Cognitive Algorithms
Lecture 5

Unsupervised Learning

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Technische Universität Berlin
Machine Learning Group

Announcements

- There will be a practice exam ("Probeklausur"), published around 1st of February
- Relevant dates 2024
  - January 9th, last course lecture
  - February 6th, recap lecture by Johannes Niediek
  - Week of February 12th, discussion of the practice exam with all tutors
  - February 19th, 14.00–16.30 written exam ("first date")
  - April 8th, 08.30–11.00 written exam ("second date")
- All relevant rooms will be announced on ISIS
- Small changes are still possible, check ISIS

Notation

Link to notation document

$$\varphi(X)\varphi(X)^\top = \begin{pmatrix} \varphi_1(\boldsymbol{x}_1) & \dots & \varphi_1(\boldsymbol{x}_n) \\ & \dots & \\ \varphi_{\tilde{d}}(\boldsymbol{x}_1) & \dots & \varphi_{\tilde{d}}(\boldsymbol{x}_n) \end{pmatrix} \begin{pmatrix} \varphi_1(\boldsymbol{x}_1) & \dots & \varphi_{\tilde{d}}(\boldsymbol{x}_1) \\ & \dots & \\ \varphi_1(\boldsymbol{x}_n) & \dots & \varphi_{\tilde{d}}(\boldsymbol{x}_n) \end{pmatrix}$$
$$= \begin{pmatrix} \sum_i \varphi_1(\boldsymbol{x}_i)\varphi_1(\boldsymbol{x}_i) & \dots & \sum_i \varphi_1(\boldsymbol{x}_i)\varphi_{\tilde{d}}(\boldsymbol{x}_i) \\ & \dots & \\ \sum_i \varphi_{\tilde{d}}(\boldsymbol{x}_i)\varphi_1(\boldsymbol{x}_i) & \dots & \sum_i \varphi_{\tilde{d}}(\boldsymbol{x}_i)\varphi_{\tilde{d}}(\boldsymbol{x}_i) \end{pmatrix}$$

This expression occurs in the derivation of ridge regression.

Notation continued

$$
\begin{aligned}
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&= \begin{pmatrix} \varphi(\boldsymbol{x}_1)^\top \varphi(\boldsymbol{x}_1) & \dots & \varphi(\boldsymbol{x}_1)^\top \varphi(\boldsymbol{x}_{\tilde{d}}) \\ & \dots & \\ \varphi(\boldsymbol{x}_{\tilde{d}})^\top \varphi(\boldsymbol{x}_1) & \dots & \varphi(\boldsymbol{x}_{\tilde{d}})^\top \varphi(\boldsymbol{x}_{\tilde{d}}) \end{pmatrix} \\
&= \begin{pmatrix} k(\boldsymbol{x}_1, \boldsymbol{x}_1) & \dots & k(\boldsymbol{x}_1, \boldsymbol{x}_{\tilde{d}}) \\ & \dots & \\ k(\boldsymbol{x}_{\tilde{d}}, \boldsymbol{x}_1) & \dots & k(\boldsymbol{x}_{\tilde{d}}, \boldsymbol{x}_{\tilde{d}}) \end{pmatrix}
\end{aligned}
$$

This expression occurs in the derivation of kernel ridge regression.
Bias and Variance questions: will be considered later!

Recap: Kernels

- Basic idea: take a known machine learning method, then replace $\boldsymbol{x}_i^\top \boldsymbol{x}_j$ by $k(\boldsymbol{x}_i, \boldsymbol{x}_j)$.

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    "compare new data to all training data points"
- How can you show that a function $k(\cdot, \cdot)$ is a kernel function?
  - Find φ such that $k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \varphi(\boldsymbol{x}_i)^T \phi(\boldsymbol{x}_j)$ or show that k is symmetric positive semi-definite

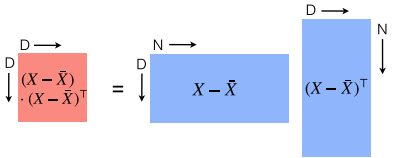
Recap: covariance matrix

Given n data points $\boldsymbol{x}_i \in \mathbb{R}^d$ in a data matrix $X \in \mathbb{R}^{d \times n}$, the empirical estimate of the **covariance matrix** is defined as

$$\bar{\Sigma} = \frac{1}{n} (X - \bar{X})(X - \bar{X})^\top$$

where $\bar{\boldsymbol{x}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i$

$$\bar{X} = (\bar{\boldsymbol{x}}, \bar{\boldsymbol{x}}, \ldots, \bar{\boldsymbol{x}}) \in \mathbb{R}^{d \times n}$$



$\bar{\Sigma}$ measures how much the data-points co-vary, for all pairs of dimensions.

Unsupervised learning

- **Supervised** algorithms
  - **Classification** and **regression**
  - Use labels in training

Approach	Labels
Binary classification	
Regression	

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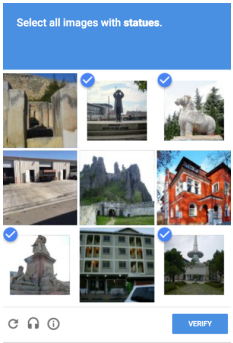
- Algorithm finds structure autonomously



Unsupervised learning

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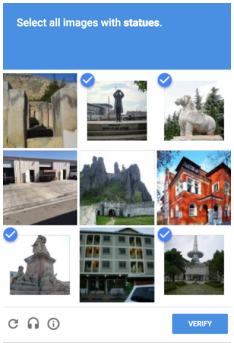
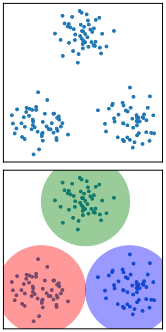
What can it be used for?

- Clustering
- Dimensionality reduction
- ...





Dimensionality reduction

In many applications...

- have high-dimensional data
- believe the data lie close to a low-dimensional subspace

→ Fewer parameters needed to account for the data properties
(the low-dimensional variables are sometimes called *hidden causes* or *latent variables*)

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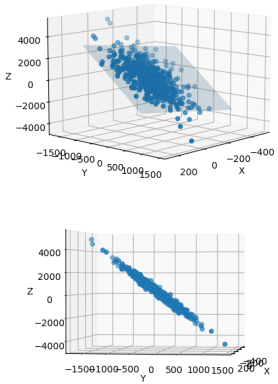

How to find a transformation $\mathbb{R}^3 \to \mathbb{R}^2$ that preserves the data structure?

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  Insights into high-dimensional structures in the data

[Xiao et al., 2017]

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- **Speeding up learning algorithms**
  Most algorithms scale badly with increasing data dimensionality
- **Data compression**
  Smaller storage requirements

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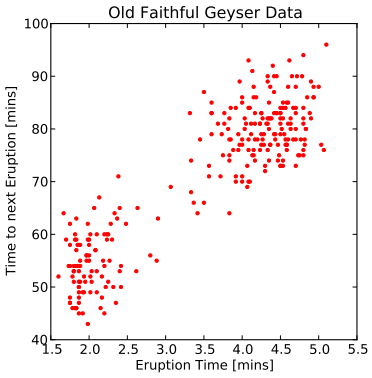
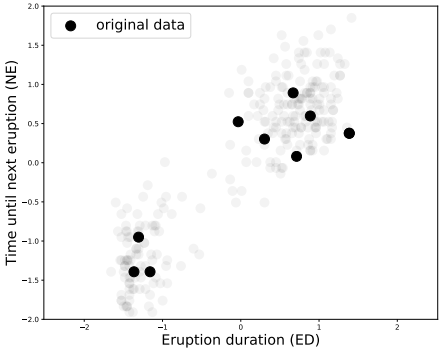
Example: Old Faithful geyser dataset

Old Faithful geyser eruption



Informal example dimensionality reduction

- High correlation between *NE* and *ED*



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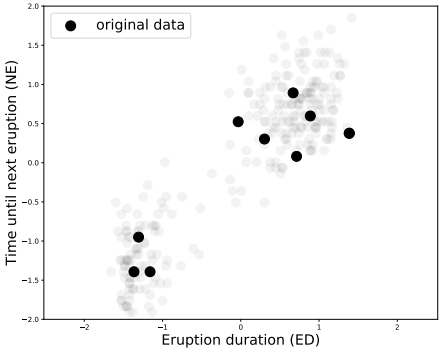
- Let's try to project data on $1D$ subspace



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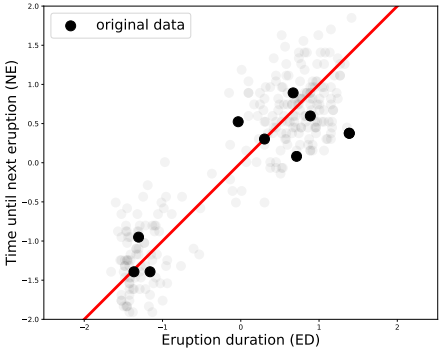

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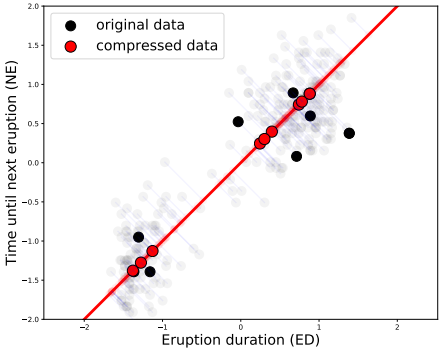

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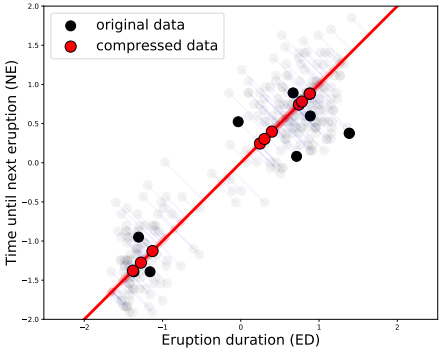

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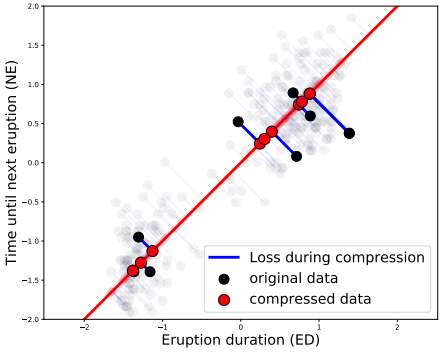

The mathematical model for linear dimensionality reduction

We have

- high-dimensional data $X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n] \in \mathbb{R}^{d \times n}$
- reason to believe they lie close to a lower-dimensional subspace

$\rightarrow$ $m < d$ parameters needed to account for the data properties
hidden causes or *latent variables* $H = [\boldsymbol{h}_1, \boldsymbol{h}_2, \ldots, \boldsymbol{h}_n] \in \mathbb{R}^{m \times n}$

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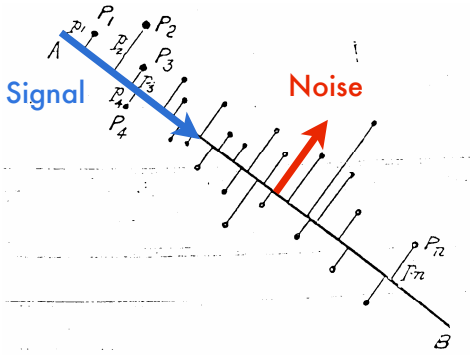
Goal: Find $m < d$ hidden causes $H \in \mathbb{R}^{m \times n}$, that explain the observed data via a (linear) *mixing* $W \in \mathbb{R}^{d \times m}$:

$$X \approx WH$$

Principal component analysis (PCA)



Adapted from Pearson [1901]

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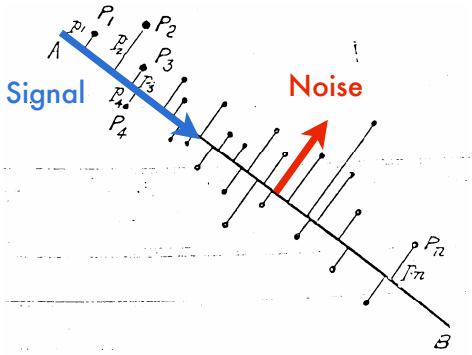

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Objective of PCA

Find a 1-dimensional subspace $\boldsymbol{w}$ that maximizes the variance of the projected data.

Equivalently: construct an orthonormal subspace such that the projected data and the original data have minimal Euclidean distance. See Bishop [2007, Section 12.1.2]

Maximizing variance

We obtained some data $X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n] \in \mathbb{R}^{d \times n}$

PCA finds a direction $\boldsymbol{w} \in \mathbb{R}^d$ such that the sample variance of the projected data $\boldsymbol{w}^\top X$ is maximal. Write $\overline{\text{Var}}$ to indicate the variance of a sample.

$$\overline{\text{Var}}(\boldsymbol{w}^T X) = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{w}^\top \boldsymbol{x}_i - \frac{1}{n}\sum_{j=1}^{n}\boldsymbol{w}^\top \boldsymbol{x}_j)^2$$

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We need to constrain $\boldsymbol{w}$ (because we can always make the variance larger by making $\|\boldsymbol{w}\|$ larger).

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This objective function is independent of the scaling of $\boldsymbol{w}$.

Note the similarity to the objective of Linear Discriminant Analysis!

$\rightarrow$ Different covariance matrices, different problem, but: same maths solve it.

$$\boldsymbol{w}_{\text{LDA}} = \underset{\boldsymbol{w}'}{\operatorname{argmax}}\, J(\boldsymbol{w}') = \underset{\boldsymbol{w}'}{\operatorname{argmax}} \frac{\boldsymbol{w}'^\top S_B \boldsymbol{w}'}{\boldsymbol{w}'^\top S_W \boldsymbol{w}'}$$

Maximizing variance

$$\underset{\boldsymbol{w}}{\text{argmax}} \frac{\boldsymbol{w}^\top S \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{w}} \tag{1}$$

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Equation 1 can be reduced to the standard eigenvalue problem:

$$S\boldsymbol{w} = \lambda \boldsymbol{w}$$

Maximizing variance

Setting $S\boldsymbol{w} = \lambda \boldsymbol{w}$ in Eq. 1, we see that the variance in direction $\boldsymbol{w}$ is given by:

$$\underset{\boldsymbol{w}}{\text{argmax}} \frac{\boldsymbol{w}^\top S \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{w}} = \frac{\boldsymbol{w}^\top \lambda \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{w}} = \lambda$$

Conclusion

- The variance of the projected data in the maximizing direction $\boldsymbol{w}$ is given by the corresponding eigenvalue

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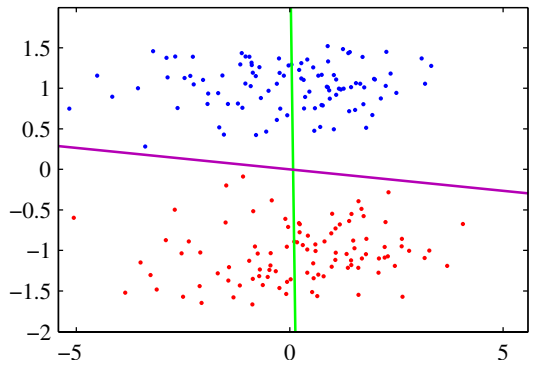
Conclusion

- The variance of the projected data in the maximizing direction $\boldsymbol{w}$ is given by the corresponding eigenvalue
- The direction of maximal variance in the data is equal to the eigenvector having the largest eigenvalue.

PCA vs. LDA

Which is which and why?



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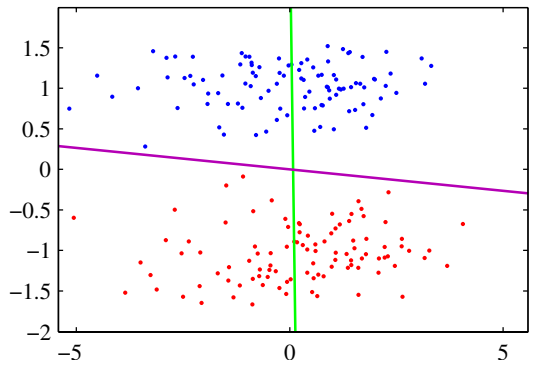

Directions found by PCA (magenta) and LDA(green) Bishop [2007]

Finding more principal components

Incremental PCA finds additional principal components, by looking at directions **orthogonal** to previous ones, that maximize variance.

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Characterization of PCA

The k first PCA basis vectors are the eigenvectors corresponding to the largest k eigenvalues

$$SW = W\Lambda,$$

where $W = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_k]$ contains the eigenvectors sorted according to their eigenvalues and Λ is a diagonal matrix containing the corresponding eigenvalues.

Recall (from linear algebra): since S is symmetric, there exist d orthogonal eigenvectors ($\boldsymbol{w}_i \perp \boldsymbol{w}_j$) and the eigenvalues are real numbers.

Encoding (from real data to latent representation)

Now that we have $W = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_k] \in \mathbb{R}^{d \times k}$, we project each data point $\boldsymbol{x}$ onto W

$$h_i = \begin{bmatrix} \boldsymbol{w}_1^T \boldsymbol{x}_i \\ \vdots \\ \boldsymbol{w}_k^T \boldsymbol{x}_i \end{bmatrix} = \begin{bmatrix} \boldsymbol{w}_1^T \\ \vdots \\ \boldsymbol{w}_k^T \end{bmatrix} \boldsymbol{x}_i = W^T \cdot \boldsymbol{x}_i$$

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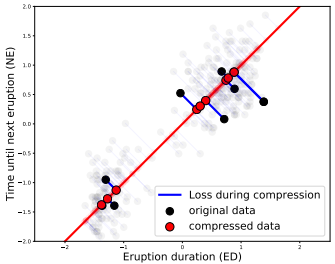

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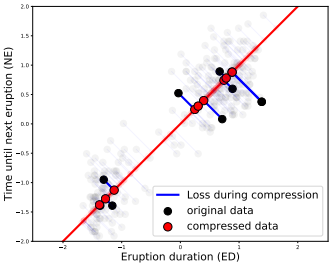
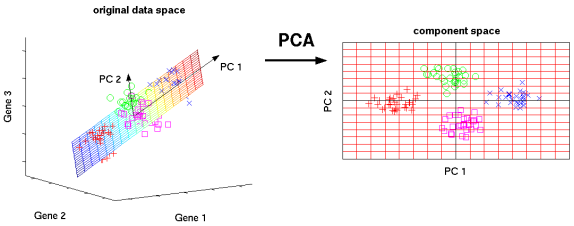
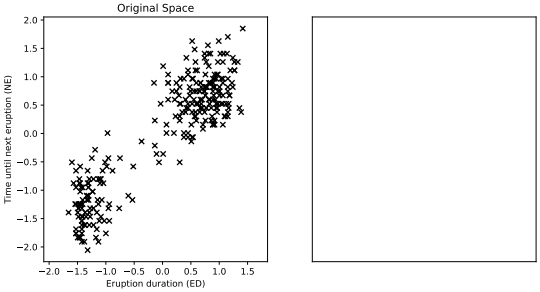


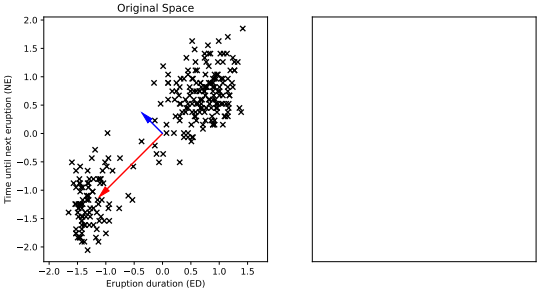


Principal Component Analysis



- PCA basis has maximum variance directions on basis vectors
  - Principal components $\boldsymbol{w}_j$ and latent representation h_{ij} do not change with increasing k

Principal Component Analysis



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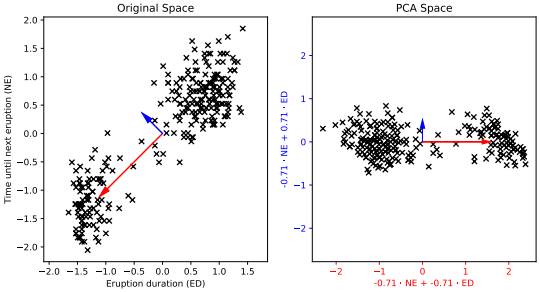

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Summary: Principal Component Analysis

1. Estimate the covariance matrix S of the data $X \in \mathbb{R}^{d \times n}$
2. Compute the eigenvectors of S
3. $W = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_k] \in \mathbb{R}^{d \times k}$ where $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_k \in \mathbb{R}^d$ are the eigenvectors corresponding to the k largest eigenvalues
4. Project the data onto W: $H = W^\top \cdot X$
5. If needed: reconstruct data by $X \approx \tilde{X} = WH$.
   This holds for all linear matrix factorization methods.

Summary: Principal Component Analysis

Algorithm 1: Principal Component Analysis

Require: data $x_1, \ldots, x_n \in \mathbb{R}^d$, number of principal components k

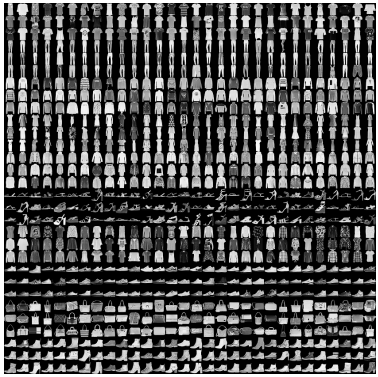
1: # Compute Sample Covariance Matrix
2: $C = 1/n\ (X - 1/n \sum_i x_i)(X - 1/n \sum_i x_i)^\top$
3: # Compute eigenvectors corresponding to the k largest eigenvalues
4: $W = \text{eig}(C)$
5: # Project data onto W
6: $H = W^\top X$
7: **return** W, H

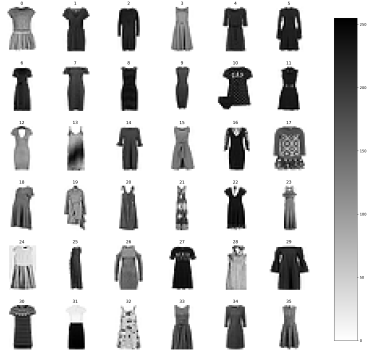
PCA on Fashion MNIST

Fashion-MNIST is a dataset of Zalando's article images consisting of 70,000 examples. Each example is a 28×28 grayscale image, associated with a label from 10 classes.

Fashion-MNIST on GitHub

PCA on Fashion MNIST





PCA on Fashion MNIST: Shirts

Figure: Eigenvectors (W)

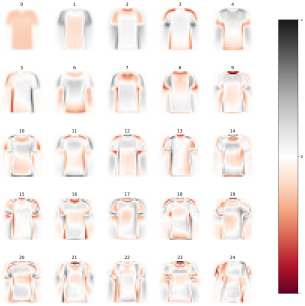
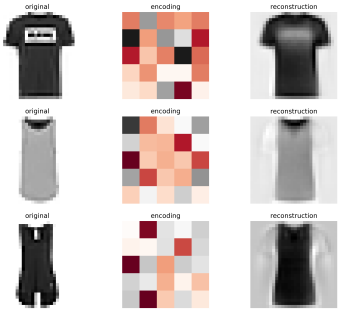


Figure: 3 examples (X, H, WH)



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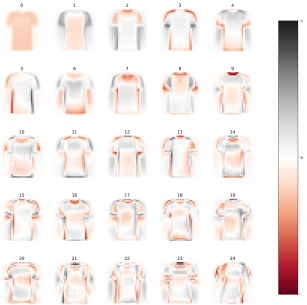

Figure: 3 examples (X, H, WH)

- Here we compress images to 25 dimensions instead of 784 (28×28), the compression ratio is 31.36.

PCA for high-dimensional data

Input: centered data $X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n] \in \mathbb{R}^{d \times n}$ with $n \ll d$

- Covariance matrix $XX^\top$ will be very large (d-by-d)
- Too few samples for a robust covariance matrix estimate

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where $\boldsymbol{\alpha} = 1/\lambda \cdot X^\top \boldsymbol{w}$ is a weighting of each data point

PCA for high-dimensional data

We can plug $\boldsymbol{w} = X\boldsymbol{\alpha}$ in and obtain

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which can be solved by [Schölkopf et al., 1998]

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Solving PCA via $X^\top X$ instead of $XX^\top$ is called **linear kernel PCA**.

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Solving PCA via $X^\top X$ instead of $XX^\top$ is called **linear kernel PCA**.

Note: if we want to use other kernels, we have to take care that data is centered in feature space, see Schölkopf et al. [1998, Appendix B] or Bishop [2007, Section 12.3].

When to use high-dimensional PCA

- If there are more dimensions than samples ($n \ll d$)
  Compute PCA on linear kernel matrix $X^\top X \in \mathbb{R}^{n \times n}$
- If there are more samples than dimensions ($d \ll n$)
  Compute PCA on covariance matrix $XX^\top \in \mathbb{R}^{d \times d}$

Wrap-up: Linear Kernel PCA

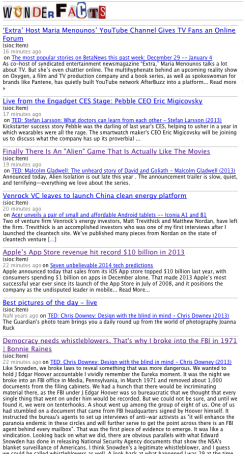
Algorithm 2: Linear Kernel PCA

Require: data $x_1, \ldots, x_n \in \mathbb{R}^d$, $n \ll d$, number of principal components k

1: # Compute Linear Kernel
2: $K = (X - 1/n \sum_i x_i)^\top (X - 1/n \sum_i x_i)$
3: # Compute eigenvectors corresponding to the k largest eigenvalues
4: $\alpha = \text{eig}(K)$
5: $W = X\alpha$
6: # Project data onto W
7: $H = W^\top X$
8: **return** W, H

Trends in text data

Let's look at some more applications of PCA!



Trends in text data

We are looking at bag-of-words data from a news web page

- We store the data in a matrix
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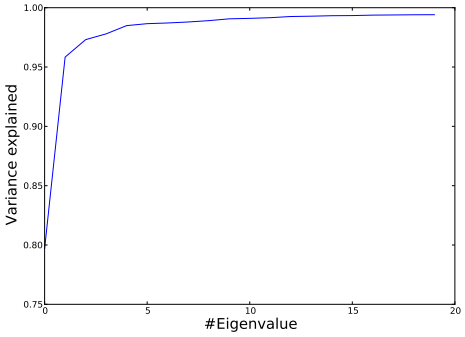

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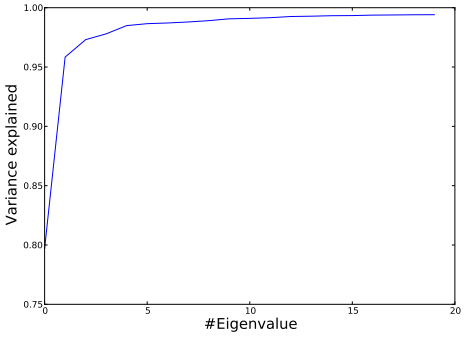
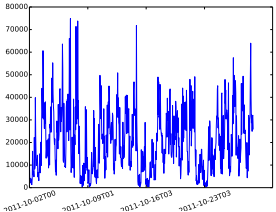
- We only need 15 principal directions to "explain" >99% of the data



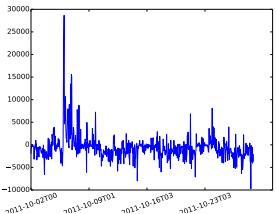
Trends in text data

First principal component



Main variance due to weekly/daily publishing activity

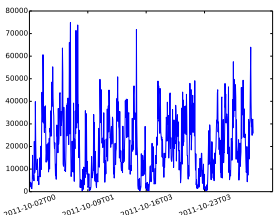
Second principal component



Spike on day of Steve Job's death

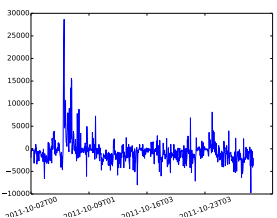
Trends in text data

First principal component



Main variance due to weekly/daily publishing activity

Second principal component



Spike on day of Steve Job's death

We can use PCA as a tool for analyzing big unlabeled data.

Non-negative matrix factorization (NMF)

- For some data PCA is not intuitive

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- Many data sets are strictly non-negative
  - Text data
  - Image data
  - Probabilistic data
- NMF is straightforward to implement
- Matrix factorization is relevant in recommender systems ("you might also like...") (more info here)

Non-negative matrix factorization

Notation: $\mathbb{R}_+ := \{x \in \mathbb{R} \,|\, x \geq 0\}$.
Given non-negative data $X \in \mathbb{R}_+^{d \times n}$ we want to find $W \in \mathbb{R}_+^{d \times m}$, $H \in \mathbb{R}_+^{m \times n}$ such that the distance between X and WH is minimal, where distance is measured as the Frobenius norm.
W and H are given by

$$\operatorname*{argmin}_{W,H} \|X - WH\|_{\text{Fro}}^2,$$

which is by definition of $\|\cdot\|_{\text{Fro}}$

$$= \operatorname*{argmin}_{W,H} \sum_{i=1}^{d} \sum_{j=1}^{n} (X_{ij} - (WH)_{ij})^2 .$$

Non-negative matrix factorization

$$\underset{W,H}{\operatorname{argmin}} \|X - WH\|_{\text{Fro}}^2 \qquad \text{such that } W \geq 0 \text{ and } H \geq 0 \text{ entry-wise}$$

Note that the constraints make the problem NP-hard and ill-posed [Gillis, 2014]. In particular, there are in general infinitely many solutions.

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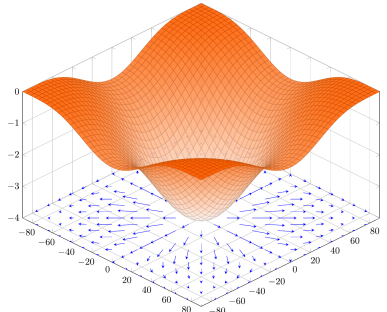
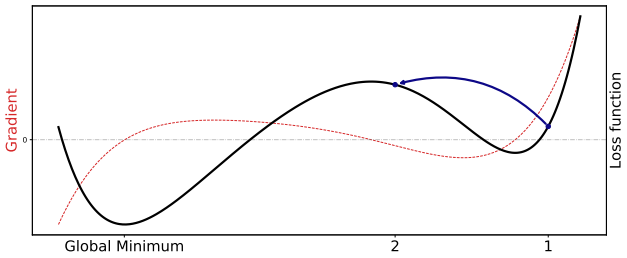


Gradient descent

Gradient descent finds **an** optimum of the loss function $\mathcal{L}(\alpha)$ by iterating

$$\alpha \leftarrow \alpha - \eta \frac{\partial \mathcal{L}(\alpha)}{\partial \alpha}$$



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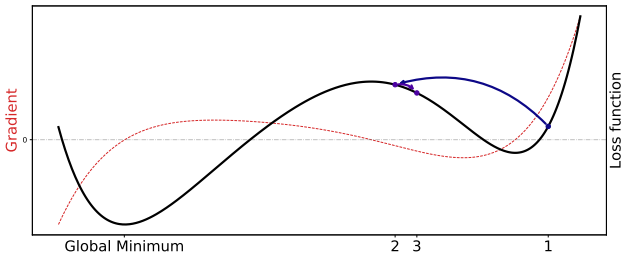

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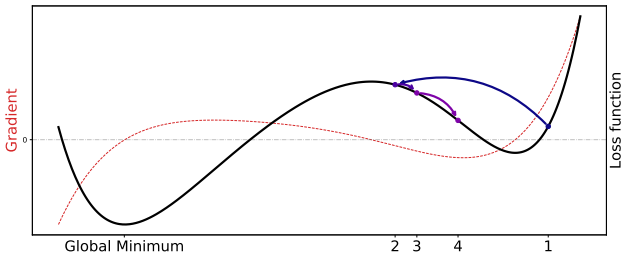

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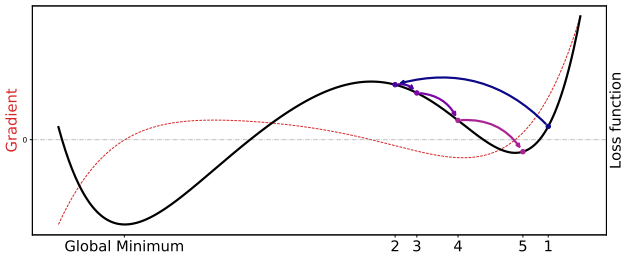

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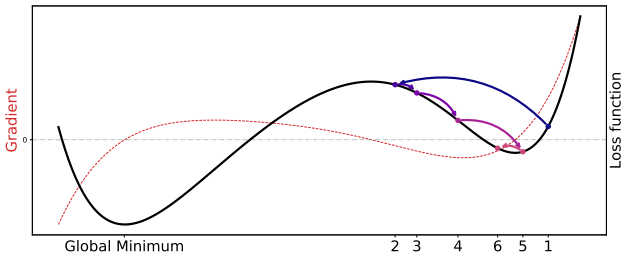

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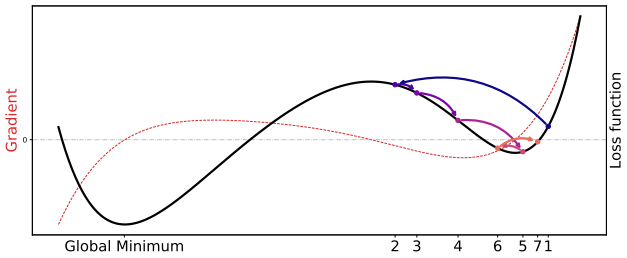

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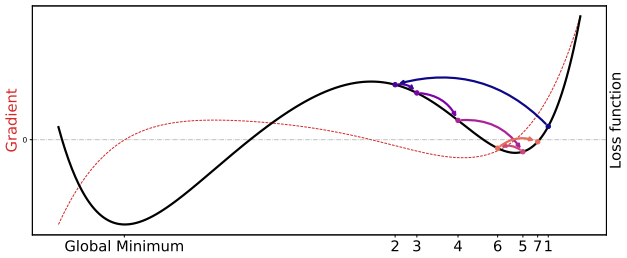

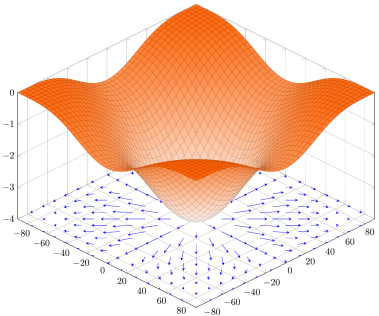

from Wikipedia

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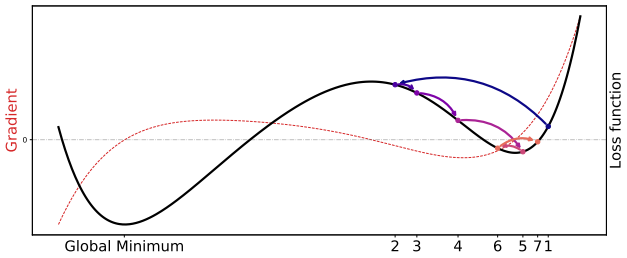

- **Not guaranteed to find global optimum**
- Adaptive η can yield improvements
- Stochastic gradient descent is basis for state-of-the-art machine learning (deep learning)

Let's do the calculations

Useful formulas (to be understood entry-wise)

$$\frac{\partial}{\partial X}\|X\|_{\text{Fro}}^2 = \frac{\partial}{\partial X}\operatorname{Tr}(XX^T)$$

$$\operatorname{Tr}(A) = \sum_i A_{ii}$$

$$\frac{\partial \operatorname{Tr}(AXB)}{\partial X} = \frac{\partial \operatorname{Tr}(B^T X^T A^T)}{\partial X} = A^T B^T$$

$$\frac{\partial \operatorname{Tr}(AXX^T A^T)}{\partial X} = 2A^T AX$$

$$\frac{\partial \operatorname{Tr}(XAX^T)}{\partial X} = XA^T + XA$$

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$$\frac{\partial \|X - WH\|_{\text{Fro}}^2}{\partial W} =$$

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Non-negative matrix factorization

Gradient descent finds a locally optimal solution by iterating

$$H \leftarrow H - \eta \left(W^\top WH - W^\top X \right)$$

$$W \leftarrow W - \eta \left(WHH^\top - XH^\top \right)$$

[2] Note that convergence has to be shown for these η.

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$$H \leftarrow H - \eta \left(W^\top WH - W^\top X \right)$$
$$W \leftarrow W - \eta \left(WHH^\top - XH^\top \right)$$

- By choosing $\eta_{ij}^H := \frac{H_{ij}}{(W^\top WH)_{ij}}$, $\eta_{ij}^W := \frac{W_{ij}}{(WHH^\top)_{ij}}$ one can transform the additive update into a multiplicative update[2] [Lee and Seung, 1999, 2000]:

$$H_{ij} \leftarrow H_{ij} \frac{(W^\top X)_{ij}}{(W^\top WH)_{ij}}$$
$$W_{ij} \leftarrow W_{ij} \frac{(XH^\top)_{ij}}{(WHH^\top)_{ij}}.$$

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NMF algorithm

Algorithm 3: Non-negative Matrix Factorization

Require: data $X = [x_1, \ldots, x_n] \in \mathbb{R}_+^{d \times n}$, number of factors k

1: # Initialize $W \in \mathbb{R}_+^{d \times k}$, $H \in \mathbb{R}_+^{k \times n}$ randomly
2: # Add a small constant $\epsilon = 10^{-19}$ to X to avoid zero-divisions
3: **for** it $\leq$ Iterations **do**
4: $\quad H = H \odot W^\top X \oslash W^\top WH$
5: $\quad W = W \odot XH^\top \oslash WHH^\top$
6: **end for**
7: **return** W, H

where

- $\odot$ is *element-wise* multiplication ($*$ in numpy)
- $\oslash$ is *element-wise* division ($/$ in numpy)

NMF on fashion MNIST: Shirts

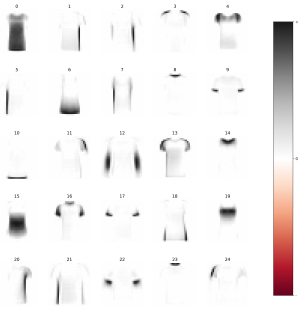


Figure: 25 main components (W)

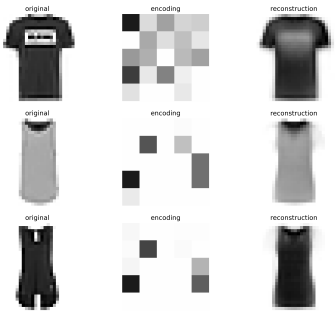


Figure: 3 examples (X, H, WH)

PCA vs. NMF - Fashion MNIST

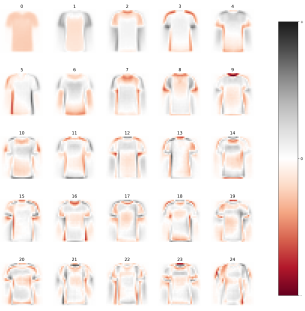


Figure: W_{PCA}

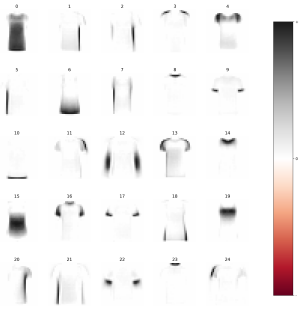
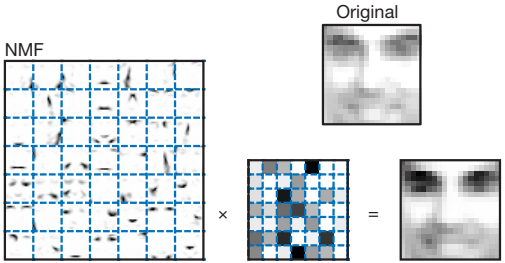
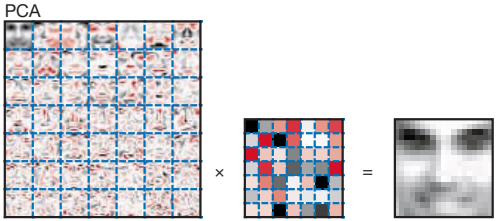


Figure: W_{NMF}

PCA vs. NMF - Face Parts

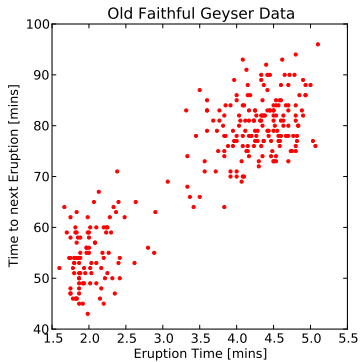




Taken from Lee and Seung [1999]

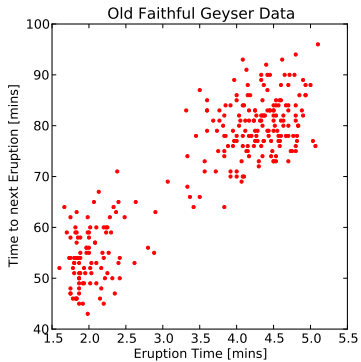
Clustering

- PCA/NMF are applied to reduce dimensionality



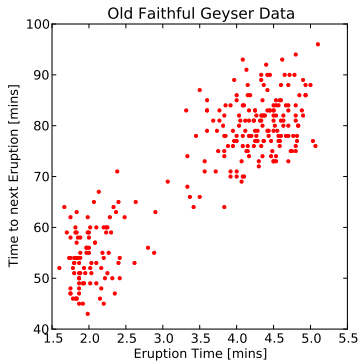
Clustering

- PCA/NMF are applied to reduce dimensionality
- Often the problem setting is different:



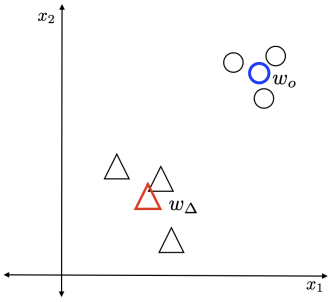
Clustering

- PCA/NMF are applied to reduce dimensionality
- Often the problem setting is different:
  - You want to categorize eruptions without labels



Clustering

Remember Lecture 2:
Psychological Models of Categorization: Prototypes



Prototypes $\boldsymbol{\mu}_\Delta$ and $\boldsymbol{\mu}_o$:

$$\boldsymbol{\mu}_\Delta = 1/n_\Delta \sum_{n}^{n_\Delta} \boldsymbol{x}_{\Delta,n}$$

$$\boldsymbol{\mu}_o = 1/n_o \sum_{n}^{n_o} \boldsymbol{x}_{o,n}$$

New data points $\boldsymbol{x}$ are assigned to their closest cluster center $\boldsymbol{\mu}^*$

$$\boldsymbol{\mu}^* = \underset{i}{\text{argmin}}(\|\boldsymbol{\mu}_i - \boldsymbol{x}\|_2)$$

K-means clustering

Objective for k-means

Find cluster centers $\boldsymbol{\mu}_1, \dots \boldsymbol{\mu}_k$ such that the sum of distances of data points to their respective cluster centers ("WCSS", "WSS"[3]) is minimized

$$L(\{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k\}, r) = \sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{\mu}_{r_i}\|^2$$

where r_i : cluster index of data point i

[3] Within cluster sum of squares

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We minimize L by re-iterating two steps

1. Assign each data point $\boldsymbol{x}_i$ to their closest cluster $\boldsymbol{\mu}_{r_i}$
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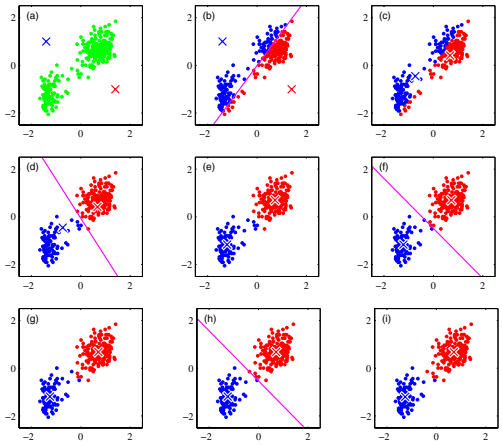
[3] Within cluster sum of squares

K-means clustering step-by-step



Re-iterate two steps:

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K-means clustering algorithm

Require: data $x_1, \ldots, x_n \in \mathbb{R}^d$, number of clusters k, iterations m.

Choose random data points as initial cluster centers $\boldsymbol{\mu}_1 \leftarrow x_{i_1}, \ldots, \boldsymbol{\mu}_k \leftarrow x_{i_k}$ where $i_j \neq i_l$ for all $j \neq l$.
$r \leftarrow \mathbf{0}_n$
$r' \leftarrow \mathbf{0}_n$
$i \leftarrow 0$
while $i < m$ **do**
    for $j \leftarrow 1$ to n **do**
        Find nearest cluster center $r'_j \leftarrow \text{argmin}_{1 \leq l \leq k} \|\boldsymbol{x}_j - \boldsymbol{\mu}_l\|_2$
    end for
    for $j \leftarrow 1$ to k **do**
        Compute new cluster center $\boldsymbol{\mu}_j \leftarrow \frac{1}{|\{l : r'_l = j\}|} \sum_{l : r'_l = j} x_l$
    end for
    if $r = r'$ **then**
        break
    end if
    $r \leftarrow r'$
    $i \leftarrow i + 1$
end while
return cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k \in \mathbb{R}^d$, assignment vector $r \in \mathbb{R}^n$

Application example: image compression

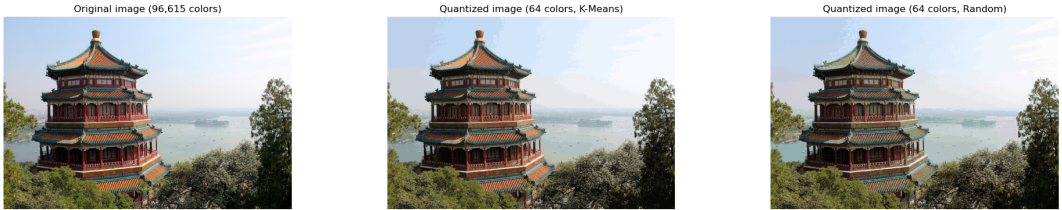
Original image (96,615 colors)

Quantized image (64 colors, K-Means)

Quantized image (64 colors, Random)

Adapted from sklearn, more information here.

Application example: image compression

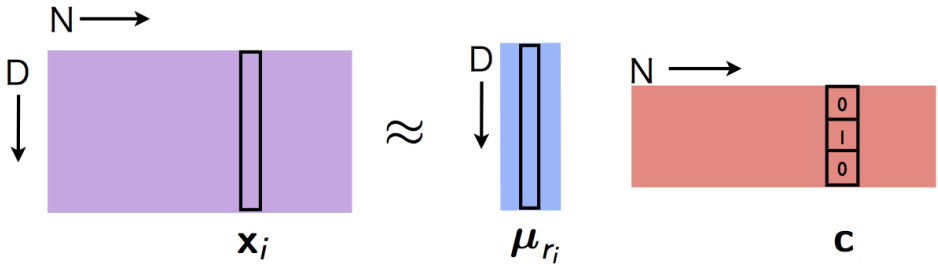


Adapted from sklearn, more information here.

- Encode color with 6 bit instead of 24 bit
- Only need one quarter of the bandwidth (and dictionary of colors)

Clustering can be seen as matrix factorization

Clustering finds an **optimal partitioning** of a data set[4]



For a clustering with k clusters, we have $\boldsymbol{\mu} \in \mathbb{R}^{D \times k}$ and $\mathbf{c} \in \{0,1\}^{k \times N}$.

[4] In the previous example, we actually used this by approximating the original colors $\boldsymbol{x}_i$ with the corresponding $\boldsymbol{\mu}_{r_i}$.

How to choose k

- Number of clusters k is critical hyper-parameter
- In supervised settings we use model selection (grid search) to optimize hyper-parameters for accuracy on test data
- How can we optimize the number of clusters?

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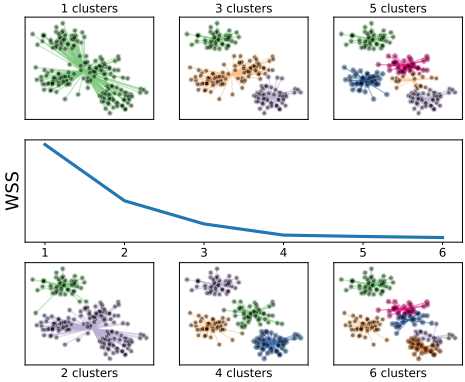
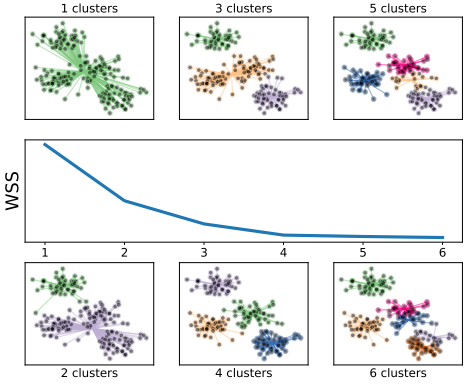
- In supervised settings we use model selection (grid search) to optimize hyper-parameters for accuracy on test data
- How can we optimize the number of clusters?



How to choose k

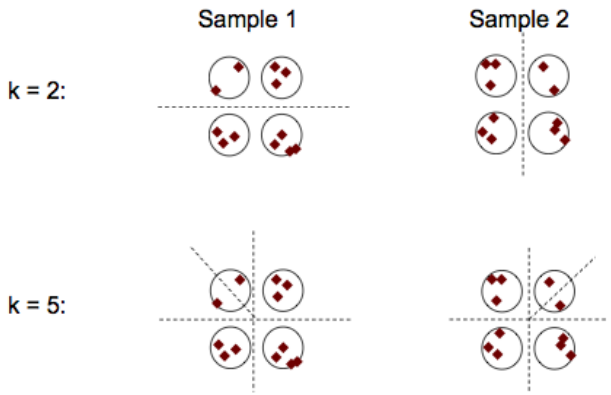
- Number of clusters k is critical hyper-parameter
- In supervised settings we use model selection (grid search) to optimize hyper-parameters for accuracy on test data
- How can we optimize the number of clusters?



→ One approach: find "elbow"; lowest k after which no real change

Clustering Instability

Number of Clusters is a critical parameter



Clusterings are unstable (i.e., converge to different results) if number of clusters is too small or too large

Summary I

- Matrix Factorization Methods
  - PCA and NMF belong to this class
  - Linearly approximate original data X with WH
- Principal Component Analysis
  - is a popular dimensionality reduction tool
  - aligns directions of maximal variance with standard basis
  - finds orthogonal directions
  - finds optimal matrix factorization
    (smallest Euclidean distance to subspace that the data is projected on)

Summary II

- Non-negative Matrix Factorization
  - works for non-negative data (count data, probabilistic data)
  - does not find orthogonal directions/uncorrelated factors
  - NMF encoding typically more sparse than PCA encoding
- Gradient Descent
  - useful for non-convex optimization
  - work-horse of Machine Learning
- K-Means Clustering
  - finds an optimal partitioning of a data set
  - K-Means requires
    - Good initialization
    - Knowledge of optimal k

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