

Statistical Natural Language Processing

Unsupervised machine learning

Çağrı Çöltekin

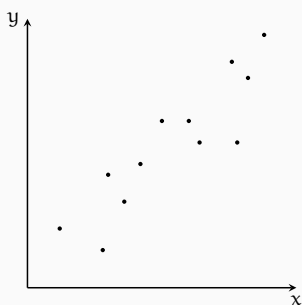
University of Tübingen
Seminar für Sprachwissenschaft

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Supervised learning

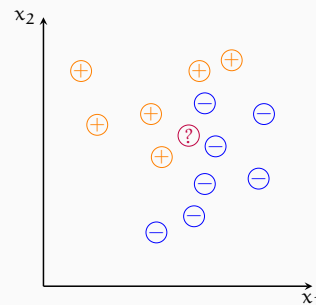
- The methods we studied so far are instances of supervised learning
- In supervised learning, we have a set of predictors \mathbf{x} , and want to predict a response or outcome variable y
- During training, we have both input and output variables
- Training consist of estimating parameters \mathbf{w}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

Supervised learning: regression



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

Supervised learning: classification



- The response (outcome) is a label. In the example: positive \oplus or negative \ominus
- 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 \mathbf{w} during training
- Often we find the parameters that minimize a loss function
 - For least-squares regression

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

- For logistic regression, the negative log likelihood

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

- 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)

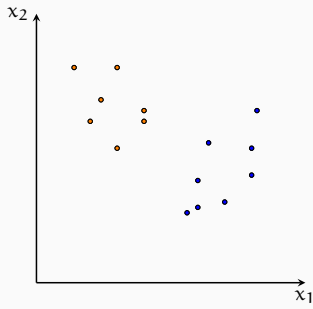
Unsupervised learning

- 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: $D(a, b) \geq 0$ for all a, b , and it $D(a, b) = 0$ iff $a = b$
 - obeys triangle inequality: $D(a, b) + D(b, c) \geq D(a, c)$
- 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:

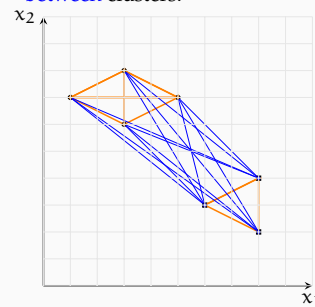
$$\|\mathbf{a} - \mathbf{b}\| = \sqrt{\sum_{j=1}^k (a_j - b_j)^2}$$

- 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.

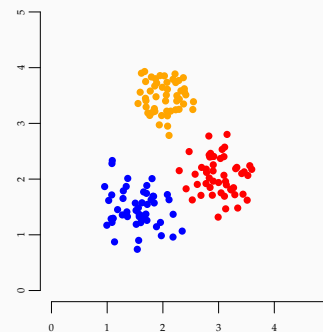
1. Randomly choose *centroids*, m_1, \dots, m_K , representing K clusters
2. Repeat until convergence
 - Assign each data point to the cluster of the nearest centroid
 - Re-calculate the centroid locations based on the assignments

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

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

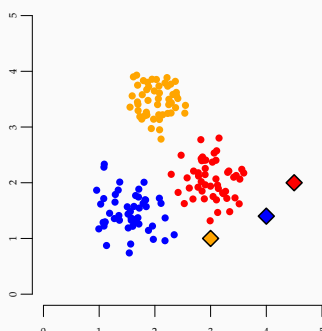
* Note the similarity with the EM algorithm

K-means clustering: visualization



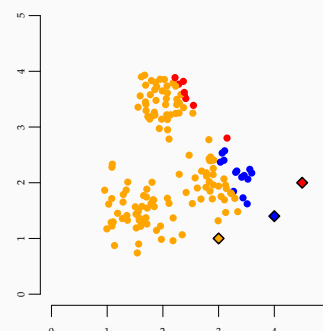
- The data
- Set cluster centroids randomly
- Assign data points to the closest centroid
- Recalculate the centroids

K-means clustering: visualization



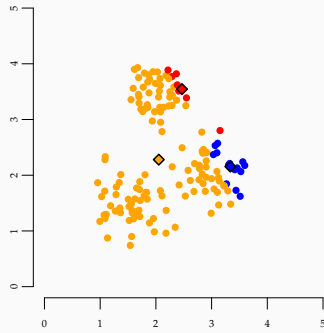
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K-means clustering: visualization



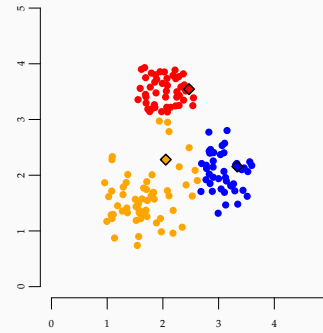
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K-means clustering: visualization



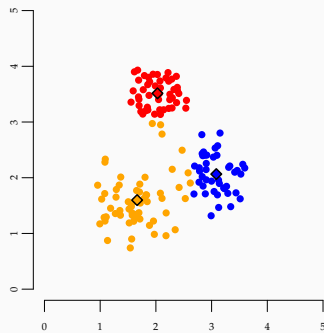
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K-means clustering: visualization



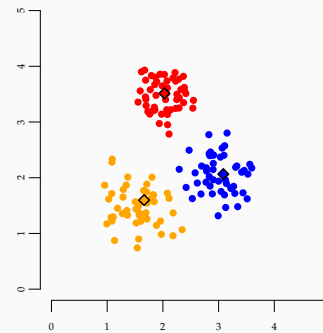
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K-means clustering: visualization



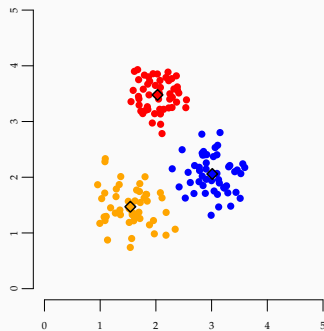
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K-means clustering: visualization



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K-means clustering: visualization



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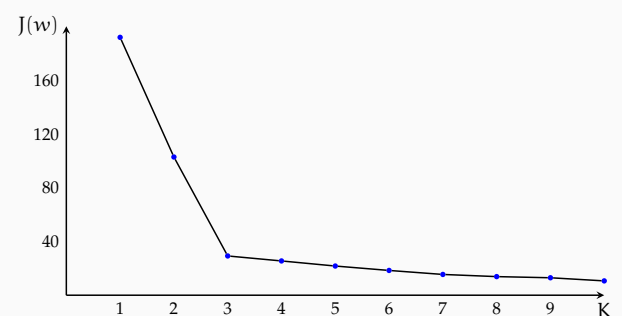
K-means: some issues

- 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

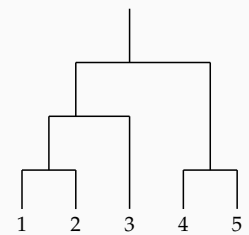
- starts with a single cluster,
- and splits until all leaves are single data points

Hierarchical clustering

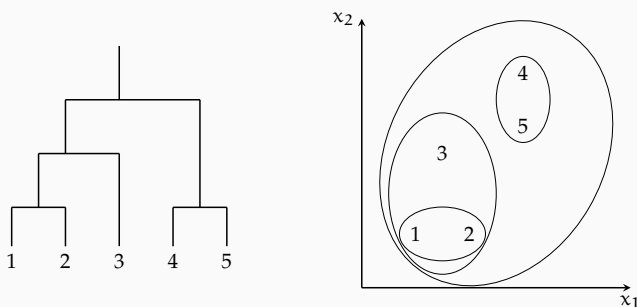
- Hierarchical clustering operates on differences (or similarities)
- The result is a binary tree called *dendrogram*
- Dendrograms are easy to interpret (especially if data is hierarchical)
- The algorithm does not commit to the number of clusters K from the start, the dendrogram can be 'cut' at any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

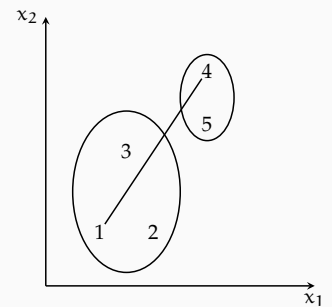


Agglomerative clustering demonstration



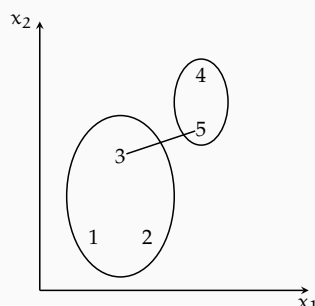
How to calculate between cluster distances

- Complete** maximal inter-cluster distance
- Single** minimal inter-cluster distance
- Average** mean inter-cluster distance
- Centroid** distance between the centroids



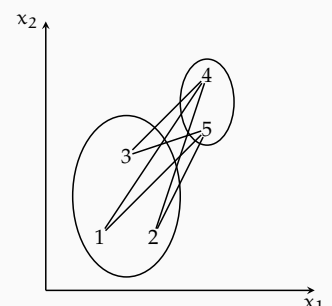
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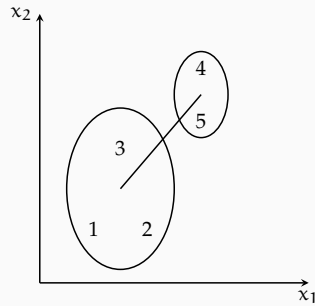
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Note: we only need distances, (feature) vectors are not necessary

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*, *B³ed 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'

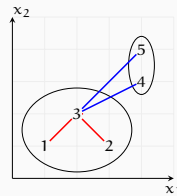
Clustering evaluation

internal metric example: silhouette

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

where

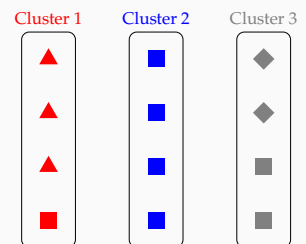
- a(i)** average distance between object i and and objects in the same cluster
- b(i)** average distance between object i and and objects in the *closest* cluster



Clustering evaluation

external metrics: general intuition

- 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

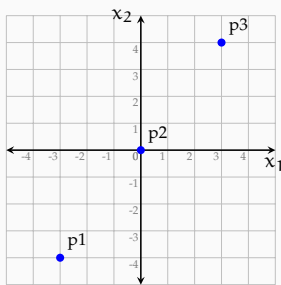
Density estimation using the EM algorithm

- The EM algorithm (or its variations) is used in learning models with latent/hidden variables
 - It is closely related to the K-means algorithm
- Initialize the parameters (e.g., randomly) of K multivariate normal distributions (μ, Σ)
 - 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



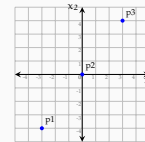
Questions:

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

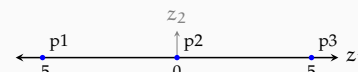
$$\Sigma = \begin{bmatrix} \frac{18}{3} & 8 \\ 8 & \frac{32}{3} \end{bmatrix}$$

- What is the correlation between x_1 and x_2 ?

PCA: A toy example (2)



What if we reduce the data to:



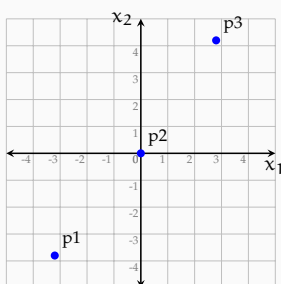
Going back to the original coordinates is easy, rotate using:

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

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

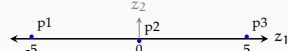
We can recover the original points perfectly. In this example the inherent dimensionality of the data is only 1.

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:

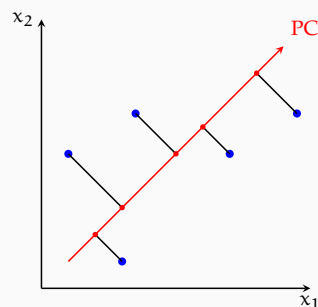
$$p1 = A \times \begin{bmatrix} -5 \\ 0 \end{bmatrix} = \begin{bmatrix} -3 \\ -4 \end{bmatrix}$$

- 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 $\Sigma = X^T X$)

$$\Sigma = U \Lambda U^T$$

- the columns of U are the principal components (eigenvectors)
- Λ is a diagonal matrix of eigenvalues

- Another option is SVD, which factorizes the input vector (k variables \times n data points) as

$$X = U D V^*$$

- U ($k \times k$) contains the eigenvectors as before,
- D ($k \times n$) diagonal matrix $D^2 = \Lambda$
- 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)

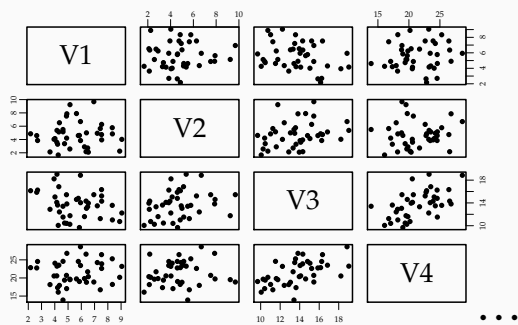
- Our data consists of ‘measurements’ from speech signal of instances of two vowels, we have 12 measurements for each vowel instance

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

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

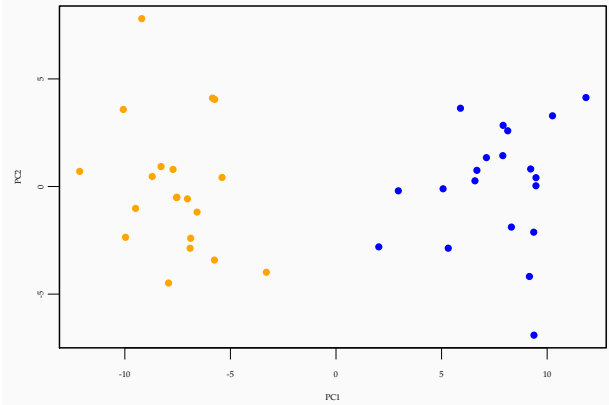
A practical example

Visualizing with pairwise scatter plots



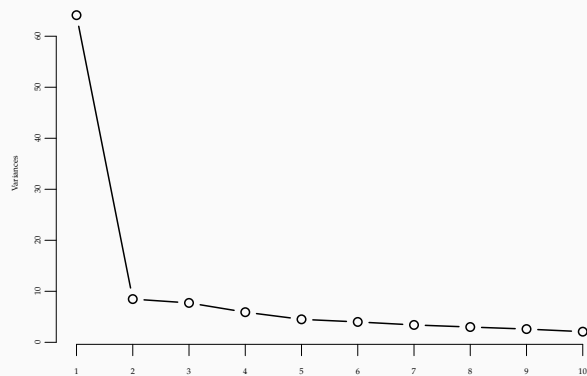
A practical example

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 $i = 1, \dots, N$.
- The variance of the projected data points (that we want to maximize) is,

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

where Σ_x is the covariance matrix of the unprojected data

Derivation of PCA by maximizing the variance (cont.)

- The problem becomes maximize

$$z_1^T \Sigma z_1$$

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

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

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

- 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