





Machine Learning *Lecture 7*

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Lecture 7 – Unsupervised Learning

- Intro Unsupervised Learning
- Clustering
- K-means clustering
- Hierarchical clustering
- DBSCAN
- Association rules



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Machine Learning Types

Supervised Learning:

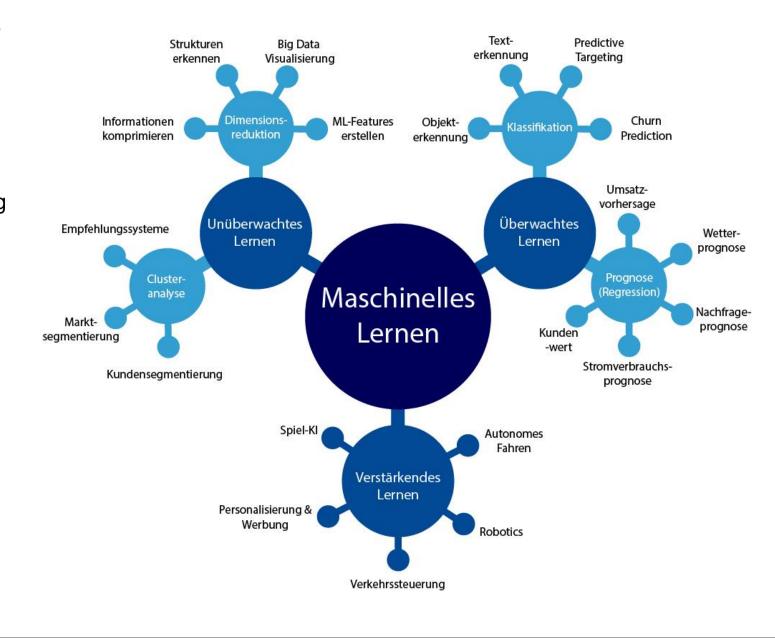
- labelled data
- Direct feedback
- Predict an outcome/future, forecasting
- E. g. predict customer churn

Unsupervised Learning:

- No labels
- No feedback
- Finding hidden structures
- E. g. cluster customers

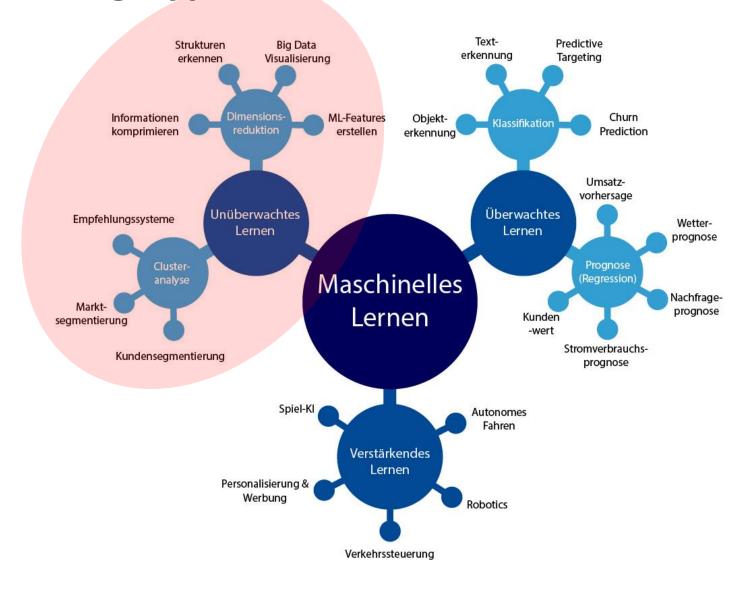
Reinforcement Learning:

- Decision process
- Reward system
- Learn a series of actions
- E. g. playing Go





Machine Learning Types

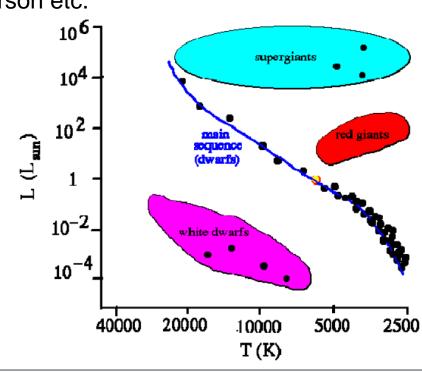




Why unsupervised learning?

- Getting enough ground truth data (a.k.a. labelled data) is expensive
- Automatic collection would be nice
- Features can update and the labels should update too
 - → e. g. color of fruit over a season; age/growth rate/weight of a person etc.

- Use cases are quite diverse, some examples:
 - Data analysis in science (e. g. grouping of genes, proteins, astronomical objects)
 - Marketing (e. g. product analysis, shopping baset analysis, grouping of customers)
 - Databases (e. g. finding similar documents)





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Unsupervised learning method to cluster data into groups

Goals:

- Clusters should be homogeneous (samples in a single cluster are similar)
- Clusters themselves should be very different

Definition:

m-clustering of $X = \{x_1, x_2, ..., x_N\}$ is a subdivision of X into m cluster $C_1, ..., C_m$ such that:

- $C_i \neq \emptyset$, i = 1, ... m
- $\bigcup_{i=1}^m C_i = X$
- $C_i \cap C_j = \emptyset, i \neq j; i, j = 1, \dots m$

The vectors x_i of cluster C_i are more similar to each other than they are to the vectors of the other clusters. This is called "hard" or "crisp" clustering.



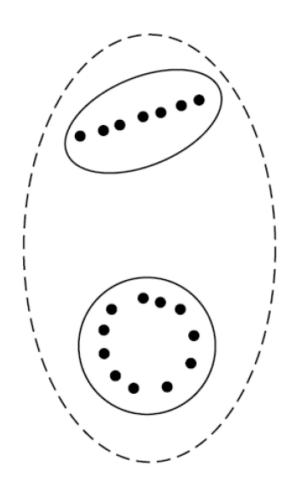
Definition (Fuzzy Clustering):

Fuzzy-clustering of $X = \{x_1, x_2, ..., x_N\}$ into m cluster $C_1, ..., C_m$ is defined by m membership functions u_i with:

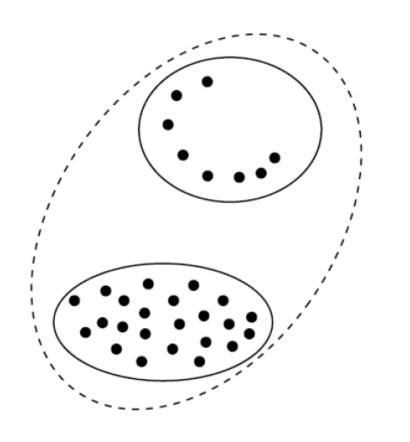
- $u_i: X \to [0,1], j = 1, ..., m$ and
- $\sum_{i=1}^{m} u_i(x_i) = 1, i = 1, ..., N$

Each vector x_i is part of several clusters at the same time, the value of this membership is quantified by u_j . Values near 1 indicate a high degree of membership to a cluster.

There are many possible solutions depending on the scale



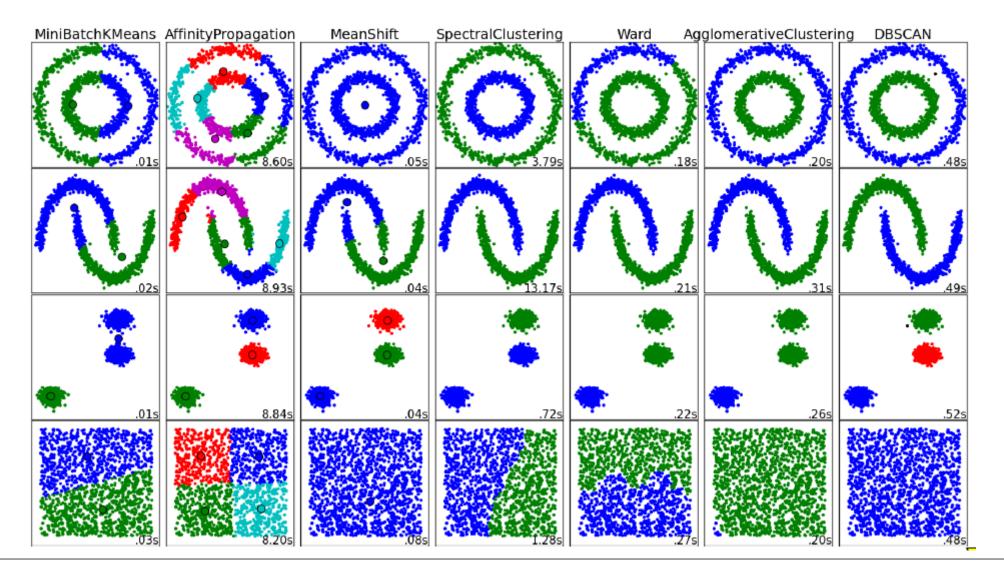
[Quelle: Theodoris et al., 2009]



- For clustering to work, you'll need:
 - Features and some pre-processing
 - Distance metric
 - Cluster criterion (grouping criterion)
 - Clustering algorithm
 - Validation and interpretation of results
 - → Depending on the selection of the above points, you'll get very different clusterings



[Quelle: http://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html]





Clustering – Similarity metrics

- Euclidean norm
- dot-product (scalar product) of two vectors x, y:

$$s_{scalar}(x,y) = x^{T}y = \sum_{i=1}^{l} x_{i}y_{i}$$

Pearson's correlation coefficient:

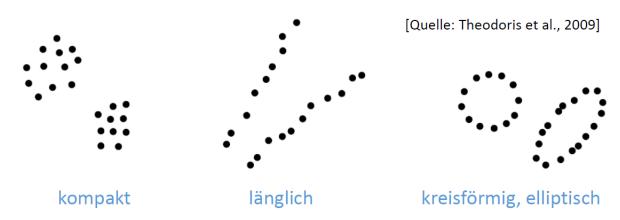
$$s_{pearson}(x,y) = \frac{x_d^T y_d}{\|x_d\| \|y_d\|},$$

with
$$x_d[x_1 - \overline{x}, ..., x_l - \overline{x}]^T$$
 and $y_d[y_1 - \overline{y}, ..., y_l - \overline{y}]^T$



Clustering – Similarity metrics

- Distance between a vector and a subset of X
 - > needed for assessing whether a vector should be assigned to a cluster C
- Several options exist:
 - Minimal dissimilarity: d(x,C) = min(d(x,y)) for all y in C
 - Maximal similarity: s(x,C) = max(s(x,y)) for all y in C
 - Average (dis)similarity or distance to a centroid average cluster coordinates)
- Depending on the cluster type, a different distance calculation might be reasonable





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K-means clustering

- K-means is a centroid-based clustering method. It is partitional
- Goal: find the k cluster centers and assign the objects to the nearest cluster center (centroids), such that the squared distances from the cluster are minimized
- NP-hard problem → we search for an approximate solution
- Number of clusters k needs to be specified (hyperparameter)
- Conceptually close the to k-nearest neighbor classification algorithm
- Some variations:
 - k-median (more robust against outliers)
 - k-medoids (centroids need to be a data sample)
 - k-means++ (choosing initial centers less randomly)
 - fuzzy c-means (allowing fuzzy cluster assignment)



K-means clustering

- The algorithm consists of the following steps:
 - Choose number of clusters k and initial centroids (usually randomly)
 - Assignment step: assign samples to the cluster with the closest (Euclidean distance) centroid
 - 3. Update step: Recalculate centroids (means) with the assignments of step 2
 - 4. Repeat steps 2 and 3 until there is no significant improvement anymore

- The algorithm is not guaranteed to find the global optimum
- It is based on spherical clusters that are separable and approximately the same size so that the mean converges towards the cluster center



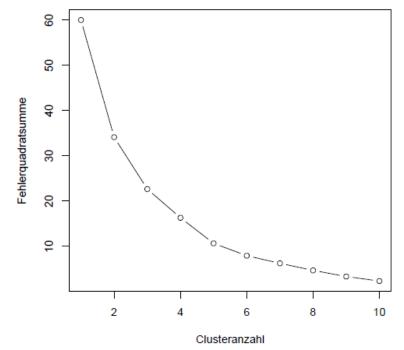
K-means clustering

- To assess "significant improvement" we need a criterion, e. g., sum of squared distances of samples to their centroids
- Since we use distance metrics standardized variables are strongly recommened!
- Initial centroids are critical to the overall result
 - > repeat algorithm several times with random initial centroids
 - → choose the best run
- The resulting clusters can be used as an additional categorical variables for further statistical methods, e. g., clustering customers and running analysis on customer clusters.



K-means clustering – Choosing k

- K is very important to the final result
- To find a good k, run the algorithm several times with different k and plot the errors

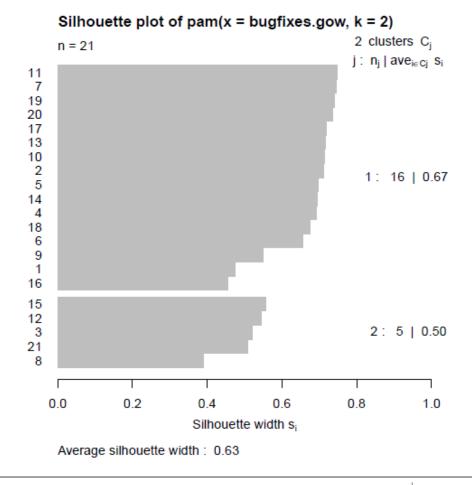


• Look out for a plateauing point or a sharp change in error trend that indicates that improvement with higher k is limited after this point.



K-means clustering – Evaluating results with silhouettes

- How good the samples are clustered can be assessed with a silhouette plots
- Silhouettes can be calculated for the overall solution or individual clusters
- Silhouette values and their approx. meaning:
 - 1.0 0.71: well clustered samples, clustering found strong structures
 - 0.7 0.51: medium and somewhat acceptable structures were found
 - 0.5 0.26: weak structures
 - <0.25: no substantial structures were found, and samples lie between clusters
- Example for n=21 samples in 2 clusters:
 - Clusters are medium (0.5) or strong clusters (0.67)
 - Average silhouette width is acceptable (0.63)
 - Individual silhouettes are >0, i. e., no samples are in wrong cluster or close to a border



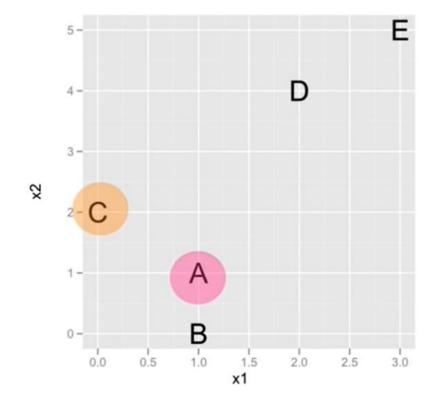


Class Assignment

Assignment:

Use K=2 with points A and C as initial cluster means and perform the k-means clustering algorithm for two iterations (Euclidean norm $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$)

— 0	i	X 1	X ₂
\overline{X}_{1}^{0}	А	1	1
	В	1	0
\overline{X}_{2}^{0}	С	0	2
2	D	2	4
	Е	3	5





Class Assignment – Solution 1/7

• Step 1 (Iteration 1): Calculate the distances between each of the cluster means and all other points

— 0	i	X 1	X ₂
\overline{X}_{1}°	A	1	1
	В	1	0
\overline{X}_{2}^{0}	С	0	2
	D	2	4
	Е	3	5

i	0	2
A	0	1.4
В	1	2.2
С	1.4	0
D	3.2	2.8
Е	4.5	4.2



Class Assignment – Solution 2/7

• Step 2 (Iteration 1): Assign each point to the cluster with the lowest distance. Use this new cluster assignment to calculate the new cluster means

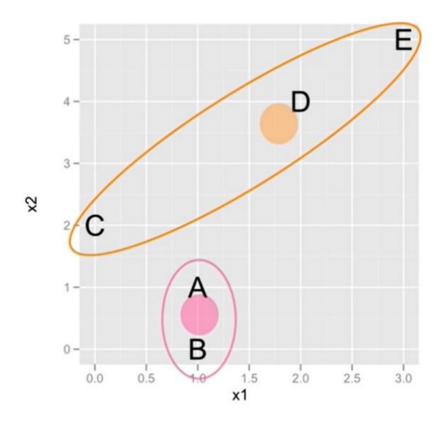
i	0	2	Cluster
А	0	1.4	1
В	1	2.2	1
С	1.4	0	2
D	3.2	2.8	2
Е	4.5	4.2	2

i	X 1	X ₂	
А	1	1	$\overline{\mathbf{X}}^{1}$
В	1	0	1
С	0	2	\overline{X}^1
D	2	4	\mathbf{X}_{2}
Е	3	5	



Class Assignment – Solution 3/7

• Iteration 1 final: Updated clusters in the graph:



$$\overline{X}_{1}^{1}=(1,0.5)$$

$$\overline{X}_{2}^{1} = (1.7, 3.7)$$



Class Assignment – Solution 4/7

• Step 3 (Iteration 2): Recalculate the distances of points to the new cluster means

i	X 1	χ_2	▼¹ /1 O 5\	i	1	2
A	1	1	$\overline{X}_{1}^{1}=(1,0.5)$	A	0.5	2.7
В	1	0	1	В	0.5	3.7
С	0	2	$\overline{X}_{2}^{1} = (1.7, 3.7)$	С	1.8	2.4
D	2	4		D	3.6	0.5
Е	3	5		Е	4.9	1.9



Class Assignment – Solution 5/7

• Step 4 (Iteration 2): Assign each point to the cluster with the lowest distance.

i	0	2	Cluster
А	0.5	2.7	1
В	0.5	3.7	1
С	1.8	2.4	1
D	3.6	0.5	2
Е	4.9	1.9	2

i	X 1	X ₂	
Α	1	1	$\overline{\mathbf{y}}^2$
В	1	0	1
С	0	2	- 2
D	2	4	X_2
Е	3	5	



Class Assignment – Solution 6/7

• Step 5 (Iteration 2): Assign each point to the cluster with the lowest distance.

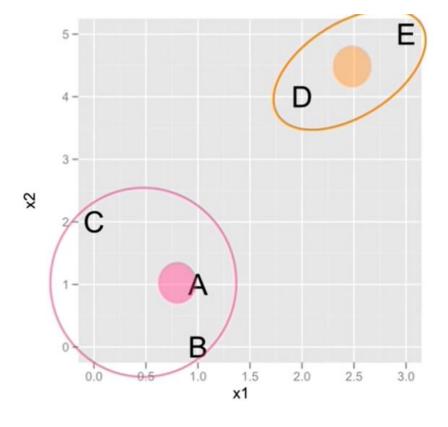
i	0	2	Cluster
А	0.5	2.7	1
В	0.5	3.7	1
С	1.8	2.4	1
D	3.6	0.5	2
Е	4.9	1.9	2

i	X 1	X ₂	
А	1	1	$\overline{\mathbf{y}}^2$
В	1	0	N ₁
С	0	2	
D	2	4	X_2
Е	3	5	



Class Assignment – Solution 7/7

Step 6 (Iteration 2): Recalculate cluster means
 → Algorithm has already converged ©



$$\overline{X}_{1}^{2} = (0.7,1)$$

$$\overline{X}_{2}^{2} = (2.5, 4.5)$$

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Hierarchical clustering

- Two types:
 - Agglomerative
 - Divisive
- In addition to homogeneous clusters, hierarchical clustering results in a hierarchical structure of the data (a dendrogram)



$$\{\{x_1\}, \{x_2\}, \{x_3\}, \{x_4\}, \{x_5\}\}$$

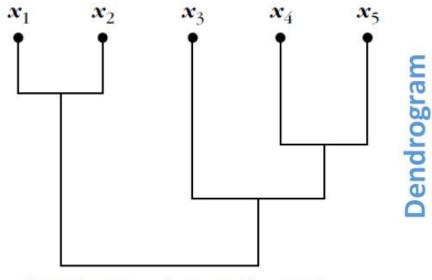
$$\{\{x_1, x_2\}, \{x_3\}, \{x_4\}, \{x_5\}\}$$

$$\{\{x_1, x_2\}, \{x_3\}, \{x_4, x_5\}\}$$

$$\{\{x_1, x_2\}, \{x_3\}, \{x_4, x_5\}\}$$

$$\{\{x_1, x_2\}, \{x_3, x_4, x_5\}\}$$

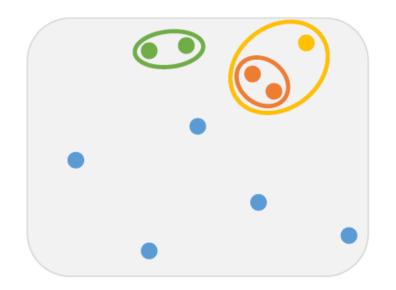
$$\{\{x_1, x_2, x_3, x_4, x_5\}\}$$

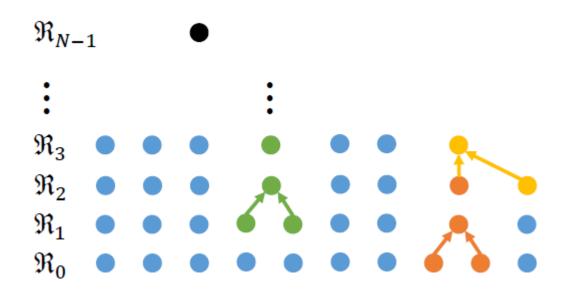


[Quelle: Theodoris et al., 2009]

Hierarchical clustering – agglomerative approach

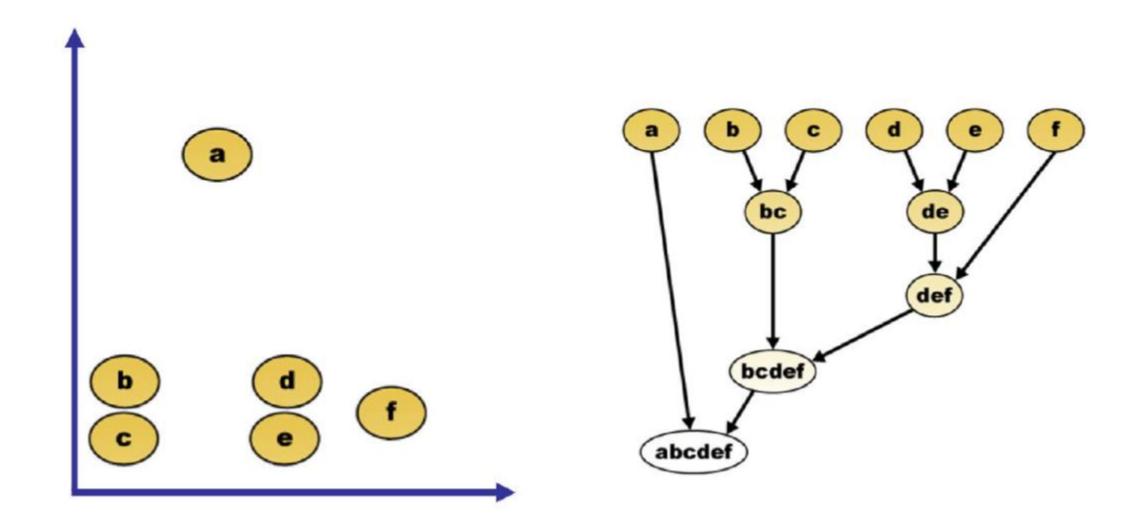
- Start with each sample in a separate cluster and then group them into larger and larger clusters until there is only one cluster left
- Grouping criterion determines how this agglomeration works:
 - Single Linkage Clustering: smallest distance between samples in clusters
 - Complete Linkage Clustering: largest distance between samples in clusters
 - Average Linkage Clustering: mean distance between samples in clusters







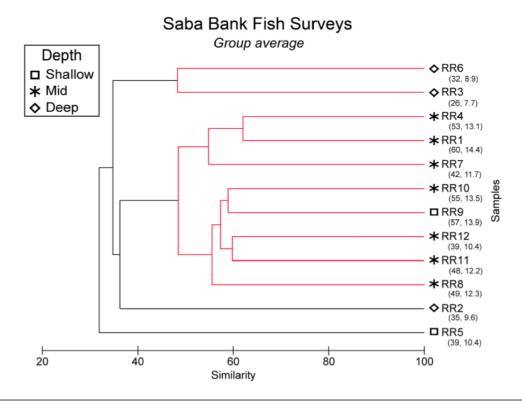
Hierarchical clustering – agglomerative approach





Hierarchical clustering – divisive approach

- Opposite of agglomerative approach: start with all samples in one cluster and recursively split until each sample is in its own cluster
- Naïve method: Search for best subdivision of a set into two clusters out of the $2^{N-1}-1$ possibilities based on some criterion.



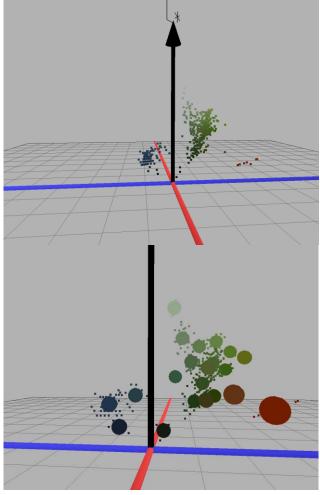


Hierarchical clustering – Remarks

- There is no way to recover from a "bad grouping" (or splitting)
- To get k clusters just stop early or cut off the appropriate branches in the dendrogram
- Example: reduce color palette to 500 colors (or even fewer)







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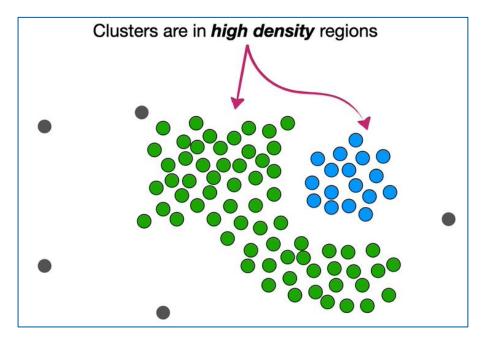
DBSCAN

• DBSCAN ... "Density-Based Spatial Clustering of Applications with Noise"

 Works well even with "nested clusters" (also in higher dimensions with the right distance metric)

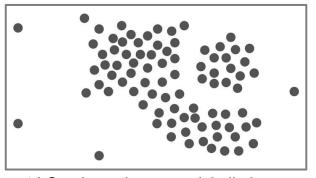
+ reduced risk of *single-link clusters*

- Sequential algorithm that also marks outliers
- Hyperparameters: distance d, min. neighbors n





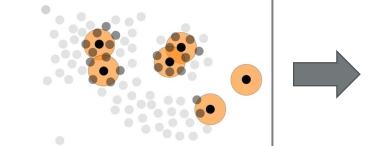
DBSCAN – Algorithm

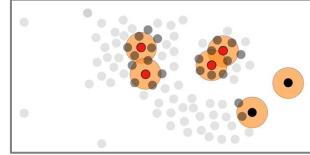


1.) Starting point: raw unlabelled points

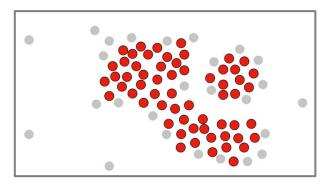


2.) Count the number of points within distance d (orange, hyperparameter) for each point

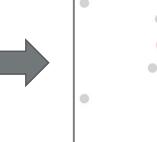




3.) Label points as "core" points (red) if they have more than n neighbors (hyperparameter, e. g. 4) within distance d, otherwise as "non-core" points (black)



4.) Each point is either core or noncore



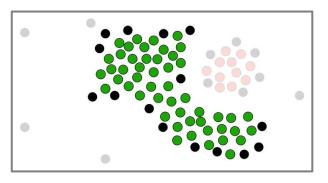
5.) Randomly pick a core point and assign it to cluster 1. Add all core points within **distance d** to that point to the cluster.



6.) Repeat step 5 for all added core points recursively until there are no more core points to add



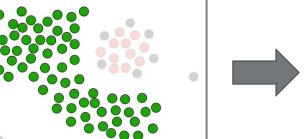
DBSCAN – Algorithm

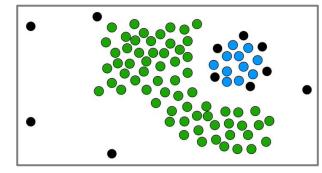


7.) Add all non-core points within distance d to cluster 1 (only once, not recursively!)

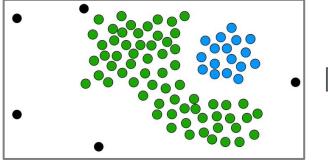


8.) That creates our first cluster (green)





9.) Like in step 5, pick a new nonclustered core point as a seed for cluster 2 (blue) and recursively add all core points closer than distance d



10.) Like in steps 7 & 8, add the noncore points and we now have our full cluster 2



11.) If there are more non-clustered core points left, repeat the steps until there are no more unclustered core points left.

All remaining non-core points are marked as outliers.



DBSCAN – Remarks

- 1. No initial number of clusters necessary
- 2. Mostly deterministic except for some non-core boundary points and cluster order
- 3. Run time complexity $O(n^2)$ but some tradeoffs can be made by using efficient memory structures (e. g. R-tree variations) and pre-calculations
- 4. Robust to outliers (we even get a list of them)
- 5. Clusters should have similar densities for the algorithm to work properly (otherwise the min neighbor parameter only fits selected clusters well)



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Association rules

- Association Rule Mining is a rule-based machine learning method that helps to uncover meaningful correlations between different products according to their co-occurrence in a data set
- in sales/marketing also called "Market Basket Analysis"

Association rules represent relationships between set of elements in transactions

(not an individual's preference)

- "Customers also bought xxx" → Recommendation
- "Frequently bought together items" → Association
- Market Basket Analysis is very simple:
 → Basic idea: check likelihood of different elements occurring together
- We use the Apriori-Algorithm
- Association rules use:
 - Support
 - Confidence
 - Lift



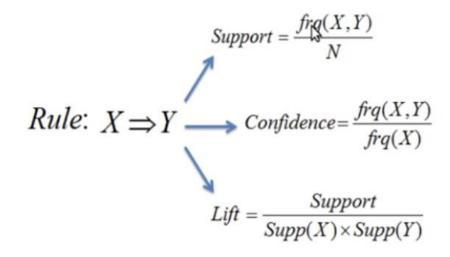
Example Use Cases:

- A and B can be placed together so that when a customer buys one of the product he doesn't have to go far away to buy the other product.
- People who buy one of the products can be targeted through an advertisement campaign to buy the other.
- Collective discounts can be offered on these products if the customer buys both of them.
- Both A and B can be packaged together.



Association rules

Rules need to meet a user-specified minimum support and minimum confidence



- Support ... (general) probability that X occurs over all transactions
- Confidence ... conditional probability of Y when X occurred/is present
- Lift ... how likely an item is purchased when another item is purchased, while controlling for how popular both items are (higher value == higher association; >1 ... "association is present")



Association rules – Apriori algorithm

Apriori principle: if an itemset is infrequent, then all its supersets must also be infrequent

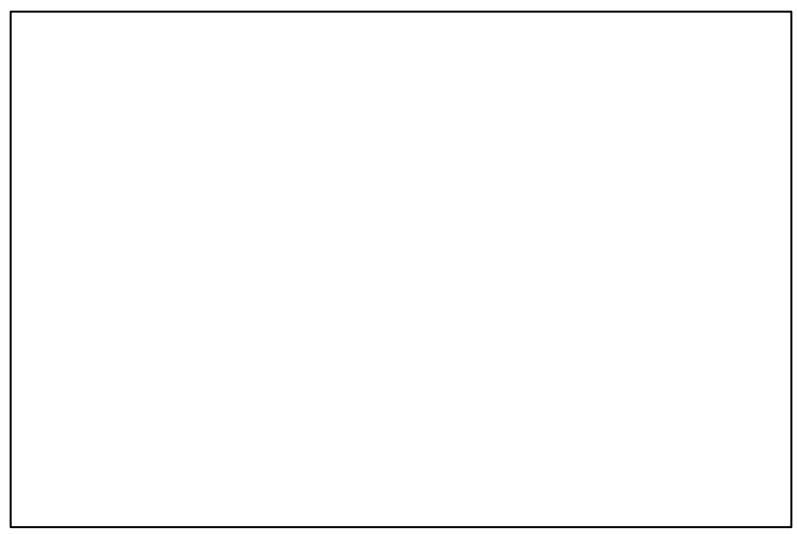
→ use this for effective pruning of possible combinations to reduce the required computational effort

Steps:

- 1. Hyperparameter Setting: set a minimum value for support and confidence. This means that we are only interested in finding rules for the items that have certain default existence (i. e. support) and have a minimum value for co-occurrence with other items (i. e. confidence)
- 2. Frequent Itemset Generation: extract all the itemsets having higher value of support than minimum threshold
 - a) Start with itemset containing only 1 element, e. g., {bread}, {butter}
 - b) Calculate the support for itemsets and only keep those itemsets that reach a specified minimum support threshold (on-the-fly-pruning see next slide for animation)
 - c) Generate all possible (non-empty) itemset combinations
 - d) Repeat step b and c until there are no more new valid itemset combinations
- **3. Strong Rule Generation:** generate all possible rules from the itemsets and only select those with confidence values higher than the minimum threshold
- **4. Order list of association rules:** order the rules by descending order of Lift



Association rules – Apriori algorithm animation (pruning via Support)



https://www.kdnuggets.com/2016/04/association-rules-apriori-algorithm-tutorial.html/2

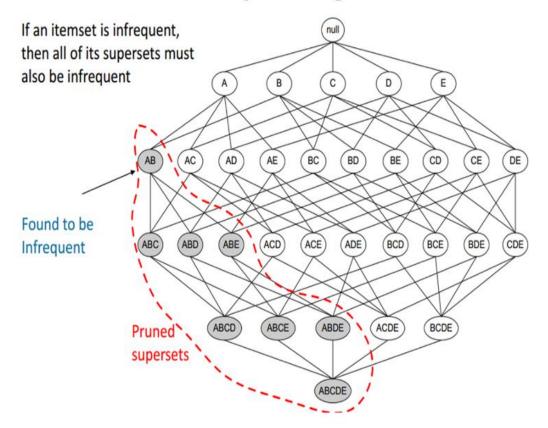


Association rules – Apriori algorithm animation (pruning via Support)

The combinations of 5items

CE BCD BCE BDE ABE ACD ACE ADE BCDE ABCD ABCE ABDE ACDE ABCDE

The Apriori Algorithm



https://www.kdnuggets.com/2019/12/market-basket-analysis.html



For this example we will use a minium support of 2 and a minimum confidence of 50%

TID	items		
T1	11, 12 , 15		
T2	12,14		
T3	12,13		
T4	11,12,14		
T5	11,13		
T6	12,13		
T7	11,13		
T8	11,12,13,15		
T9	11,12,13		



Frequent Itemset Generation:

- 1. Calculate support values and only keep those with values larger than 2 (itemset size 1)
- 2. Combine sets and check again for the support value (itemset size 2)
- 3. Combine those sets and check again for the support value (itemset size 3)

 $(\rightarrow$ Remember: we use sets, so we do not care about the order of items in an itemset)

Itemset	sup_count
I1	6
12	7
13	6
14	2
15	2

Step 1 (Level 1)

Itemset	sup_count
11,12	4
11,13	4
11,14	1
11,15	2
12,13	4
12,14	2
12,15	2
13,14	0
13,15	1
14,15	0

Itemset	sup_count
11,12	4
11,13	4
11,15	2
12,13	4
12,14	2
12,15	2
12,15	2

Step 2 (Level 2) with filtering for min support of 2

TID	items
T1	11, 12 , 15
T2	12,14
T3	12,13
T4	11,12,14
T5	11,13
T6	12,13
T7	11,13
T8	11,12,13,15
T9	11,12,13

original dataset

Itemset	sup_count
11,12,13	2
11,12,15	2

Step 3 (Level 3) with filtering for min support of 2



Strong Rule Generation:

For each frequent itemset:

- 1. Generate all combinations of possible rules with the items in your itemset
- Calculate the Confidence values
- 3. Only keep those with Confidence > min Confidence

Example for {I1, I2, I3}:

- [I1^I2]=>[I3] //confidence = sup(I1^I2^I3)/sup(I1^I2) = 2/4*100=50%
- [I1^I3]=>[I2] //confidence = sup(I1^I2^I3)/sup(I1^I3) = 2/4*100=50%
- [I2^I3]=>[I1] //confidence = sup(I1^I2^I3)/sup(I2^I3) = 2/4*100=50%
- [I1]=>[I2^I3] //confidence = sup(I1^I2^I3)/sup(I1) = 2/6*100=33%
- [I2]=>[I1^I3] //confidence = sup(I1^I2^I3)/sup(I2) = 2/7*100=28%
- [I3]=>[I1^I2] //confidence = sup(I1^I2^I3)/sup(I3) = 2/6*100=33%

Example: A confidence of 50% means that 50% of the customers, who purchased I1 and I2 also bought I3.



TID	
TID	items
T1	11, 12 , 15
T2	12,14
T3	12,13
T4	11,12,14
T5	11,13
T6	12,13
T7	11,13
T8	11,12,13,15
T9	11,12,13

original dataset

Lift:

- We now have rules of frequent itemsets where we are confident that there is a correlation
- BUT: some items are just bought very often and might create fluke rules

→ use a final ordering of rule via the Lift value to sort that out

Example:

Transaction	Support	Confidence	Lift
Canned Beer → Soda	1%	20%	1.0
Canned Beer → Berries	0.1%	1%	0.3
Canned Beer → Male Cosmetics	0.1%	1%	2.6

- Lift = 1: no actual association (because beer and soda are just bought quite often)
- Lift < 1: negative association (when somebody buys beer they are usually not buying berries)
- Lift > 1: positive association (when somebody buys beer they buy male cosmetics although the effect is small with a confidence of 1%)



Association rules – Apriori algorithm

• Drawbacks:

- Computationally expensive
 - \rightarrow time and space complexity is exponential O(2^{|D|}) with |D| being the horizontal width (= total number of items)
- Spurious associations: some rules may seem logical

Common improvements:

- Hash-based itemset counting
- Transaction reduction: A transaction that does not contain any frequent k-itemsets useless in subsequent scans
- Partitioning: An itemset that is potentially frequent must be frequent in at least one of the partitions
- Sampling: Mining on a subset of given data, lower support threshold + a method to determine the completeness
- Dynamic itemset counting: add new candidate itemsets only when all of their subsets are estimated to be frequent

Articles about association rules and Python examples:

- https://towardsdatascience.com/data-mining-market-basket-analysis-with-apriori-algorithm-970ff256a92c
- https://ml2021.medium.com/market-basket-analysis-apriori-algorithm-4fb052ffd2f2
- https://www.geeksforgeeks.org/apriori-algorithm/
- https://stackabuse.com/association-rule-mining-via-apriori-algorithm-in-python/



Final remarks on Machine Learning

 All fields of ML are evolving quite fast at the moment as more companies want to utilize their data and big-tech is investing heavily

- Selection of some current trends in ML:
 - 1. Improved security: homomorphic encryption, federated learning, private set intersection, anonymizing data etc.
 - 2. Ethics and avoiding biases in Al
 - 3. Regulation of AI (e. g. on EU-level)
 - 4. Responsible/Sustainability in AI: use less computation/simpler models to reduce CO_2 emissions
 - Few Shot, One Shot, & Zero Shot Machine Learning
 - 6. Understandable/Transparent Al
 - 7. Auto ML and democratizing Al
 - 8. Process adaptations like MLOps, DataOps, Data Governance
 - 9. Al Strategy on EU-, national- and company-level
 - 10. Tiny-ML, on-edge-inference/computing, specialized hardware (e. g. TPU)
 - 11. Multi-Modal Learning and Multi-Objective Models
 - 12. Quantum ML (hardware is not yet ready but algorithms are being adapted and software/middleware are being developed right now)



Final remarks on Machine Learning

- Some recommendations for continuous learning online:
 - https://towardsdatascience.com/
 - https://www.kdnuggets.com/
 - https://www.kaggle.com/
 - https://www.geeksforgeeks.org/
 - https://www.reddit.com/r/datascience/
 - https://machinelearningmastery.com/

and many more (also on youtube & Co)



Control Questions

You should be able to answer the following questions:

- How is unsupervised learning different from supervised and reinforcement learning?
- What is soft and hard clustering? Discuss a few use cases for clustering.
- How does k-means work and which variations do you know. Explain them and why they might make sense for a use case. What is the elbow method?
- How can you evaluate the quality of clustering results?
- What is hierarchical clustering? What two types exist? What is a dendrogram?
- How does DBSCAN work? What are it's advantages?
- What are association rules? Where would you use association rules? Benefits and drawbacks?
- How does the apriori algorithm work and which principle does it use?



Links and Sources

- C. Bishop, Pattern Recognition and Machine Learning. 2006.
- Images and content adapted from slides of Nicole Artner, TU Wien, LV "Einführung Mustererkennung"
- https://en.wikipedia.org/wiki/K-means_clustering
- https://en.wikipedia.org/wiki/K-means%2B%2B
- https://en.wikipedia.org/wiki/Silhouette_(clustering)
- https://en.wikipedia.org/wiki/Self-organizing_map
- Williams, J. T.; Carpenter, K. E.; Van Tassell, J. L.; Hoetjes, P.; Toller, W.; Etnoyer, P.; Smith, M. (2010). "Biodiversity Assessment of the Fishes of Saba Bank Atoll, Netherlands Antilles".
- https://www.kdnuggets.com/2019/12/market-basket-analysis.html
- https://en.wikipedia.org/wiki/Association_rule_learning
- https://medium.com/analytics-vidhya/association-rule-mining-concept-and-implementation-28443d16f611
- https://www.kdnuggets.com/2016/04/association-rules-apriori-algorithm-tutorial.html/2
- https://www.youtube.com/watch?v=mtkWR8sx0NA
- Distances in higher dimensions and why they loose their "meaning": https://towardsdatascience.com/the-surprising-behaviour-of-distance-metrics-in-high-dimensions-c2cb72779ea6

