

Fundamentals of machine learning

Course 4: Basics of dimension reduction

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Why dimension reduction ?

- ▶ Visualize high-dimensional data (e.g. in 2D).
- ▶ Interpret the data.
- ▶ Compress the data: advantages for storage and robustness.
- ▶ Reveal the “structure of the data”.
- ▶ Avoid the curse of dimensionality (course 2).

Learning rates & excess risk

Question

Once we have selected a model how many samples n do we need to train it ?

Learning rates & excess risk

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The answer is statistical

- ▶ Can I bound (w.h.p. or in expectation)

$$\text{excess risk} = \text{estimation error} + \text{approximation error} \leq h(n)$$

- ▶ Ideally the function $h(n) \xrightarrow[n \rightarrow +\infty]{} 0$ fast: it is called the *learning rate*

Learning rates & excess risk

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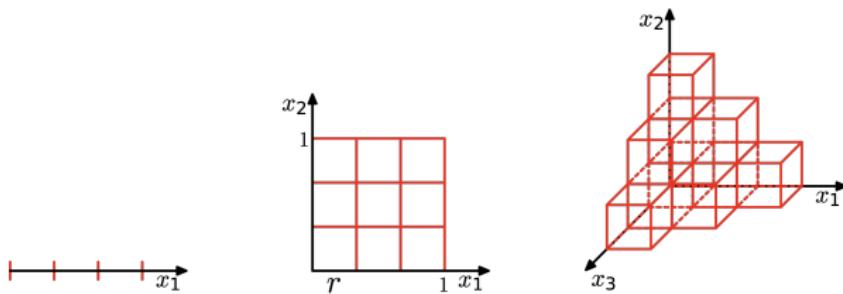
Curse of dimensionality

- ▶ If the best function f^* is only Lipschitz-continuous:

$$\mathbb{E}[\text{excess risk}] \lesssim n^{-1/d}$$

- ▶ This rate **is unavoidable** without further knowledge on f^*
- ▶ Slow rates: exponentially many samples are needed !

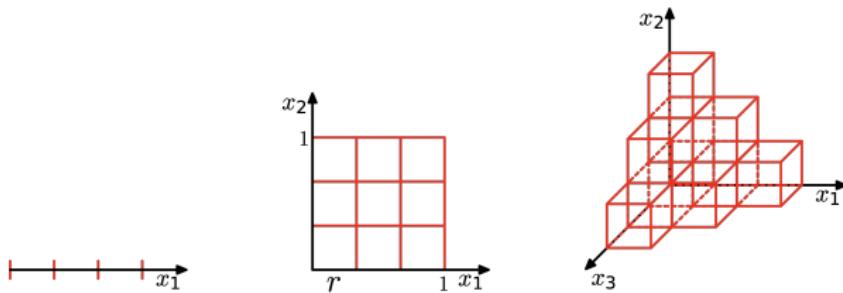
Curse of dimensionality



Think about interpolation: goal find $f : [0, 1]^d \rightarrow \mathbb{R}$

- ▶ You have n values of this function $f(x_i)$ at *sampled locations* x_i
- ▶ To find f you want to interpolate between the $f(x_i)$'s
- ▶ If f is not regular, a good approximation requires precise covering of $[0, 1]^d$ (small meshes)

Curse of dimensionality



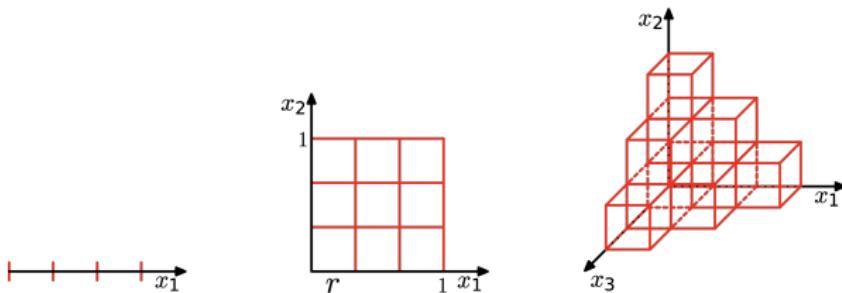
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Problem: points are isolated in high dimension

- ▶ Vol. of a hypercube with edge length $r < 1$ is r^d : quickly $\downarrow 0$ as $d \rightarrow \infty$
- ▶ To compensate you need a number of sample which **grows exponentially with d**

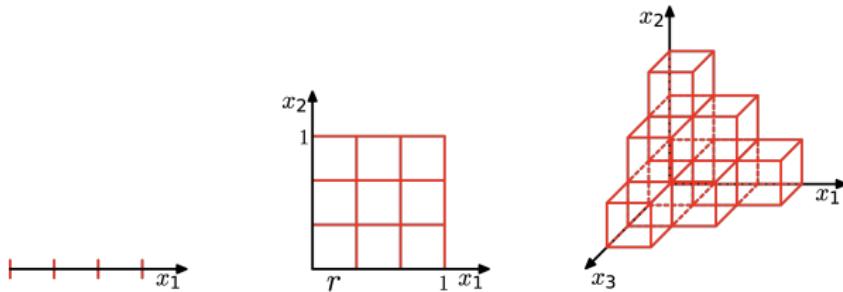
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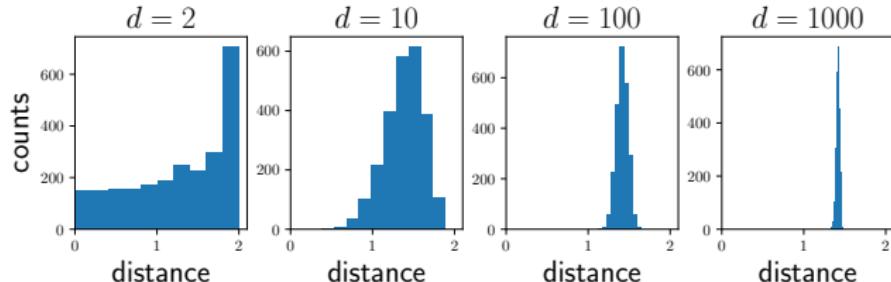
Main ideas

- ▶ Without prior on f^* the required number of samples n to estimate f^* is **exponential in d** .
- ▶ In high dim it is easy to overfit a model.
- ▶ The notion of nearest neighbors vanishes in high dim.
- ▶ Three remedies: use simple models (linear), dimensionality reduction or prior on f^*

Curse of dimensionality

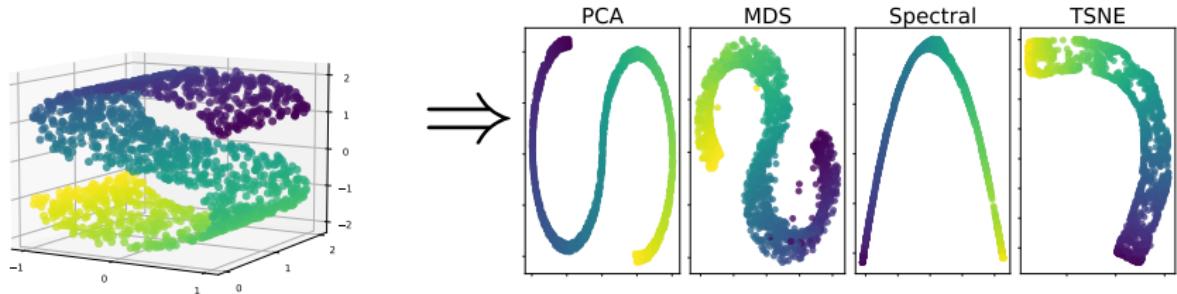


- ▶ Number of points needed to cover the hypercube cube $[0, 1]^d$ with precision r : $\left(\frac{2}{r}\right)^d$
- ▶ Distances between points become meaningless. Pairwise distances between 50 random points of \mathbb{R}^d :



The big picture

Original dataset



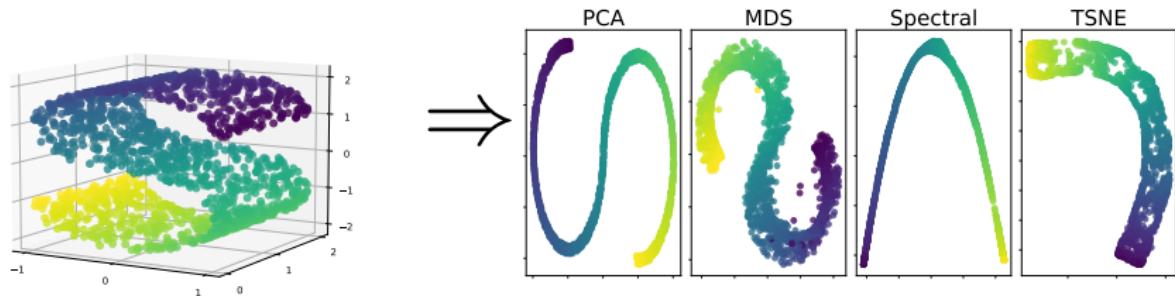
Objective

$$(\mathbf{x}_i)_{i=1}^n \quad \Rightarrow \quad (\tilde{\mathbf{x}}_i \in \mathbb{R}^k)_{i=1}^n \text{ with } k \ll d$$

- ▶ Project the data into a low dimensional space \mathbb{R}^k with $k \ll d$
- ▶ Preserve the information in the data (class, subspace, similarities)

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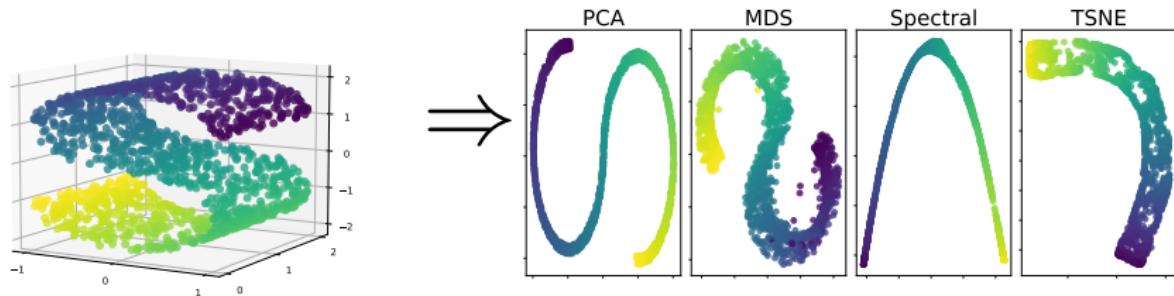
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Hyperparameters

- ▶ Linear, non linear projection ?
- ▶ Similarity between samples.

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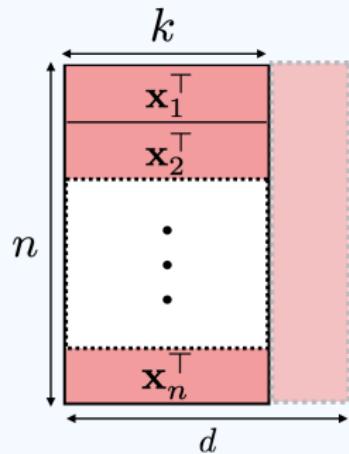
- ▶ Linear, non linear projection ?
- ▶ Similarity between samples.

Methods

- ▶ PCA, random projections.
- ▶ Non-linear methods (MDS, tSNE, Auto-Encoder)

Dimension reduction vs subsampling

Dimension reduction

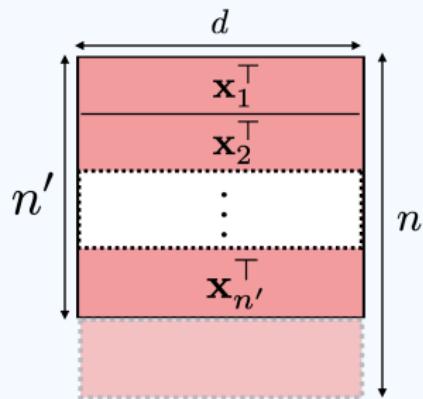


| Random projections (JL lemma)

| Feature selection

| Minimum distortion embedding, PCA

Subsampling



| Coresets

| Importance sampling

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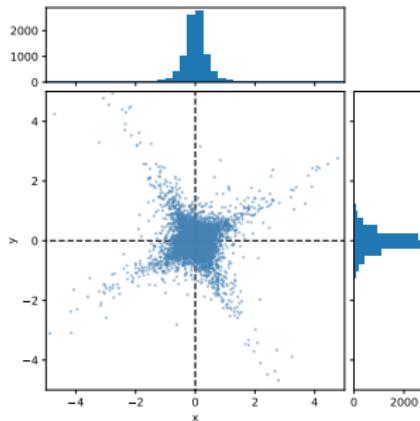
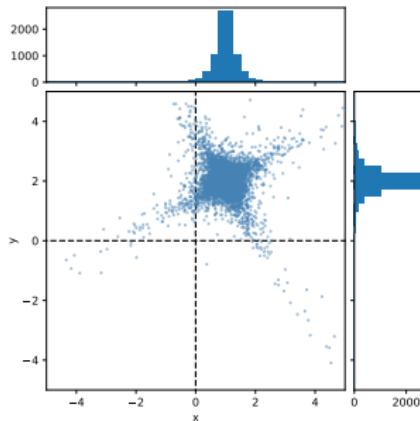
Non linear methods

Autoencoders

The principle

Setting

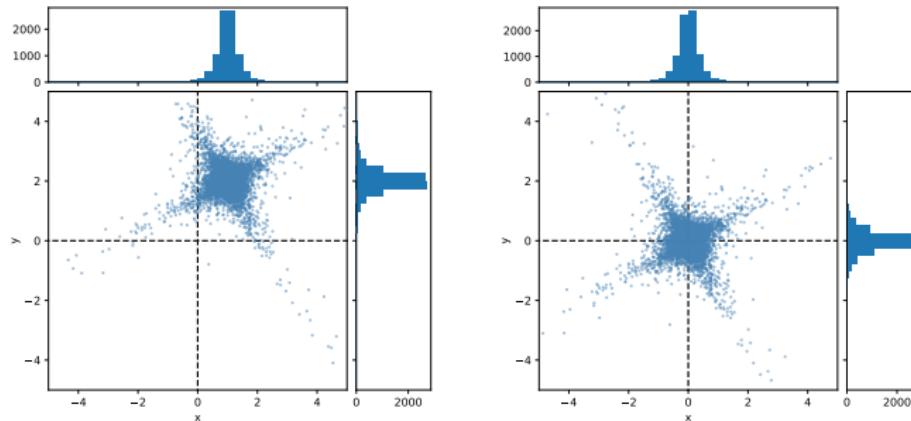
- ▶ A dataset $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$ with d big.
- ▶ Suppose for simplicity $\sum_{i=1}^n \mathbf{x}_i = 0$ (centered data), i.e. $\mathbf{X}^\top \mathbf{1}_n = 0$.



The principle

Setting

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Goal

- ▶ Find coordinates $\tilde{\mathbf{x}}_i = f(\mathbf{x}_i)$ in \mathbb{R}^k with $k \ll d$.
- ▶ The new data $(\tilde{\mathbf{x}}_i)_{i \in [n]}$ should “look like” \mathbf{X} (to be defined).
- ▶ First step: linear mapping f !

The principle of PCA

Linear mapping according to a reconstruction principle

- ▶ Find $\mathbf{U} = (\mathbf{u}_1, \dots, \mathbf{u}_k) \in \mathbb{R}^{d \times k}$ with $\mathbf{u}_n^\top \mathbf{u}_m = \delta_{nm}$ (orthonormal vectors)
- ▶ Dimension reduction via linear mapping: $\tilde{\mathbf{x}}_i = \mathbf{U}^\top \mathbf{x}_i \in \mathbb{R}^k$

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- ▶ What make a \mathbf{U} “better” than another?

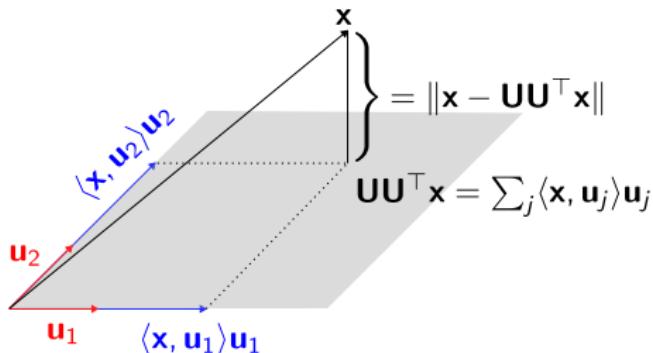
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- ▶ Reconstruction principle Pearson 1901:

$$\min_{\substack{\mathbf{U} \in \mathbb{R}^{d \times k} \\ \mathbf{U}^\top \mathbf{U} = \mathbf{I}_k}} \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{U}\tilde{\mathbf{x}}_i\|_2^2 = \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{U}\mathbf{U}^\top \mathbf{x}_i\|_2^2$$

- ▶ $\mathbf{U}\mathbf{U}^\top \mathbf{x}_i$ is the orthogonal projection of \mathbf{x}_i onto $\text{span}(\mathbf{u}_1, \dots, \mathbf{u}_k)$



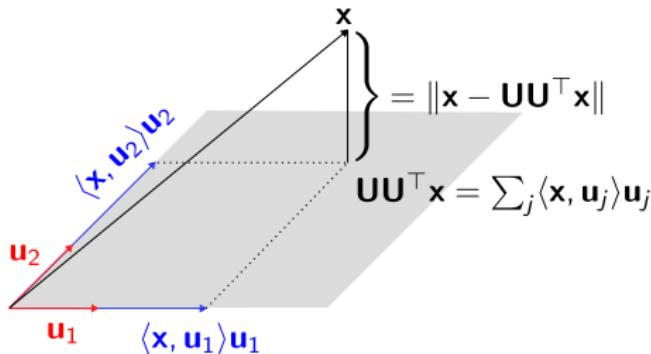
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Linear mapping according to a reconstruction principle

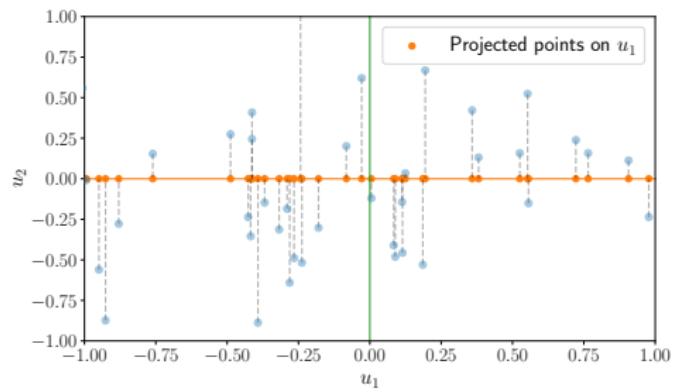
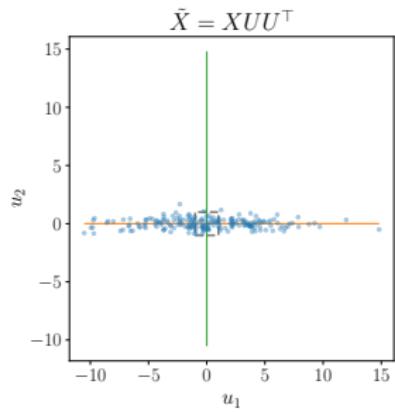
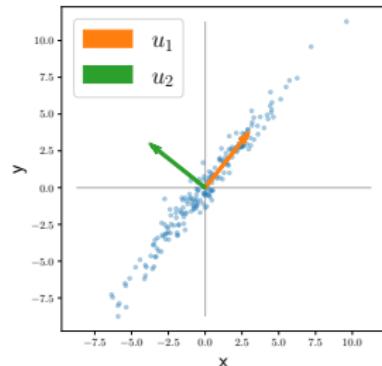
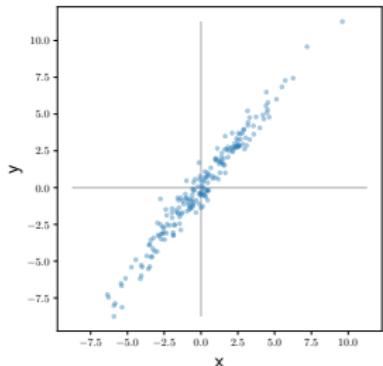
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- ▶ After finding a sol. \mathbf{U}^* , $\mathbf{x}_i \approx \sum_{j=1}^k \langle \mathbf{x}_i, \mathbf{u}_j^* \rangle \mathbf{u}_j^*$ (equality when $k = d$).



Illustration



Variance interpretation

Equivalent problem

- The PCA problem is equivalent to the *non-convex* quadratic problem (board):

$$\max_{\substack{\mathbf{U} \in \mathbb{R}^{d \times k} \\ \mathbf{U}^\top \mathbf{U} = \mathbf{I}_k}} \frac{1}{n} \sum_{i=1}^n \|\mathbf{U}^\top \mathbf{x}_i\|_2^2 = \text{tr} \left(\mathbf{U}^\top \underbrace{\left(\frac{1}{n} \mathbf{X}^\top \mathbf{X} \right)}_{\hat{\Sigma}} \mathbf{U} \right)$$

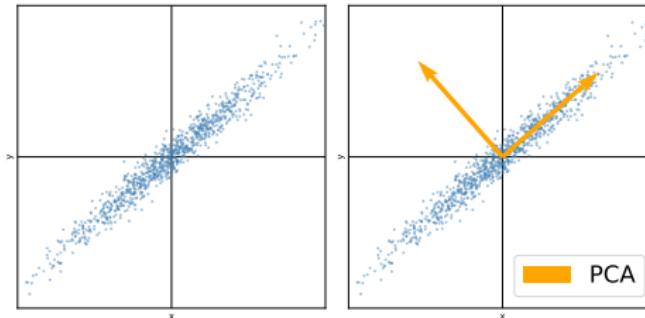
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- Equivalent to maximizing the **variance of the projected samples** $\tilde{\mathbf{x}}_i$.



- Empirical covariance matrix $\widehat{\Sigma} = \frac{1}{n} \mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{d \times d}$

Recap: Two views on PCA

The PCA is the linear mapping $\mathbf{x} \mapsto \tilde{\mathbf{x}} = \mathbf{U}\mathbf{x} \in \mathbb{R}^k$ that (equivalently):

- ▶ minimizes the reconstruction error

$$\min_{\substack{\mathbf{U} \in \mathbb{R}^{d \times k} \\ \mathbf{U}^\top \mathbf{U} = \mathbf{I}_k}} \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{U}\mathbf{U}^\top \mathbf{x}_i\|^2$$

- ▶ maximizes the variance of the projected data

$$\max_{\substack{\mathbf{U} \in \mathbb{R}^{d \times k} \\ \mathbf{U}^\top \mathbf{U} = \mathbf{I}_k}} \frac{1}{n} \sum_{i=1}^n \|\mathbf{U}\mathbf{x}_i\|^2$$

Now how do we compute this optimal \mathbf{U} ?

Ky-Fan theorem

Fan 1949

Let $\mathbf{A} \in \mathbb{R}^{d \times d}$ **symmetric** with eigenvalues $\lambda_1 \geq \dots \geq \lambda_d$ and $k \leq d$. Then $\sum_{i=1}^k \lambda_i$ (*resp.* $\sum_{i=1}^k \lambda_{d+i-1}$) is the maximum (*resp.* minimum) of $\text{tr}(\mathbf{U}^\top \mathbf{A} \mathbf{U})$ over $\{\mathbf{U} \in \mathbb{R}^{d \times k}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}_k\}$. In particular

$$\max_{\mathbf{U} \in \mathbb{R}^{d \times k}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}_k} \text{tr}(\mathbf{U}^\top \mathbf{A} \mathbf{U}) = \sum_{i=1}^k \lambda_i. \quad (1)$$

The solution of (1) is given by $\mathbf{U}^* = (\mathbf{u}_1, \dots, \mathbf{u}_k)$ where $\mathbf{u}_1, \dots, \mathbf{u}_k$ are eigenvectors of \mathbf{A} associated to the top- k eigenvalues.

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Consequences for PCA

- ▶ Solution of PCA: find the k largest eigenvalues of $\widehat{\Sigma} = \frac{1}{n} \mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{d \times d}$.
- ▶ Solution $\mathbf{U}^* = (\mathbf{u}_1^*, \dots, \mathbf{u}_k^*)$ associated to the top- k eigenvalues of $\widehat{\Sigma}$.
- ▶ $\mathbf{u}_1^* \in \mathbb{R}^d, \dots, \mathbf{u}_k^* \in \mathbb{R}^d$ are called *principal components*.

Ky-Fan theorem

Fan 1949 (proof on board)

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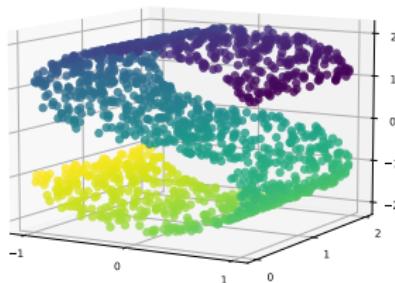
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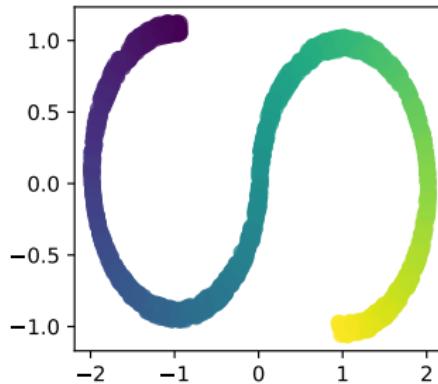
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Example with 3D data

- ▶ Simple 3D data.

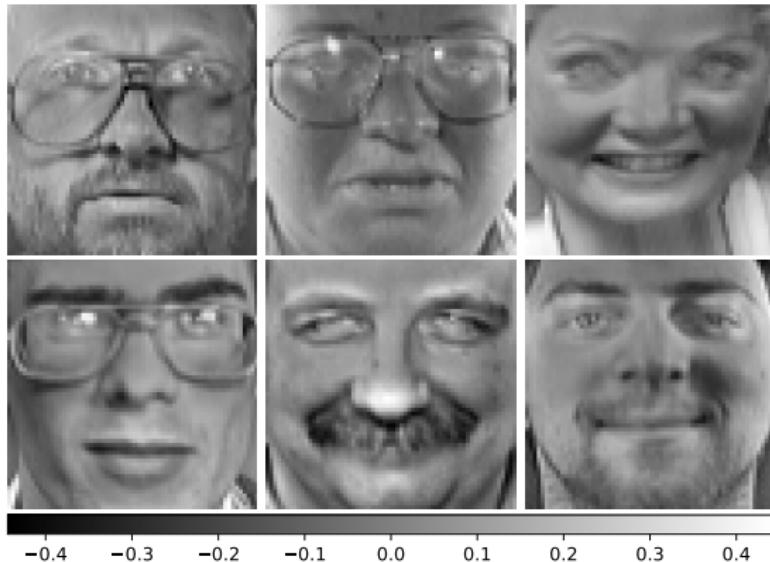


- ▶ Projection onto the two firsts principal components ($d = 3 \rightarrow k = 2$).
PCA



Example with eigenfaces

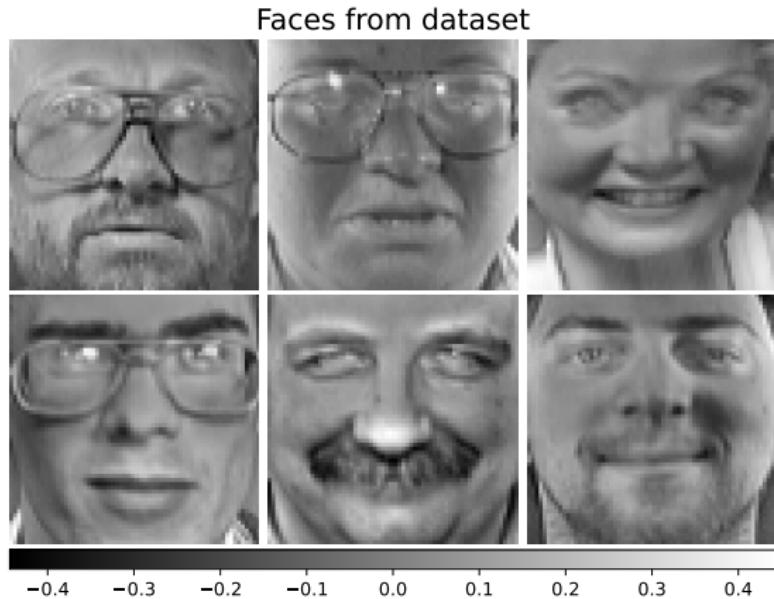
Faces from dataset



Setting

- ▶ Each image is a vector $\mathbf{x}_i \in \mathbb{R}^{4096}$ ($d = 4096$ pixels), $n = 400$ images.

Example with eigenfaces



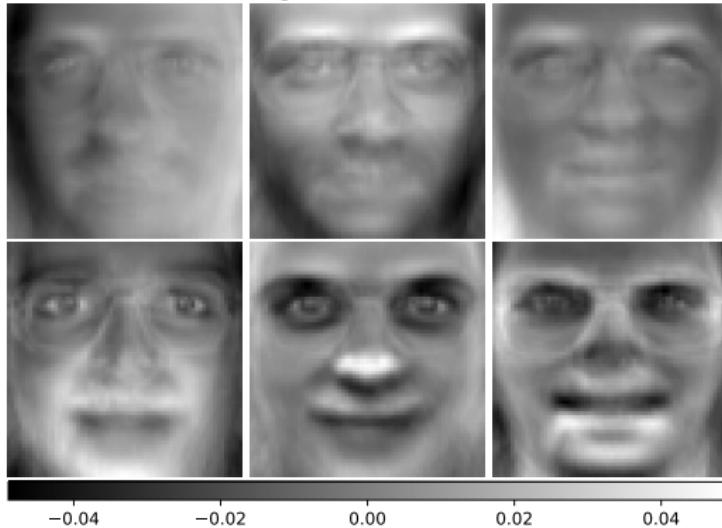
Setting

- ▶ Each image is a vector $\mathbf{x}_i \in \mathbb{R}^{4096}$ ($d = 4096$ pixels), $n = 400$ images.
- ▶ Find k “standard faces”: principal components $\mathbf{u}_1^*, \dots, \mathbf{u}_k^* \in \mathbb{R}^d$.
- ▶ Idea: explain images via $\mathbf{x}_i \approx \sum_{j=1}^k \langle \mathbf{x}_i, \mathbf{u}_j^* \rangle \mathbf{u}_j^*$, in other words
image $\approx \alpha_1 \times \text{eigenface 1} + \dots + \alpha_k \times \text{eigenface } k$

Example with eigenfaces

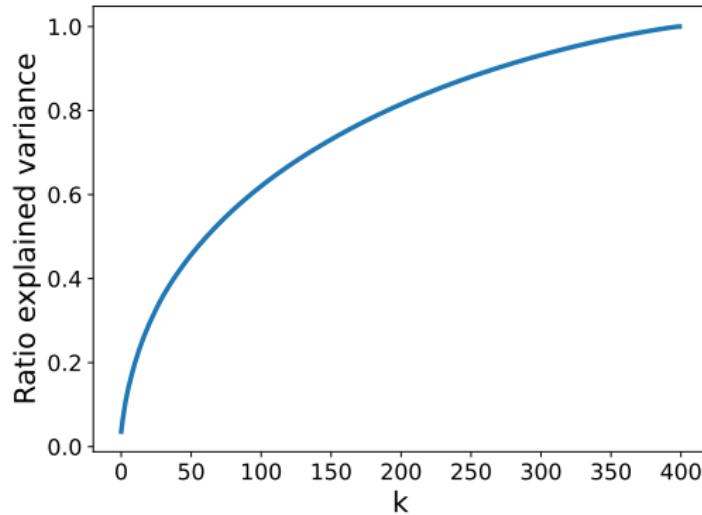
- ▶ Result with $k = 6$

Eigenfaces - SVD



Example with eigenfaces

- ▶ How to choose k ? ratio explained variance: $r = \sum_{i=1}^k \lambda_i / \sum_{i=1}^d \lambda_i$



- ▶ Explanation:

$$r = \sum_{i=1}^k \lambda_i / \sum_{i=1}^d \lambda_i = \text{tr} \left((\mathbf{U}^*)^\top \widehat{\Sigma} (\mathbf{U}^*) \right) / \text{tr}(\widehat{\Sigma})$$

$$= \frac{1}{n} \sum_{i=1}^n \|\tilde{\mathbf{x}}_i\|_2^2 / \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i\|_2^2$$

How to compute the PCA?

The “naive” way

- ▶ Find the eigenvalue decomposition of $\widehat{\Sigma} = \frac{1}{n} \mathbf{X}^\top \mathbf{X} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top$
- ▶ Compute $\widehat{\Sigma}$: $\mathcal{O}(nd^2)$ operations.
- ▶ Eigenvalue decomposition : $\mathcal{O}(d^3)$ operations.
- ▶ Keep only the k -largest eigenvalues associated to k eigenvectors.
- ▶ Space complexity: $\mathcal{O}(d^2)$
- ▶ Time complexity: $\mathcal{O}(nd^2 + d^3)$

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The right way

- ▶ Compute the singular value decomposition (SVD) of \mathbf{X} !

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One of the most useful tool in linear algebra

Singular value decomposition

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$. Then \mathbf{X} can be decomposed as

$$\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^\top \tag{2}$$

where $\mathbf{U} \in \mathbb{R}^{n \times n}$, $\mathbf{V} \in \mathbb{R}^{d \times d}$ are *unitary* ($\mathbf{U}^\top \mathbf{U} = \mathbf{U}\mathbf{U}^\top = \mathbf{I}_n$, $\mathbf{V}^\top \mathbf{V} = \mathbf{V}\mathbf{V}^\top = \mathbf{I}_d$) and $\Sigma \in \mathbb{R}^{n \times d}$ is a rectangular diagonal matrix with *non-negative* real numbers $(\sigma_i)_{i \in [\min\{n,d\}]}$ on the diagonal, called *singular values*.

One of the most useful tool in linear algebra

Singular value decomposition

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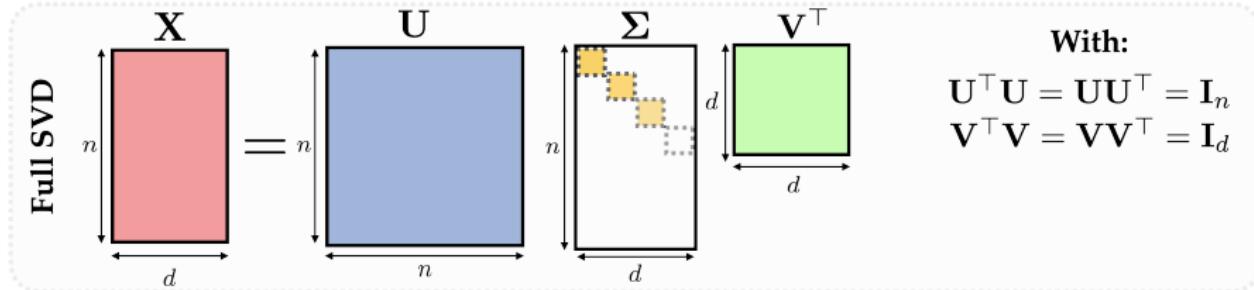
$$\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^\top \tag{2}$$

where $\mathbf{U} \in \mathbb{R}^{n \times n}$, $\mathbf{V} \in \mathbb{R}^{d \times d}$ are *unitary* ($\mathbf{U}^\top \mathbf{U} = \mathbf{U}\mathbf{U}^\top = \mathbf{I}_n$, $\mathbf{V}^\top \mathbf{V} = \mathbf{V}\mathbf{V}^\top = \mathbf{I}_d$) and $\Sigma \in \mathbb{R}^{n \times d}$ is a rectangular diagonal matrix with *non-negative* real numbers $(\sigma_i)_{i \in [\min\{n,d\}]}$ on the diagonal, called *singular values*.

Properties

- ▶ $\text{rank}(\mathbf{X}) = \text{number of non-zero } \sigma'_i$ s.
- ▶ The *columns* of \mathbf{V} are eigenvectors of $\mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{d \times d}$.
- ▶ The *columns* of \mathbf{U} are eigenvectors of $\mathbf{X}\mathbf{X}^\top \in \mathbb{R}^{n \times n}$.
- ▶ We have $\sigma_i = \sqrt{\text{eigenvalue}_i(\mathbf{X}^\top \mathbf{X})} = \sqrt{\text{eigenvalue}_i(\mathbf{X}\mathbf{X}^\top)}$.
- ▶ We have the relations $\mathbf{X}\mathbf{v}_i = \sigma_i\mathbf{u}_i$, $\mathbf{X}^\top \mathbf{u}_i = \sigma_i\mathbf{v}_i$.

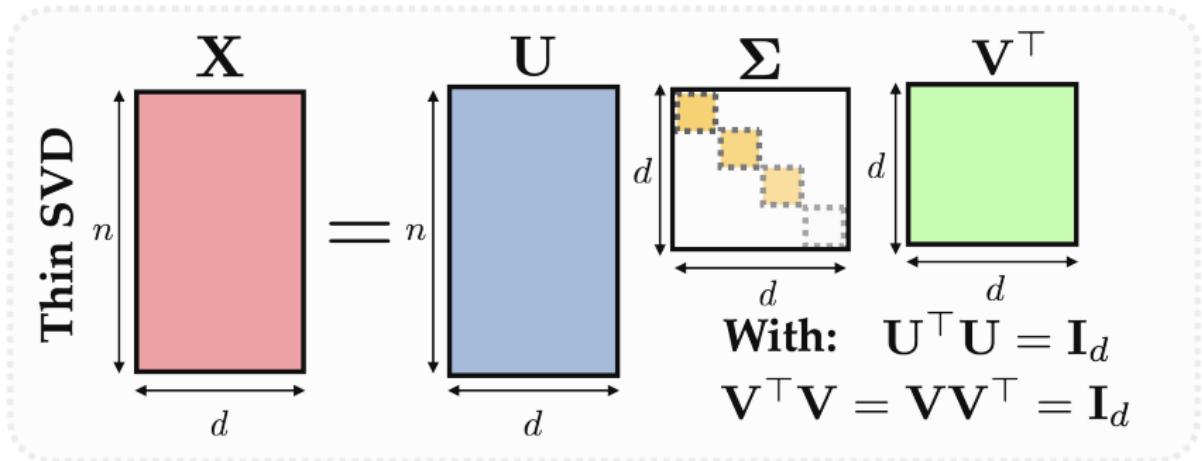
SVD: many flavors



Full SVD (image in case $n \geq d$)

- ▶ Generalizes eigenvalue decomposition for non-symmetric matrices.
- ▶ Complexity: $\mathcal{O}(nd \min\{n, d\})$ (Golub–Reinsch algorithm see [Cline and Dhillon 2006](#)).
- ▶ To find the eigenvalues of $\mathbf{X}^\top \mathbf{X}$ or $\mathbf{X}\mathbf{X}^\top$ we do not even have to compute these matrices !

SVD: many flavors

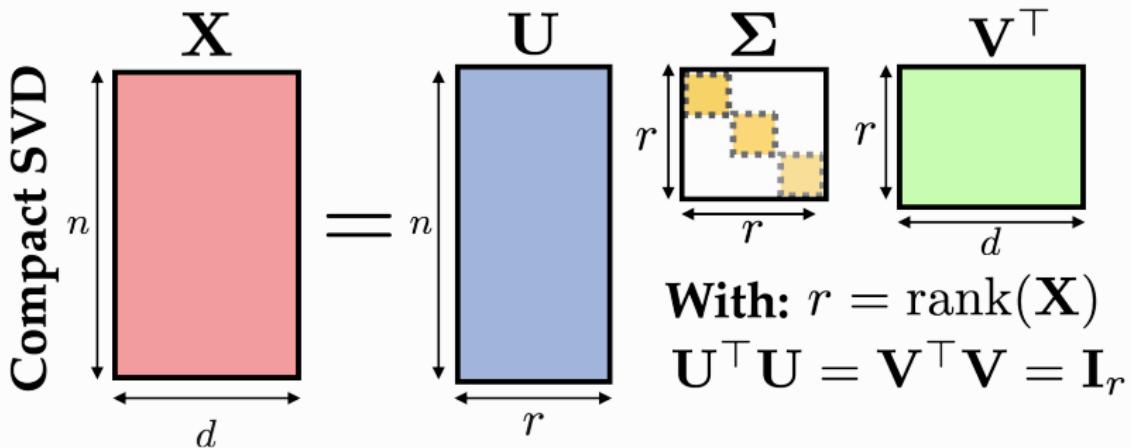


Thin SVD

- If we write $\mathbf{U} = (\mathbf{u}_1, \dots, \mathbf{u}_n)$, $\mathbf{V} = (\mathbf{v}_1, \dots, \mathbf{v}_d)$ the full SVD, then Thin SVD gives:

$$\mathbf{X} = \sum_{i=1}^{\min\{n,d\}} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$$

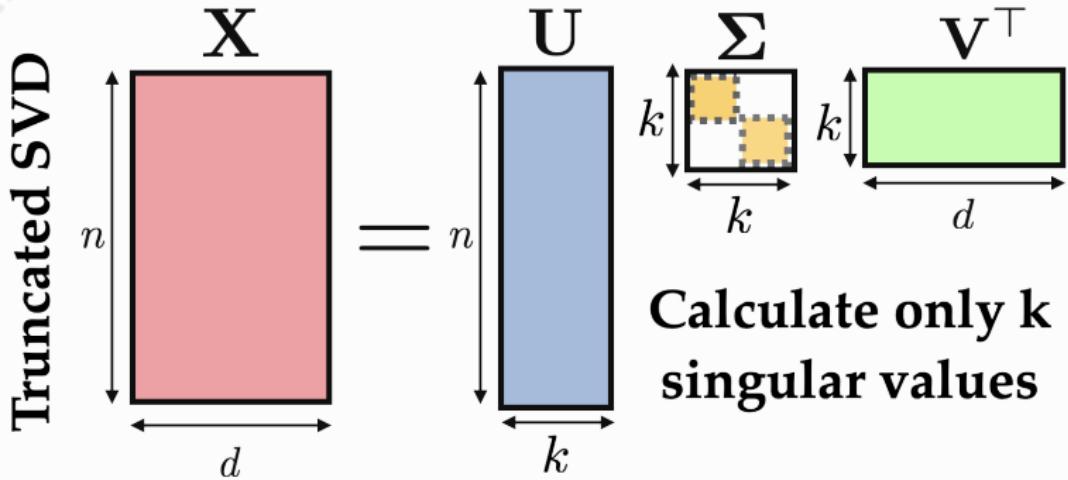
SVD: many flavors



Compact SVD

- ▶ Keep only the non-zero singular values. In particular $r = \text{rank}(\mathbf{X})$.
- ▶ The pseudo-inverse of \mathbf{X} is given by $\mathbf{X}^\dagger = \mathbf{V}\Sigma^{-1}\mathbf{U}^\top$.

SVD: many flavors



Truncated SVD

- ▶ Best rank- k approximation of \mathbf{X} (in the sense of $\|\cdot\|_F$, $\|\cdot\|_{2\rightarrow 2}$).
- ▶ The solution of the PCA is given by $\mathbf{V} \in \mathbb{R}^{d \times k}$.
- ▶ The embedding $(\tilde{\mathbf{x}}_i)_{i \in [n]}$ in low dim of PCA is given by $\mathbf{U}\Sigma \in \mathbb{R}^{n \times k}$.
- ▶ Efficient algorithms $\mathcal{O}(ndk)$ Halko, Martinsson, and Tropp 2011.

PCA: a recap

- ▶ Dimension reduction $\mathbb{R}^d \rightarrow \mathbb{R}^k$ via a linear mapping.
- ▶ Defined with a matrix \mathbf{U} with orthonormal columns.
- ▶ Follows a reconstruction principle.
- ▶ Maximizes the variance of the projected samples.
- ▶ Used for compression, interpretation, robustness.
- ▶ Can be computed with SVD in $\mathcal{O}(ndk)$ time.

A word on Kernel PCA

From PCA...

- ▶ PCA solves $\max_{\substack{\mathbf{U} \in \mathbb{R}^{d \times k} \\ \mathbf{U}^\top \mathbf{U} = \mathbf{I}_k}} \text{tr}(\mathbf{U}^\top (\mathbf{X}^\top \mathbf{X}) \mathbf{U})$.
- ▶ Eigenvalue decomposition of $\mathbf{X}^\top \mathbf{X} = \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top \in \mathbb{R}^{d \times d}$.
- ▶ Same non-zero eigenvalues than $\mathbf{X} \mathbf{X}^\top = (\langle \mathbf{x}_i, \mathbf{x}_j \rangle)_{ij} \in \mathbb{R}^{n \times n}$ (**exercise**).

A word on Kernel PCA

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... to Kernel PCA Schölkopf, Smola, and Müller 2005

- ▶ PCA in a *high-dimensional non-linear* embedding $\Phi(\mathbf{x})$ of the data.
- ▶ *Kernel trick:* embedding is *implicit* we only need $\mathbf{K} = (\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle)_{ij}$.
- ▶ Kernel PCA: eigenvalue decomposition of $\mathbf{K} \in \mathbb{R}^{n \times n}$.
- ▶ More powerful but expensive for large n .

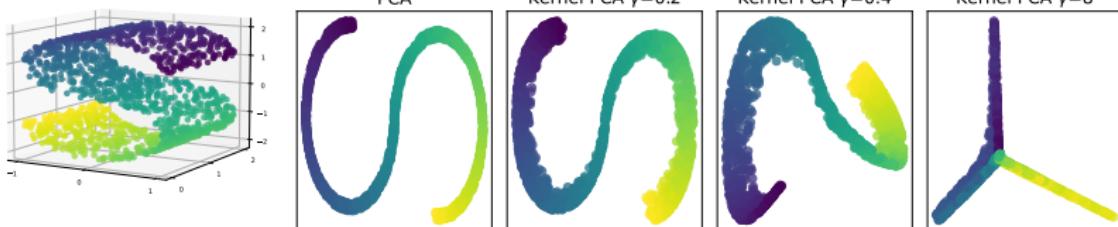
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A more general setting: dictionary learning

From PCA...

- ▶ One principle of PCA is to represent a sample as a linear combination $\mathbf{x} \approx \sum_{j=1}^k \alpha_j \mathbf{d}_j$ with $\mathbf{d}_j \in \mathbb{R}^d$.
- ▶ PCA: $\alpha_j = \langle \mathbf{x}, \mathbf{u}_j^* \rangle$, $\mathbf{d}_j = \mathbf{u}_j^*$ principal component.

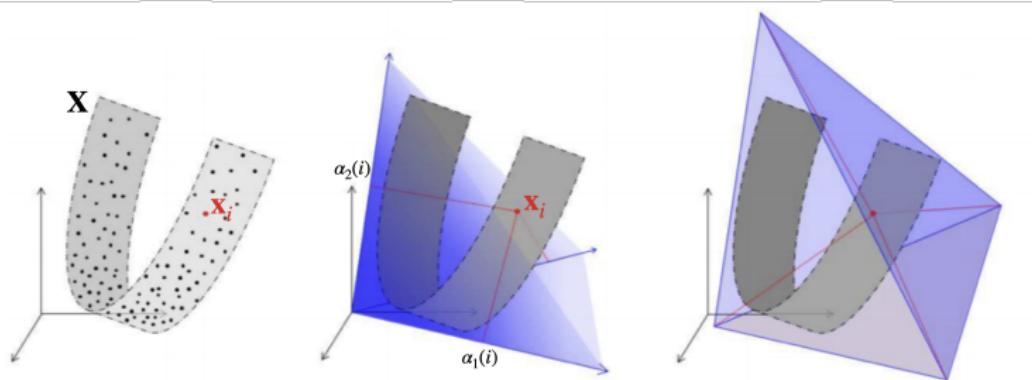
A more general setting: dictionary learning

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- ▶ PCA: $\alpha_j = \langle \mathbf{x}, \mathbf{u}_j^* \rangle$, $\mathbf{d}_j = \mathbf{u}_j^*$ principal component.

... to dictionary learning (DL)

- ▶ Represent \mathbf{x} in another “base”: $\mathbf{x} \approx \mathbf{D}\boldsymbol{\alpha}$ (e.g. Fourier/Wavelet basis).
- ▶ $\mathbf{D} \in \mathbb{R}^{d \times k}$ is the *dictionary*. k might be bigger than d ! (overcomplete)
- ▶ $\boldsymbol{\alpha} \in \mathbb{R}^k$ is the representation of \mathbf{x} in the dictionary \mathbf{D} .



A more general setting: dictionary learning

Find the representation

- ▶ Given a point \mathbf{x} and a dictionary \mathbf{D} :

$$\hat{\boldsymbol{\alpha}} = \arg \min_{\boldsymbol{\alpha} \in C} \|\mathbf{x} - \mathbf{D}\boldsymbol{\alpha}\|_2^2 \quad (3)$$

- ▶ When $C = \mathbb{R}^k$, $\mathbf{D}^\top \mathbf{D} = \mathbf{I}_k$ then $\hat{\boldsymbol{\alpha}} = \mathbf{D}^\top \mathbf{x}$.
- ▶ Can also be used with different losses than $\|\cdot\|_2^2$.

A more general setting: dictionary learning

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- Can also be used with different losses than $\|\cdot\|_2^2$.

Learn the representation and the dictionary

- Given a dataset $\mathbf{x}_1, \dots, \mathbf{x}_n$, learn the dictionary and the representations

$$\hat{\mathbf{D}}, \hat{\boldsymbol{\alpha}_1}, \dots, \hat{\boldsymbol{\alpha}_n} = \arg \min_{\substack{\mathbf{D} \in \mathcal{D} \\ \boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_n \in C}} \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i\|_2^2. \quad (4)$$

- When $C = \mathbb{R}^k$, $\mathcal{D} = \{\mathbf{D} \in \mathbb{R}^{d \times k}, \mathbf{D}^\top \mathbf{D} = \mathbf{I}_k\}$ we retrieve the PCA.
- But various possibilities Mairal et al. 2009 !
- Scikit-learn implementation : `sklearn.decomposition.DictionaryLearning`

One example

Sparse dictionary learning

- Given a dataset $\mathbf{x}_1, \dots, \mathbf{x}_n$, learn the dictionary and the representations

$$\widehat{\mathbf{D}}, \widehat{\boldsymbol{\alpha}}_1, \dots, \widehat{\boldsymbol{\alpha}}_n = \arg \min_{\substack{\mathbf{D} \in \mathcal{D} \\ \boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_n \in C}} \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i\|_2^2. \quad (5)$$

- Take $\mathcal{D} = \{\mathbf{D} \in \mathbb{R}^{d \times k} : \forall i, \|\mathbf{d}_i\|_2 = 1\}$ (normalized columns).
- Take $C = \{\boldsymbol{\alpha} : \|\boldsymbol{\alpha}\|_1 \leq \lambda\}$ sparsity promoting regularization.
- Example $d = 2, k = 3$ (not dimension reduction !!)

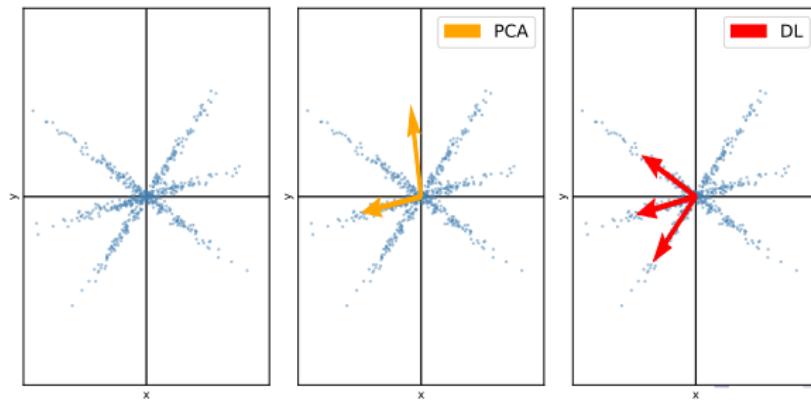


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General setting

Preserve the pairwise distances Agrawal, Ali, and Boyd 2021

- ▶ A dataset $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n), \mathbf{x}_i \in \mathbb{R}^d$.
- ▶ Find a dataset $\tilde{\mathbf{X}} = (\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n), \tilde{\mathbf{x}}_i \in \mathbb{R}^k, k \ll d$ such that

$$\forall(i,j), \text{similarity}_{\mathbb{R}^d}(\mathbf{x}_i, \mathbf{x}_j) \approx \text{similarity}_{\mathbb{R}^k}(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_j) \text{ or}$$

$$\forall(i,j), \text{dissimilarity}_{\mathbb{R}^d}(\mathbf{x}_i, \mathbf{x}_j) \approx \text{dissimilarity}_{\mathbb{R}^k}(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_j)$$

- ▶ Optional: find a mapping $f : \mathbb{R}^d \rightarrow \mathbb{R}^k, \tilde{\mathbf{x}}_i = f(\mathbf{x}_i)$.

General setting

Preserve the pairwise distances Agrawal, Ali, and Boyd 2021

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- ▶ Optional: find a mapping $f : \mathbb{R}^d \rightarrow \mathbb{R}^k, \tilde{\mathbf{x}}_i = f(\mathbf{x}_i)$.

Example with $\|\cdot\|_2^2$

- ▶ Can we find $\delta \in [0, 1]$ and $f : \mathbb{R}^d \rightarrow \mathbb{R}^k$ such that

$$(1 - \delta) \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 \leq \|f(\mathbf{x}_i) - f(\mathbf{x}_j)\|_2^2 \leq (1 + \delta) \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 ? \quad (6)$$

One necessary result

The notion of distortion Matoušek 2013

- ▶ Consider two metric spaces (X, d_X) and (Y, d_Y) . A function $f : X \rightarrow Y$ is called a μ -embedding if, $\exists r > 0$, such that

$$\forall (\mathbf{x}, \mathbf{x}') \in X, \quad r \cdot d_X(\mathbf{x}, \mathbf{x}') \leq d_Y(f(\mathbf{x}), f(\mathbf{x}')) \leq \mu \times r \cdot d_X(\mathbf{x}, \mathbf{x}'). \quad (7)$$

- ▶ The smallest $\mu > 1$ such that (7) is called the *distortion*.

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Example

- ▶ Not always possible to have low distortion !
- ▶ Every embedding of the n -point equilateral space $X = K_n$ (every two points have distance 1) into the Euclidean plane $(\mathbb{R}^2, \|\cdot\|_2)$ has distortion at least $\Omega(\sqrt{n})$.

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Example

- ▶ Not always possible to have low distortion !
- ▶ Every embedding of the n -point equilateral space $X = K_n$ (every two points have distance 1) into the Euclidean plane $(\mathbb{R}^k, \|\cdot\|_2)$ has distortion at least $\Omega(n^{1/k})$.

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Johnson-Lindenstrauss lemma

Johnson and Lindenstrauss 1984

Let $0 < \delta < 1$ and *any* dataset $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$. Providing that

$$k > 8\delta^{-2} \log(n),$$

there is a matrix $\mathbf{A} \in \mathbb{R}^{k \times d}$, such that,

$$\forall (i, j) \in \llbracket n \rrbracket^2, (1 - \delta) \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 \leq \|\mathbf{A}\mathbf{x}_i - \mathbf{A}\mathbf{x}_j\|_2^2 \leq (1 + \delta) \|\mathbf{x}_i - \mathbf{x}_j\|_2^2.$$

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Important comments

- ▶ The mapping is linear + works for any dataset !
- ▶ k does not depend on the dimension d !
- ▶ Magical: \mathbf{A} can be drawn randomly: $A_{ij} \sim \mathcal{N}(0, \frac{1}{k})$.
- ▶ This is tight in some sense [Larsen and Nelson 2017](#).
- ▶ Caveat: $n = 300$ samples, $\delta = 10\%$ already requires $k > 4560$.

Johnson-Lindenstrauss in practice

- ▶ Real dataset in $\mathbb{R}^{38 \times 7129}$, $\delta = 0.15$.
- ▶ For various choices of k , draw random Gaussian $A \sim \mathcal{N}(0, \frac{1}{k}) \in \mathbb{R}^{k \times d}$.
- ▶ Compare distances between \mathbf{Ax}_i s to distances between \mathbf{x}_i s.

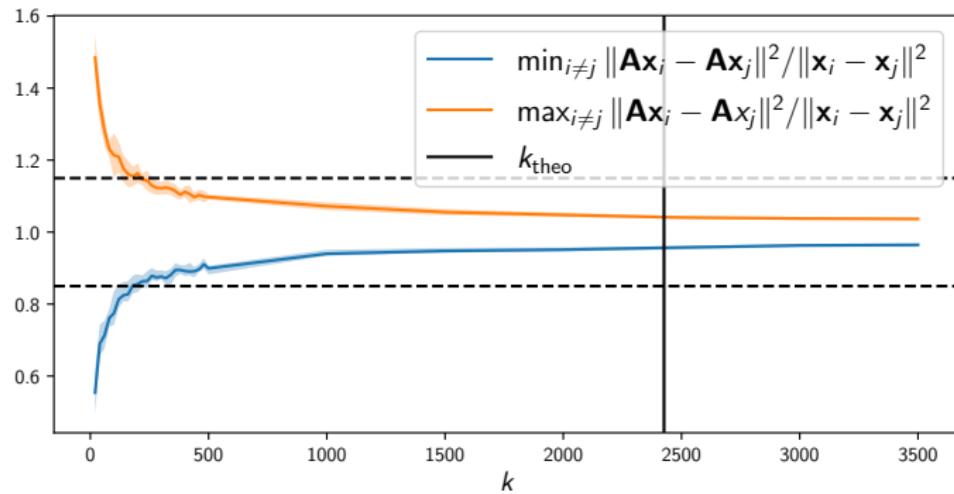


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Multidimensional scaling (MDS)

Learn from pairwise distances

- ▶ Distances in the big space: $D_{ij} = d(\mathbf{x}_i, \mathbf{x}_j)$ for some “metric” D .
- ▶ Find $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n \in \mathbb{R}^k$ that minimizes:

$$\text{stress}_D(\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n) = \sum_{i \neq j} (D_{ij} - \|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|_2)^2 \quad (9)$$

- ▶ Eq. (9) usually called *stress minimization*: $\|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|_2 \approx D_{ij}$.
- ▶ Can also be used for embedding nodes \mathbf{x}_i of a graph (not only Euclidean).
- ▶ Can be solved with eigenvalue decomposition.
- ▶ No map from the high dim space to the lower dim space.

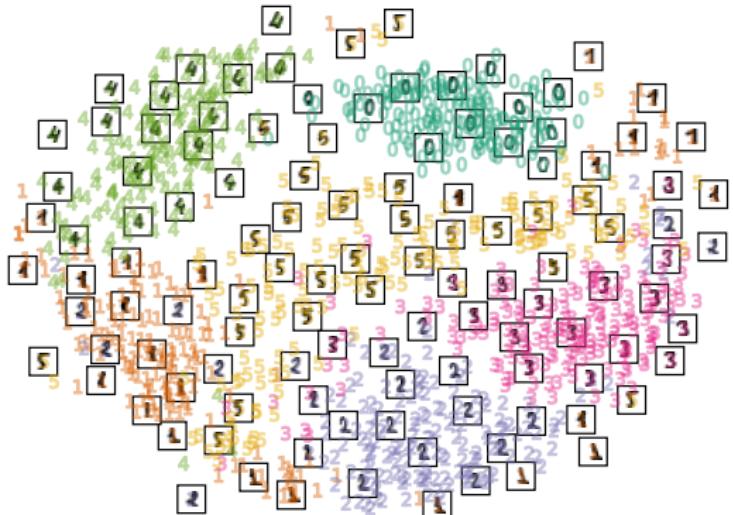
Multidimensional scaling (MDS)

- With digits dataset:

A selection from the 64-dimensional digits dataset

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

MDS embedding (time 2.959s)



Stochastic neighbor embedding (SNE)

Learn from pairwise similarities

- ▶ One of the most used algorithm G. E. Hinton and Roweis 2002.
- ▶ Similarities in the high-dim space:

$$P_{ij} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|_2^2/2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|_2^2/2\sigma_i^2)}, P_{ii} = 0.$$

- ▶ Similarities in the low-dim space:

$$Q_{ij} = \frac{\exp(-\|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|_2^2)}{\sum_{k \neq i} \exp(-\|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_k\|_2^2)}, Q_{ii} = 0.$$

- ▶ SNE: find $(\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n)$ that minimizes $\text{KL}(\mathbf{P}|\mathbf{Q}) = \sum_{ij} P_{ij} \log(\frac{P_{ij}}{Q_{ij}})$.
- ▶ σ_i local scaling, tuned with *entropic affinities* with fixed *perplexity* Vladymyrov and Carreira-Perpinan 2013.
- ▶ t-SNE variant for the kernel \mathbf{Q} (t-Student) Van der Maaten and G. Hinton 2008.

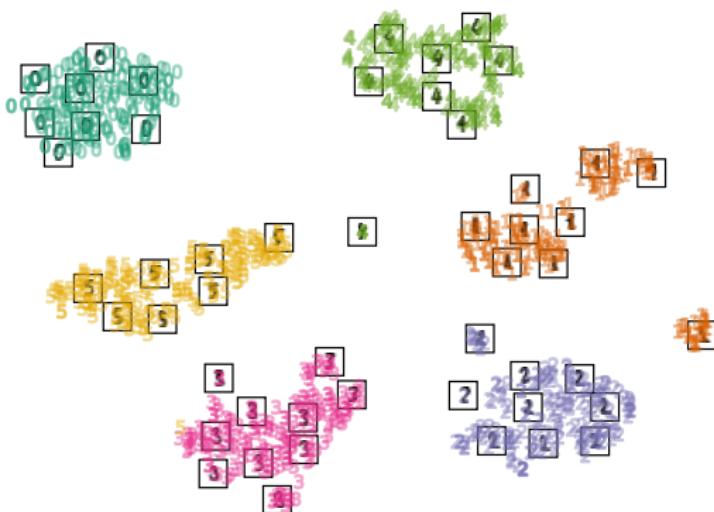
Stochastic neighbor embedding (SNE)

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

t-SNE embedding (time 1.324s)



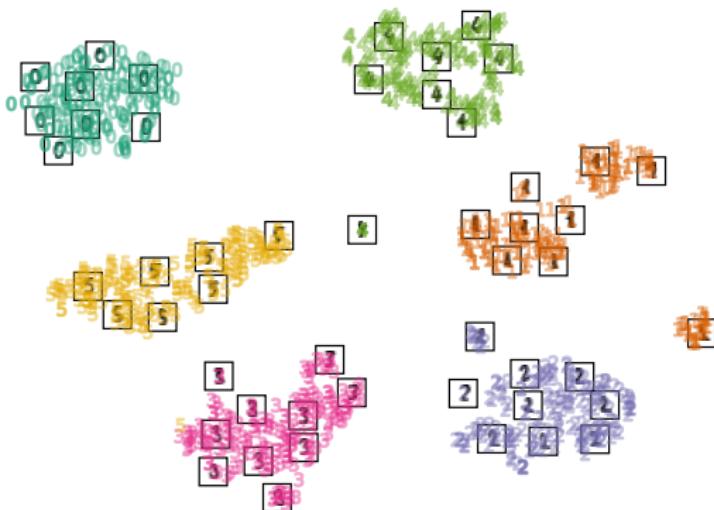
Stochastic neighbor embedding (SNE)

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3	4	4	6	0	5	7	4	5	4
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t-SNE embedding (time 1.324s)



Stochastic neighbor embedding (SNE)

On the perplexity parameter

- ▶ $(\sigma_i)_i$ local scalings are found so that:

$$\forall i \in \llbracket n \rrbracket, H(P_{i,:}) = - \sum_j P_{ij} \log(P_{ij}) = \log(\text{perp})$$

Stochastic neighbor embedding (SNE)

On the perplexity parameter

- ▶ $(\sigma_i)_i$ local scalings are found so that:

$$\forall i \in \llbracket n \rrbracket, H(P_{i,:}) = - \sum_j P_{ij} \log(P_{ij}) = \log(\text{perp})$$

Be aware of ...

- ▶ (T)SNE has tendency to show non-existent clusters for small perplexity
- ▶ (T)SNE struggles in high-dim! In practice: PCA first.
- ▶ No geometrical relations between clusters.
- ▶ Difficult to interpret, sensitive to perplexity.
- ▶ No mapping from the high dim space to the lower dim space.

t-SNE perp=3



t-SNE perp=50



t-SNE perp=200



t-SNE perp=500



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Principal component analysis

The principle of PCA

Singular value decomposition

Minimum distortion embedding

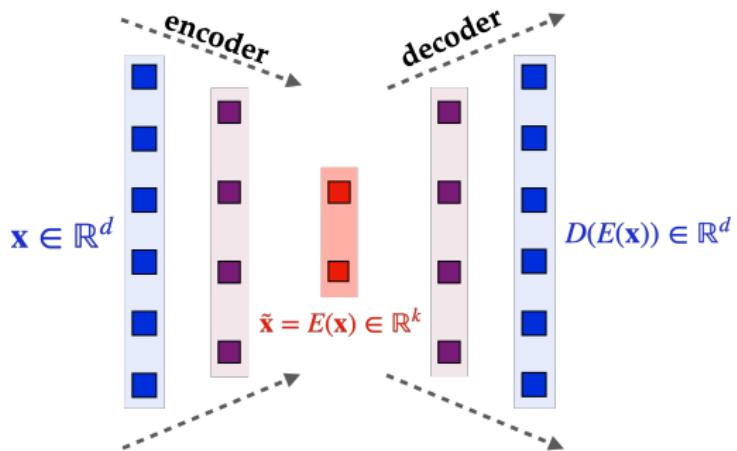
General setting

Random projections

Non linear methods

Autoencoders

Autoencoders



Principle

- ▶ Send the point x from \mathbb{R}^d to \mathbb{R}^k with an *encoder* E .
- ▶ Map back the *code/latent variable* $E(x)$ to the original space with a *decoder* D .
- ▶ Decoded code should be close to the original point.
- ▶ Code dimension $k \ll$ original dimension d .
- ▶ Autoencoder: E and D are neural networks!

Learning autoencoders

- ▶ Architecture of E and D is fixed (number of layers, non-linearity, type of layers)
- ▶ Typical fully-connected neural networks are a combination of matrix multiplication + bias with pointwise non-linearity:

$$g_K \circ \dots \circ g_1 \text{ where } g_k(\mathbf{x}) = \sigma(\mathbf{W}_k \mathbf{x} + \mathbf{b}_k)$$

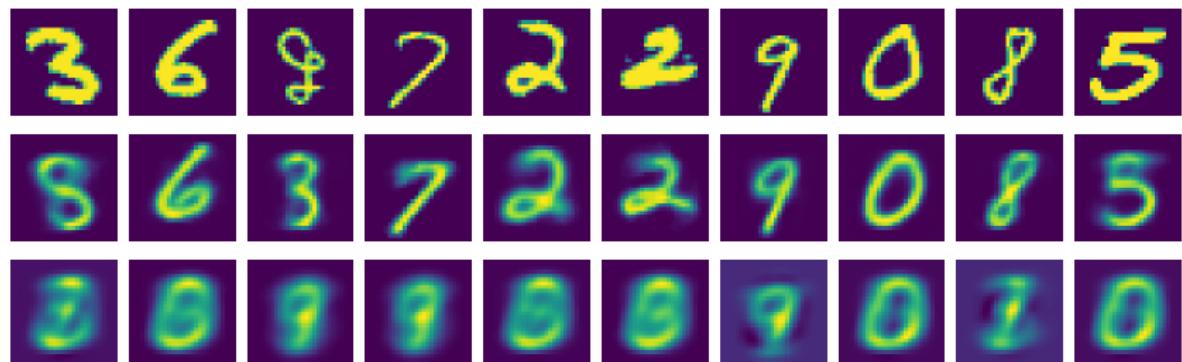
- ▶ Weights are learned by solving:

$$\min_{D,E} \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - D(E(\mathbf{x}_i))\|_2^2$$

- ▶ Optimisation is performed with first-order methods (SGD, Adam).

Autoencoder application to MNIST

- ▶ MNIST data: 28×28 images (784 pixels)
- ▶ Compressed into \mathbb{R}^2 with Autoencoder or PCA



Top: original, middle: autoencoder, bottom: PCA.

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