Statistical Natural Language Processing

Unsupervised machine learning

Çağrı Çöltekin

University of Tübingen
Seminar für Sprachwissenschaft

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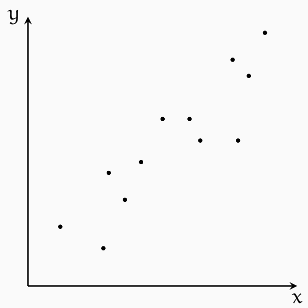
Supervised learning

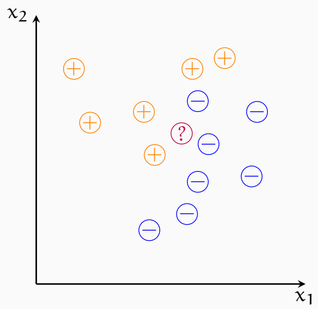
- The methods we studied so far are instances of supervised learning
- In supervised learning, we have a set of predictors x, and want to predict a response or outcome variable y
- During training, we have both input and output variables
- Training consist of estimating parameters $\boldsymbol{w}$ of a model
- During prediction, we are given x and make predictions based on model we learned

Supervised learning: regression



- The response (outcome) variable (y) is a quantitative variable.
- Given the features (x) we want to predict the value of y

Supervised learning: classification



- The response (outcome) is a label. In the example: positive + or negative −
- Given the features (x_1 and x_2), we want to predict the label of an unknown instance ?

Supervised learning: estimating parameters

- Most models/methods estimate a set of parameters $\boldsymbol{w}$ during training
- Often we find the parameters that minimize a loss function
  - For least-squares regression

$$J(w) = \sum_i (\hat{y}_i - y_i)^2 + \|\boldsymbol{w}\|$$

  - For logistic regression, the negative log likelihood

$$J(w) = -\log \mathcal{L}(w) + \|\boldsymbol{w}\|$$

- If the loss function is *convex*, we can find a *global* minimum. Sometimes with an analytic solution, sometimes using search methods such as *gradient descent*

Today's lecture

- *Clustering*: find related groups of instances
- *Density estimation*: find a probability distribution that explains the data
- *Dimensionality reduction*: find an accurate/useful lower dimensional representation of the data

…and soon

- Unsupervised learning in ANNs (RBMs, autoencoders)

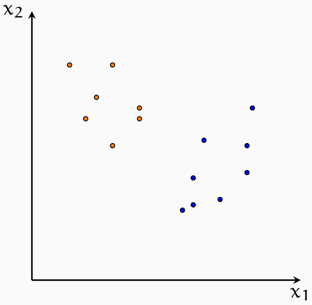
Unsupervised learning

- In unsupervised learning, we do not have labels in our training data
- Our aim is to find useful patterns/structure in the data
  - for exploratory study of the data
  - for augmenting / complementing supervised methods
- Close relationships with 'data mining', 'data science / analytics', 'knowledge discovery'
- All unsupervised methods can be cast as graphical models with hidden variables
- Evaluation is difficult: we do not have 'true' labels/values

Clustering: why do we do it?

- The aim is to find groups of instances/items that are similar to each other
- Applications include
  - Clustering languages, dialects for determining their relations
  - Clustering (literary) texts, for e.g., authorship attribution
  - Clustering words for e.g., better parsing
  - Clustering documents, e.g., news into topics
  - …

Clustering in two dimensional space



- Unlike classification, we do not have labels
- We want to find 'natural' groups in the data
- Intuitively, similar or closer data points are grouped together

Similarity and distance

- The notion of distance (similarity) is important in clustering. A distance measure D,
  - is symmetric: $D(a, b) = D(b, a)$
  - non-negative: $D(a, b) \geqslant 0$ for all a, b, and it $D(a, b) = 0$ iff $a = b$
  - obeys triangle inequality: $D(a, b) + D(b, c) \geqslant D(a, c)$
- The choice of distance is application specific
- We will often face with defining distance measures between linguistic units (letters, words, sentences, documents, ...)

Distance measures in Euclidean space

- Euclidean distance:

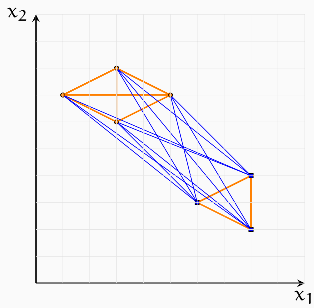
$$\|\mathbf{a} - \mathbf{b}\| = \sqrt{\sum_{j=1}^{k}(a_j - b_j)^2}$$

- Manhattan distance:

$$\|\mathbf{a} - \mathbf{b}\|_1 = \sum_{j=1}^{k}|a_j - b_j|$$

How to do clustering

Most clustering algorithms try to minimize the scatter within each cluster. Which is equivalent to maximizing the scatter between clusters.



$$\sum_{k=1}^{K}\sum_{a\in C_k}\sum_{b\in C_k} d(a, b)$$

$$\sum_{k=1}^{K}\sum_{a\in C_k}\sum_{b\notin C_k} d(a, b)$$

K-means algorithm

K-means is a popular method for clustering.

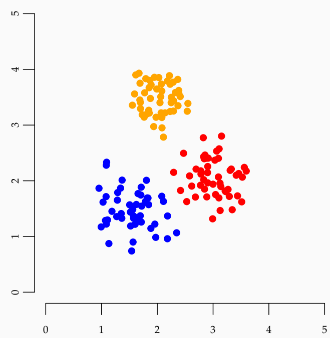
1. Randomly choose *centroids*, $m_1, \ldots, m_K$, representing K clusters
2. Repeat until convergence
   - Assign each data point to the cluster of the nearest centroid
   - Re-calculate the centroid locations based on the assignments

Effectively, we are finding a *local minimum* of the sum of squared Euclidean distance within each cluster

$$\frac{1}{2}\sum_{k=1}^{K}\sum_{a \, in \, C_k}\sum_{b\in C_k} \|a - b\|^2$$

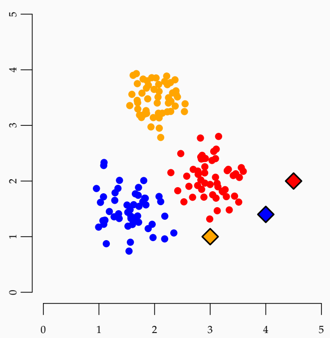
* Note the similarity with the EM algorithm

K-means clustering: visualization



- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



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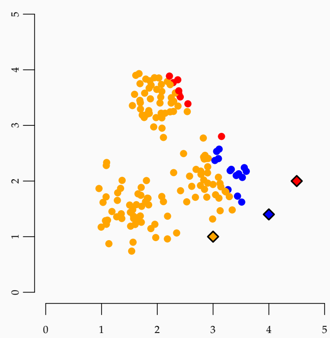

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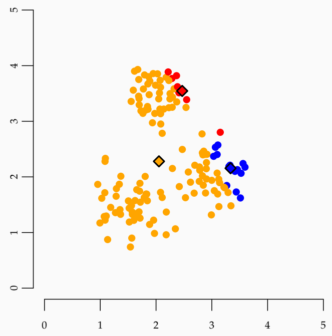

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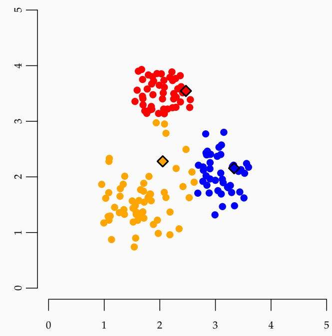

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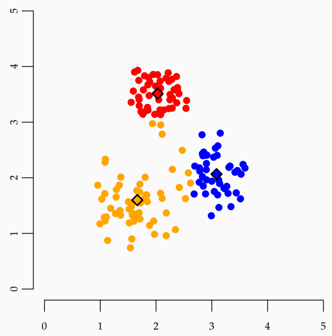
K-means clustering: visualization



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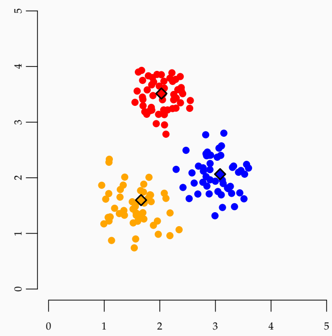

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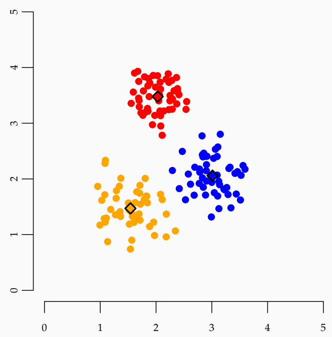
K-means clustering: visualization



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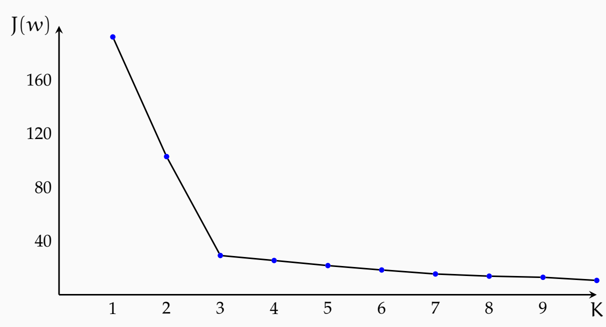
K-means: some issues

- K-means requires the data to be in an Euclidean space
- K-means is sensitive to outliers
- The results are sensitive to initialization
  - There are some smarter ways to select initial points
  - One can do multiple initializations, and pick the best (with lowest within-group squares)
- It works well with approximately equal-size round-shaped clusters
- We need to specify number of clusters in advance

How many clusters?

- The number of clusters is defined for some problems, e.g., classifying news into a fixed set of topics/interests
- For others, there is no clear way to select the best number of clusters
- The error (within cluster scatter) always decreases with increasing number of clusters, using a test set or cross validation is not useful either
- A common approach is clustering for multiple K values, and picking where there is an 'elbow' in the graph against the error function

How many clusters?



This plot is sometimes called a *scree plot*.

K-medoids

- K-medoids algorithm is an alternation of K-means
- Instead of calculating centroids, we try to find most typical data point (medoids) at each iteration
- K-medoids can work with distances, does not need feature vectors to be in an Euclidean space
- It is less sensitive to outliers
- It is computationally more expensive than K-means

Hierarchical clustering

- Instead of a flat division to clusters as in K-means, hierarchical clustering builds a hierarchy based on similarity of the data points
- There are two main 'modes of operation':

Bottom-up or *agglomerative* clustering
- starts with individual data points,
- merges the clusters until all data is in a single cluster

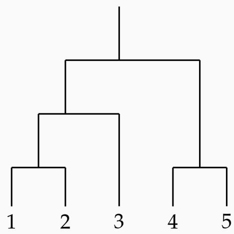
Top-down or *divisive* clustering
- starts with a single cluster,
- and splits until all leaves are single data points

Hierarchical clustering

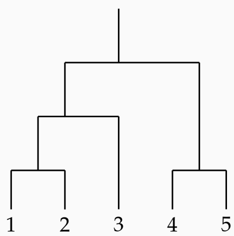
- Hierarchical clustering operates on differences (or similarities)
- The result is a binary tree called *dendrogram*
- Dendrograms are easy to interpret (especially if data is hierarchical)
- The algorithm does not commit to the number of clusters K from the start, the dendrogram can be 'cut' at any height for for determining the clusters

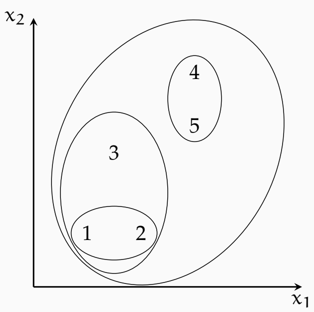
Agglomerative clustering

1. Compute the similarity/distance matrix
2. Assign each data point to its own cluster
3. Repeat until no clusters left to merge
   - Pick two clusters that are most similar to each other
   - Merge them into a single cluster



Agglomerative clustering demonstration





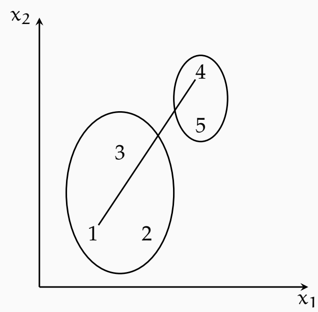
How to calculate between cluster distances

Complete maximal inter-cluster distance

Single minimal inter-cluster distance

Average mean inter-cluster distance

Centroid distance between the centroids



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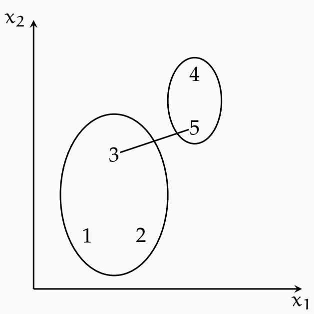

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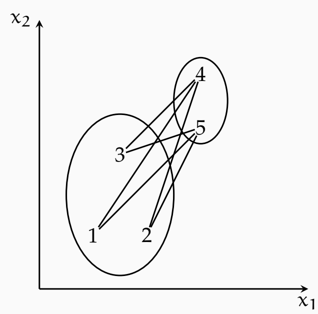

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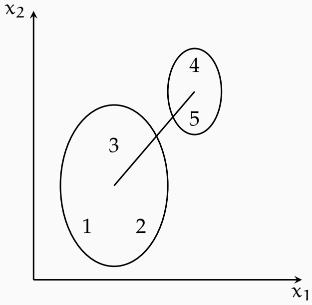


Note: we only need distances, (feature) vectors are not necessary

Clustering evaluation

Evaluating clustering results is often non-trivial

- Internal evaluation is based a metric that aims to indicate 'good clustering': e.g., *Dunn index*, *gap statistic*, *silhouette*
- External metrics can be useful if we have labeled *test* data: e.g., *V-measure*, B^3*ed F-score*
- The results can be tested on the target application: e.g., word-clusters evaluated based on their effect on parsing accuracy
- Human judgments, manual evaluation – 'looks good to me'

Clustering evaluation

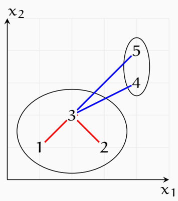
internal metric example: silhouette

$$s_i = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

where

$a(i)$ average distance between object i and and objects in the same cluster

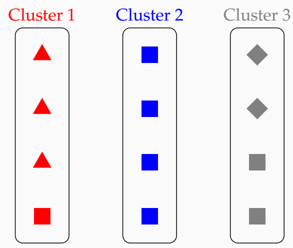
$b(i)$ average distance between object i and and objects in the *closest* cluster



Clustering evaluation

external metrics: general intution

- We want clusters that contain members of a single gold-standard class (homogeneity)
- We want all members of a class to be in a single cluster (completeness)



Note the similarity with precision and recall.

Clustering: some closing notes

- We do not have proper evaluation procedures for clustering results (for unsupervised learning in general)
- Clustering is typically unstable, slight changes in the data or parameter choices may change the results drastically
- Approaches against instability include some validation methods, or producing 'probabilistic' dendrograms by running clustering with different options

Density estimation

- K-means treats all data points in a cluster equally
- A 'soft' version of K-means is density estimation for Gaussian mixtures, where
  - We assume the data comes from a mixture of K Gaussian distributions
  - We try to find the parameters of each distribution (instead of centroids) that maximizes the likelihood of the data
- Unlike K-means, mixture of Gaussians assigns probabilities for each data point belonging to one of the clusters
- It is typically estimated using the expectation-maximization (EM) algorithm

Density estimation using the EM algorithm

- The EM algorithm (or its variations) is used in learning models with latent/hidden variables
- It is closely related to the K-means algorithm

1. Initialize the parameters (e.g., randomly) of K multivariate normal distributions (μ, Σ)
2. Iterate until convergence:

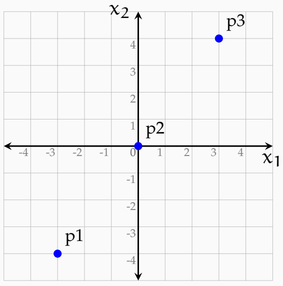
E-step Given the parameters, compute the membership 'weights', the probability of each data point belonging to each distribution

M-step Re-estimate the mixture density parameters using the calculated membership weights in the E-step

Principal component Analysis

- Principal component analysis (PCA) is a method of *dimensionality reduction*
- PCA maps the original data into a lower dimensional space by a linear transformation (rotation)
- The transformed lower-dimensional variables retain most of the variation (=information) in the input
- PCA can be used for
  - visualization
  - data compression
  - reducing dimensionality of features for other machine learning methods
  - eliminating noise

PCA: a toy example



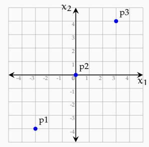
Questions:

- How many dimensions do we have?
- How many dimensions do we need?
- Short divergence: calculate the covariance matrix

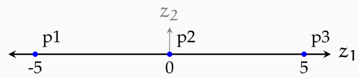
$$\Sigma = \begin{bmatrix} \frac{18}{3} & 8 \\ 8 & \frac{32}{3} \end{bmatrix}$$

  – What is the correlation between x_1 and x_2?

PCA: A toy example (2)



What if we reduce the data to:



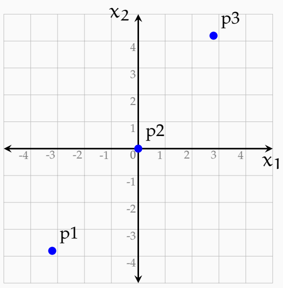
Going back to the original coordinates is easy, rotate using:

$$A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} = \begin{bmatrix} \frac{3}{5} & -\frac{4}{5} \\ \frac{4}{5} & \frac{3}{5} \end{bmatrix}$$

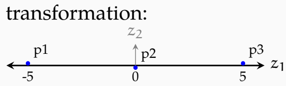
$$p1 = A \times \begin{bmatrix} -5 \\ 0 \end{bmatrix} = \begin{bmatrix} -3 \\ -4 \end{bmatrix} \quad p1 = A \times \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad p1 = A \times \begin{bmatrix} 5 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

We can recover the original points perfectly. In this example the inherent dimensionality of the data is only 1.

PCA: A toy example (3)



- What if the variables were not perfectly but strongly correlated?
- We could still do a similar transformation:



- Discarding z_2 results in a small reconstruction error:

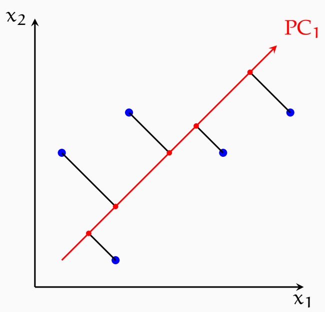
$$p1 = A \times \begin{bmatrix} -5 \\ 0 \end{bmatrix} = \begin{bmatrix} -3 \\ -4 \end{bmatrix}$$

- Note: z_1 (also z_2) is a linear combination of original variables

Why do we want to reduce the dimensionality

- Visualizing high-dimensional data becomes possible
- If we use the data for other ML methods,
  – we reduce the computation time
  – we may avoid 'the curse of dimensionality'
- Decorrelation is useful in some applications
- We compress the data (in a lossy way)
- We eliminate noise (assuming a high signal to noise ratio)

Different views on PCA



- Find the direction of the largest variance
- Find the projection with the least reconstruction error
- Find a lower dimensional latent Gaussian variable such that the observed variable is a mapping of the latent variable to a higher dimensional space (with added noise)

How to find PCs

- When viewed as *maximizing variance* or *reducing the reconstruction error*, we can write the appropriate objective function and find the vectors that minimize it
- In latent variable interpretation, we can use EM as in estimating mixtures of Gaussians
- The principle components are the eigenvectors of the correlation matrix, where large eigenvalues correspond to components with large variation
- A numerically stable way to obtain principal components is doing *singular value decomposition* (SVD) on the input data

PCA as matrix factorization (eigenvalue decomposition)

- One can compute PCA by decomposing the covariance matrix as (note $\mathbf{\Sigma} = \mathbf{X}^T\mathbf{X}$)

$$\mathbf{\Sigma} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$$

  – the columns of $\mathbf{U}$ are the principal components (eigenvectors)
  – $\mathbf{\Lambda}$ is a diagonal matrix of eigenvalues
- Another option is SVD, which factorizes the input vector (k variables $\times$ n data points) as

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^*$$

  – $\mathbf{U}$ ($k \times k$) contains the eigenvectors as before,
  – $\mathbf{D}$ ($k \times n$) diagonal matrix $\mathbf{D}^2 = \mathbf{\Lambda}$
  – $\mathbf{V}^*$ is a $n \times n$ unitary matrix

* The above is correct for standardized variables, otherwise the formulas get slightly more complicated.

A practical example

(with simplified/fake data)

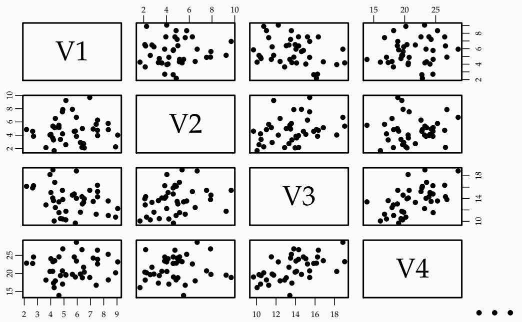
- Our data consists of 'measurements' from speech signal of instances of two vowels, we have 12 measurements for each vowel instance

$$\begin{bmatrix} 5.19 & 4.33 & 14.76 & 30.08 & 14.73 & 7.06 & 15.56 & 24.46 & 8.51 & \ldots \\ 2.99 & 5.25 & 11.69 & 19.27 & 18.02 & 11.04 & 13.34 & 38.13 & 8.70 & \ldots \\ 6.25 & 6.05 & 13.88 & 19.26 & 17.81 & 6.95 & 12.58 & 39.74 & 9.58 & \ldots \\ 7.24 & 5.43 & 15.15 & 18.93 & 15.69 & 10.18 & 14.89 & 34.86 & 10.03 & \ldots \\ 6.07 & 6.27 & 13.34 & 17.60 & 19.98 & 11.04 & 13.28 & 36.02 & 8.66 & \ldots \\ & & & & \ldots & & & & & \end{bmatrix}$$

- How do we visualize this data?
- Are all 12 variables useful?

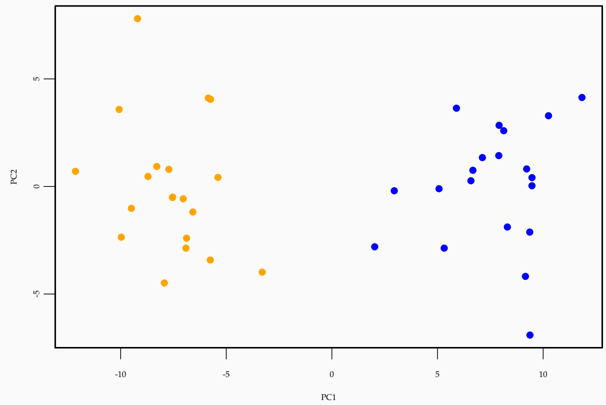
A practical example

Visualizing with pairwise scatter plots



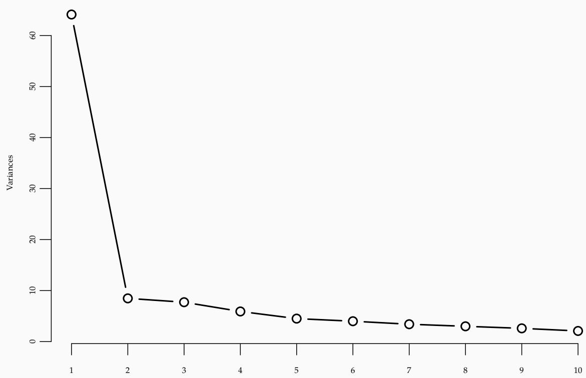
A practical example

Plotting the first two principal components



A practical example

How many components to keep? (scree plot)



Some practical notes on PCA

- Variables need to be centered
- Scales of the variables matter, standardizing may be a good idea depending on the units/scales of the individual variables
- The sign/direction of the principal component (vector) is not important
- If there are more variables than the data points, we can still calculate the principal components, but there will be at most $n - 1$ PCs
- PCA will be successful if variables are correlated, there are extensions for dealing with nonlinearities (e.g., kernel PCA, ICA, t-SNE)

Summary

- In unsupervised learning, we do not have labels. Our aim is to find/exploit (latent) structure in the data
- Unsupervised methods try to discover 'hidden' structure in the data

  Clustering finds groups in the data
  Density estimation estimates parameters of latent probability distributions
  Dimensionality reduction transforms the data in a low dimensional space while keeping most of the information in the original data

Next:

Mon Artificial neural networks (ANNs)
Wed Deadline for assignment 3, assignment 4 will be out

Derivation of PCA by maximizing the variance

- We focus on the first PC (z_1), which maximizes the variance of the data onto itself
- We are interested only on the direction, so we choose z_1 to be a unit vector ($\|z_1\| = 1$)
- Remember that to project a vector onto another, we simply use dot product, So the projected data points are zx_i for $i = 1, \ldots, N$.
- The variance of the projected data points (that we want to maximize) is,

$$\sigma_{z_1} = \frac{1}{N}\sum_{i}^{N}(z_1 x_i - z_1 \bar{x}_i)^2 = z_1^T \Sigma z$$

where Σ_x is the covariance matrix of the unprojected data

Derivation of PCA by maximizing the variance (cont.)

- The problem becomes maximize

$$z_1^T \Sigma z$$

with the constraint $\|z_1\| = z_1^T z_1 = 1$

- Turning it into a unconstrained optimization problem with Lagrange multipliers, we minimize

$$z_1^T \Sigma z + \lambda_1(1 - z_1^T z_1)$$

- Taking the derivative and setting it to 0 gives us

$$\Sigma z_1 = \lambda_1 z_1$$

Note: by definition, z_1 is an eigenvector of Σ, and λ_1 is the corresponding eigenvalue

- z_1 is the first principal component, we can now compute the second principal component with the constraint that it has to be orthogonal to the first one