Clustering

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Einführung Machine Learning

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Data Generating Processes Revisited

Recap

It is useful to think of our datasets as samples from **data generating processes** for the input X and the conditional output Y|X.

- **MNIST**
  X: people write digits $\rightarrow$ people take standardized photos thereof.
  Y|X: different people label the same photo X.
- **Weather**
  X: the weather acts on sensors in weather stations.
  Y|X: the weather evolves from X and is measured again 5 hours later.

Using samples from these data generating processes, supervised learning aims at learning something about the conditional processes, i.e how Y depends on X.

Using samples from these data generating processes, **unsupervised learning** aims at learning something about the input generator, i.e how X is generated.

Goals of Unsupervised Learning

- **Exploratory Data Analysis**: Is there an informative way to visualize the data? Can we discover subgroups among the variables or among the observations?
- **Data Processing**: Can we separate signal from noise (denoising)? Can we efficiently compress the data?
- **Uncovering Hidden "Causes" of Observations**: Can we uncover hidden structure in the data? Does the data lie on a low-dimensional manifold?
- **Generating Artificial Data**: Can we generate high-quality novel data samples, e.g. images, text or music?

For the assessment of unsupervised learning there are often no clear objective guidelines.

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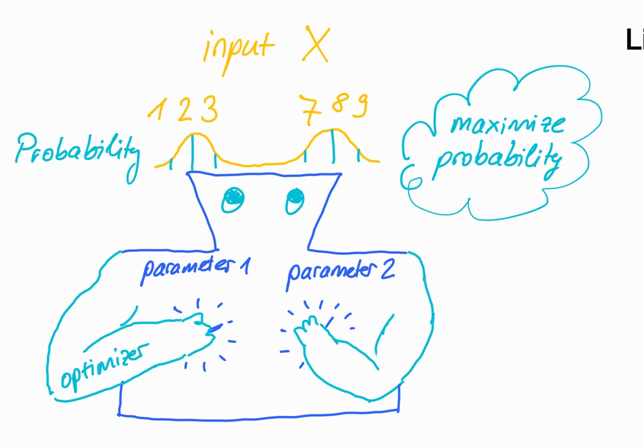
How Does Unsupervised Learning Work?

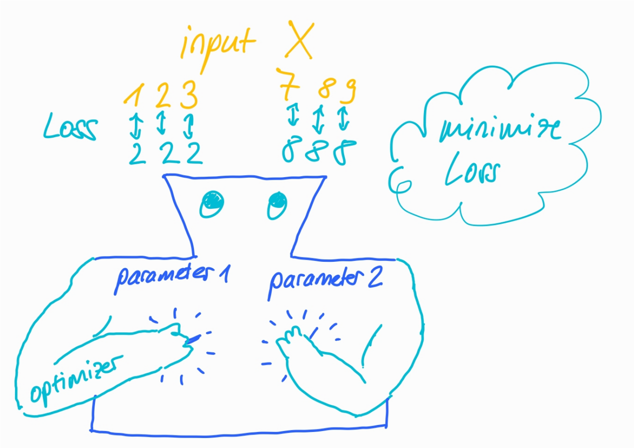


Likelihood Maximizing Machine

- We specify
  1. the training data
  2. the family of probability distributions (model)
  3. the optimizer
- The machine changes the parameters with the help of the optimizer until the likelihood of the parameters is maximal.

E.g.: Gaussian Mixture Model (not further discussed here)

How Does Unsupervised Learning Work?



Loss Minimizing Machine

- We specify
  1. the training data
  2. the function family (model)
  3. the loss function $L(x)$
  4. the optimizer
- The machine changes the parameters with the help of the optimizer until the loss is minimal.

E.g.: K-Means Clustering

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K-Means Clustering

- $C_1, \ldots, C_K$ contain the indices of the observations in each cluster.
- K needs to be chosen.
- Every observation with index $i = 1, \ldots, n$ is in exactly one cluster.
- Goal:

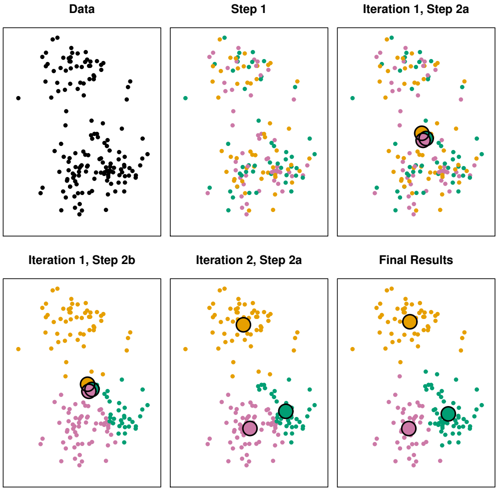
$$\underset{C_1,\ldots,C_K}{\text{minimize}} \sum_{k=1}^{K} W(C_k) \tag{1}$$

where $W(C_k)$ measures the dissimilarity between observations in cluster k, e.g. *squared Euclidean distance*

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = 2 \sum_{i \in C_k} \sum_{j=1}^{p} (x_{ij} - \bar{x}_{kj})^2$$

with $|C_k|$ the number of observations in cluster k and cluster mean $\bar{x}_{kj} = \frac{1}{|C_k|} \sum_{i \in C_k} x_{ij}$.

K-Means Clustering

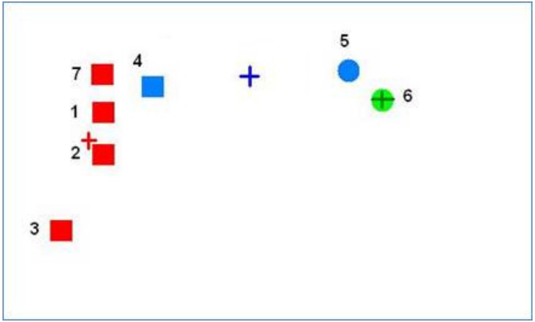


K-Means Clustering Algorithm

1. Randomly assign a number, from 1 to K, to each to the observations.
2. Iterate until the cluster assignments stop changing.
   (a) For each of the K clusters, compute the cluster *centroid* $\bar{x}_{kj} = \frac{1}{|C_k|} \sum_{i \in C_k} x_{ij}$ for $j = 1, \ldots, p$.
   (b) Assign each observation to the cluster whose centroid is closest.

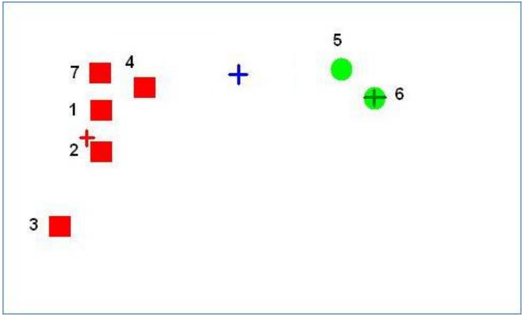
K-Means Empty Cluster Example

Start



Clusters are indicated with colors, centroids with crosses

Next Iteration



Clusters can become empty

Adapted from `http://user.ceng.metu.edu.tr/~tcan/ceng465_f1314/Schedule/KMeansEmpty.html`

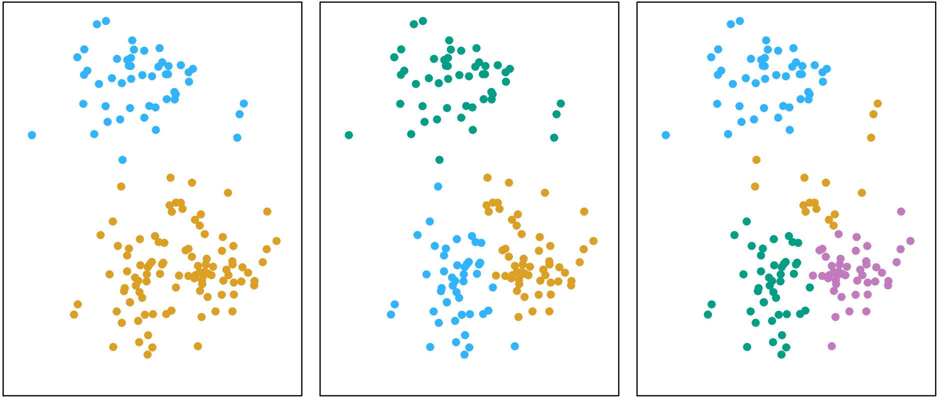
Dependence on the Initial Condition

K-Means Clustering performed six times on the same data set with different random assignments. Above the plot is the value of the loss function (in Equation 1 on slide 8) at convergence.

Three different local optima were obtained. Those labelled in red all achieve the same solution.

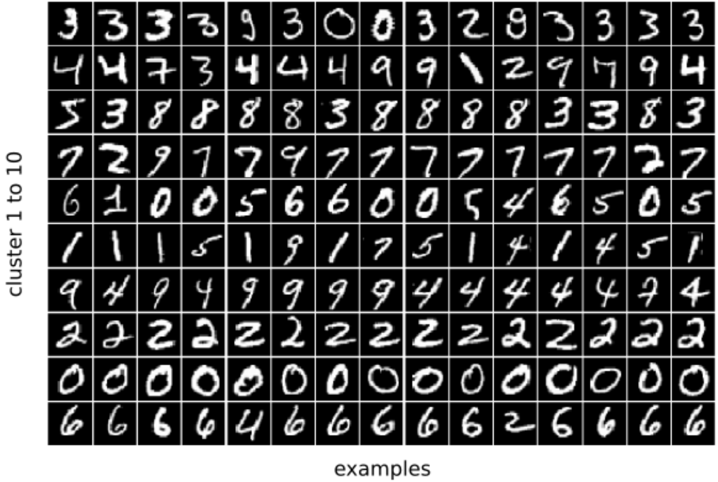
Choosing *k* in K-Means Clustering

K=2 K=3 K=4



Some of the figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani

K-Means Clustering of MNIST Images



- All images in the same row are in the same cluster according to one run of K-Means clustering with 10 clusters.
- Some clusters contain images alsmost exclusively from one class; other clusters contain images from a few different classes.

Quiz

Richtig oder falsch?

- Am Ende von K-Means Clustering ist jeder Datenpunkt in genau einem Cluster.
- Das Resultat von K-Means Clustering hängt nur von k und dem Verschiedenheitsmass $W(C_k)$ ab.

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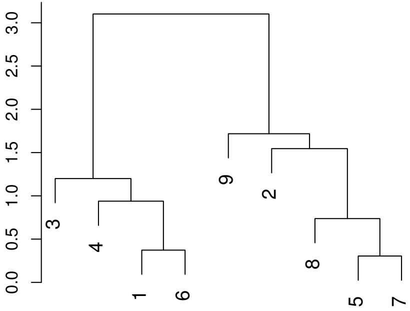
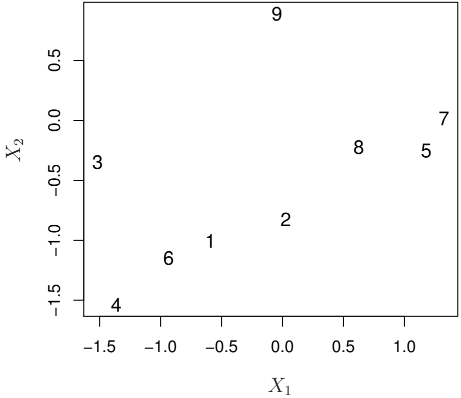
Hierarchical Clustering

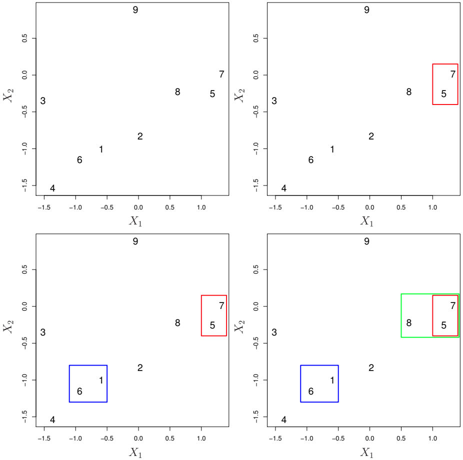
Organize data in a tree called **dendrogram**





The height of the fusion of two branches indicates how different the observations in the two branches are.

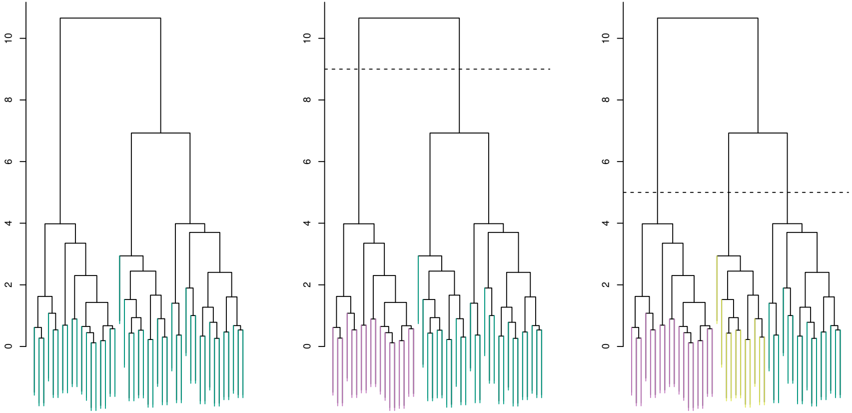
Hierarchical Clustering Algorithm



Euclidean distance, complete linkage

1. Begin with n observations and a measure of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster.
2. For $i = n, n-1, \ldots, 2$:
   (a) Examine all pairwise dissimilarities among the i clusters and fuse the most similar pair. The dissimilarity of this pair indicates the height in the dendrogram at which the fusion is placed.
   (b) Compute the new pairwise inter-cluster dissimilarities among the $i-1$ remaining clusters.

Clustering with a Dendrogram



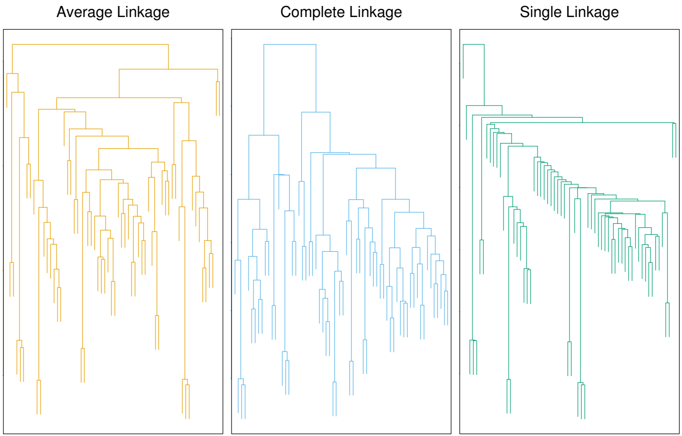
The coloured leaves indicate the class identity. The length of the leaves has no meaning.

Cut the dendrogram at different heights to get different clusterings.

Linkage: Measuring Distances Between Sets

Linkage	Description
Complete	**Maximal intercluster dissimilarity**. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the largest of these dissimilarities.
Single	**Minimal intercluster dissimilarity**. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the smallest of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	**Mean intercluster dissimilarity**. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the average of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in **undesirable inversions** (i.e. clusters are fused at a height below either of the individual clusters).

The Effect of the Linkage



Average and complete linkage tend to yield more balanced clusters.

Small Decisions with Big Consequences

- What type of dissimilarity measure should be used?
  Euclidean distance is not the most natural for many types of data.
- Should the observations or features be standardized (e.g. variance 1)?
  Scaling can be seen as changing the dissimilarity measure.
- In the case of hierarchical clustering:
  - What type of linkage should be used?
  - Where should we cut the dendrogram?
- In the case of K-means clustering: how should be choose k?

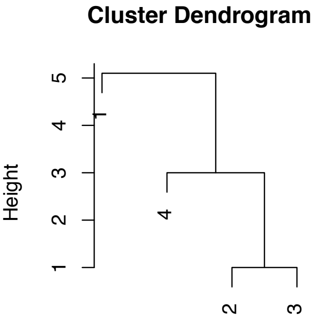
[...] we must be careful about how the results of a clustering analysis are reported. These results should not be taken as the absolute truth about a data set. Rather, they should constitute a starting point for the development of a scientific hypothesis and further study, preferably on an independent data set.

Quiz

Richtig oder falsch?

Stellen Sie sich ein Problem mit 4 Datenpunkten vor:
$x_1 = 1, x_2 = 4, x_3 = 5, x_4 = 7$.

- Nach dem ersten Schritt von hierarchischem Clustering mit euklidschem Verschiedenheitsmass finden wir die 3 Cluster $\{1\}, \{2, 3\}, \{4\}$.
- Mit complete linkage ist der euklidsche Abstand zwischen Cluster $\{1\}$ und $\{2, 3\}$ gleich $\sqrt{(1-5)^2} = 4$.
- Das Dendrogram rechts ist das Resultat von hierarchischem Clustering der 4 Datenpunkte..
- Nachbarn im Dendrogram (beispielsweise 1 und 4) sind Datenpunkte, welche nahe beieinander liegen.



Terminology

- **Supervised Learning**: learn $p(Y|X)$
- **Semi-Supervised Learning**: learn $p(Y|X)$ with typically a small fraction of the data having labels given explicitly by humans and the rest unlabeled, e.g. many images, but only some with labels.
- **Self-Supervised Learning**: learn $p(Y|X)$ where Y is not a label given explicitly by humans (or other supervisors). *Example: auto-regressive models like weather prediction.*
- **Unsupervised Learning**: learn $p(X)$.
  In unsupervised learning one is often more interested in a hidden representation of the data than in plain fitting of $p(X)$, e.g. if the data seems to be clustered, what is the cluster identity of a given point.
  If X is multidimensional one learns sometimes parts of $p(X)$ in a self-supervised manner, e.g. $p(X) = p(X_1)p(X_2|X_1)$.