Cognitive Algorithms
Lecture 5

Unsupervised Learning

Klaus-Robert Müller, **Ali Hashemi**, **Lorenz Vaitl**,
Augustin Krause, Joanina Oltersdorff, Ken Schreiber

Berlin Institute of Technology
Dept. Machine Learning

Today's agenda

Recap

Unsupervised Learning

PCA

PCA Applications

NMF

Clustering

Summary

Recap: Kernels

What is a kernel function?

$\rightarrow k(x_i, x_j) = \varphi(x_i) \cdot \varphi(x_j)^T$

Why are kernels useful?

$\rightarrow$ Implicitly work in high-dimensional space

$\rightarrow$ Thanks to representer theorem, work on space spanned by data

How can you show that a function $k(\cdot, \cdot)$ is a kernel function?

$\rightarrow$ Find $\phi(\cdot)$ s.t. $k(x_i, x_j) = \phi(x_i)^T \phi(x_j)$ or show that $k(\cdot, \cdot)$ is PSD

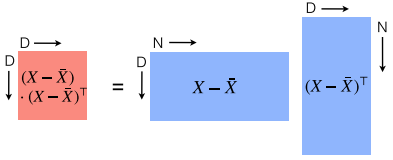
Recap: Covariance Matrices

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

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

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

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



Unsupervised learning

Supervised algorithms

- **Classification** and **regression**
- Labels for training

But labels not always given e.g.

- Mixtures of different speakers in an audio recording
- Complex artefacts in experimental recordings

Unsupervised algorithms

- No labels for training

	y
(Binary) Classification	$\in \{+1, -1\}$
Regression	$\in \mathbb{R}$
Unsupervised	$\in \emptyset$ don't exist

Unsupervised learning

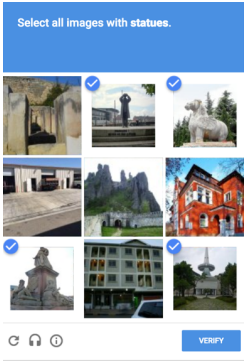
Why unsupervised learning

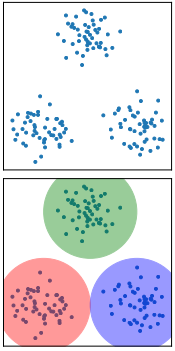
- No need for human made labels
- Algorithm finds structure autonomously

What can it be used for?

- Clustering
- Dimensionality Reduction

⋮





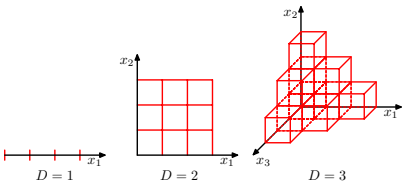
Dimensionality Reduction

In many applications, we have

- high-dimensional data
- reason to believe they lie close to a lower dimensional subspace

$\rightarrow$ Fewer parameters needed to account for the data properties
hidden causes or *latent variables*

Curse of Dimensionality



[Bishop, 2007]

解释数据属性、隐藏原因或潜在变量所需的参数更少

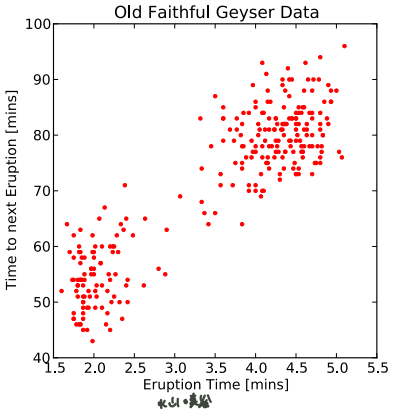
Why Dimensionality Reduction

- **Visualization**:
  Insights into high-dimensional structures in the data
- **Better Generalization**:
  Fewer dimensions $\rightarrow$ smaller chance of overfitting
- **Speeding up** learning algorithms:
  Most algorithms scale badly with increasing data dimensionality
- **Data compression**:
  Less storage requirements

[Xiao et al., 2017]

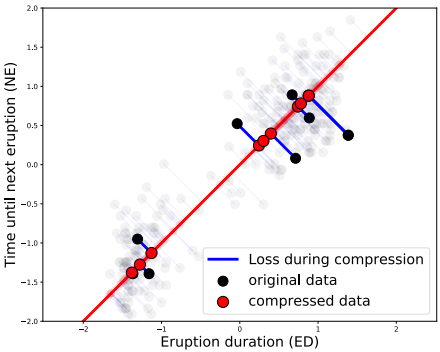
Example: Old Faithful Geyser Dataset

Old Faithful Geyser



Informal example dimensionality reduction

- High correlation between *NE* and *ED*
- Let's try to project data on $1D$ subspace
- Relatively good representation



The mathematical model for linear dimensionality reduction

We have

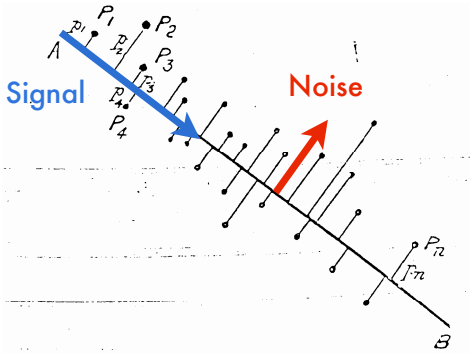
- high-dimensional data $X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n] \in \mathbb{R}^{d \times n}$
- reason to believe they lie close to a lower dimensional subspace

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

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

$$X \approx WH$$

Principal Component Analysis (PCA)



Adapted from Pearson [1901]

has the following two equivalent objectives: find the direction $\boldsymbol{w}$ that minimizes the

noise and maximizes the signal

or equivalently

find the line $\boldsymbol{w}$ that maximizes the variance within the data set

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 estimated variance of the projected data $\boldsymbol{w}^\top X$ is maximal

$$
\begin{aligned}
\overline{\mathrm{Var}}(\boldsymbol{w}^T X) &= \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{w}^\top \boldsymbol{x}_i - \frac{1}{n}\sum_{j=1}^{n}\boldsymbol{w}^\top \boldsymbol{x}_j)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{w}^\top \boldsymbol{x}_i - \boldsymbol{w}^\top \frac{1}{n}\sum_{j=1}^{n}\boldsymbol{x}_j)^2 = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{w}^\top (\boldsymbol{x}_i - \bar{\boldsymbol{x}}))^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{w}^\top (\boldsymbol{x}_i - \bar{\boldsymbol{x}}) \cdot (\boldsymbol{x}_i - \bar{\boldsymbol{x}}))^\top \boldsymbol{w} \\
&= \boldsymbol{w}^\top \underbrace{\left(\frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{x}_i - \bar{\boldsymbol{x}})) \cdot (\boldsymbol{x}_i - \bar{\boldsymbol{x}}))^\top\right)}_{\text{Empirical covariance matrix } \bar{\Sigma}} \boldsymbol{w}
\end{aligned}
$$

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 variance of the projected data $\boldsymbol{w}^\top X$ is maximal
Let's assume centered data for easier notation [1]

$$\begin{aligned} \overline{\mathrm{Var}}(\boldsymbol{w}^T X) &= \boldsymbol{w}^\top \underbrace{\left(\frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i \cdot \boldsymbol{x}_i^\top \right)}_{\text{Empirical Covariance matrix } \bar{\Sigma}} \boldsymbol{w} \\ &\propto \boldsymbol{w}^\top \underbrace{XX^\top}_{\text{Scatter matrix } S} \boldsymbol{w} \end{aligned}$$

And: we need to constrain $\boldsymbol{w}$

[1] i.e. we assume $\bar{\boldsymbol{x}} = 0$

Maximizing variance

PCA finds a direction $\boldsymbol{w} \in \mathbb{R}^d$ such that the variance of the projected data $\boldsymbol{w}^T X$ is maximal

$$\underset{w}{\operatorname{argmax}} \frac{\boldsymbol{w}^\top S \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{w}}$$

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

Maximizing variance

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

Set the derivative w.r.t $\boldsymbol{w}$ to zero:

$$\frac{\partial}{\partial \boldsymbol{w}} \frac{\boldsymbol{w}^\top S \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{w}} = \frac{(\boldsymbol{w}^\top \boldsymbol{w}) 2S\boldsymbol{w} - (\boldsymbol{w}^\top S \boldsymbol{w}) 2\boldsymbol{w}}{(\boldsymbol{w}^\top \boldsymbol{w})^2} \stackrel{!}{=} 0$$

$$\Rightarrow \underbrace{(\boldsymbol{w}^\top S \boldsymbol{w})}_{\text{scalar}} \boldsymbol{w} = \underbrace{(\boldsymbol{w}^\top \boldsymbol{w})}_{\text{scalar}} S\boldsymbol{w}$$

$$\Rightarrow \underbrace{\frac{\boldsymbol{w}^\top S \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{w}}}_{\equiv \lambda} \boldsymbol{w} = S\boldsymbol{w}$$

$\rightarrow$ Eq. 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:

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

The variance of the projected data in an eigendirection $\boldsymbol{w}$ 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?

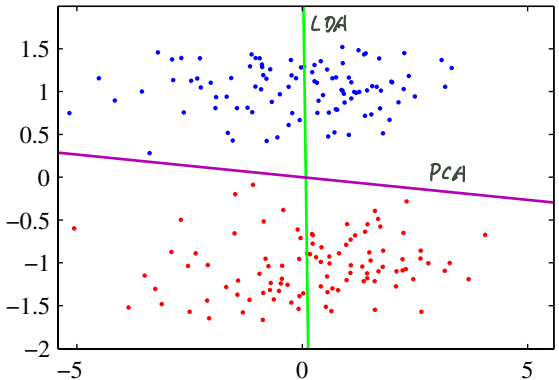


Figure: Directions found by PCA (magenta) and LDA(green) Bishop [2007]

Finding more Principal Components

Incremental PCA then finds additional principal components, by looking at directions **orthogonal** to previous ones, that maximize variance. It can be shown that:

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

$$SW = W\Lambda$$

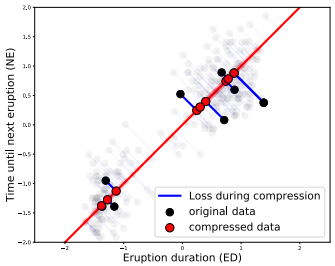
where $W = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_k]$ contains the eigenvectors sorted according to their eigenvalues and Λ is a diagonal matrix containing the corresponding eigenvalues.

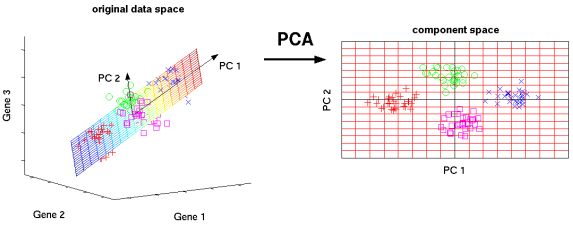
Recall theory of eigenvectors:
Since S is symmetric, there exist d orthogonal eigenvectors!
$\rightarrow \boldsymbol{w}_i \perp \boldsymbol{w}_j$

Encoding (from real data to latent representation)

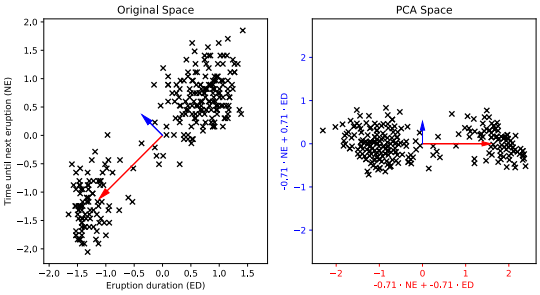
Now that we have $W = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_k] \in \mathbb{R}^{d \times k}$, we project each data point $\boldsymbol{x}$ onto W

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





Principal Component Analysis



- PCA aligns maximum variance directions with standard basis
  - → Variance along each dimension is **uncorrelated**
  - → PCs $\boldsymbol{w}_j$ and latent representation h_{ij} do not change with increasing k

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: $H = W^\top \cdot X$

* If needed[2]: reconstruct data by $X \approx \tilde{X} = WH$

[2] This holds for all Linear Matrix Factorization methods

Summary: Principal Component Analysis

Algorithm 1: Principal Component Analysis

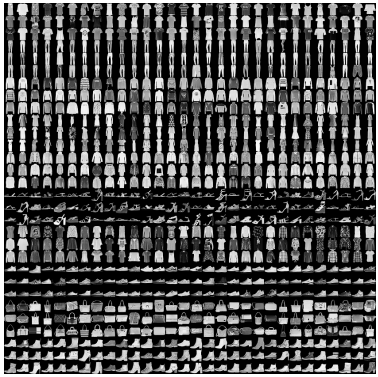
Require: data $x_1, \ldots, x_n \in \mathbb{R}^d$, number of principal components k

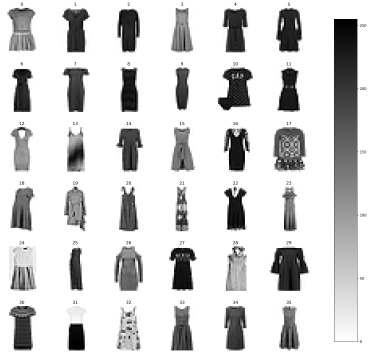
1: # Compute Sample Covariance Matrix
2: $C = 1/n\ (X - 1/n \sum_i x_i)(X - 1/n \sum_i x_i)^\top$
3: # Compute eigenvectors corresponding to the k largest eigenvalues
4: $W = \text{eig}(C)$
5: # Project data onto W
6: $H = W^\top X$
7: **return** W, H

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.

PCA on Fashion MNIST





PCA on Fashion MNIST: Shirts

Figure: Eigenvectors (W)

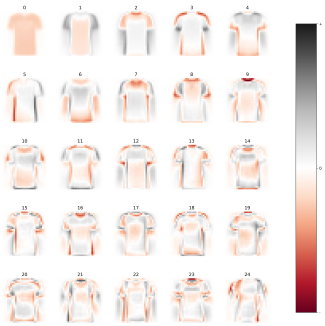


Figure: 3 examples (X, H, WH)

Here we compress images to 25 dimensions instead of 784 (28×28)

$\rightarrow$ more than factor 31

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 $n \ll d$

$\rightarrow$ Covariance matrix $XX^\top$ will be very large (d-by-d)

$\rightarrow$ Too few samples for a robust covariance matrix estimate

We know the direction of maximal variance $\boldsymbol{w}$ must lie in the span of the data (for $\lambda \neq 0$):

$$\lambda \boldsymbol{w} = XX^\top \boldsymbol{w} \;\rightarrow\; \boldsymbol{w} = X\boldsymbol{\alpha}$$

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

$$\begin{aligned} XX^\top \boldsymbol{w} &= \lambda \boldsymbol{w} \\ XX^\top X\boldsymbol{\alpha} &= \lambda X\boldsymbol{\alpha} \\ \underbrace{X^\top X}_{K}\underbrace{X^\top X}_{K}\boldsymbol{\alpha} &= \lambda \underbrace{X^\top X}_{K}\boldsymbol{\alpha} \\ KK\boldsymbol{\alpha} &= \lambda K\boldsymbol{\alpha} \end{aligned}$$

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

$$K\boldsymbol{\alpha} = \lambda\boldsymbol{\alpha}.$$

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 features space $\rightarrow$ more complicated

When should we use a kernel for PCA ?

If there are more dimensions than samples ($n \ll d$)

$\rightarrow$ Compute PCA on linear kernel matrix $X^\top X \in \mathbb{R}^{n \times n}$

If there are more samples than dimensions ($d \ll n$)

$\rightarrow$ Compute PCA on covariance matrix $XX^\top \in \mathbb{R}^{d \times d}$

Wrap-up: Linear Kernel PCA

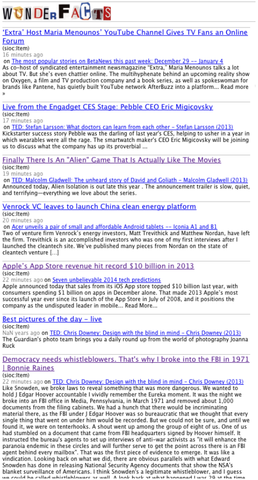
Algorithm 2: Linear Kernel PCA

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!


WONDERFACTS

'Extra' Host Maria Menounos' YouTube Channel Gives TV Fans an Online Forum
(sioc:Item)
16 minutes ago
on The most popular stories on BetaNews this past week: December 29 -- January 4
As co-host of syndicated entertainment newsmagazine "Extra," Maria Menounos talks a lot about TV. But she's even chattier online. The multihyphenate behind an upcoming reality show on Oxygen, a film and TV production company and a book series, as well as spokeswoman for brands like Pantene, has quietly built YouTube network AfterBuzz into a platform... Read more »

Live from the Engadget CES Stage: Pebble CEO Eric Migicovsky
(sioc:Item)
17 minutes ago
on TED: Stefan Larsson: What doctors can learn from each other - Stefan Larsson (2013)
Kickstarter success story Pebble was the darling of last year's CES, helping to usher in a year in which wearables were all the rage. The smartwatch maker's CEO Eric Migicovsky will be joining us to discuss what the company has up its proverbial ...

Finally There Is An "Alien" Game That Is Actually Like The Movies
(sioc:Item)
19 minutes ago
on TED: Malcolm Gladwell: The unheard story of David and Goliath - Malcolm Gladwell (2013)
Announced today, Alien Isolation is out late this year . The announcement trailer is slow, quiet, and terrifying—everything we love about the series.

Venrock VC leaves to launch China clean energy platform
(sioc:Item)
20 minutes ago
on Acer unveils a pair of small and affordable Android tablets -- Iconia A1 and B1
Two of venture firm Venrock's energy investors, Matt Trevithick and Matthew Nordan, have left the firm. Trevithick is an accomplished investors who was one of my first interviews after I launched the cleantech site. We've published many pieces from Nordan on the state of cleantech venture [...]

Apple's App Store revenue hit record $10 billion in 2013
(sioc:Item)
22 minutes ago on Seven unbelievable 2014 tech predictions
Apple announced today that sales from its iOS App store topped $10 billion last year, with consumers spending $1 billion on apps in December alone. That made 2013 Apple's most successful year ever since its launch of the App Store in July of 2008, and it positions the company as the undisputed leader in mobile... Read More...

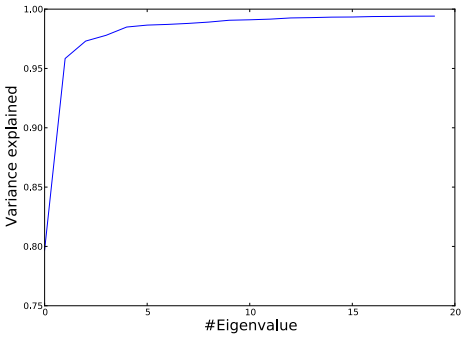
Best pictures of the day - live
(sioc:Item)
NaN years ago on TED: Chris Downey: Design with the blind in mind - Chris Downey (2013)
The Guardian's photo team brings you a daily round up from the world of photography Joanna Ruck

Democracy needs whistleblowers. That's why I broke into the FBI in 1971 | Bonnie Raines
(sioc:Item)
22 minutes ago on TED: Chris Downey: Design with the blind in mind - Chris Downey (2013)
Like Snowden, we broke laws to reveal something that was more dangerous. We wanted to hold J Edgar Hoover accountable I vividly remember the Eureka moment. It was the night we broke into an FBI office in Media, Pennsylvania, in March 1971 and removed about 1,000 documents from the filing cabinets. We had a hunch that there would be incriminating material there, as the FBI under J Edgar Hoover was so bureaucratic that we thought that every single thing that went on under him would be recorded. But we could not be sure, and until we found it, we were on tenterhooks. A shout went up among the group of eight of us. One of us had stumbled on a document that came from FBI headquarters signed by Hoover himself. It instructed the bureau's agents to set up interviews of anti-war activists as "it will enhance the paranoia endemic in these circles and will further serve to get the point across there is an FBI agent behind every mailbox". That was the first piece of evidence to emerge. It was like a vindication. Looking back on what we did, there are obvious parallels with what Edward Snowden has done in releasing National Security Agency documents that show the NSA's blanket surveillance of Americans. I think Snowden's a legitimate whistleblower, and I guess

Trends in Text Data

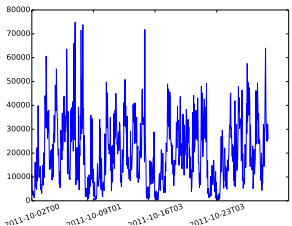
We are looking at Bag-Of-Words data from news web pages wunderfacts.com, in October 2011

- We store the data in a matrix $X \in \mathbb{R}^{d \times t}$
  The entry $X_{dt} = 10$ tells us: word d was counted 10 times in time bin t
- Let's apply PCA and look at the explained variance ($\text{ev}_i = \frac{\sum_{j=1}^{i} \lambda_i}{\sum_{l=1}^{d} \lambda_l}$)
- We only need 15 principal directions to explain >99% of the data



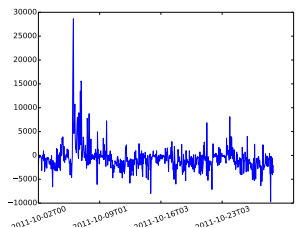
Trends in Text Data

First Principal Component



Main Variance due to weekly/daily publishing activity

Second Principal Component



Spike on day of Steve Job's death

$\rightarrow$ We can use PCA as a tool for analysing big unlabelled data

Non-Negative Matrix Factorization (NMF)

- For some data PCA is not intuitive
- Example: Non-negative data
  - Principal directions will have negative entries
  - This can be hard to interpret
- Many data sets are strictly non-negative
  - Text data
  - Image data
  - Probabilistic data
- NMF is straightforward to implement
- Applicable to Recommender Systems (more info here)

Non-Negative Matrix Factorization

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

$$\underset{W,H}{\operatorname{argmin}} ||X - WH||_{\text{Fro}}^2 = \underset{W,H}{\operatorname{argmin}} \sum_{d=1}^{d} \sum_{n=1}^{n} (X_{dn} - (WH)_{dn})^2$$

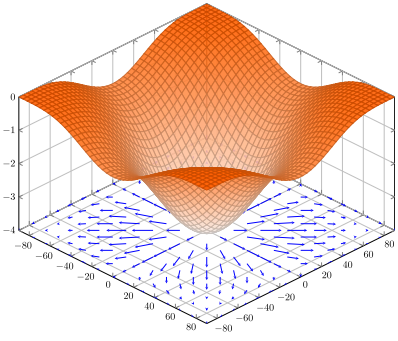
Non-Negative Matrix Factorization

$$\underset{W,H}{\operatorname{argmin}} ||X - WH||^2_{\text{Fro}} \qquad \text{s.t. } W \geq 0 \text{ and } H \geq 0$$

Note that the constraints make the problem NP-hard and Ill-posed [Gillis, 2014].

Note

Whenever the problem is too hard just follow the gradients!

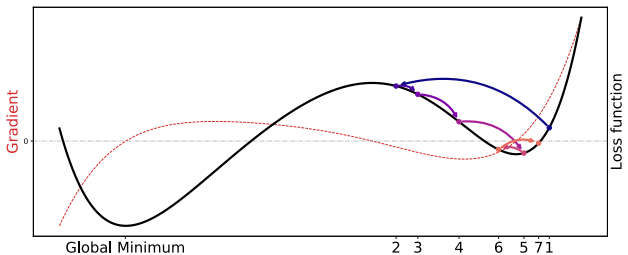


from Wikipedia

Gradient Descent

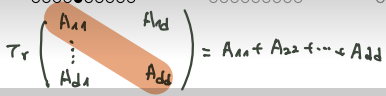
Gradient descent finds **an** optimum of Loss $\mathcal{L}(\alpha)$ by iterating

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



- **Not guaranteed to find global optimum**
- Adaptive η can yield improvements
- Stochastic Gradient Descent is basis for State of the Art ML

Tr is the trace of the matrix



Using

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

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

$$\frac{\partial\,\text{Tr}(AXX^TA^T)}{\partial X} = 2A^TAX$$

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

$$\frac{\partial\,\text{Tr}(AXB)}{\partial X} = \frac{\partial\,\text{Tr}(B^TX^TA^T)}{\partial X} = A^TB^T$$

$$\frac{\partial||X - WH||_{\text{Fro}}^2}{\partial H} = 2(W^TWH - W^TX)$$

$$\frac{\partial||X - WH||_{\text{Fro}}^2}{\partial W} = 2(WHH^T - XH^T)$$

Non-Negative Matrix Factorization

Gradient descent finds an optimal solution by iterating

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

$$\eta_{ij}^H := \frac{H_{ij}}{(W^T W H)_{ij}}$$

- By choosing η wisely one can transform the additive updates into multiplicative ones [Lee and Seung, 1999, 2000]:

$$H = H \odot W^\top X \oslash W^\top WH \qquad H_{ij} \leftarrow H_{ij} \frac{(W^T X)_{ij}}{(W^T W H)_{ij}}$$
$$W = W \odot XH^\top \oslash WHH^\top \qquad W_{ij} \leftarrow W_{ij} \frac{(XH^T)_{ij}}{(WHH^T)_{ij}}$$

where

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

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

NMF on Fashion MNIST: Shirts

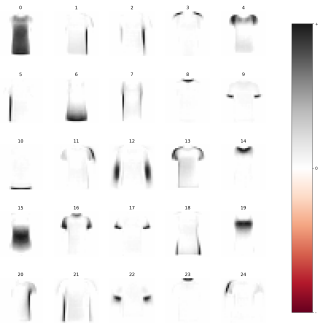


Figure: 25 main components (W)

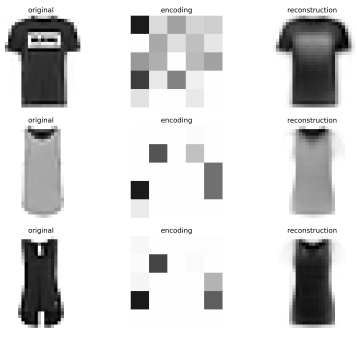


Figure: 3 examples (X, H, WH)

PCA vs. NMF - Fashion Mnist

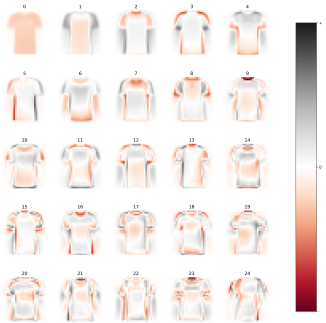


Figure: W_{PCA}

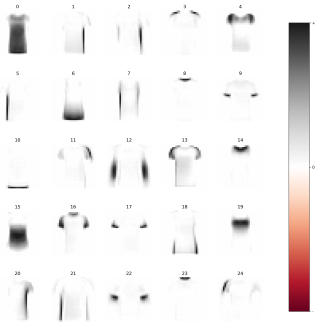
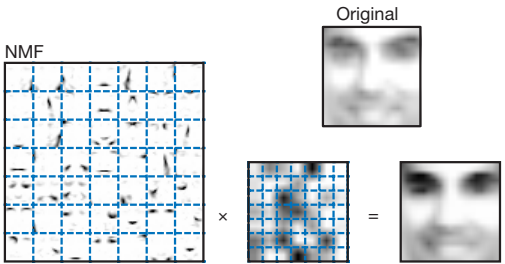
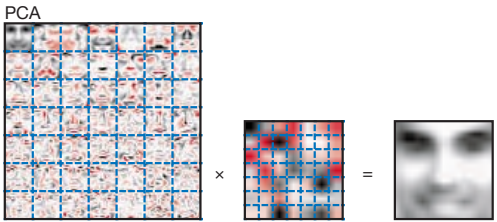


Figure: W_{NMF}

PCA vs. NMF - Face Parts





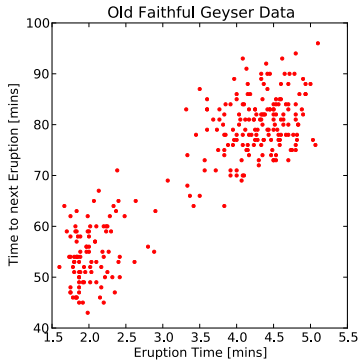
Taken from Lee and Seung [1999]

Clustering

PCA/NMF are applied to reduce dimensionality

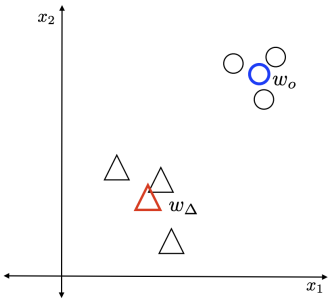
Often the problem setting is different:

- 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: 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[3]) is minimized

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

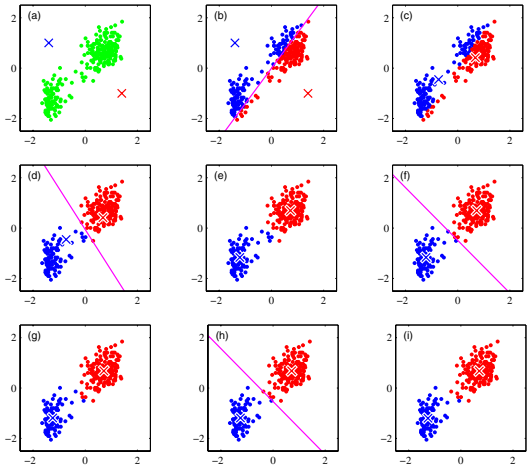
where r_i : cluster index of data point i

We minimize L by re-iterating two steps:

1. Assign each data point $\boldsymbol{x}_i$ to their closest cluster $\boldsymbol{\mu}_{r_i}$
2. Update $\boldsymbol{\mu}_r$ to the mean of the members in that cluster r

[3]Within Cluster Sum of Squares

K-means Clustering Step-by-Step



Re-iterate two steps:

1. Assign each $\boldsymbol{x}_i$ to closest cluster $\boldsymbol{\mu}_{r_i}$
2. Update $\boldsymbol{\mu}_r$ to mean of members in cluster r

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 $r'_j \leftarrow \operatorname{argmin}_{1 \leq l \leq k} \|\boldsymbol{x}_j - \boldsymbol{\mu}_l\|_2$
    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 (colors: RGB 3 channels [0, 255])

Quantized image (16 colors, K-Means)

Quantized image (16 colors, Random)

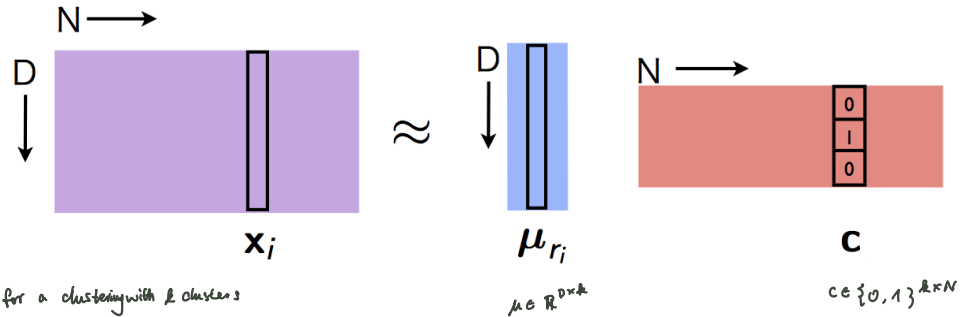
Adapted from sklearn

Encode color with one nibble (4 bit) instead of 3 Byte (24 bit)

$\rightarrow$ only need $1/6^{th}$ of the bandwidth ($+$ dictionary of colors)

Clustering can be seen as Matrix Factorization

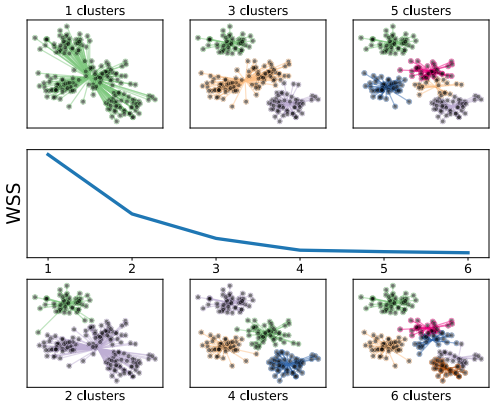
Clustering finds an **optimal partitioning** of a data set [4]



[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

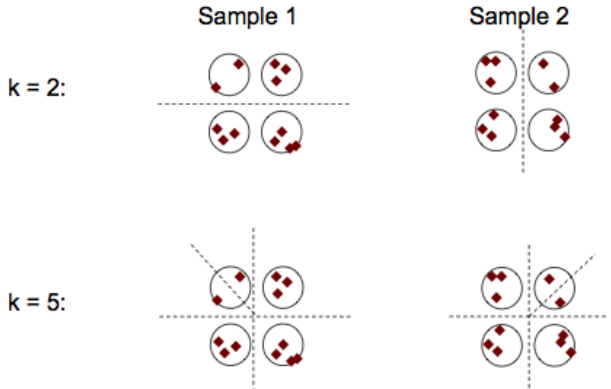
- Number of clusters k is critical hyper-parameter
- In supervised settings we use model selection (grid search) to optimize hyper-parameters for accuracy on test data
- How can we optimize the number of clusters?



$\rightarrow$ One approach: find "elbow"; Lowest k after which no real change

Clustering Instability

Number of Clusters is a critical parameter



Clusterings are instable (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 $\approx WH$

Principal Component Analysis

- is a popular dimensionality reduction tool
- aligns directions of maximal variance with standard basis
- finds orthogonal directions
- finds optimal matrix factorization

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

Summary II

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

References

C. M. Bishop. *Pattern Recognition and Machine Learning (Information Science and Statistics)*. 2007.

N. Gillis. The why and how of nonnegative matrix factorization. *Regularization, Optimization, Kernels, and Support Vector Machines*, 12(257):257–291, 2014.

D. D. Lee and H. S. Seung. Learning the parts of objects by non-negative matrix factorization. *Nature*, 401(6755):788–91, 1999. doi: $10.1038/44565$.

D. D. Lee and H. S. Seung. Algorithms for non-negative matrix factorization. In *In NIPS*, pages 556–562. MIT Press, 2000.

K. Pearson. Liii. on lines and planes of closest fit to systems of points in space. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 2(11):559–572, 1901.

B. Schölkopf, A. J. Smola, and K.-R. Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*, 10(6):1299–1319, 1998.

H. Xiao, K. Rasul, and R. Vollgraf. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms. 08 2017.

References

C. M. Bishop. *Pattern Recognition and Machine Learning (Information Science and Statistics)*. 2007.

N. Gillis. The why and how of nonnegative matrix factorization. *Regularization, Optimization, Kernels, and Support Vector Machines*, 12(257):257–291, 2014.

D. D. Lee and H. S. Seung. Learning the parts of objects by non-negative matrix factorization. *Nature*, 401(6755):788–91, 1999. doi: $10.1038/44565$.

D. D. Lee and H. S. Seung. Algorithms for non-negative matrix factorization. In *In NIPS*, pages 556–562. MIT Press, 2000.

K. Pearson. Liii. on lines and planes of closest fit to systems of points in space. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 2(11):559–572, 1901.

B. Schölkopf, A. J. Smola, and K.-R. Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*, 10(6):1299–1319, 1998.

H. Xiao, K. Rasul, and R. Vollgraf. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms. 08 2017.