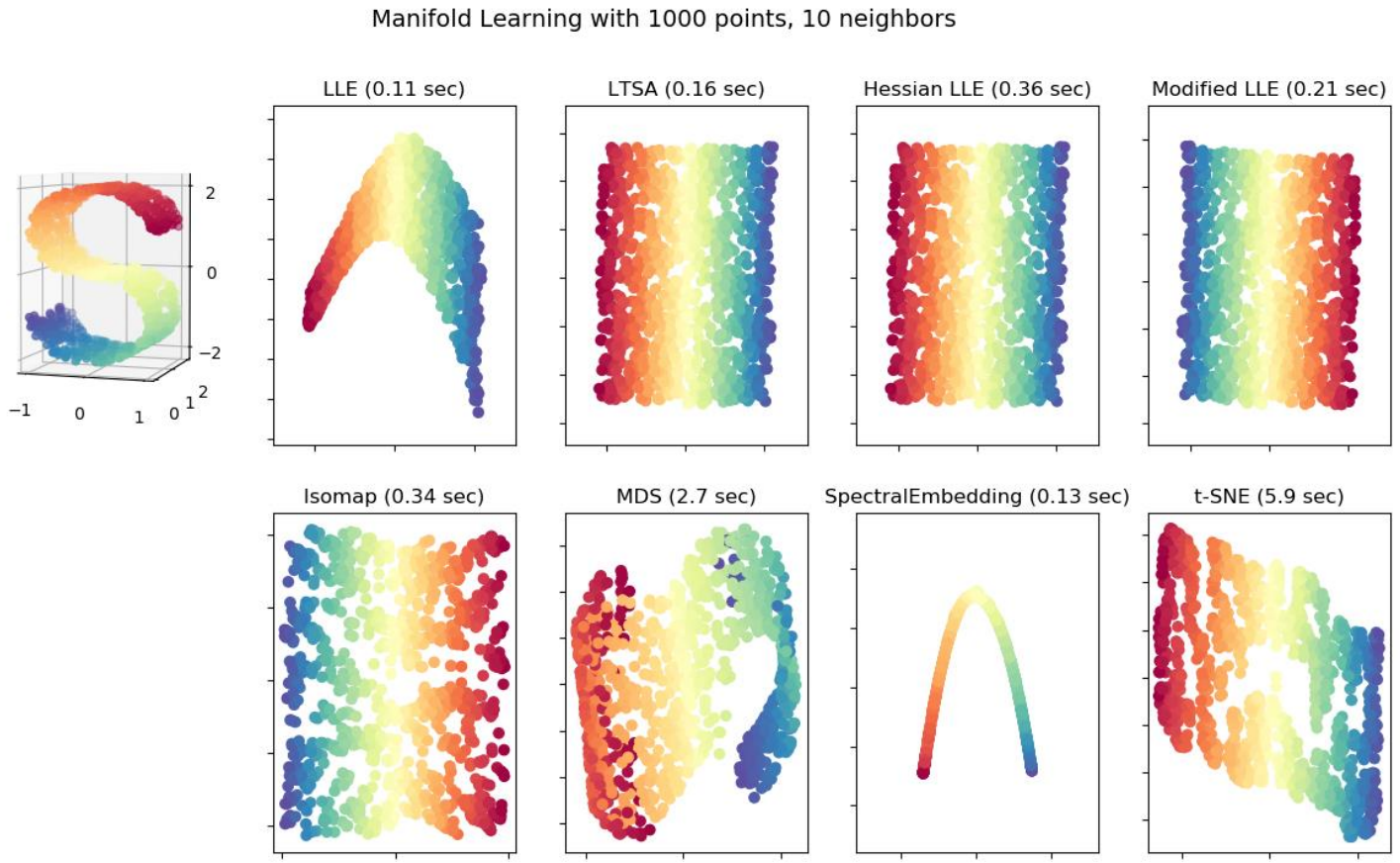
- quite slow
- Requires retraining if new points are added

No Free Lunch

For more complex manifolds you need more complex data



There are many other approaches



https://scikit-learn.org/stable/auto_examples/manifold/plot_compare_methods.html

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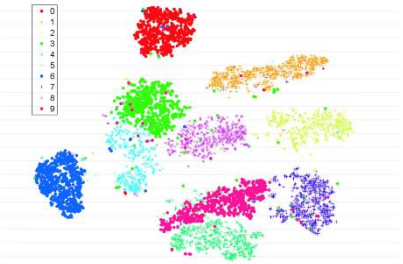
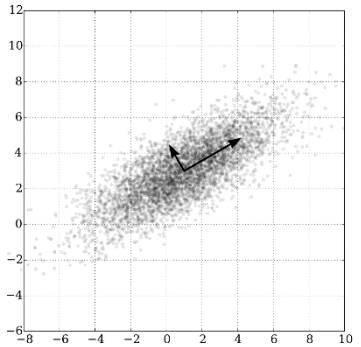
Dimension reduction: take home messages

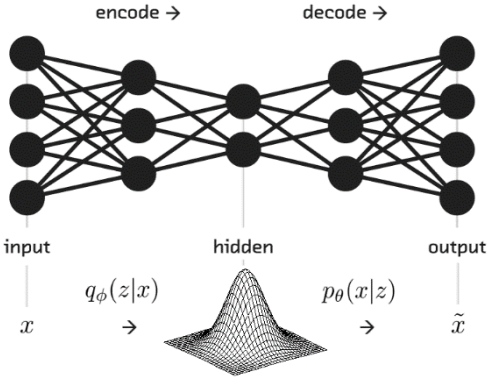
- Start with tSNE – it works surprisingly good



- PCA helps if data is linear



- There are also neural networks based embeddings



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