Clustering I

COMP5318 Machine Learning and Data Mining

semester 1, 2023, week 9

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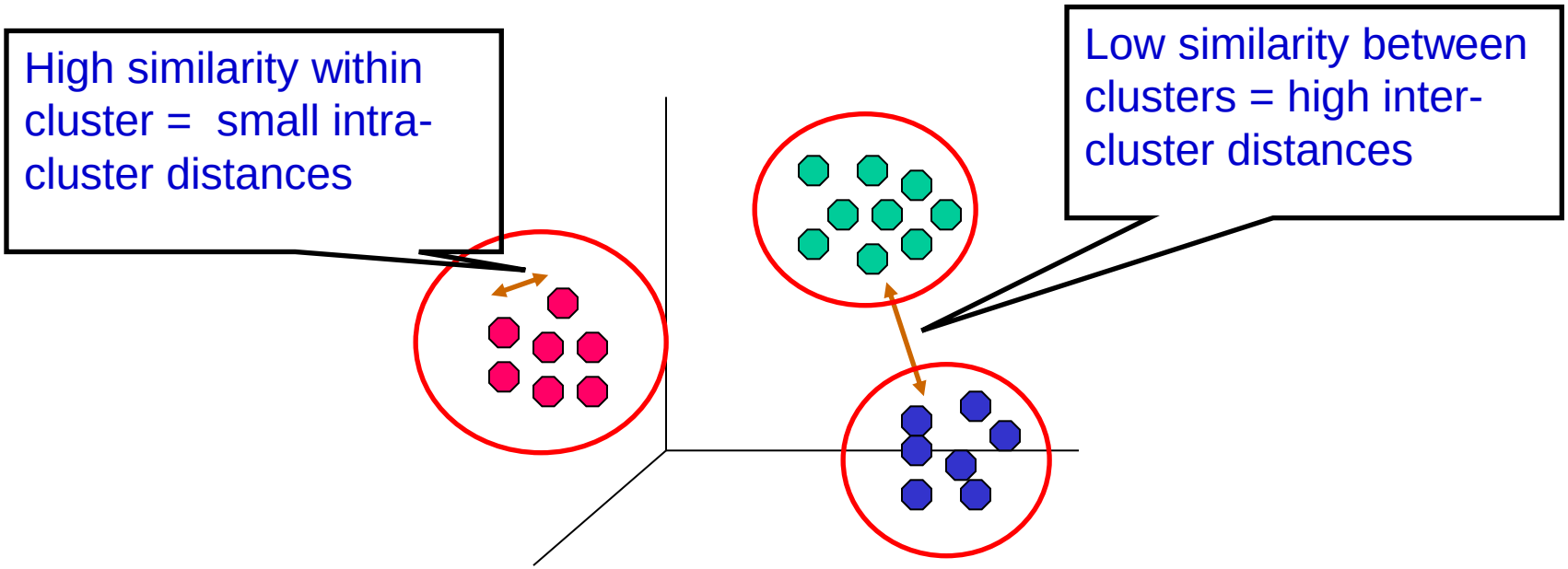
Reference: Tan ch.7.1-7.3, 8.2, Witten ch.4.8, Müller & Guido: ch.3.5, Geron: ch.9

Outline

- Introduction
  - Definition and applications
  - Distance measures and distance between clusters
  - Taxonomy
- Partitional clustering: K-means algorithm
- Model-based clustering: GMM
- Hierarchical clustering: agglomerative and divisive

What is clustering?

- The process of dividing the data objects (items, examples) into groups (called clusters) so that the objects from the same group are:
  - similar to each other within the cluster
  - dissimilar to the objects in other clusters
- The similarity is computed using a distance measure



Clustering is unsupervised learning

- Clustering is unsupervised learning: no labels
- Given:
  - A set of unlabeled examples (input vectors)
  - k – desired number of clusters (may not be given)
- Task: Cluster (group) the examples into k clusters (groups)

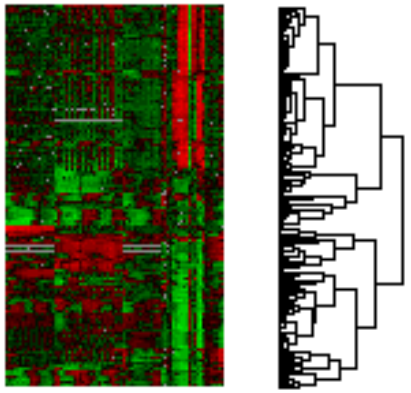
- Supervised vs unsupervised learning
  - Supervised – the class labels are given; the goal is to build a classifier that can be used to predict the class of new (unlabelled) examples
  - Unsupervised – there are no class labels; the goal is to group similar examples together.

Applications of clustering

- Clustering is used
  - As a stand-alone tool to group data
  - As a building block for other algorithms - e.g. a pre-processing tool for dimensionality reduction – using the cluster center to represent all data points in the cluster

Clustering applications

- Ex.1: Targeted marketing
  - Segment customers into groups with distinct characteristics and use this knowledge to develop targeted marketing campaigns
  - Data – purchase history, browsing history, demographic data
  - Targeted campaigns are cheaper than mass-campaigns
- Ex. 2: Customer loyalty
  - Analyse customer behavior and find groups of customer who are likely to defect, e.g. to another medical insurance, electricity or phone company
- Ex. 3: Gene clustering
  - Find genes with similar structure and functionality – important for understanding diseases and finding effective treatments
  - Data: microarray – from thousands of genes, analysed simultaneously



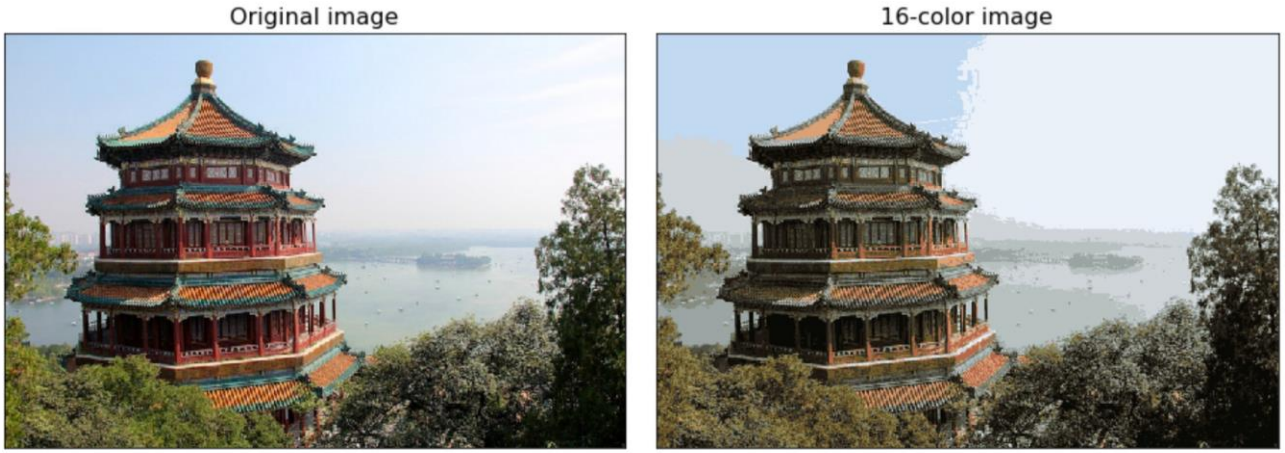
Clustering applications (2)

- Ex. 3: Document clustering
  - Find groups of documents that are similar to each other based on their content
  - Applications:
    - Patent documents assessment: group similar patent documents to make the evaluation of a new patent document easier
    - Personalized news recommendations

- Ex. 4: Clustering for understanding eating habits and dietary patterns of a particular cohorts (e.g. of young Australians)
  - Group 1: People who skip breakfast, care about weight, do not exercise regularly; eat high protein, low fat and high sugar diet; eat out because they enjoy the social aspect; snack after dinner
  - Group 2: …
  - Use this knowledge to promote good eating habits and changes in government policies

Clustering applications (3)

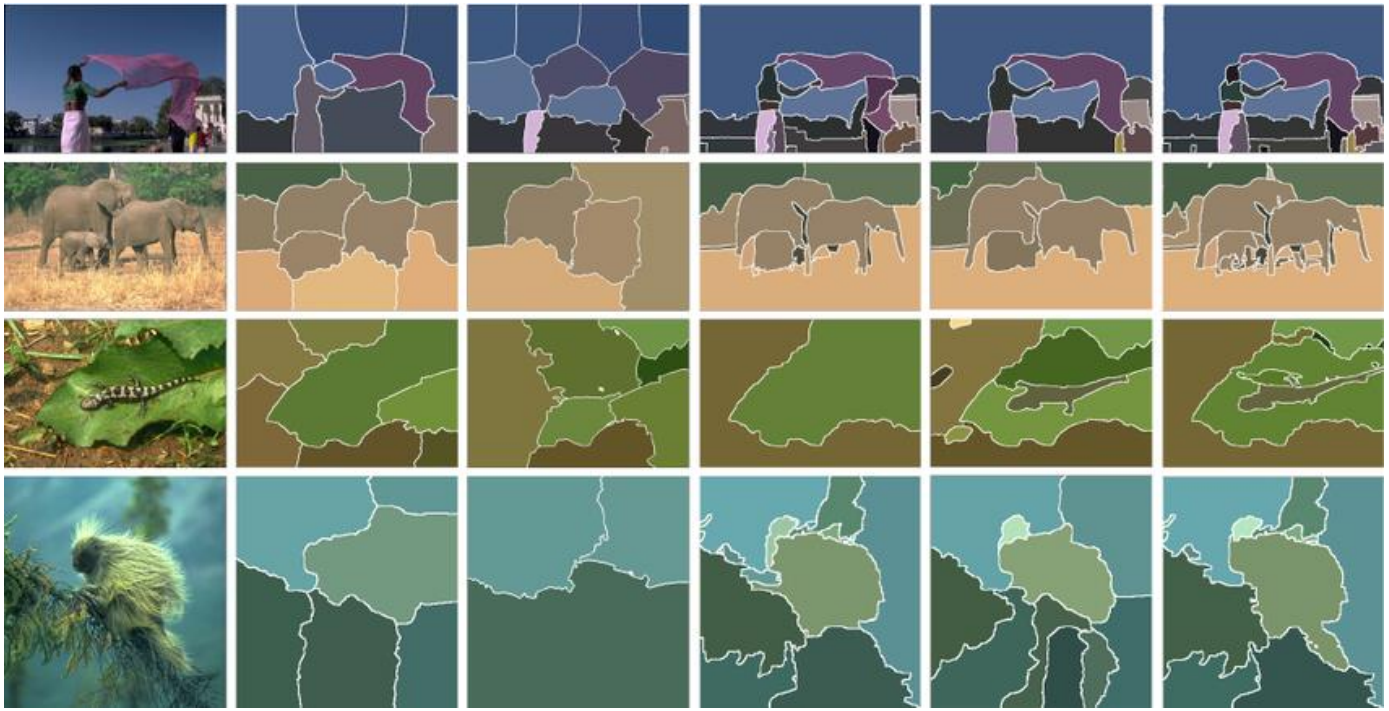
- Color compression
  - Reduce the number of colors in an image – smaller storage requirements
- Cluster the pixels and then replace them with the color of their cluster centroids – smaller number of colors used, smaller storage requirements
- See the tutorial exercises



16 million colors 16 colors

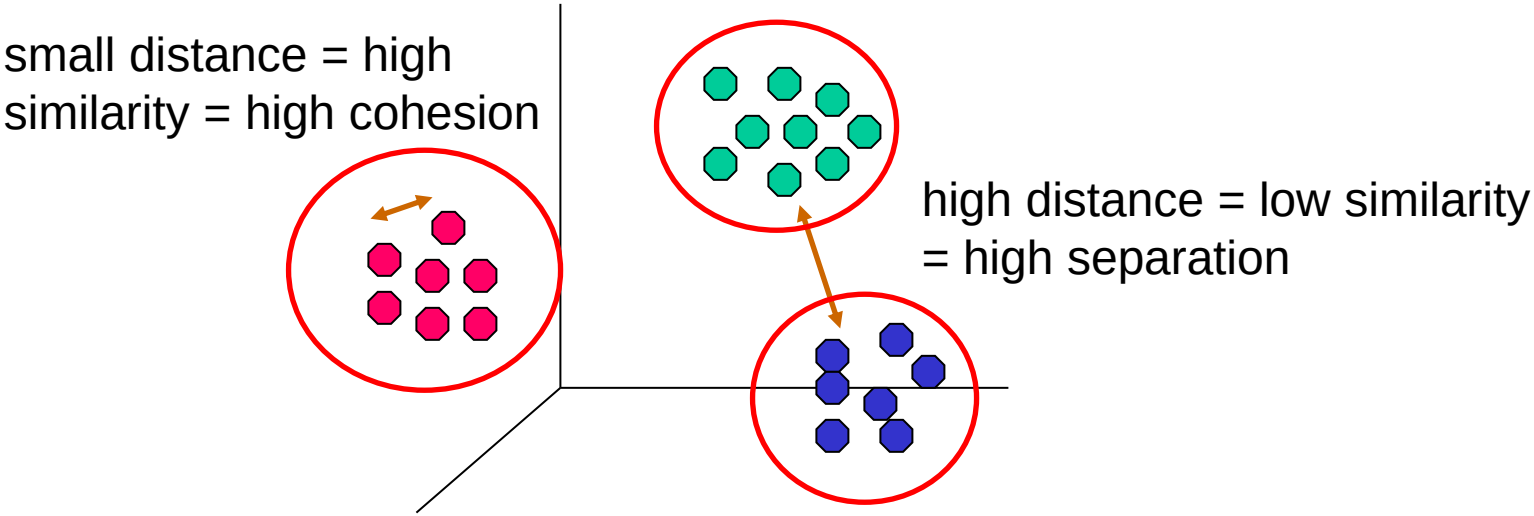
Clustering applications (4)

- Image segmentation
  - Partition an image into segments based on similar colors



Good clustering

- A good clustering will produce clusters with
  - High cohesion (i.e. high similarity within the cluster)
  - High separation (i.e. low similarity between the clusters)
- How to evaluate the quality of the clustering – next week



Measuring similarity between data points

- Similarity between 2 data points A and B is measured using a distance measure
  - If the distance D(A,B) is high -> A and B are dissimilar
  - If the distance D(A,B) is low -> A and B are similar
- Various similarity measures – see lecture 1b
  - Euclidean and Manhattan distance
  - Cosine similarity
  - Many others

Euclidean and Manhattan distance - revision

- 2 examples (data points): A = [a_1, a_2,..., a_n], B = [b_1, b_2,..., b_n]
- e.g. A= [1, 3, 5], B=[1, 6, 9]

- Euclidean distance

$$D(A,B) = \sqrt{(a_1 - b_1)^2 + (a_2 - b_2)^2 + ... + (a_n - b_n)^2}$$

$$D(A,B) = \sqrt{(1-1)^2 + (3-6)^2 + (5-9)^2} = 5$$

- Manhattan distance

$$D(A,B) = |a_1 - b_1| + |a_2 - b_2| + ... + |a_n - b_n|$$

D(A,B)=|1-1|+|3-6|+|5-9|=7

Cosine distance - revision

- Cosine similarity

$$\cos(A,B) = \frac{A.B}{\|A\| \, \|B\|} = \frac{\sum_i^n a_i b_i}{sqrt(\sum_i^n {a_i}^2) \; sqrt(\sum_i^n {b_i}^2)}$$

- Geometric representation: measures the angle between A and B
  - Cosine similarity = 1 => angle(A,B)=0º
  - Cosine similarity = 0 => angle (A,B)=90º

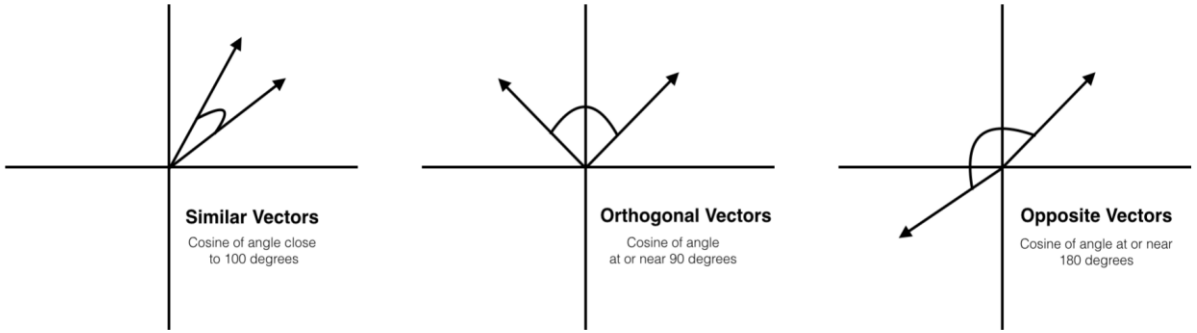


Image from https://deepai.org/machine-learning-glossary-and-terms/cosine-similarity

Cosine distance – revision (2)

- A= [3,2,0,5,0,0,0,2,0,0]
- B = [1,0,0,0,0,0,0,1,0,2]

$$A.B = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$$

$$\|A\| = \sqrt{3^2 + 2^2 + 0^2 + 5^2 + 0^2 + 0^2 + 0^2 + 2^2 + 0^2 + 0^2} = \sqrt{42} = 6.481$$

$$\|B\| = \sqrt{1^2 + 0^2 + 0^2 + 0^2 + 0^2 + 0^2 + 0^2 + 1^2 + 0^2 + 2^2} = \sqrt{6} = 2.245$$

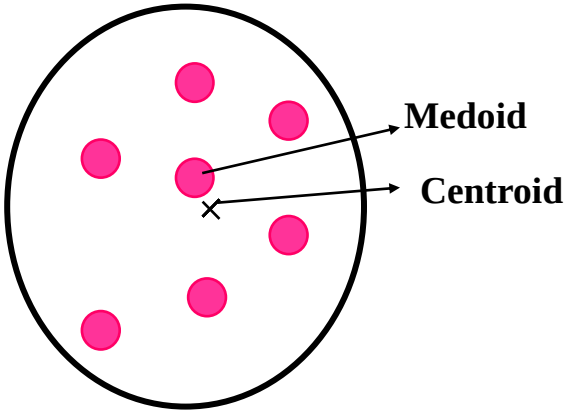
=> cos(*A,B*) = 0.3150

Centroid and medoid of a cluster

- Consider a cluster with N points {p1,..,pN}
- Centroid C – the "middle" of the cluster
  - Typically not an actual data point in the cluster

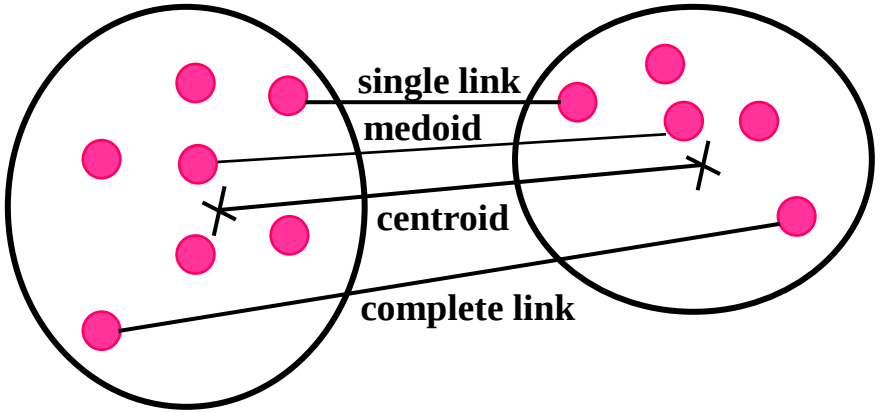
$$C = \frac{\sum_{i=1}^{N} p_i}{N}$$

- Medoid M – the centrally located data point in the cluster



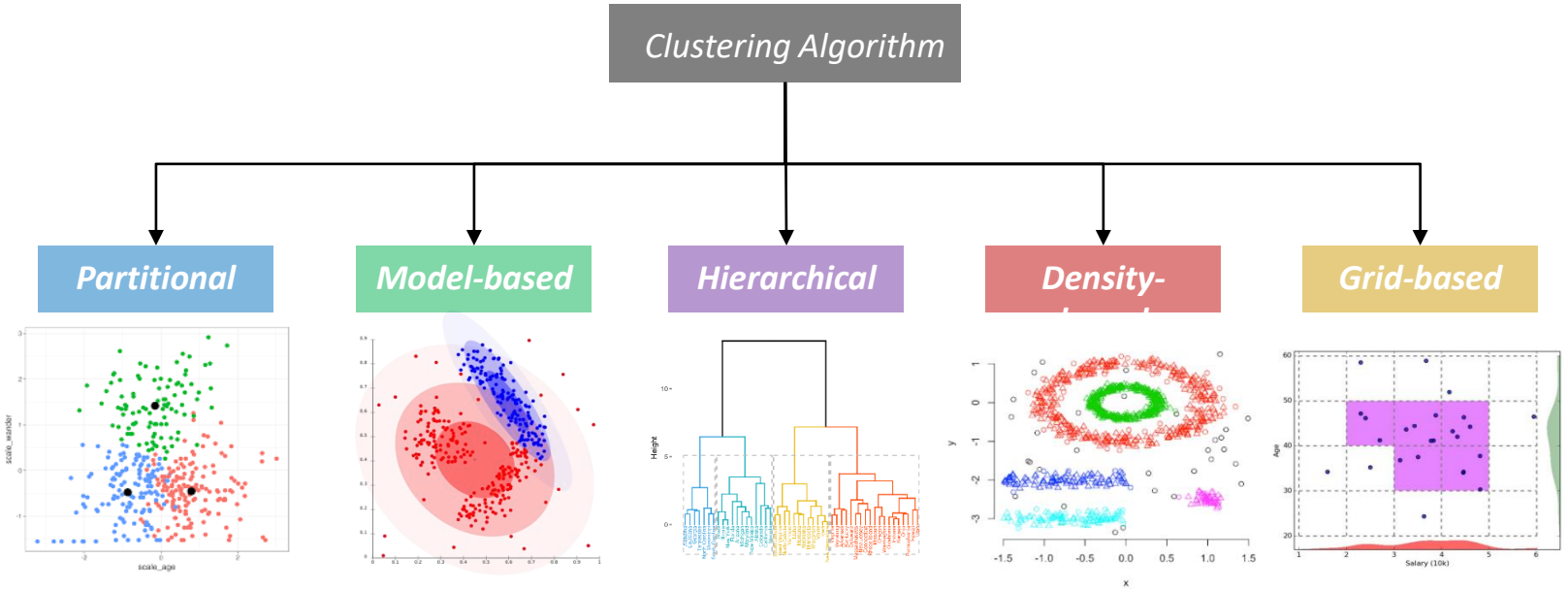
Distance between clusters

- Centroid – the distance between the centroids
- Medoid – the distance between the medoids
- Single link (MIN) – The smallest pairwise distance between elements from each cluster
- Complete link (MAX) – the largest pairwise distance between elements from each cluster
- Average link – the average pairwise distance between elements from each cluster

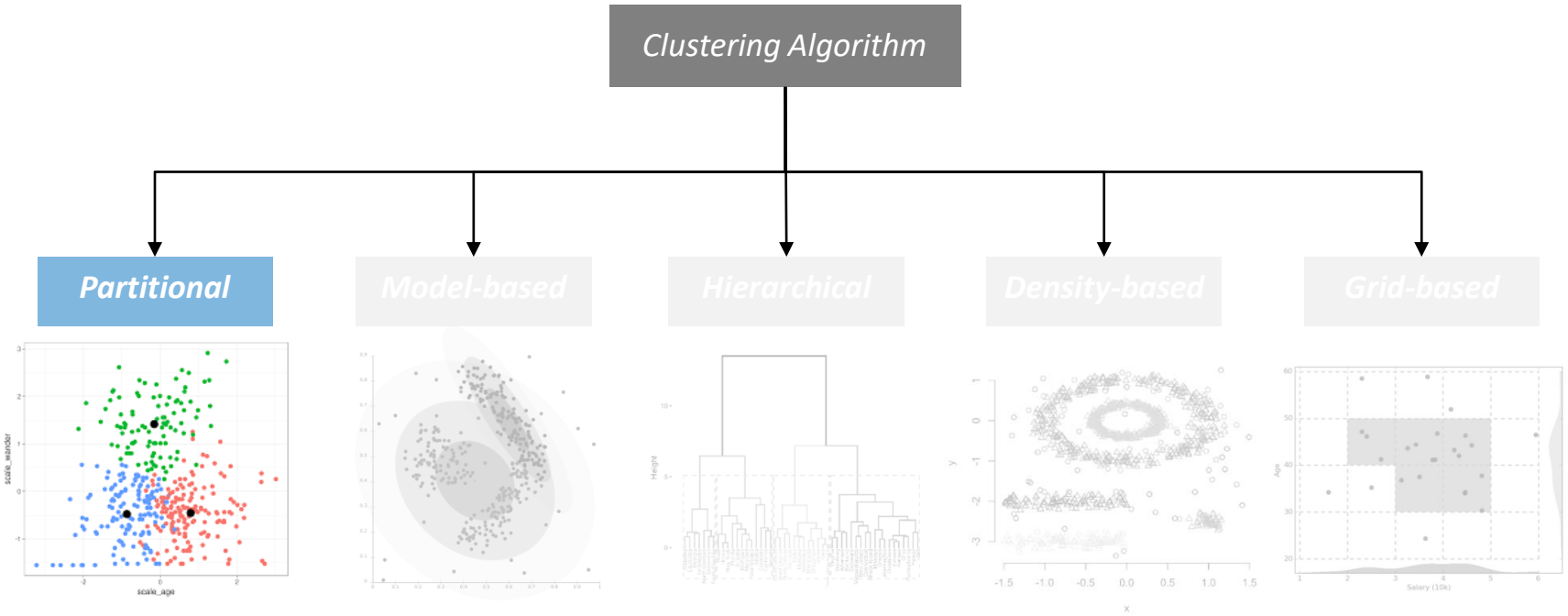


Taxonomy of clustering algorithms

- Partitional – k-means, k-medoids; create 1 set of clusters
- Model-based – GMM
- Hierarchical - agglomerative and divisive; create a nested set of clusters
- Density-based – DBSCAN; regions with high density form clusters
- Grid-based – CLIQUE; density-based but divides the space into grid cells and forms clusters from cells that are sufficiently dense



K-Means clustering algorithm

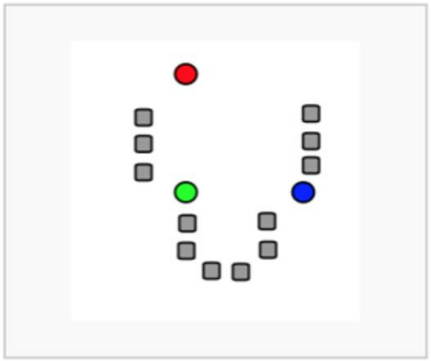


K-Means clustering algorithm

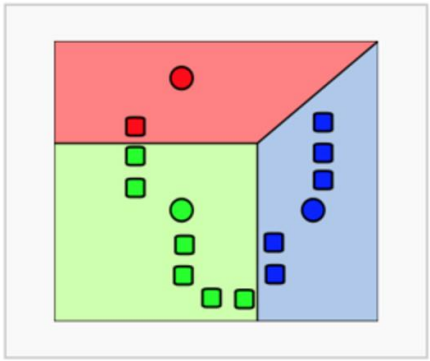
- Partitional clustering algorithm
- Very popular and widely used
- Requires the number of clusters k to be specified
- 3 main steps:
  - Choose k examples as the initial centroids of the clusters
  - Form k clusters by assigning each example to the closest centroid
  - At the end of each epoch:
    - Re-compute the centroid of the clusters
    - Check if the stopping condition is satisfied: centroids do not change. If yes – stop; otherwise, repeat steps 2 and 3 using the new centroids.

Pseudo code and example

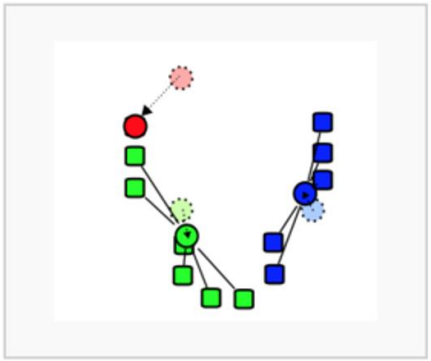
1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change



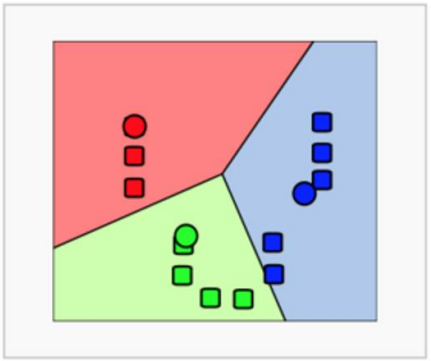
Step 1: Choose initial centroids



Step 2: Assign data points to the cluster of the closest centroid



Step 3: End of epoch:
-Recompute centroids
-Check if stopping condition is satisfied – yes, stop; no - repeat from step 2



Step 4: Assign data points to the cluster of the closest centroid

K-means - more details

- The initial centroids are typically chosen randomly
- The algorithm is sensitive to the initial centroids – different clusters will be produced – see next slides
- “Closeness” is measured by a distance measure
- Most of the convergence happens in the first few epochs
- Often the stopping condition is changed from “Until centroids do not change” to ‘Until relatively few points change clusters’
- Complexity is O(n*k*i*d)
  - n - number of points, k - number of clusters, i - number of iterations, d - number of attributes

K-Means task

- Given: 5 items with the distance between them
- Task: Use the K-means algorithm to cluster them into 2 clusters. The initial centroids are A and B. Show the clusters after the first epoch.

	A	B	C	D	E
A	0	2	7	10	1
B	2	0	3	4	6
C	7	3	0	5	9
D	10	4	5	0	1
E	1	6	9	1	0

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

Solution

- Initial centroids: A and B
- cluster1 – the cluster of A
- cluster2 – the cluster of B

	A	B	C	D	E
A	0	2	7	10	1
B	2	0	3	4	6
C	7	3	0	5	9
D	10	4	5	0	1
E	1	6	9	1	0

Epoch1 – start:

- A is assigned to cluster1 (centroid)
- B is assigned to cluster2 (centroid)

- C:
  d(C, A)=7, d(C, B)=3
  => C is assigned to cluster2

- D:
  d(D, A)=10, d(D, B)=4
  => D is assigned to cluster2

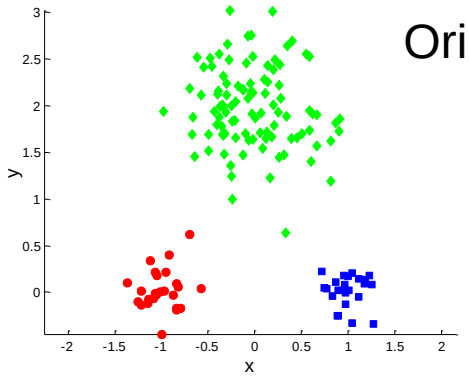
- E:
  d(E, A)=1, d(E, B)=6
  => E is assigned to cluster1

End of epoch 1, clusters are:

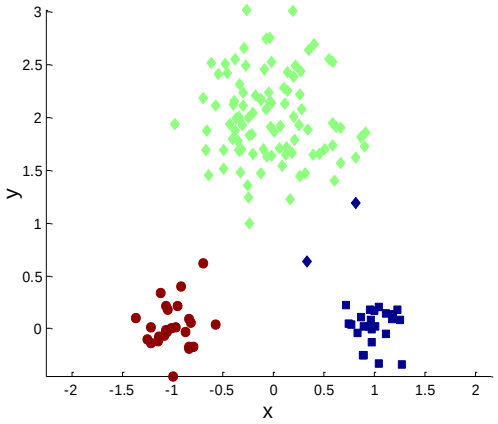
- {A, E} and {B, C, D}

Sensitive to initial centroids

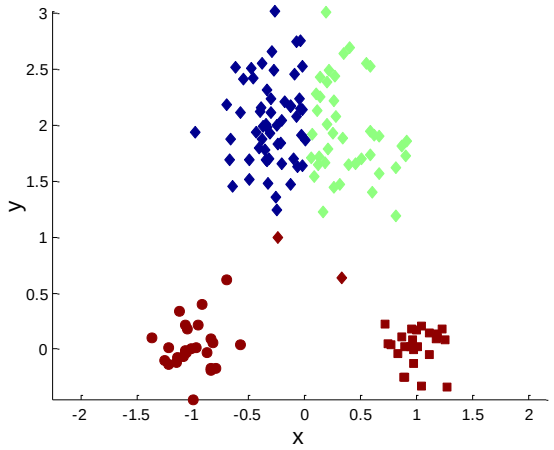
- Different random initialisation -> different result



Original data

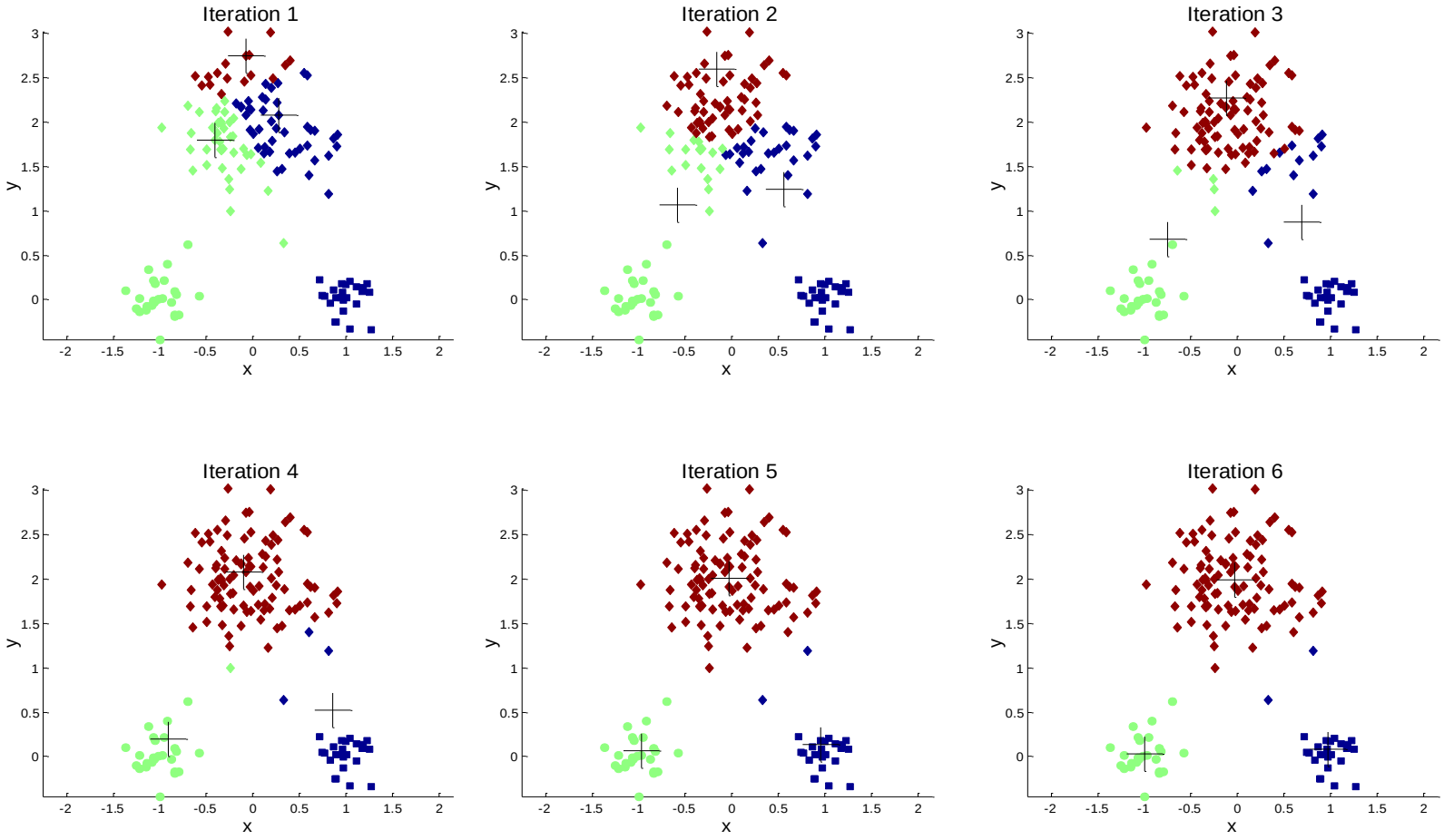


Initialisation 1 - good clustering

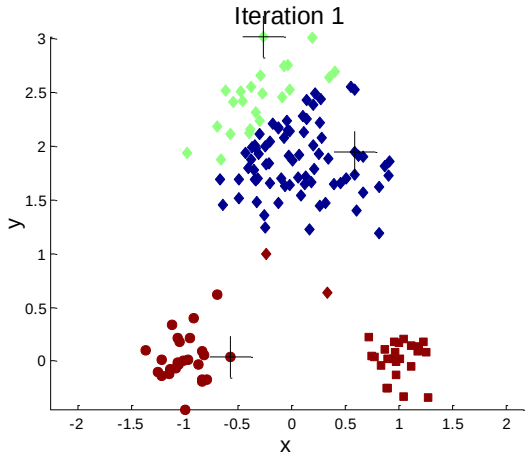


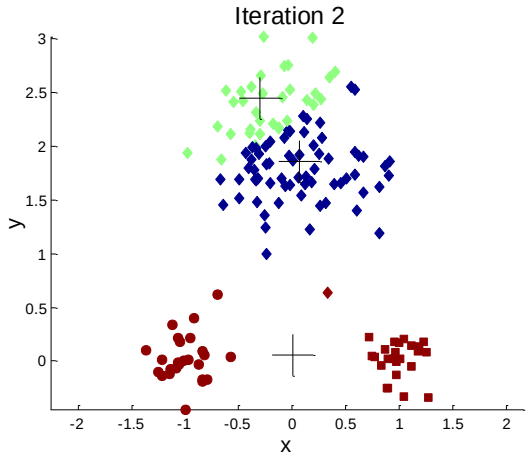
Initialisation 2 - bad clustering

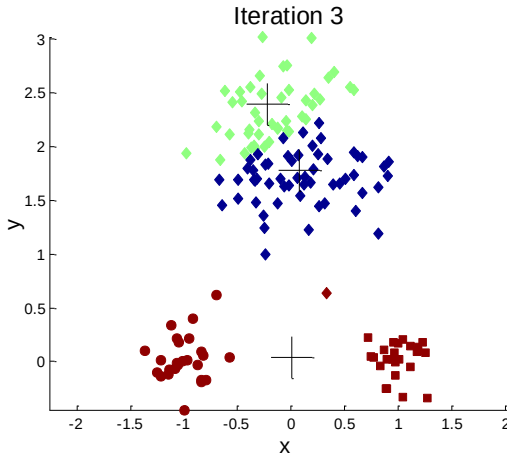
Good initial centroids

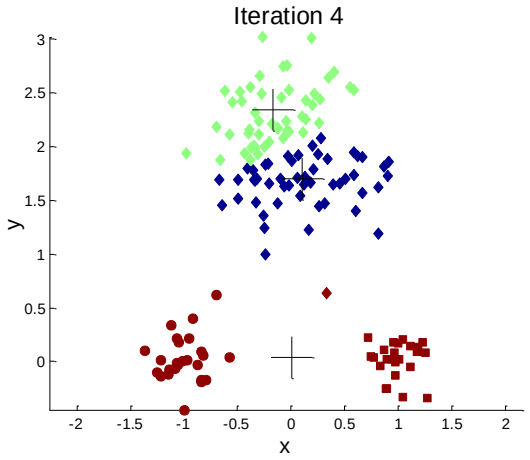


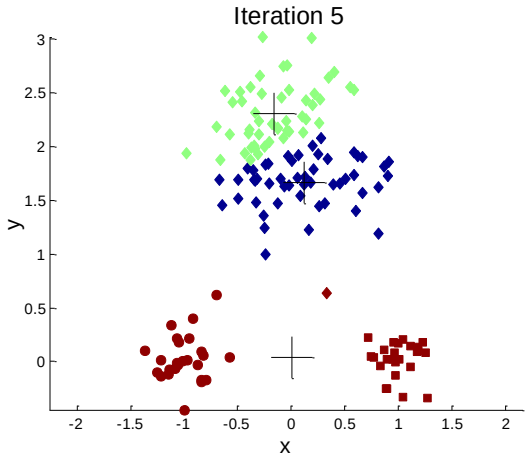
Poor initial centroids











Selecting good initial centroids

- Method 1: Run K-means several times with different randomly selected initial centroids; evaluate each clustering using SSE, select the clustering with the smallest Sum of Squared Error (SSE)
- SSE:
  - For each point, the error is the distance to the closest centroid
  - To get SSE, we square these errors and sum them

$$SSE = \sum_{i=1}^{k} \sum_{\mathrm{X} \in K_i} d(c_i, \mathbf{x})^2$$

c_i are the centroids, k - number of clusters, x – data points

- Method 2: K-means++

K-means++

- K-means++ is a variation of K-means which uses a new method for selecting the initial centroids; the rest is the same as the standard K-means
- Centroid selection:
  - Select centroids incrementally, until k centroids have been selected
  - At every step, each point has a probability to be selected as a centroid that is proportional to the square of its distance to its closest centroid
  - => Selects points that are farthest away from the current centroids – selects well-separated points
  - Can select outliers, but outliers are rare by definition
- Works well in practice

K-means++ pseudocode for centroid selection

- Selection of initial centroids in K-means++:

1: For the first centroid, pick one of the points at random.
2: **for** i=1 to *number of trials* **do**
3: Compute the distance, d(x), of each point to its closest centroid.
4: Assign each point a probability proportional to each point's d(x)2.
5: Pick new centroid from the remaining points using the weighted probabilities.
6: **end for**

K-means issues: Handling empty clusters

- K-means can yield empty clusters – no points are allocated to a cluster during the assignment step – the cluster consists only of the initial centroid
- Solution: choose different initial centroid – strategies:
  - Choose the point that is farthest away from any current centroid
  - Use the K-means++ approach (similar idea)
  - Choose a point from the cluster that has the highest SSE
    - This will typically split the cluster and reduce the overall SSE of the clustering
- If there are several empty clusters, the above can be repeated several times

K-means issues: Outliers

- When there are outliers, the resulting cluster centroids are less representative and the SSE is higher
- Solution: remove outliers before clustering
- Caution: for some clustering applications outliers are important and should not be removed, e.g.:
  - Data compression: all points need to be clustered
  - Financial analysis – unusually profitable customers can be the most interesting
- Alternatively, remove outliers as a post-processing step after clustering – keep track of SSE contributed by each point, eliminate points with unusually high contributions, especially over multiple runs

- Various techniques for identifying outliers - out scope for this course, see Tan ch.9

Variations: Bisecting K-means

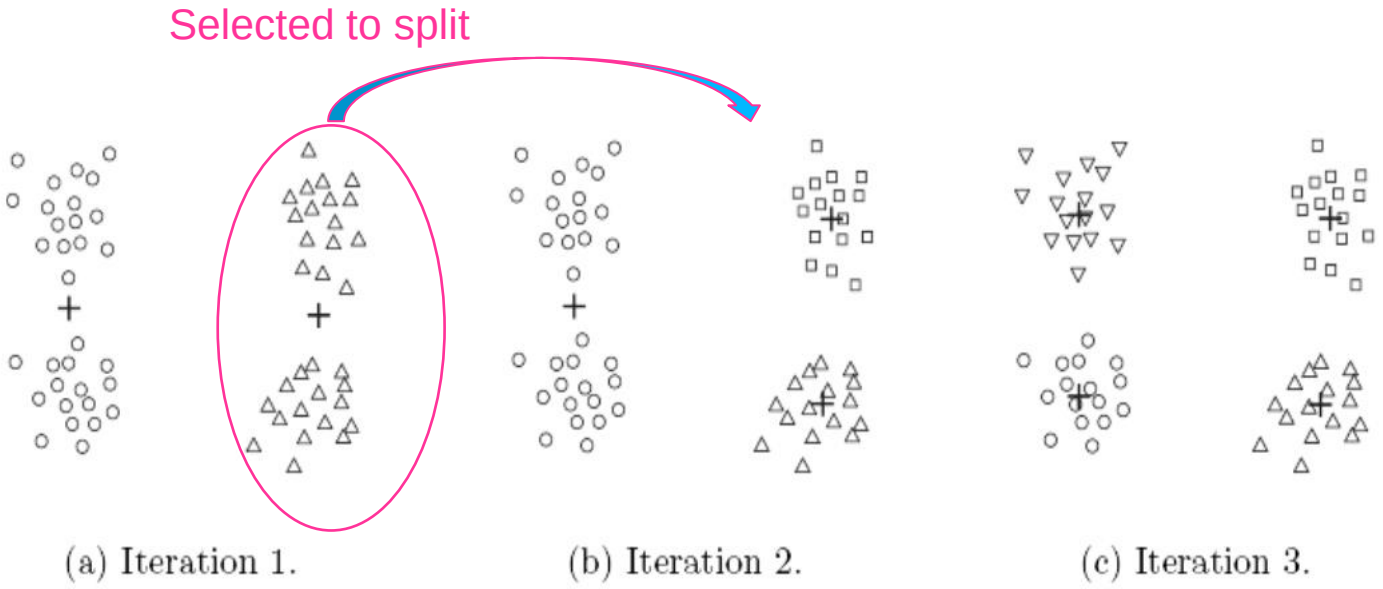
- Extension of k-means
- Main idea: to obtain k clusters, split the data into 2 clusters, select one of these clusters to split further and so one until k clusters are obtained

1: Initialize the list of clusters to contain the cluster containing all points.
2: **repeat**
3: Select a cluster from the list of clusters
4: **for** $i = 1$ to *number_of_iterations* **do**
5: Bisect the selected cluster using basic K-means
6: **end for**
7: Add the two clusters from the bisection with the lowest SSE to the list of clusters.
8: **until** Until the list of clusters contains K clusters

Different ways: the largest cluster, the cluster with the largest SSE, or based on both size and SSE

Bisecting K-means - Example

- Less sensitive to initialization problems

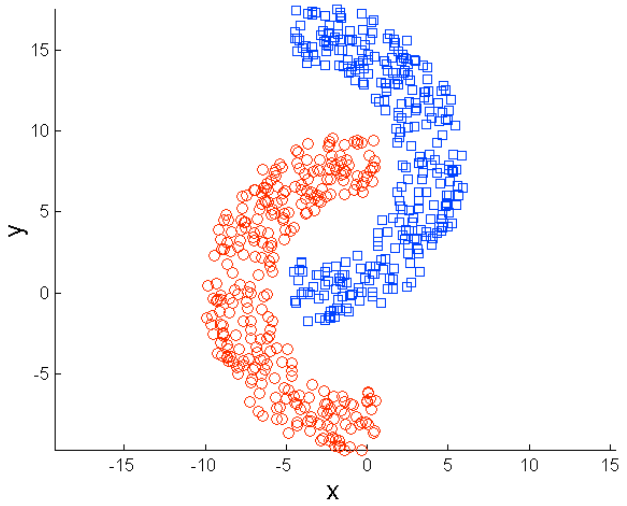


K-means and different types of clusters

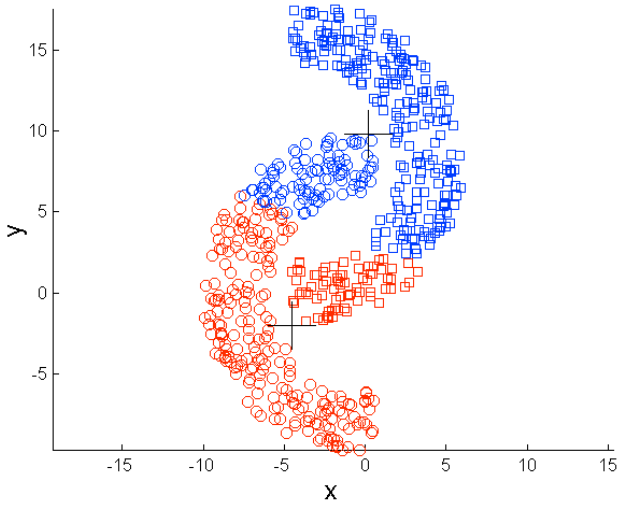
- K-means works well if the clusters are spherical, of equal density, equal size and are well separated

K-means on clusters with non-spherical shapes

- Doesn't work well for natural clusters with complex (non-spherical) shape



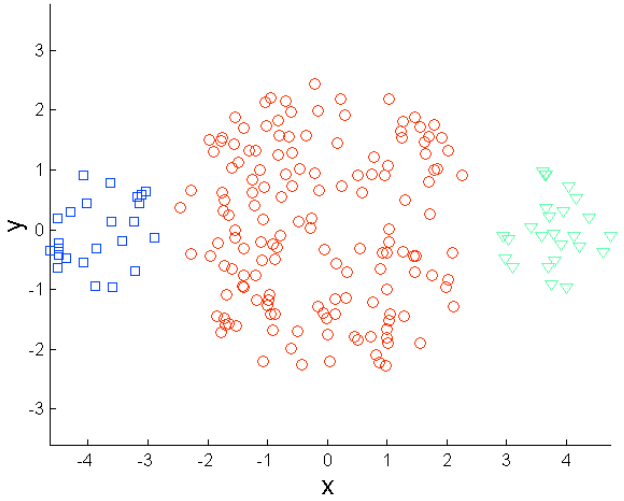
Original points



K-means (2 Clusters)

K-means on clusters with different size

- Doesn't work well for natural clusters with vastly different size
- 3 natural clusters, the second one is much bigger than the first and third
- K-Means cannot find the natural clusters – it splits the largest



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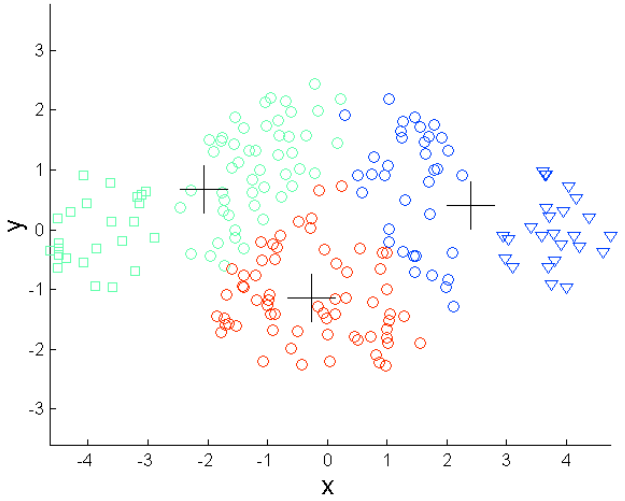
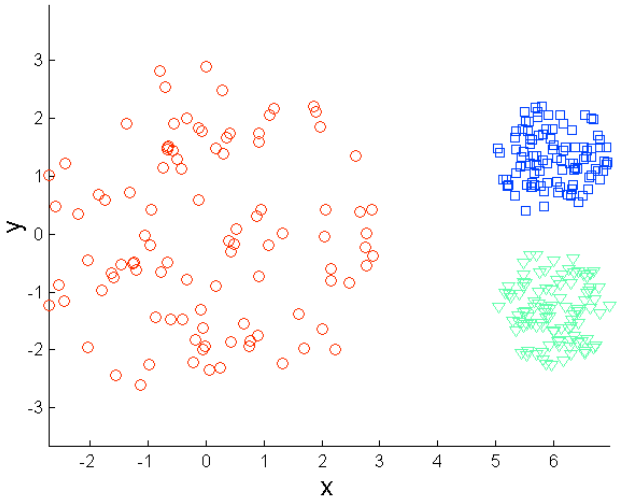


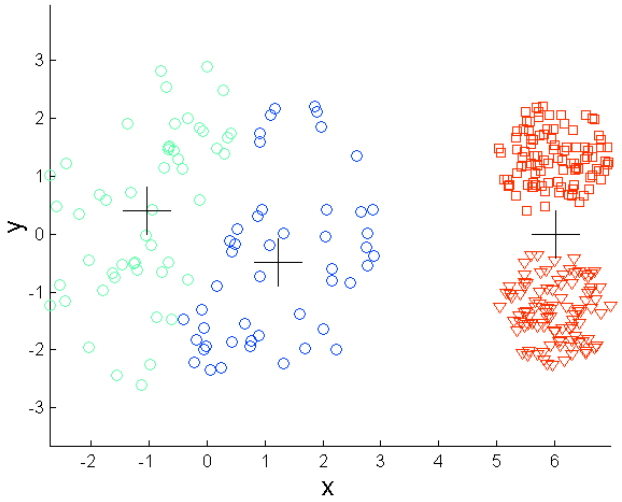
K-means (3 Clusters)

K-means on clusters with different density

- Doesn't work well for natural clusters with different density
- 3 natural clusters, 2 of them are much denser than the other
- K-Means cannot find the natural clusters – it splits the large cluster



Original points

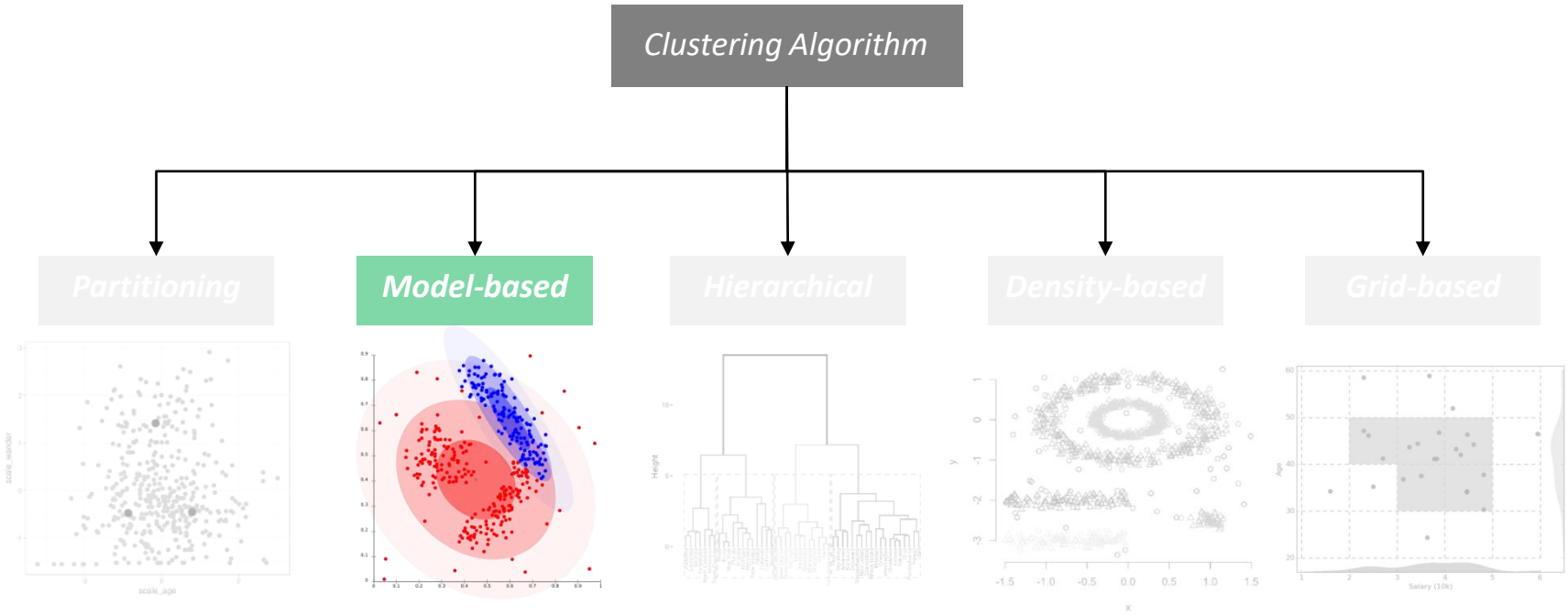


K-means (3 clusters)

K-Means - strengths and weaknesses

- Simple and very popular
- Relatively efficient, even though multiple runs are required
- Sensitive to centroid initialization
- Not sensitive to the order in which the input examples are applied
- Does not work well for clusters with non-spherical shape, different sizes and different density
- Does not work well for data containing outliers
  - Pre-processing is needed - outlier detection and removal
- Different variations – e.g. bisecting K-means and K-means++
  - Both reduce sensitivity to initialization (choice of initial centroids)

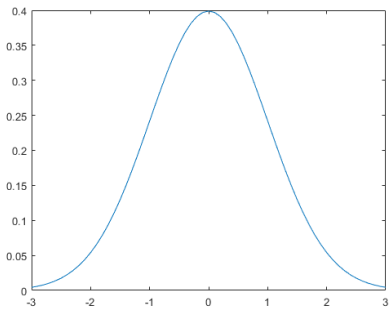
Model-based: GMM



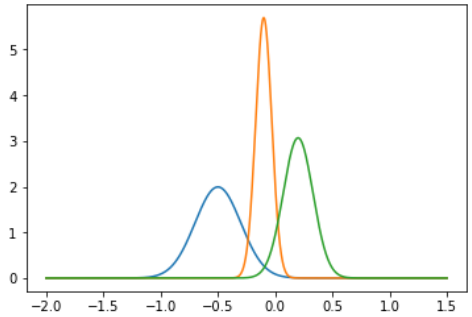
Gaussian mixture model clustering

- Gaussian Mixture Model (GMM) clustering is a probabilistic clustering
- It assumes that the data is generated by a mixture of normal (Gaussian) distributions

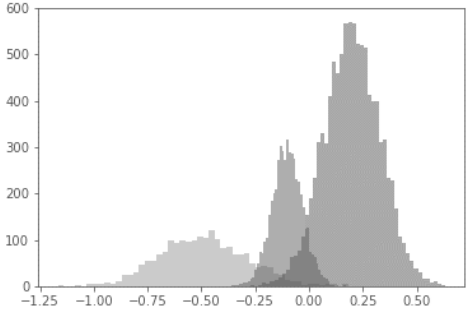
Normal distribution



3 normal distributions



Randomly generated data for these NDs



ND = normal distribution

- *ND1:* $\mu = 0.5, \sigma = 0.2$
- *ND2:* $\mu = -0.1, \sigma = 0.07$
- *ND3:* $\mu = 0.2, \sigma = 0.13$

- *2000 data samples for ND1*
- *5000 data samples for ND2*
- *10000 data samples for ND3*

- Probability density function for a normal distribution with mean μ and standard deviation σ:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

GMM Algorithm

- We assume that the data is generated by a mixture of *k* Gaussian (normal) distributions. Each distribution has 2 parameters: μ and σ.
- One distribution corresponds to 1 cluster
- We don't know the parameters μ and σ of the distributions; starting from random initial values we iteratively estimate them from the data
- After each estimation, we compute the probability of each example to belong to each distribution (cluster)
- Using the probabilities, we re-compute the parameters, until they don't change

GMM Algorithm

Algorithm 9.2 EM algorithm.

1: Select an initial set of model parameters.
(As with K-means, this can be done randomly or in a variety of ways.)
2: **repeat**
3: **Expectation Step** For each object, calculate the probability that each object belongs to each distribution, i.e., calculate $prob(distribution\ j|\mathbf{x}_i, \Theta)$.
4: **Maximization Step** Given the probabilities from the expectation step, find the new estimates of the parameters that maximize the expected likelihood.
5: **until** The parameters do not change.
(Alternatively, stop if the change in the parameters is below a specified threshold.)

GMM and K-Means correspondence

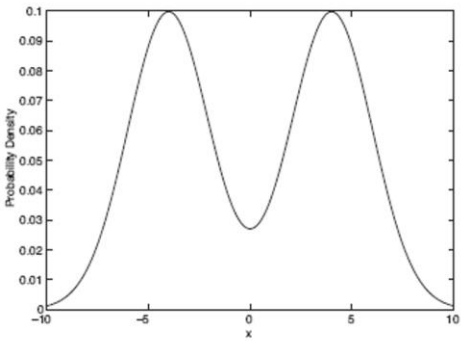
- Expectation step in GMM -> Assigning each object to a cluster in K-means
  - In K-means – crisp assignment, in GMM – probabilistic; each object is assigned to each cluster with a certain probability

- Maximization step in GMM -> Computing the cluster centroid in K-Means
  - In GMM we compute the parameters of the distributions

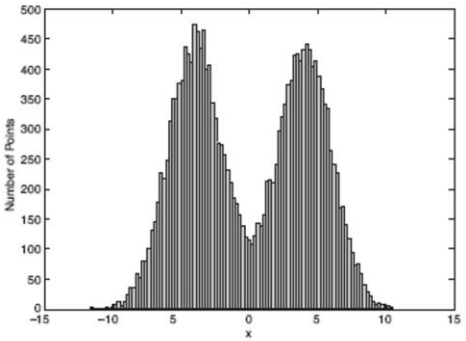
Algorithm 9.2 EM algorithm.

1: Select an initial set of model parameters.
(As with K-means, this can be done randomly or in a variety of ways.)
2: **repeat**
3: **Expectation Step** For each object, calculate the probability that each object belongs to each distribution, i.e., calculate $prob(distribution\ j|\mathbf{x}_i, \Theta)$.
4: **Maximization Step** Given the probabilities from the expectation step, find the new estimates of the parameters that maximize the expected likelihood.
5: **until** The parameters do not change.
(Alternatively, stop if the change in the parameters is below a specified threshold.)

Example



(a) Probability density function for the mixture model.



(b) 20,000 points generated from the mixture model.

- 1-dim data x (20 000 points), generated by 2 Gaussian distributions: distribution 1 and distribution 2
- For simplicity, let's assume that we know the standard deviations σ_1 and σ_2 and that both are the same: $\sigma_1 = \sigma_2 = 2$

- Step 1: Initial guesses for μ_1 and μ_2 : $\mu_1 = -2$, $\mu_2 = 3$
- => initial parameters of the 2 distributions: $\theta_1=(-2,2)$, $\theta_2=(3,2)$
- Set of parameters for the entire mixture model: $\theta = (\theta_1, \theta_2)$

Example (2)

- Step 2: Expectation step
  - Compute the probability that a point x_i came from each distribution *j* (j=1,2)

$$P(distribution\ j|x_i, \theta) = \frac{w_j\ P(x_i|\theta_j)}{w_1\ P(x_i|\theta_1) + w_2\ P(x_i|\theta_2)}$$

w_j are the weights of each distribution (the probability for distribution j to generate the example); all weights should sum to 1, i.e. $w_1+w_2=1$.

For our example we assume that $w_1=w_2=0.5$:

$$P(distribution\ j|x_i, \theta) = \frac{0.5\ P(x_i|\theta_j)}{0.5\ P(x_i|\theta_1) + 0.5\ P(x_i|\theta_2)}$$

  - E.g. for point $x_i = 0$: $P(x_i|\theta_1) = 0.12$, $P(x_i|\theta_2) = 0.06$ (calculated using the probability density function of normal distribution)
  - => $P(distribution\ 1|\mathrm{x} = 0, \theta) = \frac{0.12}{0.12+0.06} = 0.66$

$$P(distribution\ 2|\mathrm{x} = 0, \theta) = \frac{0.06}{0.12+0.06} = 0.33$$

  - We compute these probabilities for all n = 20 000 points

Example (3)

- Step 3: Maximization step – compute new estimates for μ_1 and μ_2

$$\mu_1 = \sum_{i=1}^{n} x_i \frac{P(distribution\ 1|x_i, \theta)}{\sum_{i=1}^{n} P(distribution\ 1|x_i, \theta)}, \quad \mu_2 = \sum_{i=1}^{n} x_i \frac{P(distribution\ 2|x_i, \theta)}{\sum_{i=1}^{n} P(distribution\ 2|x_i, \theta)}$$

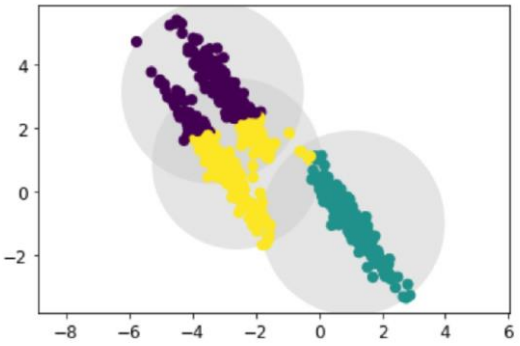
- Notice that the new estimate for the mean μ is the weighted average of the points, where the weights are the probabilities that the points belong to the distribution

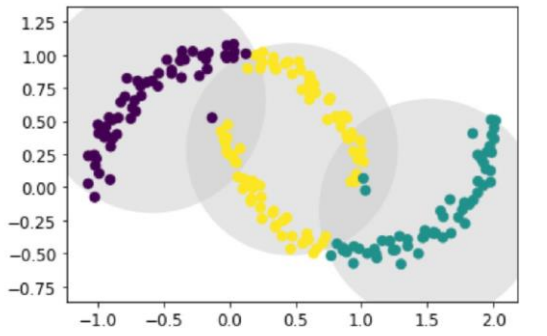
- Repeat the expectation and maximization steps until the estimates for μ_1 and μ_2 don't change or change very little

- After convergence, each point is assigned to the cluster with the highest probability

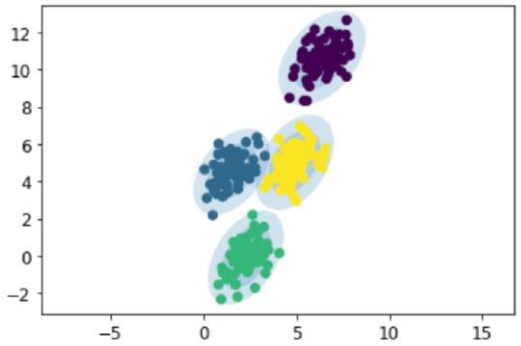
GMM vs K-means

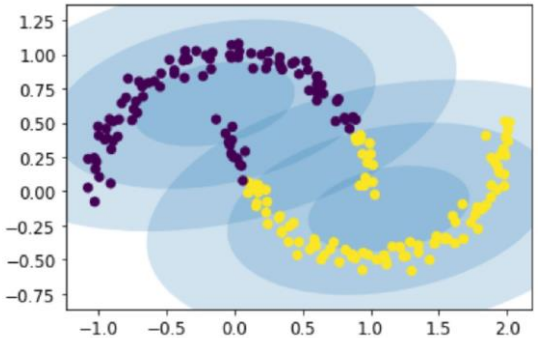
- GMM can be seen as a generalization of K-means
- It is more flexible – it allows for elliptical clusters rather than circular and for probabilistic assignment to each cluster rather than crisp – see the tutorial notes
  - K-means:





  - GMM:





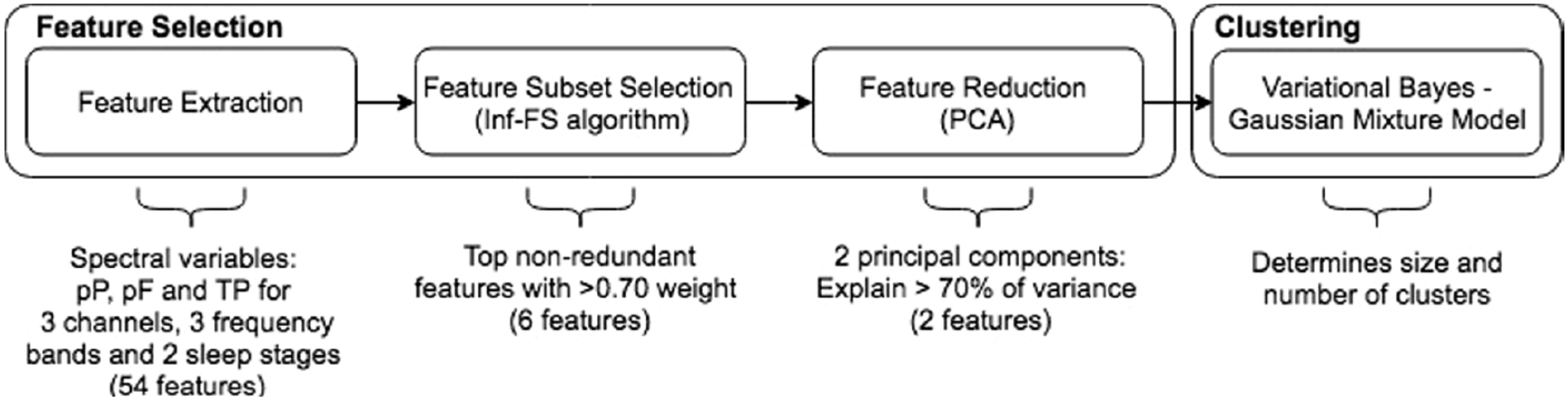
GMM example

- Clustering of people with insomnia based on EEG data

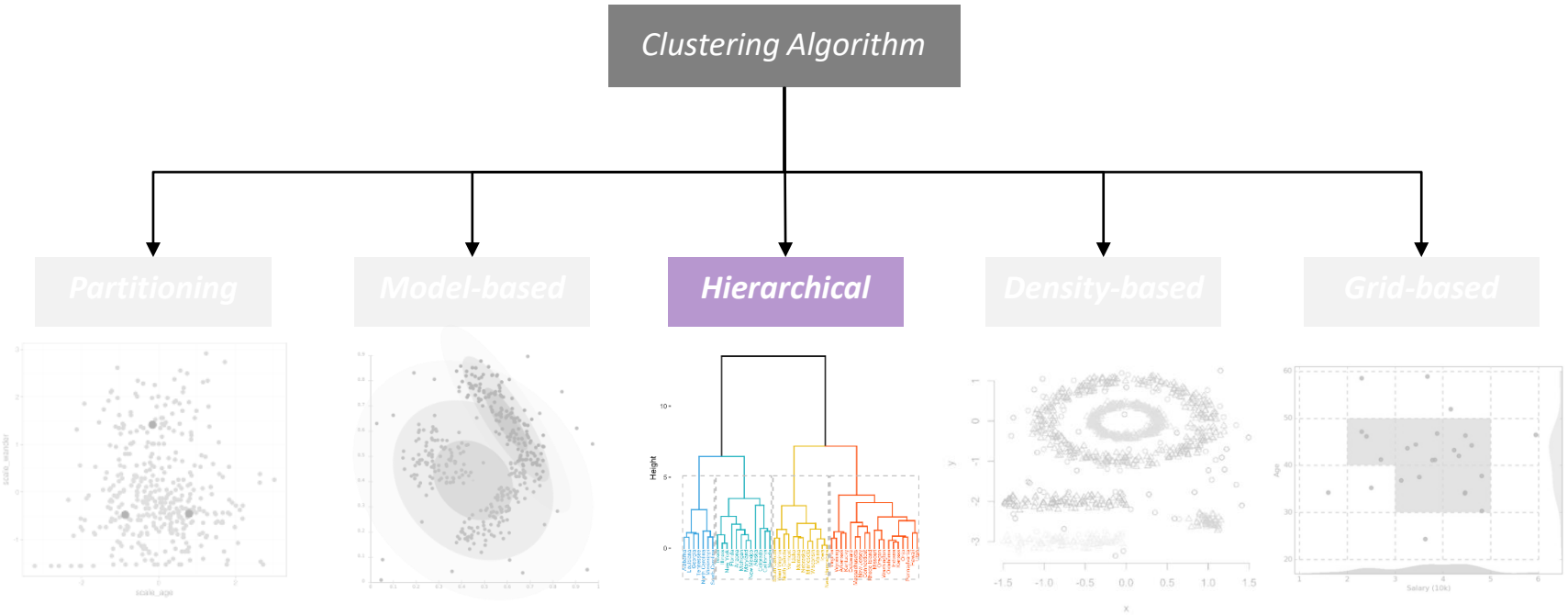
- https://www.sciencedirect.com/science/article/abs/pii/S0950705119303387

Data-driven cluster analysis of insomnia disorder with physiology-based qEEG variables ☆

Stephen McCloskey [a], Bryn Jeffries [a, b], Irena Koprinska [a], Christopher B. Miller [b, c], Ronald R. Grunstein [b, c]

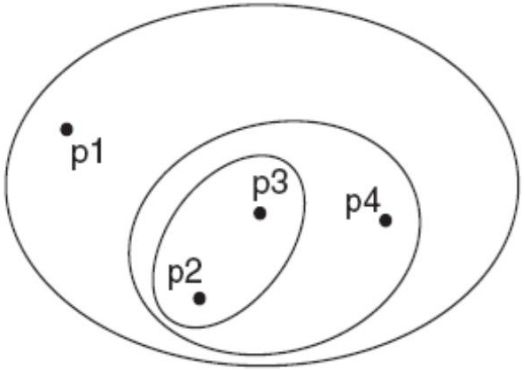


Hierarchical clustering

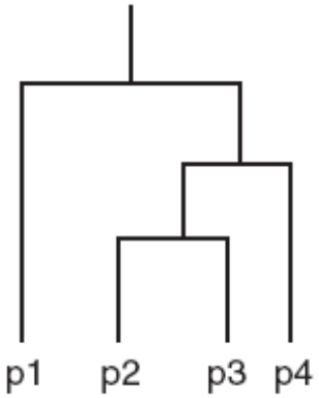


Hierarchical clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram – a tree like diagram that records the sequences of merges



Nested clusters



Dendrogram

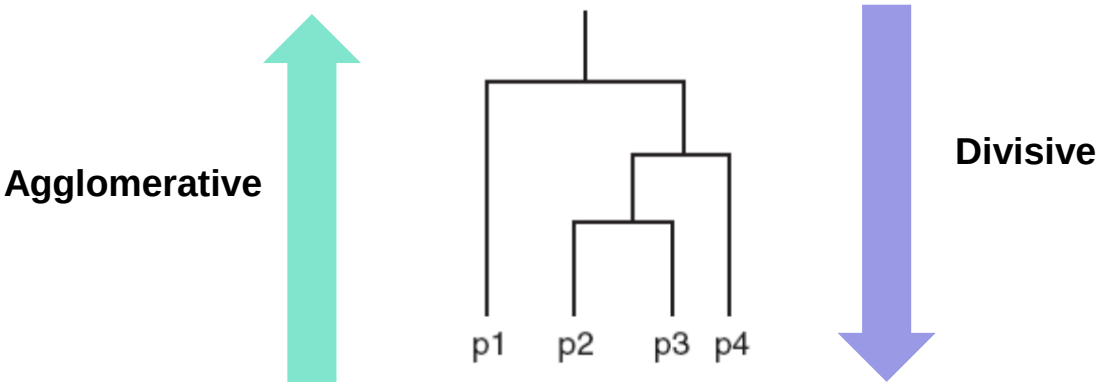
Strengths of hierarchical clustering

- No need to specify the number of clusters in advance
- A desired number of clusters can be obtained by ‘cutting’ the dendrogram at different levels

- The dendrogram provides a useful visualization – an interpretable description of the clustering process
- The dendrogram may reveal a meaningful taxonomy

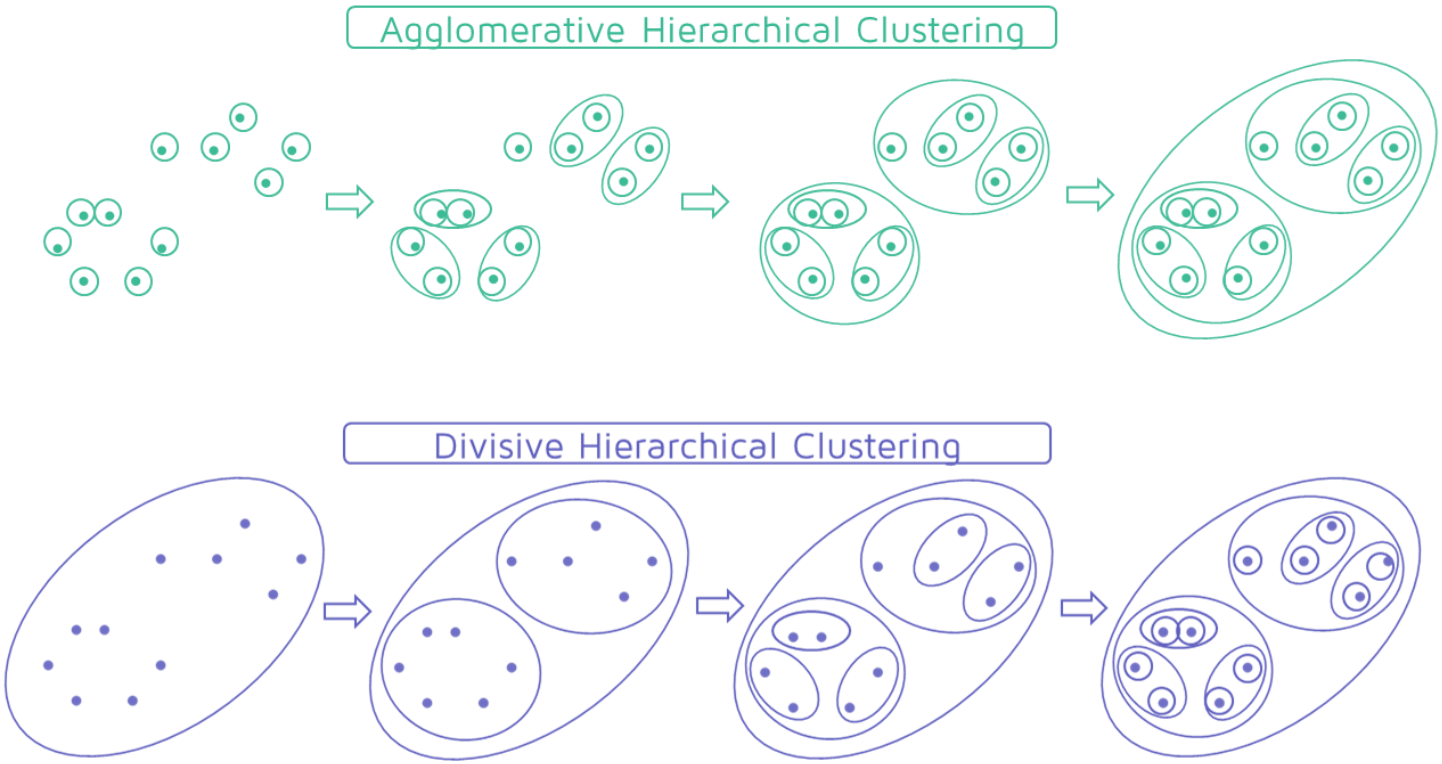
Two approaches: agglomerative and divisive

- Agglomerative (bottom-up) – merges clusters iteratively
  - Start with each item in its own cluster; iteratively merge clusters until all items belong to one cluster
- Divisive (top-down) – splits a cluster iteratively
  - Place all items in one cluster; iteratively split clusters in two until all items are in their own cluster
- Divisive is less popular than agglomerative; we will focus on agglomerative



Agglomerative and divisive clustering - diagrams

- Agglomerative (bottom-up) – merges clusters iteratively
- Divisive (top-down) – splits a cluster iteratively



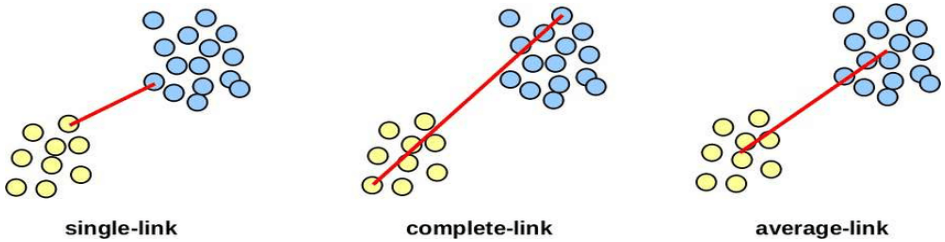
Agglomerative hierarchical clustering

- Agglomerative is the most popular hierarchical clustering algorithm
- The key operation is computing the distance between two clusters (the proximity matrix)
- There are different versions of how the clusters are merged at each step; we will use the version that merges the 2 closest clusters

1. Compute the proximity matrix
2. Let each data point be a cluster
3. **Repeat**
4. Merge the two closest clusters
5. Update the proximity matrix
6. **Until** only a single cluster remains

Distance between clusters

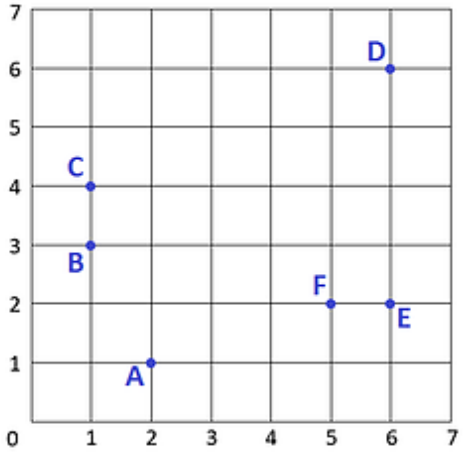
- Hierarchical clustering typically uses the following distance measures:
  - Single link (MIN)
  - Complete link (MAX)
  - Average link
  - Ward's method – the distance between 2 clusters is the increase in SSE that results when the 2 clusters are merged



	The distance between 2 clusters is:
Single link (MIN)	the **smallest** distance between an element in one cluster and an element in the other
Complete link (MAX)	the **largest** distance between an element in one cluster and an element in the other
Average link	the **average** distance between each element in one cluster and each element in the other

Agglomerative clustering - example

- Given are 6 data points. Apply agglomerative hierarchical clustering to cluster them using the single-link distance between clusters and the Manhattan distance between data points.



Data points

Algorithm:

Compute the distance matrix

Let each data point be a cluster

Repeat

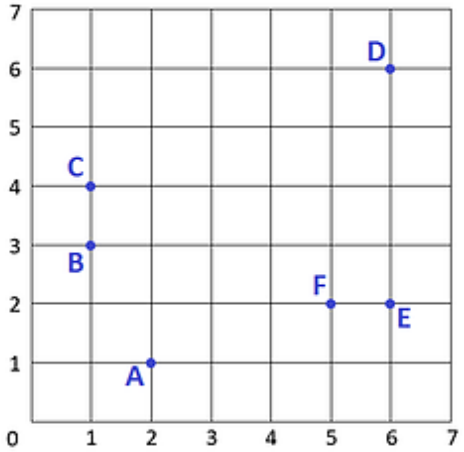
Merge the two closest clusters

Update the proximity matrix

Until only a single cluster remains

Step 1

- Step 1: Compute the distance matrix using the Manhattan distance



Data points

	A	B	C	D	E	F
A	x	3	4	9	5	4
B		x	1	8	6	5
C			x	7	7	6
D				x	4	5
E					x	1
F						x

Distance matrix

Algorithm:

Compute the distance matrix

Let each data point be a cluster

Repeat

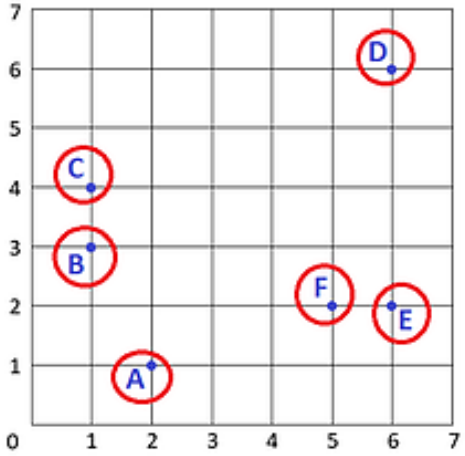
Merge the two closest clusters

Update the proximity matrix

Until only a single cluster remains

Step 2

- Step 2: Let each data point be a cluster



Data points

	A	B	C	D	E	F
A	x	3	4	9	5	4
B		x	1	8	6	5
C			x	7	7	6
D				x	4	5
E					x	1
F						x

Distance matrix

Algorithm:

Compute the distance matrix

Let each data point be a cluster

Repeat

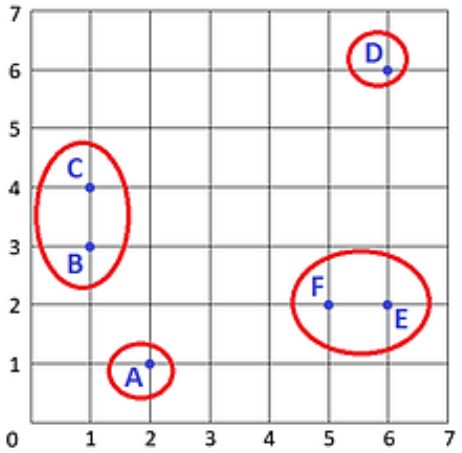
Merge the two closest clusters

Update the proximity matrix

Until only a single cluster remains

Step 3 part 1

- Step 3: Merge the 2 closest clusters and update the distance matrix
  - There are 2 pairs of clusters with the smallest distance of 1: (B and C) and (E and F) – we can merge them



Data points

	A	B	C	D	E	F
A	x	3	4	9	5	4
B		x	1	8	6	5
C			x	7	7	6
D				x	4	5
E					x	1
F						x

Distance matrix (not updated)

Algorithm:

Compute the distance matrix

Let each data point be a cluster

Repeat

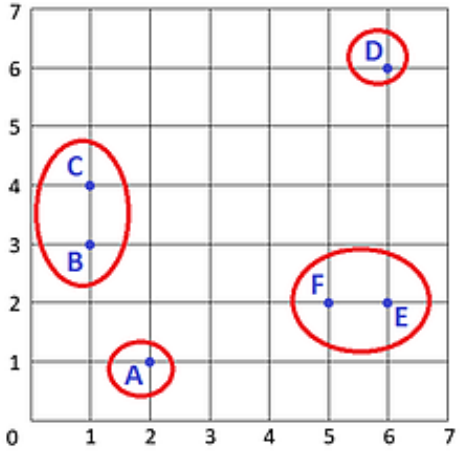
Merge the two closest clusters

Update the proximity matrix

Until only a single cluster remains

Step 3 part 2

- Step 3: Merge the 2 closest clusters and update the distance matrix
  - B and C are merged; E and F are merged
  - Now we can update the distance matrix using the single-link distance



Data points

	A	B, C	D	E, F
A	x	3	9	4
B, C		x	7	5
D			x	4
E, F				x

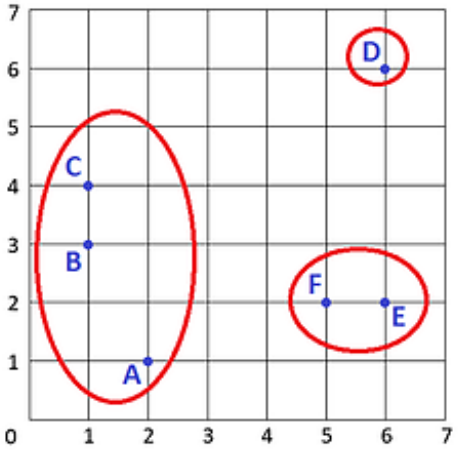
Distance matrix (updated)

Algorithm:

Compute the distance matrix
Let each data point be a cluster
Repeat
    Merge the two closest clusters
    Update the proximity matrix
Until only a single cluster remains

Step 4

- Step 4: Merge the 2 closest clusters and update the distance matrix (repeat until we have only 1 cluster)



Data points

	A	B, C	D	E, F
A	x	3	9	4
B, C		x	7	5
D			x	4
E, F				x

Distance matrix (not updated)

- Merge {A} with {B,C} (smallest distance)

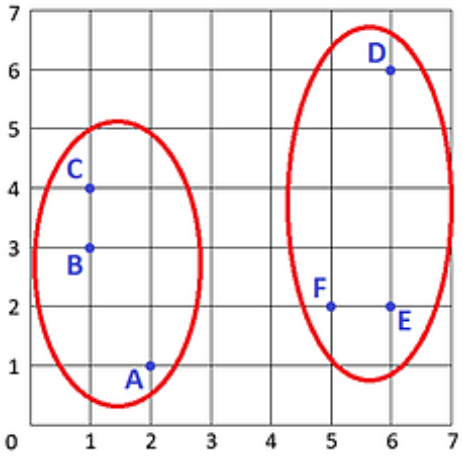
	A, B, C	D	E, F
A, B, C	x	7	4
D		x	4
E, F			x

Distance matrix (updated)

- Update the distance matrix

Step 5

- Step 5: Merge the 2 closest clusters and update the distance matrix (repeat until we have only 1 cluster)



Data points

	A, B, C	D	E, F
A, B, C	x	7	4
D		x	4
E, F			x

Distance matrix (not updated)

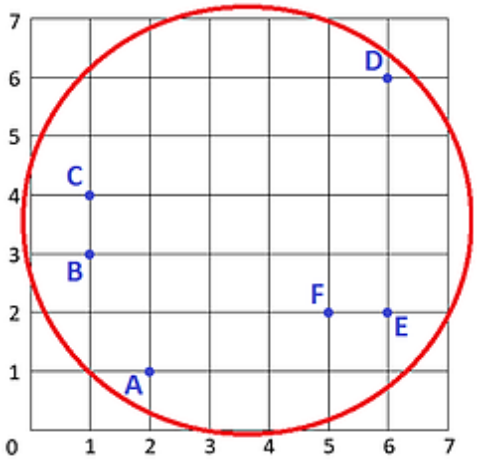
	A, B, C	D, E, F
A, B, C	x	4
D, E, F		x

Distance matrix (updated)

- The smallest distance is 4 in 2 cases:
  - 1) {A,B,C} and {E,F}
  - 2) {D} and {E,F}
- There is an overlap – both involve {E,F} – which one to merge first? We need a rule to resolve ties; assume random choice – we select 2)
- Merge {D} with {E,F} and update the distance matrix

Step 6 - finish

- Step 6: Merge {A,B,C} with {D,E,F}
- Finish – all items belong to the same cluster
- Draw the dendrogram



Data points

	A, B, C	D, E, F
A, B, C	x	4
D, E, F		x

Distance matrix (not updated)

	A, B, C, D, E, F
A, B, C, D, E, F	x

Distance matrix (updated)

Algorithm:

Compute the distance matrix

Let each data point be a cluster

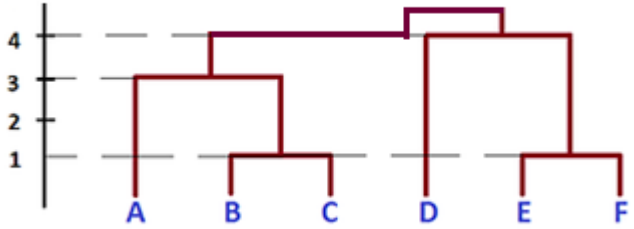
Repeat

Merge the two closest clusters

Update the proximity matrix

Until only a single cluster remains

- Note: The last 2 merges are both at distance 4



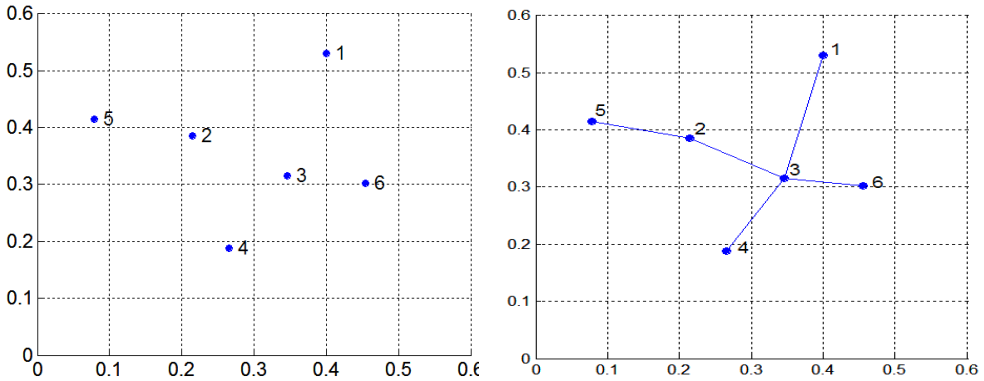
Dendrogram

Divisive hierarchical clustering

- Less popular
- Can be implemented based on computing the minimum spanning tree

Algorithm 7.5 MST Divisive Hierarchical Clustering Algorithm

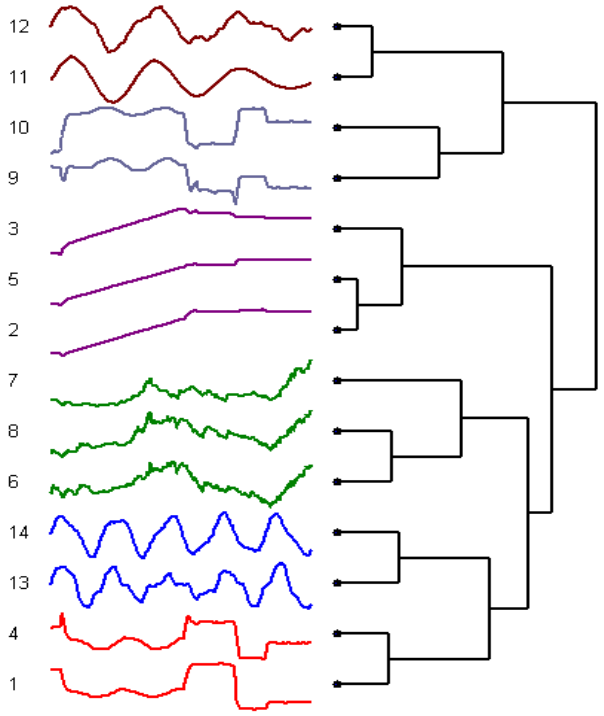
1: Compute a minimum spanning tree for the proximity graph.
2: **repeat**
3: Create a new cluster by breaking the link corresponding to the largest distance (smallest similarity).
4: **until** Only singleton clusters remain



Minimum spanning tree

Hierarchical clustering – example

- Using hierarchical clustering to cluster time series
- The similarity between two time series can be calculated using correlation or other measures

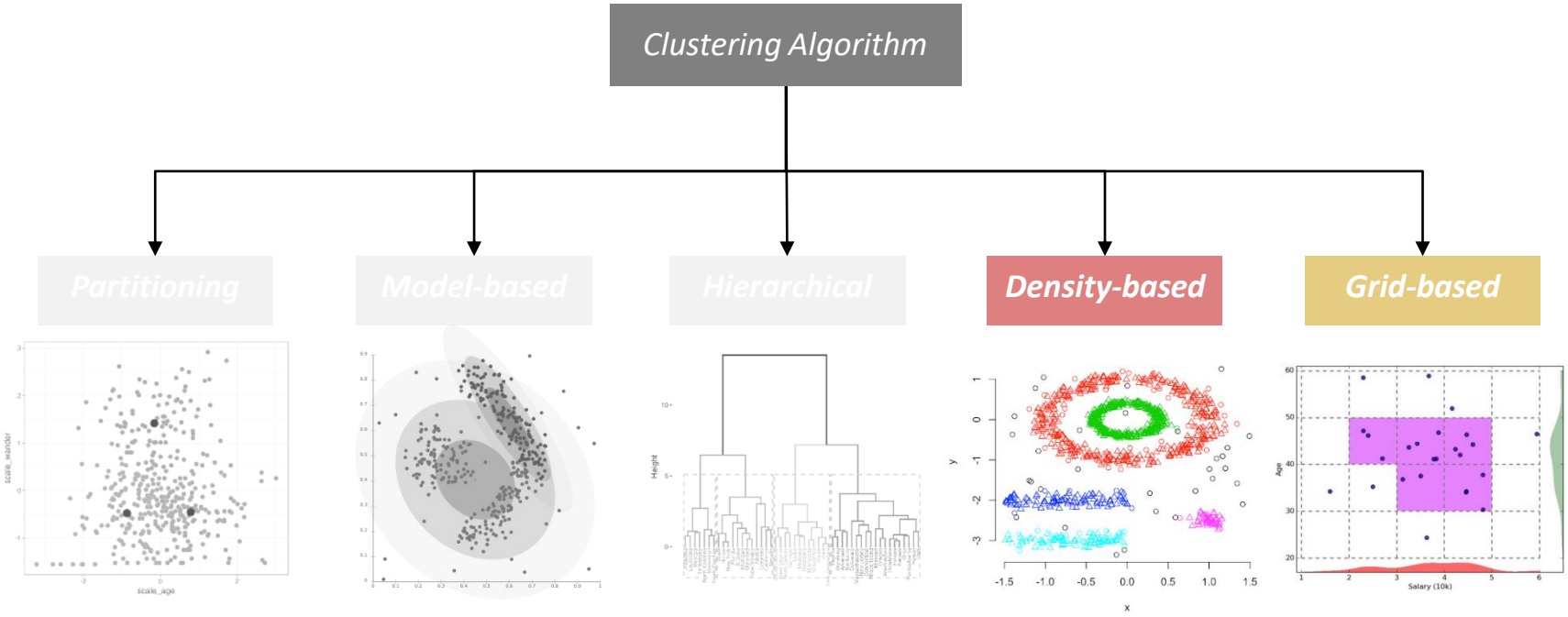


Hierarchical clustering – strengths and limitations

- Especially suitable for tasks with natural nesting relationships between clusters (taxonomies, hierarchies)
- Does not require the number of clusters to be specified in advance
- Computationally expensive which limits its applicability to high dimensional data
  - Space complexity: $O(n^2)$, n - number of examples (storing the distance matrix and dendrogram)
  - Time complexity: $O(n^3)$ – n levels; at each of them n^2 distance matrices must be searched and updated
- Not incremental – assumes all data is present
- Sensitive to noise and outliers
  - Outliers are more problematic for the Ward's method as they increase the SSE and less problematic for the single, complete and average link
  - Outliers tend to form single clusters that do not merge with any other clusters until later in the process; they can be removed by discarding small clusters

Next week - preview

- Next week: Clustering II
  - Density-based and grid-based clustering
  - Evaluating clustering results



+ Evaluating clustering