

Cognitive Algorithms Lecture 5

Unsupervised Learning

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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](#)

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

This expression occurs in the derivation of ridge regression.

Notation continued

$$\begin{aligned}\varphi(X)^\top \varphi(X) &= \begin{pmatrix} \varphi_1(\mathbf{x}_1) & \dots & \varphi_{\tilde{d}}(\mathbf{x}_1) \\ \dots & & \dots \\ \varphi_1(\mathbf{x}_n) & \dots & \varphi_{\tilde{d}}(\mathbf{x}_n) \end{pmatrix} \begin{pmatrix} \varphi_1(\mathbf{x}_1) & \dots & \varphi_1(\mathbf{x}_n) \\ \dots & & \dots \\ \varphi_{\tilde{d}}(\mathbf{x}_1) & \dots & \varphi_{\tilde{d}}(\mathbf{x}_n) \end{pmatrix} \\ &= \begin{pmatrix} \varphi(\mathbf{x}_1)^\top \varphi(\mathbf{x}_1) & \dots & \varphi(\mathbf{x}_1)^\top \varphi(\mathbf{x}_{\tilde{d}}) \\ \dots & & \dots \\ \varphi(\mathbf{x}_{\tilde{d}})^\top \varphi(\mathbf{x}_1) & \dots & \varphi(\mathbf{x}_{\tilde{d}})^\top \varphi(\mathbf{x}_{\tilde{d}}) \end{pmatrix} \\ &= \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \dots & k(\mathbf{x}_1, \mathbf{x}_{\tilde{d}}) \\ \dots & & \dots \\ k(\mathbf{x}_{\tilde{d}}, \mathbf{x}_1) & \dots & k(\mathbf{x}_{\tilde{d}}, \mathbf{x}_{\tilde{d}}) \end{pmatrix}\end{aligned}$$

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 $\mathbf{x}_i^\top \mathbf{x}_j$ by $k(\mathbf{x}_i, \mathbf{x}_j)$.
 - Mercer's theorem: if k is symmetric positive semi-definite, then there is some $\varphi : \mathcal{X} \rightarrow \mathcal{F}$ such that $k(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^\top \varphi(\mathbf{x}_j)$.
 - Why are kernels useful?
 - Implicitly work in high-dimensional space
 - Representer theorem: for minimizer of *regularized* error function, have $f(\mathbf{x}) = \sum_i \alpha_i k(\mathbf{x}, \mathbf{x}_i)$.
“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 $k(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^\top \varphi(\mathbf{x}_j)$ or show that k is symmetric positive semi-definite

Recap: covariance matrix

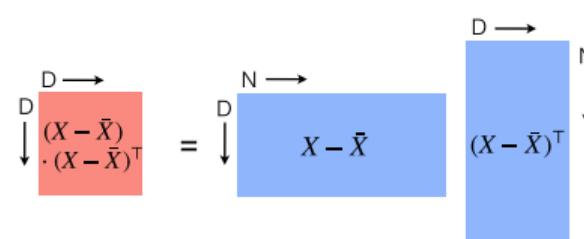
Given n data points $x_i \in \mathbb{R}^d$ in a data matrix $X \in \mathbb{R}^{d \times n}$, the empirical estimate of the **covariance matrix** is defined as

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

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

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

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



Unsupervised learning

■ Supervised algorithms

- Classification and regression
 - Use labels in training
- But labels not always given e.g.
- Mixtures of different speakers in an audio recording
 - Complex artifacts in experimental recordings

■ Unsupervised algorithms

- No labels for training

Approach	Labels
Binary classification	$\in \{+1, -1\}$
Regression	$\in \mathbb{R}$
Unsupervised	Do not exist!

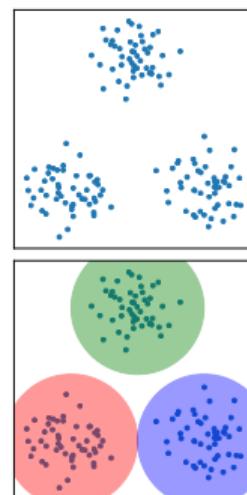
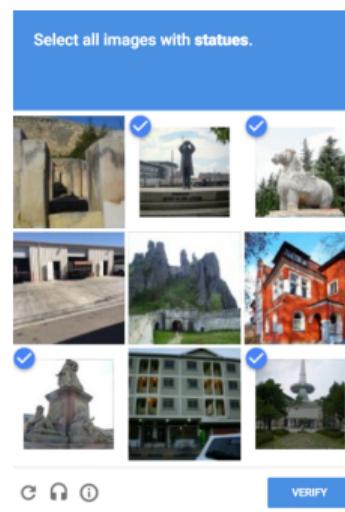
Unsupervised learning

Why unsupervised learning?

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

What can it be used for?

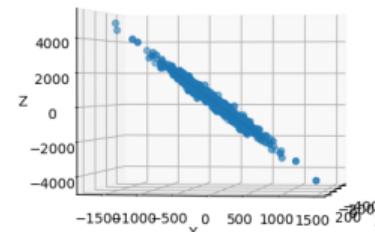
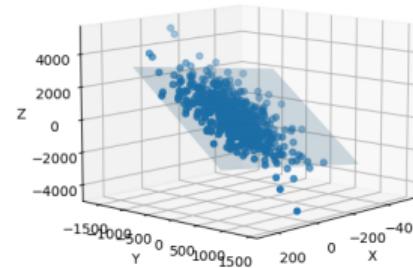
- Clustering
- Dimensionality reduction
- ...



Dimensionality reduction

In many applications...

- 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*)



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

Why dimensionality reduction?

- **Visualization**

Insights into high-dimensional structures in the data

- **Better Generalization**

Fewer dimensions → more robust parameter estimation

- **Speeding up learning algorithms**

Most algorithms scale badly with increasing data dimensionality

- **Data compression**

Smaller storage requirements

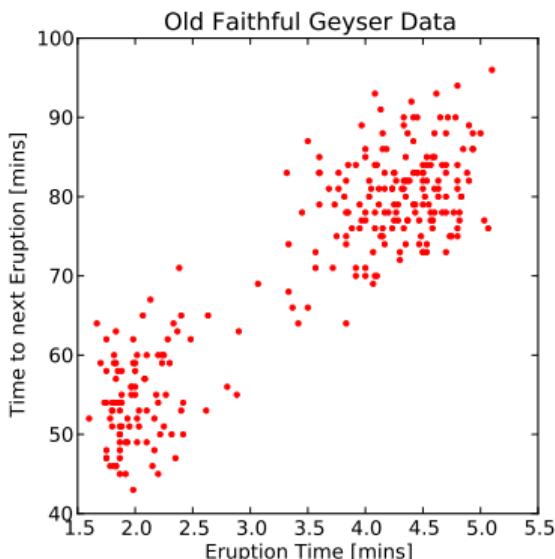


[Xiao et al., 2017]

Example: Old Faithful geyser dataset

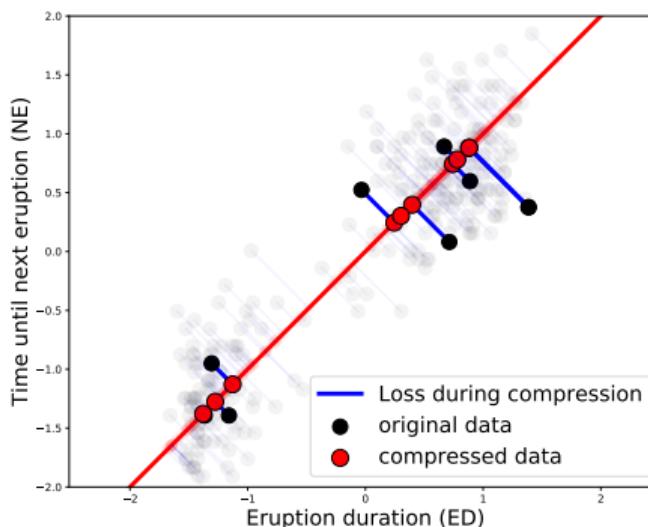


Old Faithful geyser eruption



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

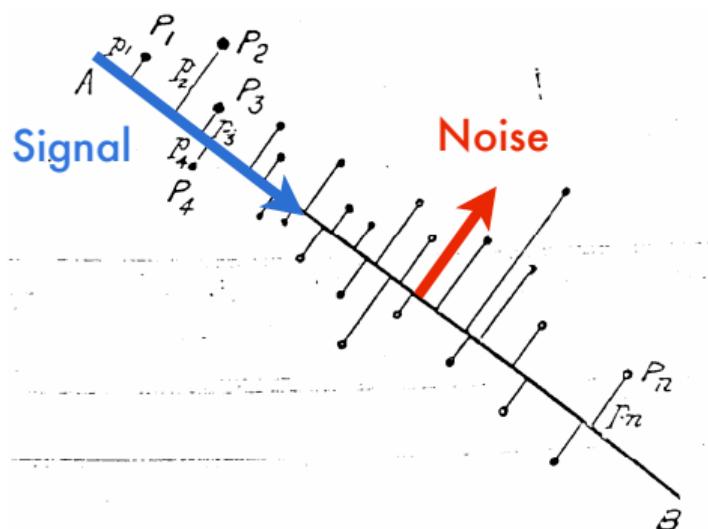
We have

- high-dimensional data $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
- reason to believe they lie close to a lower-dimensional subspace
 - $m < d$ parameters needed to account for the data properties
 - hidden causes* or *latent variables* $H = [\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_n] \in \mathbb{R}^{m \times n}$

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

$$X \approx WH$$

Principal component analysis (PCA)



Adapted from Pearson [1901]

Objective of PCA

Find a 1-dimensional subspace 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 $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$

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

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

Maximizing variance

We obtained some data $X = [x_1, x_2, \dots, x_n] \in \mathbb{R}^{d \times n}$

PCA finds a direction $w \in \mathbb{R}^d$ such that the variance of the projected data $w^\top X$ is maximal
Let's assume centered data for easier notation ¹

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

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

¹i.e. we assume $\bar{x} = 0$

Maximizing variance

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

$$\operatorname{argmax}_{\mathbf{w}} \frac{\mathbf{w}^\top S \mathbf{w}}{\mathbf{w}^\top \mathbf{w}}$$

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

Note the similarity to the objective of Linear Discriminant Analysis!

→ Different covariance matrices, different problem, but: same maths solve it.

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

Maximizing variance

$$\operatorname{argmax}_{\mathbf{w}} \frac{\mathbf{w}^T S \mathbf{w}}{\mathbf{w}^T \mathbf{w}} \quad (1)$$

Set the derivative with respect to \mathbf{w} to zero:

$$\begin{aligned} \frac{\partial}{\partial \mathbf{w}} \frac{\mathbf{w}^T S \mathbf{w}}{\mathbf{w}^T \mathbf{w}} &= \frac{(\mathbf{w}^T \mathbf{w}) 2 S \mathbf{w} - (\mathbf{w}^T S \mathbf{w}) 2 \mathbf{w}}{(\mathbf{w}^T \mathbf{w})^2} \stackrel{!}{=} 0 \\ \Rightarrow \underbrace{(\mathbf{w}^T S \mathbf{w})}_{\text{scalar}} \mathbf{w} &= \underbrace{(\mathbf{w}^T \mathbf{w})}_{\text{scalar}} S \mathbf{w} \\ \Rightarrow \underbrace{\frac{\mathbf{w}^T S \mathbf{w}}{\mathbf{w}^T \mathbf{w}}}_{\equiv \lambda} \mathbf{w} &= S \mathbf{w} \end{aligned}$$

Equation 1 can be reduced to the standard eigenvalue problem:

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

Maximizing variance

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

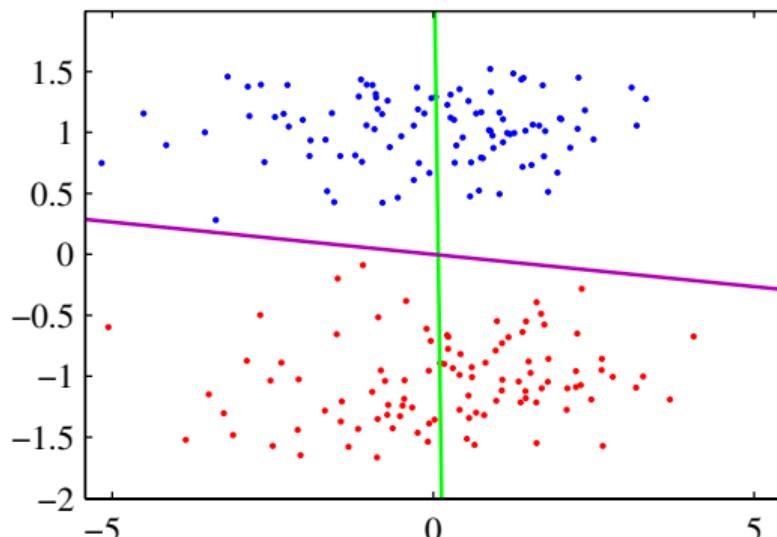
$$\operatorname{argmax}_{\mathbf{w}} \frac{\mathbf{w}^T S \mathbf{w}}{\mathbf{w}^T \mathbf{w}} = \frac{\mathbf{w}^T \lambda \mathbf{w}}{\mathbf{w}^T \mathbf{w}} = \lambda$$

Conclusion

- The variance of the projected data in the maximizing direction \mathbf{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?



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.

Characterization of PCA

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

$$SW = W\Lambda,$$

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

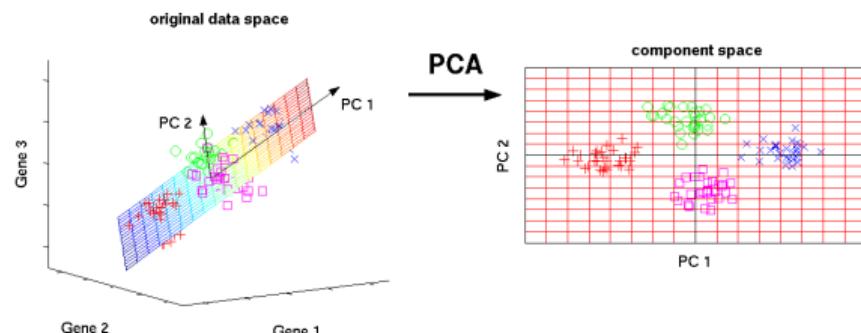
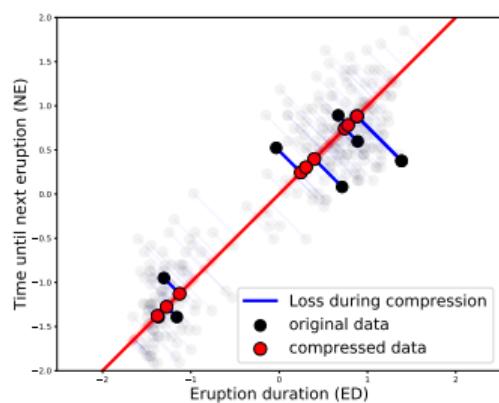
Recall (from linear algebra): since S is symmetric, there exist d orthogonal eigenvectors ($\mathbf{w}_i \perp \mathbf{w}_j$) and the eigenvalues are real numbers.

Encoding (from real data to latent representation)

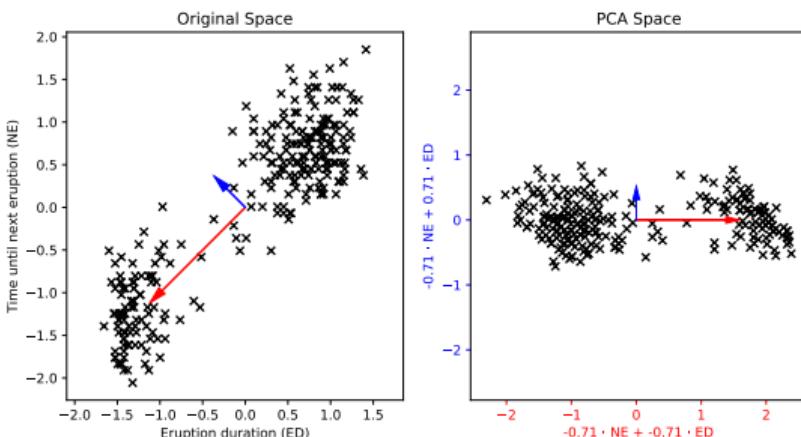
Now that we have

$W = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_k] \in \mathbb{R}^{d \times k}$, we project each data point \mathbf{x} onto W

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



Principal Component Analysis



- PCA basis has maximum variance directions on basis vectors
 - Principal components 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 $W = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_k] \in \mathbb{R}^{d \times k}$ where $\mathbf{w}_1, \dots, \mathbf{w}_k \in \mathbb{R}^d$ 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 $x_1, \dots, x_n \in \mathbb{R}^d$, number of principal components k

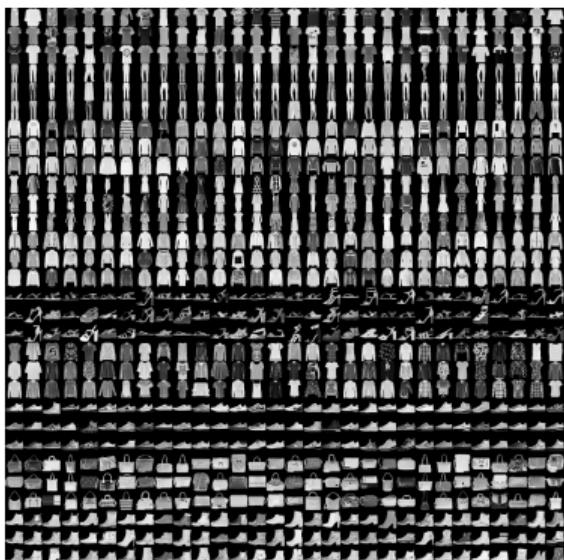
- 1: # Compute Sample Covariance Matrix
 - 2: $C = 1/n (X - 1/n \sum_i x_i)(X - 1/n \sum_i x_i)^\top$
 - 3: # Compute eigenvectors corresponding to the k largest eigenvalues
 - 4: $W = \text{eig}(C)$
 - 5: # Project data onto W
 - 6: $H = W^\top X$
 - 7: **return** W, H
-

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)

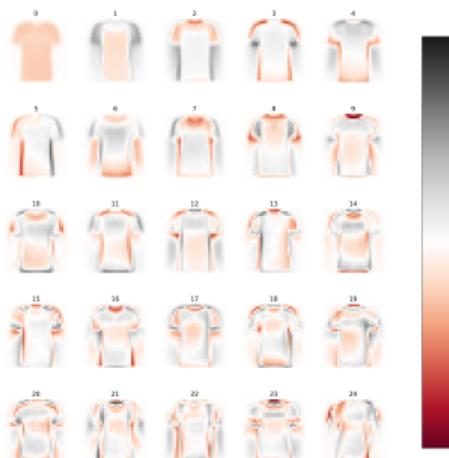
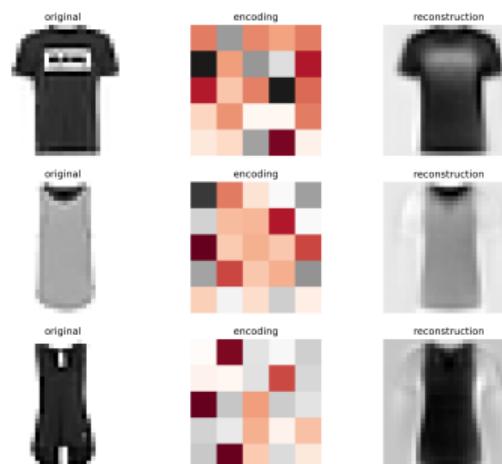


Figure: 3 examples (X, H, WH)



- 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 $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$ with $n \ll d$

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

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

$$\lambda \mathbf{w} = XX^\top \mathbf{w} \rightarrow \mathbf{w} = X\alpha,$$

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

PCA for high-dimensional data

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

$$\begin{aligned} \mathbf{X}\mathbf{X}^\top \mathbf{w} &= \lambda \mathbf{w} \\ \mathbf{X}\mathbf{X}^\top X\alpha &= \lambda X\alpha \\ \underbrace{\mathbf{X}^\top \mathbf{X}}_K \underbrace{\mathbf{X}^\top X\alpha}_K &= \lambda \underbrace{\mathbf{X}^\top X\alpha}_K \\ KK\alpha &= \lambda K\alpha \end{aligned}$$

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

$$K\alpha = \lambda\alpha.$$

Solving PCA via $\mathbf{X}^\top \mathbf{X}$ instead of $\mathbf{X}\mathbf{X}^\top$ 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 $x_1, \dots, x_n \in \mathbb{R}^d$, $n \ll d$, 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

[See More]

16 minutes ago

on [TED: Maria Menounos: Extra stories as BuzzNews this past week](#) - December 29 -- BuzzNews

As Co-host of syndicated entertainment newsmagazine "Extra," Maria Menounos talks a lot about TV. But she's even chattier online. The multipathlete behind an upcoming reality show on Oxygen, a new production company and a book series, as well as spokeswoman for branch-lick Partners, has quietly built YouTube network AmazeBlaze into a platform... Read more

Live from the Engadget CES Stage: Pebble CEO Eric Migicovsky

[See More]

19 minutes ago

on [TED: Stephan Larsson: What doctors can learn from each other](#) - Stephan Larsson (2011)

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 in its proverbial...

Finally There Is An "Alien" Game That Is Actually Like The Movies

[See More]

19 minutes ago

on [TED: Malcolm Gladwell: The unheard story of David and Goliath](#) - Malcolm Gladwell (2011)

Acknowledging that Alien isolation is out there 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

[See More]

20 minutes ago

or [TED: A pair of real and affordable Android tablets - Jessie AI and S1](#)

Two of venture firm Venrock's energy investors, Matt Trewhick and Matthew Nordan, have left the firm. Trewhick is an accomplished investor who was one of my first interviewees after I started this website. We've published many pieces from Nordan on the state of cleantech venture I...

Apple's App Store revenue hit record \$10 billion in 2013

[See More]

22 minutes ago

on [TED: Seven unbelievable 2014 tech predictions](#)

Apple announced today that sales from its App Store topped \$10 billion last year, which is up 50% from 2012. It's the first time Apple has hit that mark. 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

[See More]

23 minutes ago

on [TED: Chris Dorney: Design with the mind in mind - Chris Dorney \(2013\)](#)

The Guardian's photo team brings you a daily round up from the world of photography. Journa

Ruck

Democracy needs whistleblowers. That's why I broke into the FBI in 1973

[See More]

1 hour ago

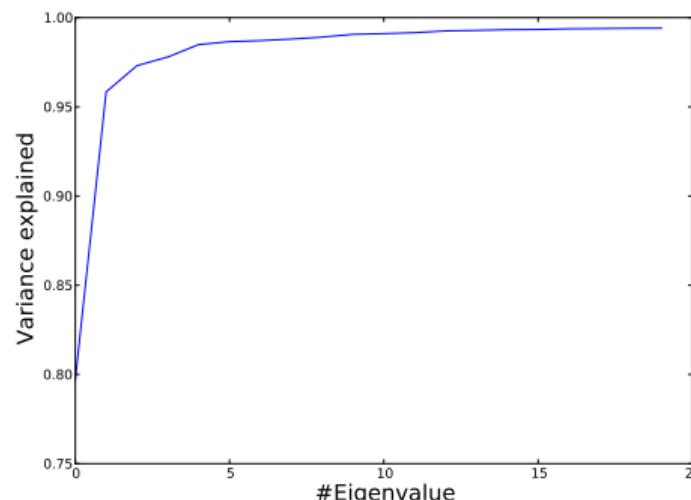
on [TED: Chris Dorney: Design with the mind in mind - Chris Dorney \(2013\)](#)

Like Snowden, we broke laws to reveal something that was more dangerous. We waited to tell J Edgar Hoover accountable I vividly remember his famous moment. He was the right we probably had to do it. We had to break into the FBI. We had to steal over 100,000 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 organization had to have a file on us. So we went to the FBI and we found that when we found it, we were on terrorist hooks. A shoot 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 informed him that he had to do something about the AIDS epidemic. He had to do something about the paroxysm epidemic 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 red thread through the entire film. I think that's what makes it so powerful. I think that's what 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 we could be called whistleblowers to us. A look back at what happened last night in the

Trends in text data

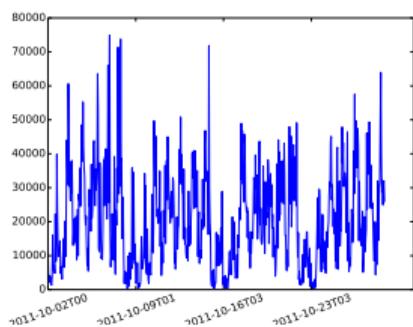
We are looking at bag-of-words data from a news web page

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



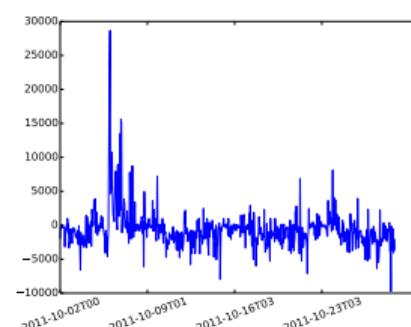
Trends in text data

First principal component



Main variance due to weekly/daily publishing activity

Second principal component



Spike on day of Steve Job's death

We can use PCA as a tool for analyzing big unlabeled 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
- Matrix factorization is relevant in recommender systems ("you might also like. . .") ([more info here](#))

Non-negative matrix factorization

Notation: $\mathbb{R}_+ := \{x \in \mathbb{R} \mid x \geq 0\}$.

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 $\|\cdot\|_{\text{Fro}}$

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

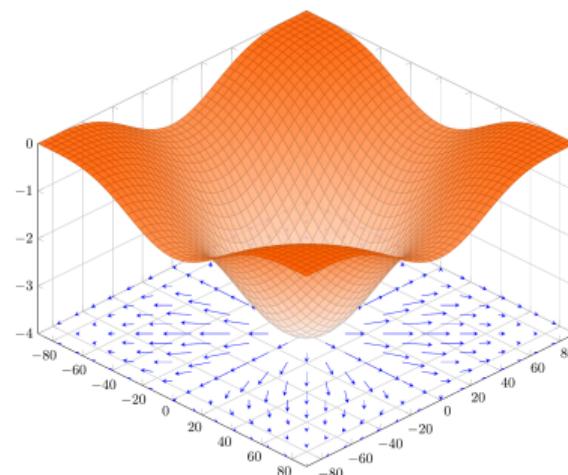
Non-negative matrix factorization

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

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

Note

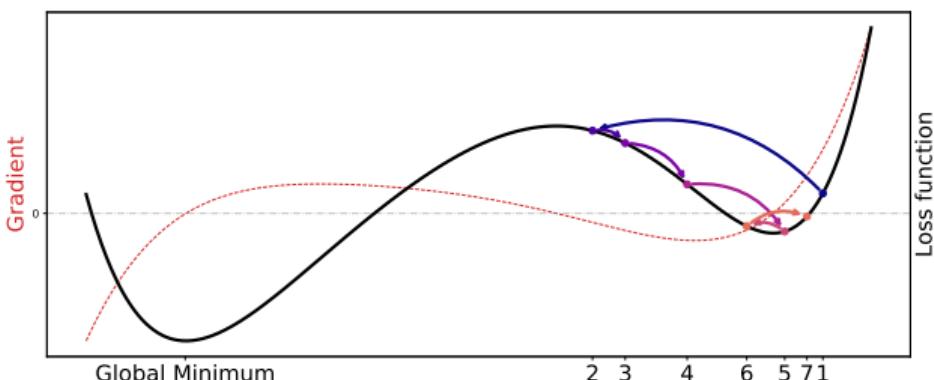
Whenever the problem is too hard, just follow the gradients!



Gradient descent

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

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



- 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)

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

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

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

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

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

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

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

Non-negative matrix factorization

Gradient descent finds a locally optimal solution by iterating

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

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

- 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 update² [Lee and Seung, 1999, 2000]:

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

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

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

NMF algorithm

Algorithm 3: Non-negative Matrix Factorization

Require: data $X = [x_1, \dots, x_n] \in \mathbb{R}_+^{d \times n}$, 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** $it \leq \text{Iterations}$ **do**
 - 4: $H = H \odot W^\top X \oslash W^\top WH$
 - 5: $W = W \odot XH^\top \oslash WHH^\top$
 - 6: **end for**
 - 7: **return** W, H
-

where

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

NMF on fashion MNIST: Shirts

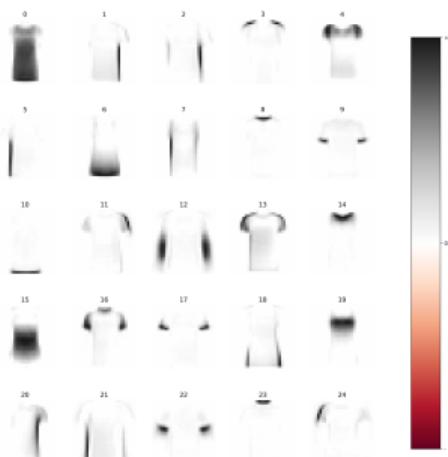


Figure: 25 main components (W)

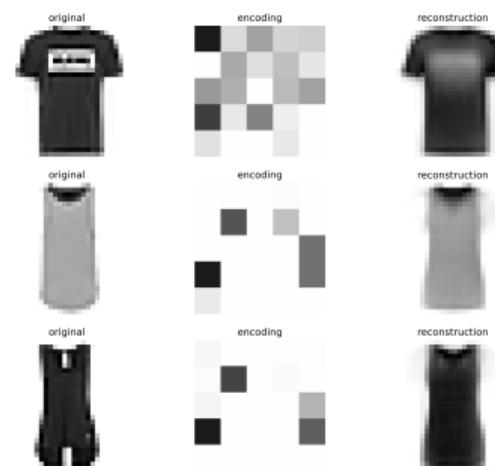


Figure: 3 examples (X, H, WH)

PCA vs. NMF - Fashion MNIST

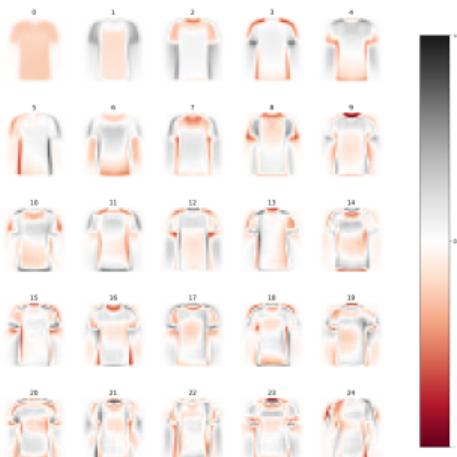
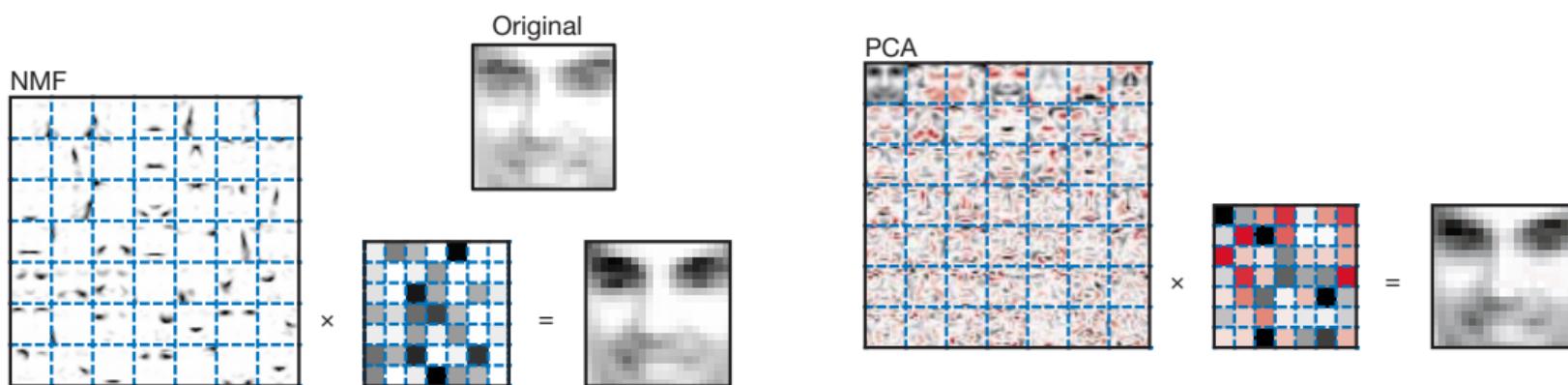


Figure: W_{PCA}



Figure: W_{NMF}

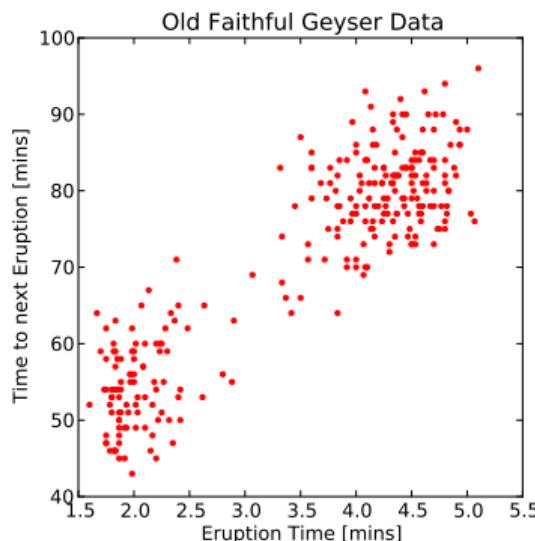
PCA vs. NMF - Face Parts



Taken from Lee and Seung [1999]

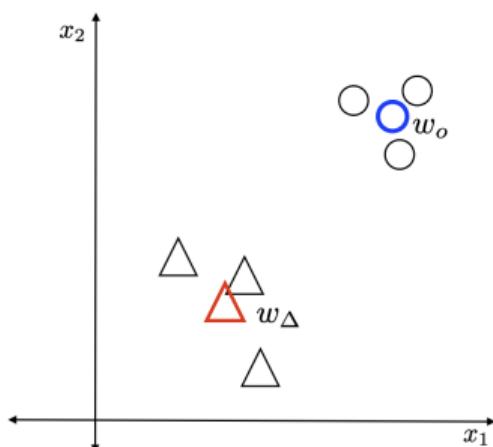
Clustering

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



Clustering

Remember Lecture 2:
Psychological Models of Categorization: Prototypes



Prototypes μ_Δ and μ_o :

$$\mu_\Delta = \frac{1}{n_\Delta} \sum_{n=1}^{n_\Delta} x_{\Delta,n}$$

$$\mu_o = \frac{1}{n_o} \sum_{n=1}^{n_o} x_{o,n}$$

New data points x are assigned to their closest cluster center μ^*

$$\mu^* = \operatorname{argmin}_i (\|\mu_i - x\|_2)$$

K-means clustering

Objective for k-means

Find cluster centers μ_1, \dots, μ_k such that the sum of distances of data points to their respective cluster centers ("WCSS", "WSS"³) is minimized

$$L(\{\mu_1, \dots, \mu_k\}, r) = \sum_{i=1}^n \|x_i - \mu_{r_i}\|^2$$

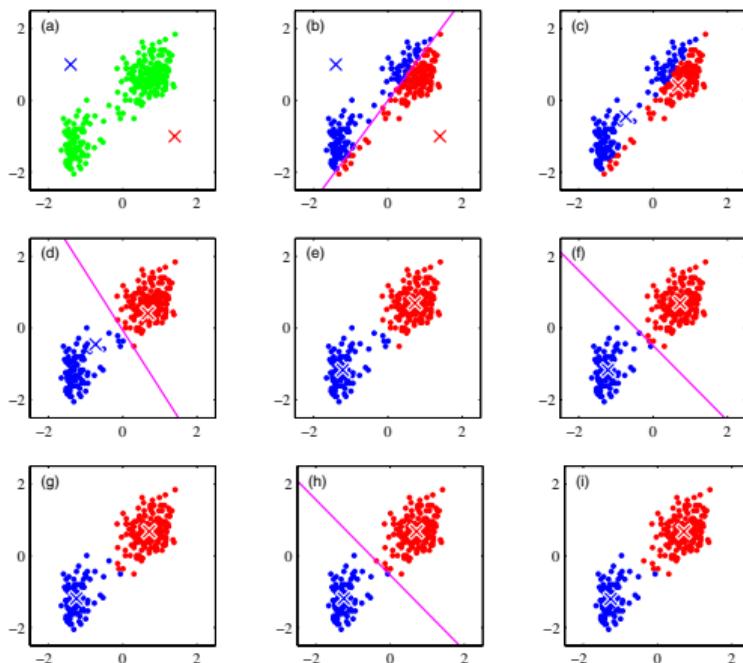
where r_i : cluster index of data point i

We minimize L by re-iterating two steps

- 1 Assign each data point x_i to their closest cluster μ_{r_i}
- 2 Update μ_r to the mean of the members in that cluster r

³Within cluster sum of squares

K-means clustering step-by-step



Re-iterate two steps:

- 1 Assign each x_i to closest cluster μ_r
- 2 Update μ_r to mean of members in cluster r

K-means clustering algorithm

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

```
1: Choose random data points as initial cluster centers  $\mu_1 \leftarrow x_{i_1}, \dots, \mu_k \leftarrow x_{i_k}$  where  $i_j \neq i_l$  for all  $j \neq l$ .  
2:  $r \leftarrow \mathbf{0}_n$   
3:  $r' \leftarrow \mathbf{0}_n$   
4:  $i \leftarrow 0$   
5: while  $i < m$  do  
6:   for  $j \leftarrow 1$  to  $n$  do  
7:     Find nearest cluster center  $r'_j \leftarrow \operatorname{argmin}_{1 \leq l \leq k} \|x_j - \mu_l\|_2$   
8:   end for  
9:   for  $j \leftarrow 1$  to  $k$  do  
10:    Compute new cluster center  $\mu_j \leftarrow \frac{1}{|\{l : r'_l = j\}|} \sum_{l : r'_l = j} x_l$   
11:   end for  
12:   if  $r = r'$  then  
13:     break  
14:   end if  
15:    $r \leftarrow r'$   
16:    $i \leftarrow i + 1$   
17: end while  
18: return cluster centers  $\mu_1, \dots, \mu_k \in \mathbb{R}^d$ , assignment vector  $r \in \mathbb{R}^n$ 
```

Application example: image compression

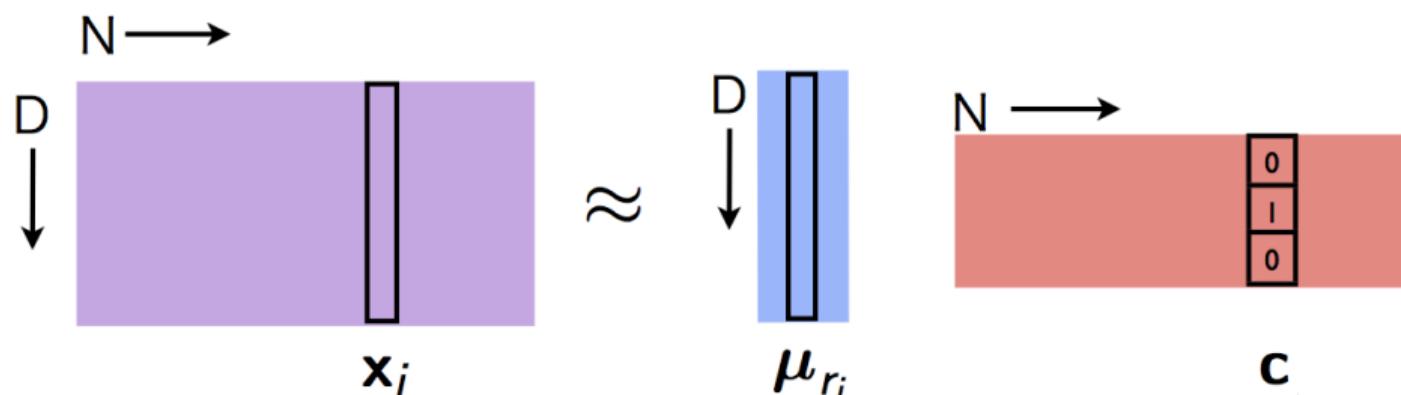


Adapted from sklearn, [more information here](#).

- 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 set⁴

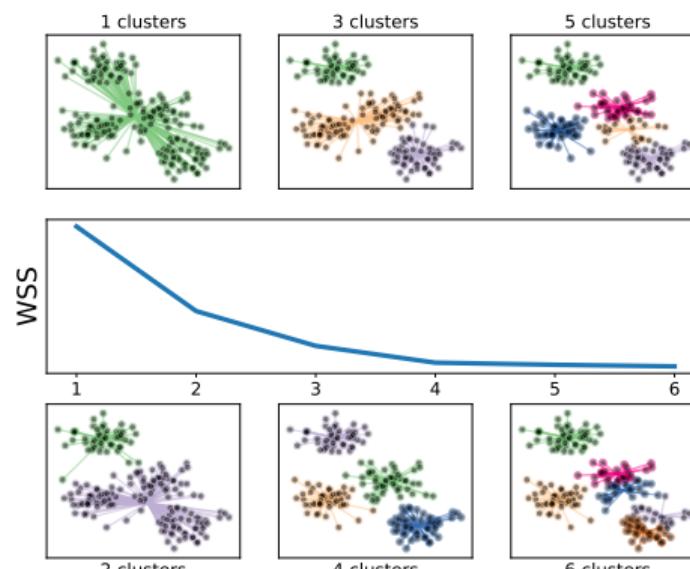


For a clustering with k clusters, we have $\mu \in \mathbb{R}^{D \times k}$ and $\mathbf{c} \in \{0, 1\}^{k \times N}$.

⁴In the previous example, we actually used this by approximating the original colors \mathbf{x}_i with the corresponding μ_{r_i} .

How to choose k

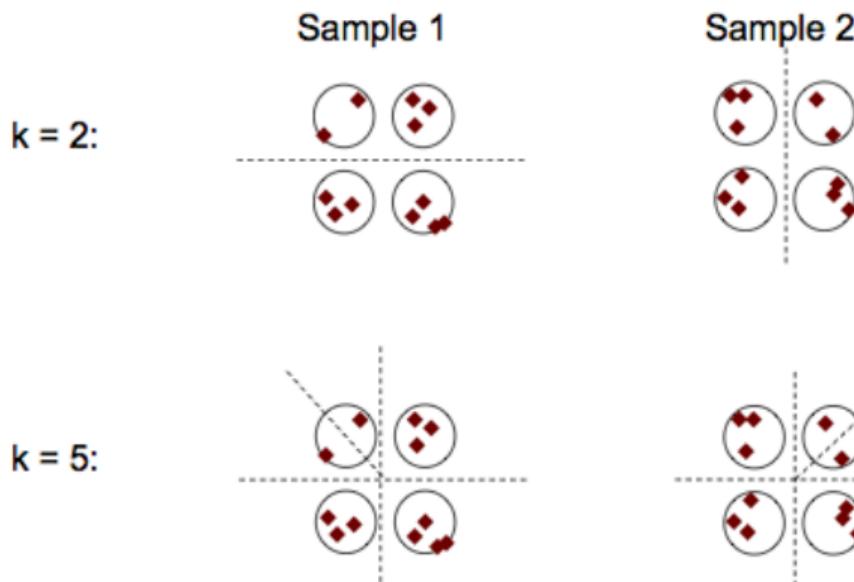
- Number of clusters k is critical hyper-parameter
- In supervised settings we use model selection (grid search) to optimize hyper-parameters for accuracy on test data
- How can we optimize the number of clusters?



→ 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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