Unsupervised learning

- Unsupervised learning:
  - Data with no target attribute. Describe hidden structure from unlabeled data.
  - Explore the data to find some intrinsic structures in them.
- Clustering: the task of grouping a set of objects in such a way that objects in the same group (called a cluster) are more similar to each other than to those in other clusters.
- Useful for
  - Automatically organizing data.
  - Understanding hidden structure in data.
  - Preprocessing for further analysis.

Murdered Delhi Woman's Last Instagram Photo With Her Live-in Partner Was Captioned "Happy Days"

NDTV · 1 hour ago

- **Details Of Shraddha Murder Case | CNN-News18 Reports From Aftab's Home | English News | News18**
  CNN-News18 · 14 hours ago
- **Man Who Killed Partner 'Used To See Her Face' After Keeping Head In Fridge**
  NDTV · 22 hours ago
- **Delhi murder: Shraddha Walkar story is not as distant from us as we might think**
  The Indian Express · 17 hours ago · Opinion
- **Opinion | Why did Aftaab brutally murder live-in partner Shraddha?**
  India TV News · 17 hours ago · Opinion

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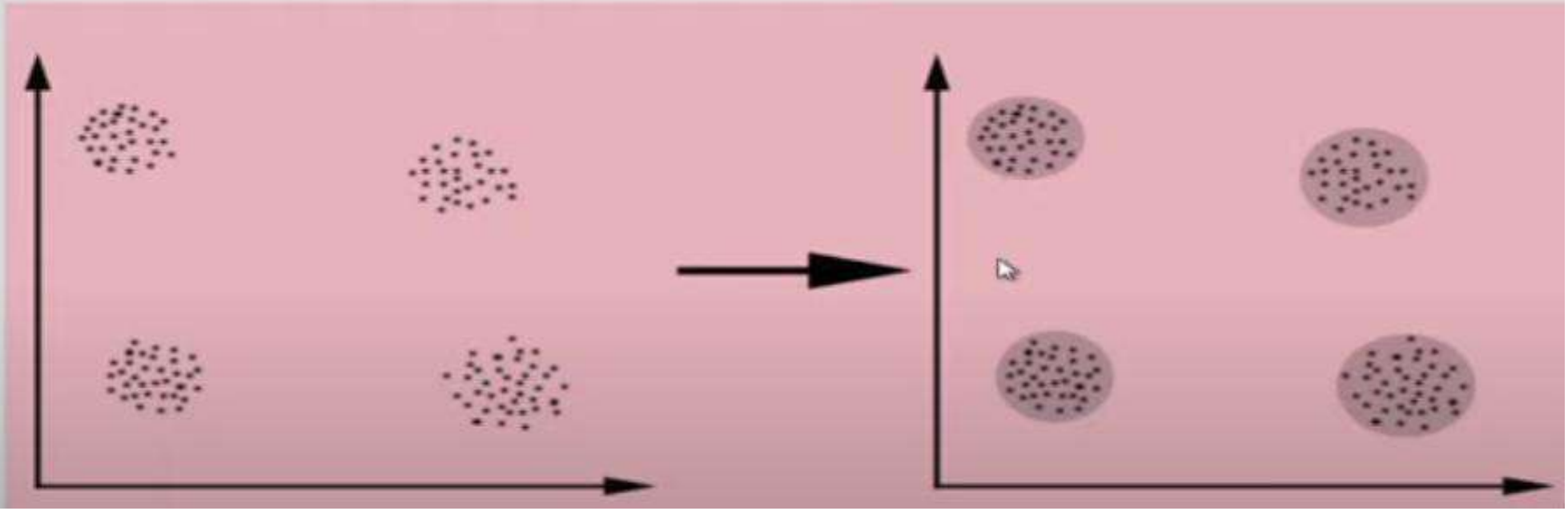
Other Applications

- Biology: classification of plants and animal kingdom given their features
- Marketing: Customer Segmentation based on a database of customer data containing their properties and past buying records
- Clustering weblog data to discover groups of similar access patterns.

An illustration

- This data set has four natural clusters.



Aspects of clustering

- A clustering algorithm such as
  - Partitional clustering eg, kmeans
  - Hierarchical clustering eg, AHC
  - Mixture of Gaussians
- A distance or similarity function
  - such as Euclidean, Minkowski, cosine
- Clustering quality
  - Inter-clusters distance $\Rightarrow$ maximized
  - Intra-clusters distance $\Rightarrow$ minimized

The quality of a clustering result depends on the algorithm, the distance function, and the application.

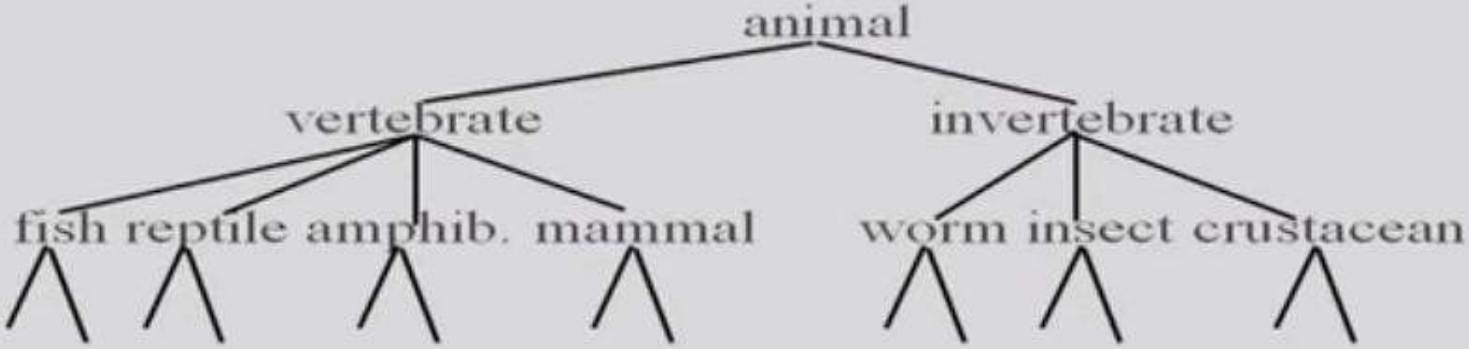
Major Clustering Approaches

- Partitioning: Construct various partitions and then evaluate them by some criterion
- Hierarchical: Create a hierarchical decomposition of the set of objects using some criterion
- Model-based: Hypothesize a model for each cluster and find best fit of models to data
- Density-based: Guided by connectivity and density functions
- Graph-Theoretic Clustering

Partitioning Algorithms

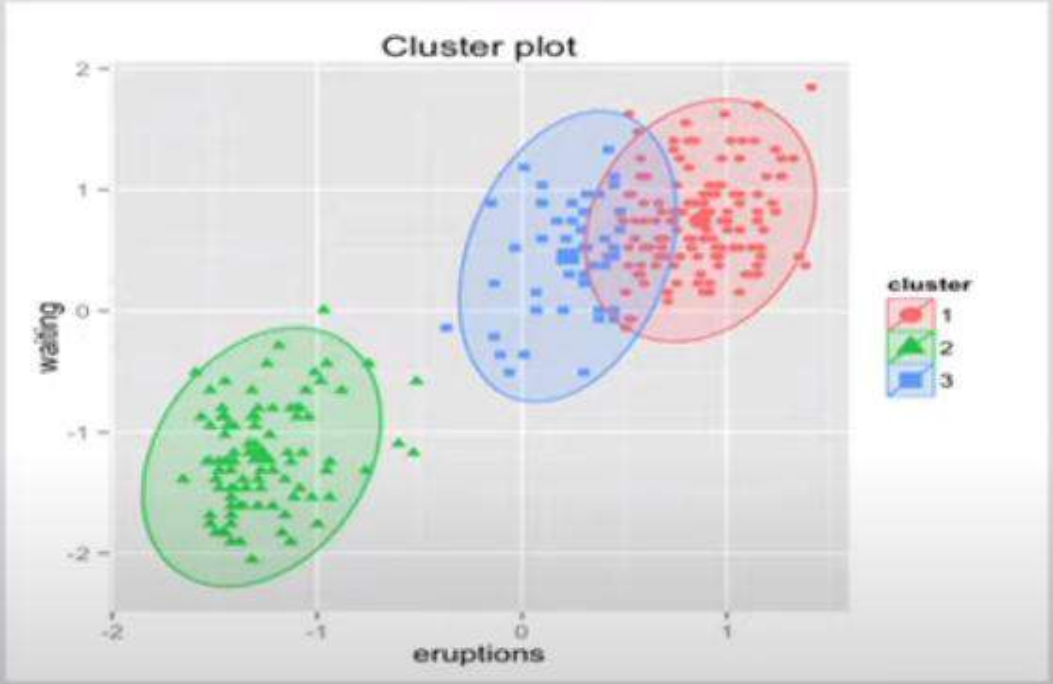
- Partitioning method: Construct a partition of a database D of m objects into a set of k clusters
- Given a k, find a partition of k *clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic method: *k-means* (MacQueen, 1967)

Hierarchical Clustering



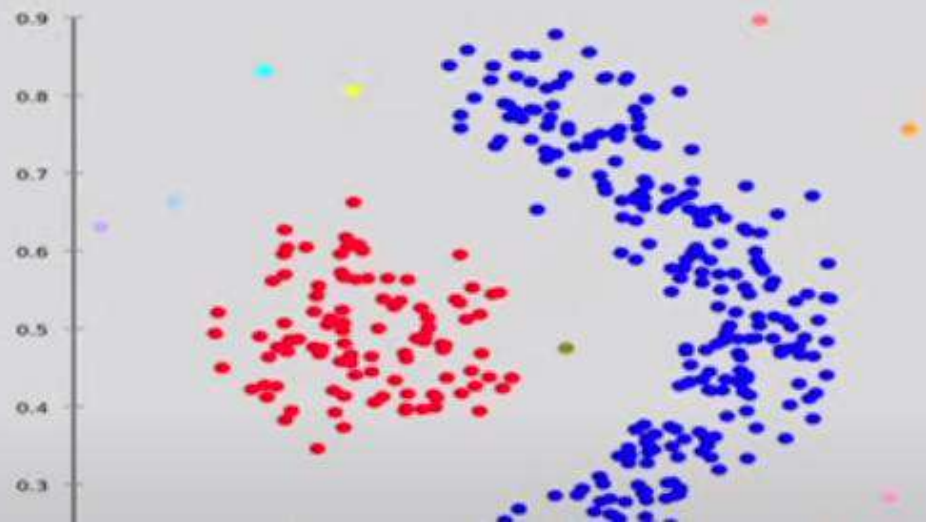
- Produce a nested sequence of clusters.
- One approach: recursive application of a partitional clustering algorithm.

Model Based Clustering



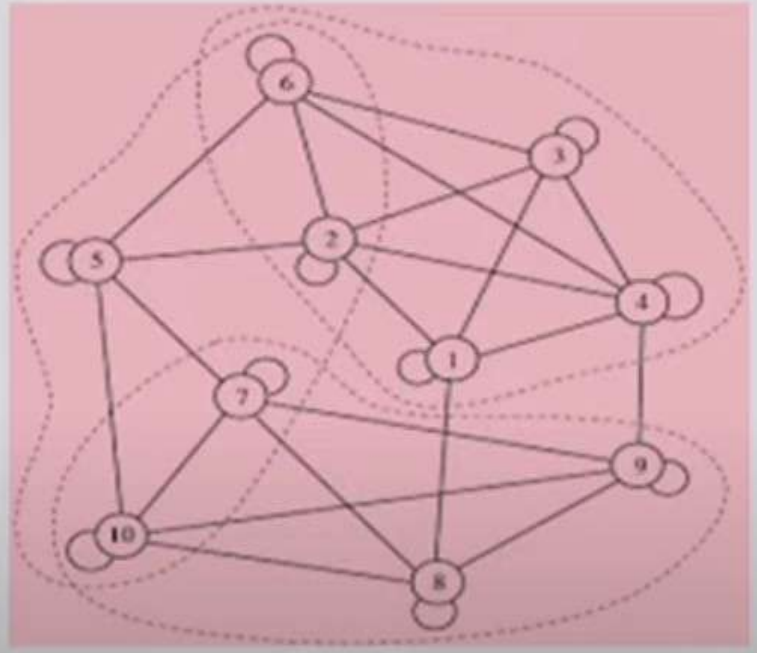
- A model is hypothesized
- e,g., Assume data is generated by a mixture of underlying probability distributions
- Fit the data to model

Density based Clustering



- Based on density connected points
- Locates regions of high density separated by regions of low density
- e.g., DBSCAN

Graph Theoretic Clustering



- Weights of edges between items (nodes) based on similarity
- E.g., look for minimum cut in a graph

(Dis)similarity measures

- Distance metric (scale-dependent)
  - Minkowski family of distance measures

$$d(\boldsymbol{x_i}, \boldsymbol{x_j}) = \left(\sum_{s=1}^{m} |x_{is} - x_{js}|^p \right)^{1/p}$$

Manhattan (p=1), Euclidean (p=2)

  - Cosine distance

$$\text{cosine}(x_i, x_j) = \frac{x_i . x_j}{||x_i||. ||x_i||}$$

(Dis)similarity measures

- Correlation coefficients (scale-invariant)
- Mahalanobis distance

$$d(x_i, x_i) = \sqrt{(x_i - x_j)\Sigma^{-1}(x_i - x_j)}$$

- Pearson correlation

$$r(x_i, x_j) = \frac{Cov(x_i, x_j)}{\sigma_{x_i}\sigma_{x_j}}$$

Quality of Clustering

- Internal evaluation:
  - assign the best score to the algorithm that produces clusters with high similarity within a cluster and low similarity between clusters, e.g., Davies-Bouldin index

$$DB = \frac{1}{n}\sum_{i=1}^{k}\max_{j\neq i}\frac{\sigma_i + \sigma_j}{d(c_i, c_j)}$$

- External evaluation:
  - evaluated based on data such as known class labels and external benchmarks, eg, Rand Index, Jaccard Index, f-measure

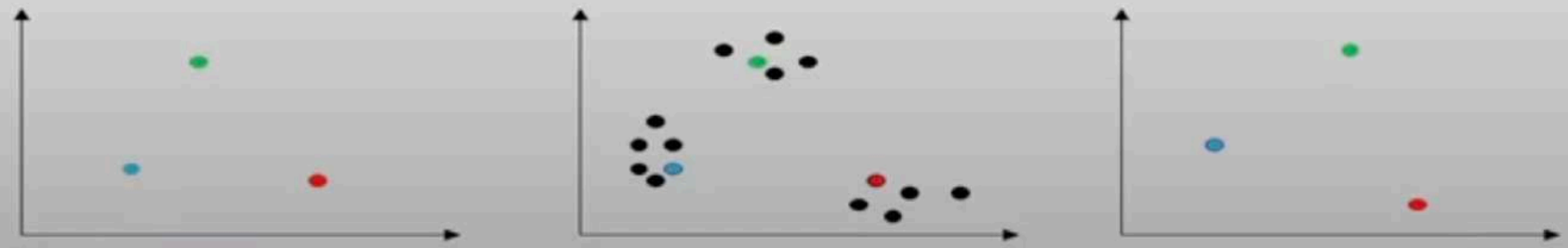
$$RI = \frac{TP + TN}{TP + FP + FN + TN}$$

$$J(A, B) = \frac{|A \cap B|}{|A \cup B|} = \frac{TP}{TP + FP + FN}$$

K-means algorithm

Given *k*

1. Randomly choose *k* data points (seeds) to be the initial cluster centres
2. Assign each data point to the closest cluster centre
3. Re-compute the cluster centres using the current cluster memberships.
4. If a convergence criterion is not met, go to 2.



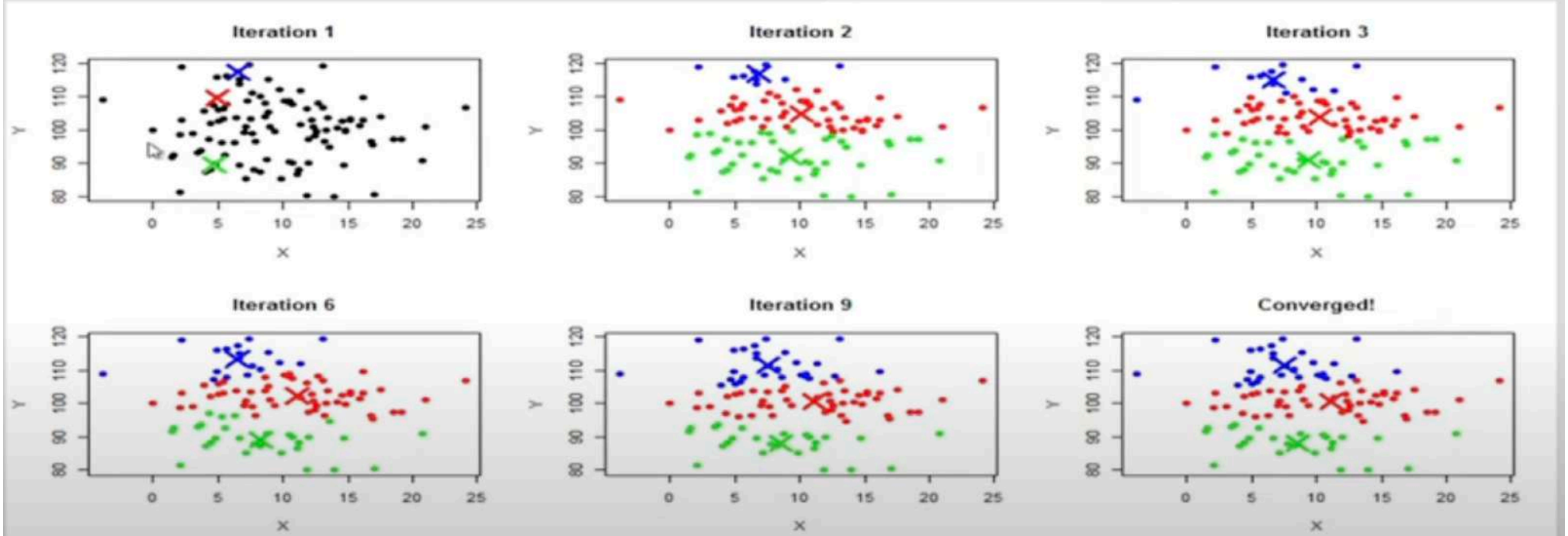
Stopping/convergence criterion

OR

1. no re-assignments of data points to different clusters
2. no (or minimum) change of centroids
3. minimum decrease in the *sum of squared error*

$$SSE = \sum_{i=1}^{k} \sum_{x \in S_i} \|x_i - \mu_i\|^2$$

Kmeans illustrated



Similarity / Distance measures

- Distance metric (scale-dependent)
  - Minkowski family of distance measures

$$d(\boldsymbol{x}_i, \boldsymbol{x}_j) = \left(\sum_{s=1}^{n} |x_{is} - x_{js}|^p \right)^{1/p}$$

Manhattan (p=1), Euclidean (p=2)

  - Cosine distance

Time Complexity

- Computing distance between two items is $O(n)$ where n is the dimensionality of the vectors.
- Reassigning clusters: $O(km)$ distance computations, or $O(kmn)$.
- Computing centroids: Each item gets added once to some centroid: $O(mn)$.
- Assume these two steps are each done once for t iterations: $O(tknm)$.

Advantages

- Fast, robust easy to understand.
- Relatively efficient: O(tkmn)
- Gives best result when data set are distinct or well separated from each other.

Disadvantages

- Requires apriori specification of the number of cluster centers.
- Hard assignment of data points to clusters
- Euclidean distance measures can unequally weight underlying factors.
- Applicable only when mean is defined i.e. fails for categorical data.
- Only local optima

K-Means on RGB image

$x_1=\{r_1, g_1, b_1\}$

$x_2=\{r_2, g_2, b_2\}$

...

$x_i=\{r_i, g_i, b_i\}$

...

Classifier (K-Means)

Classification Results

$x_1 \rightarrow C(x_1)$

$x_2 \rightarrow C(x_2)$

...

$x_i \rightarrow C(x_i)$

...

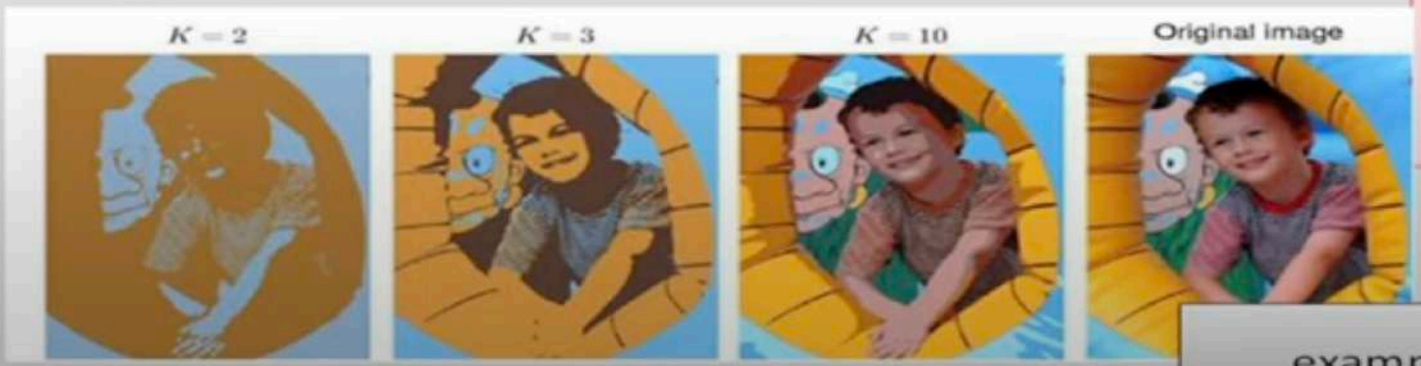
Cluster Parameters

θ_1 for C_1

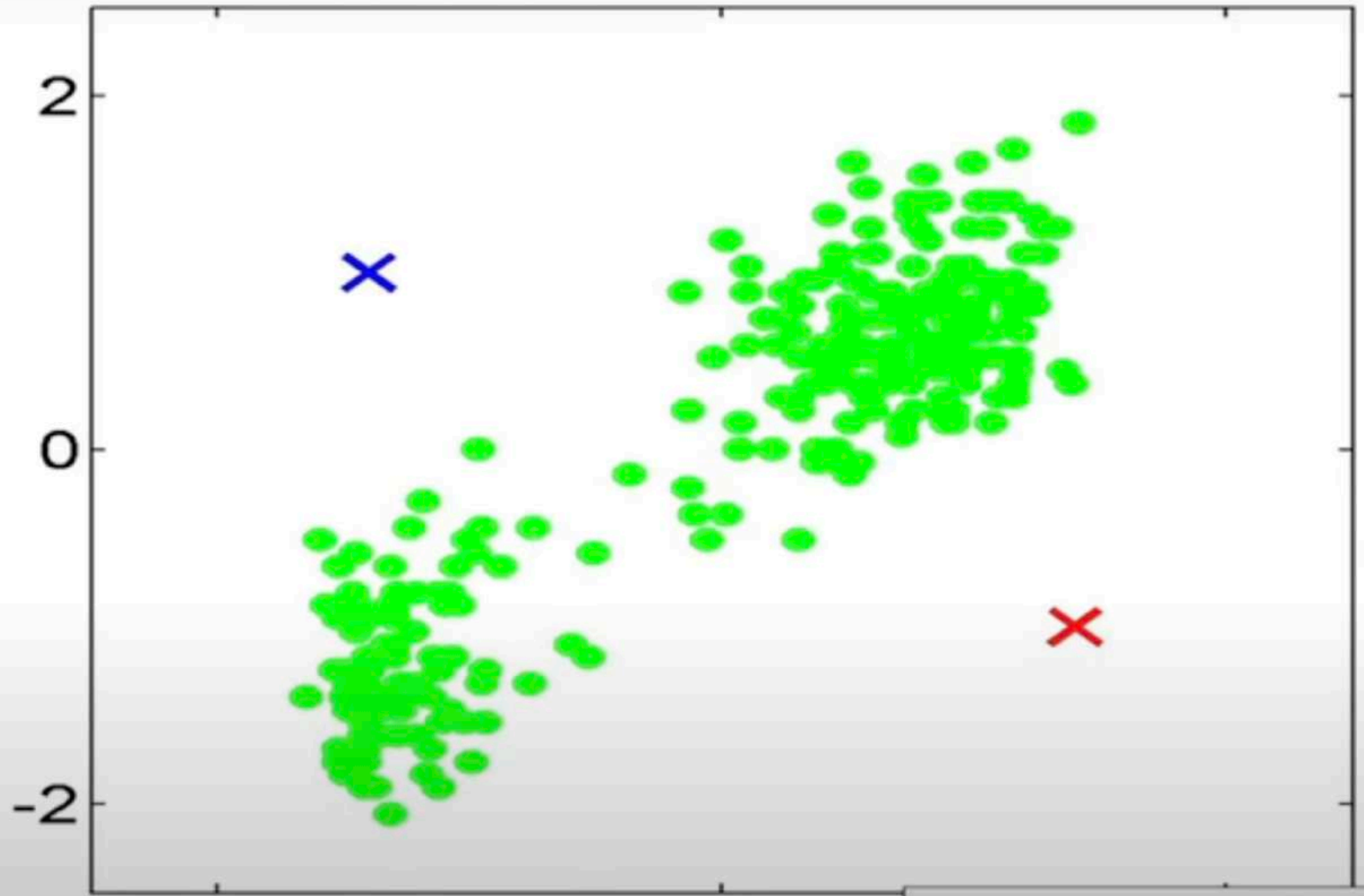
θ_2 for C_2

...

θ_k for C_k



example from Bishop's Book



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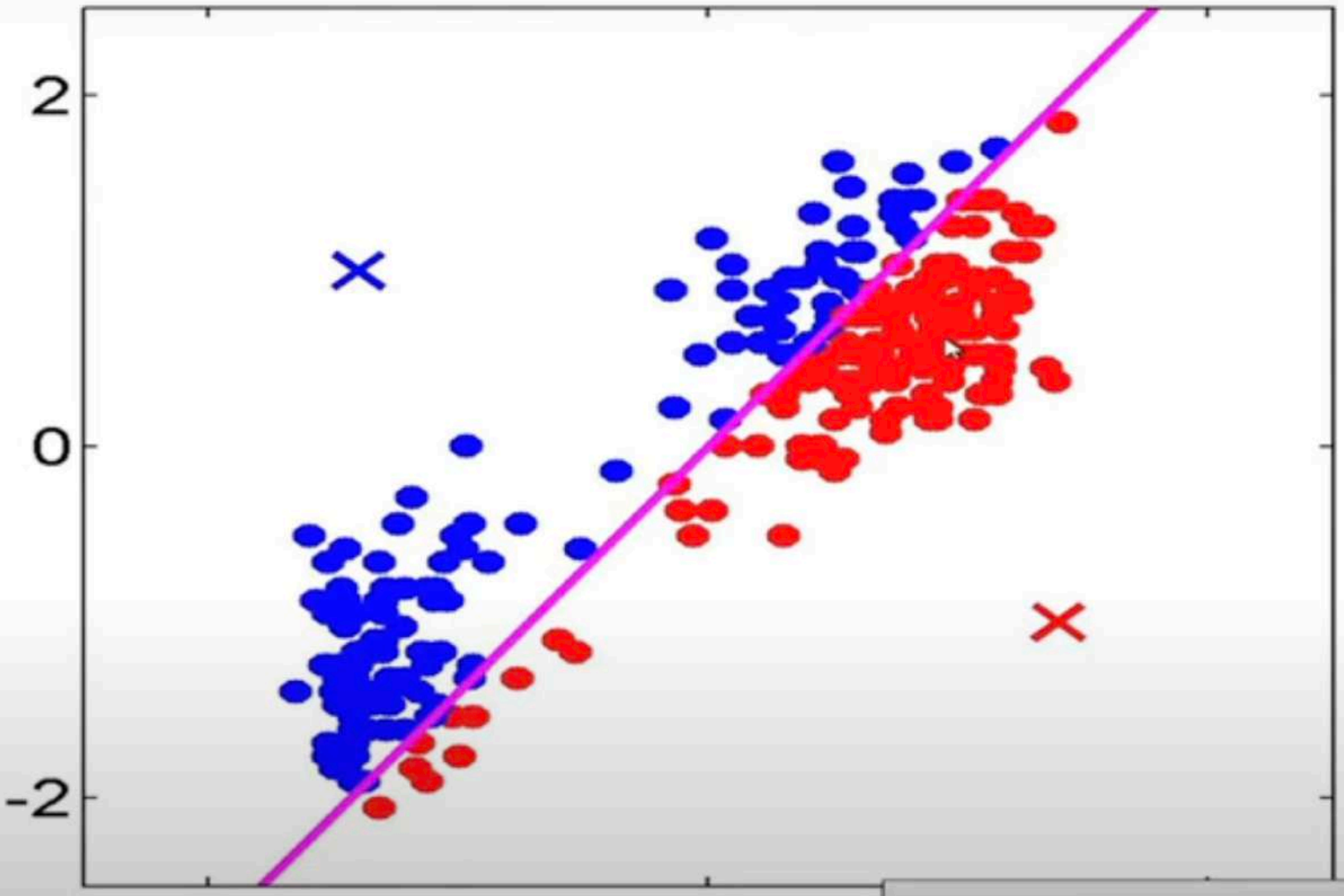

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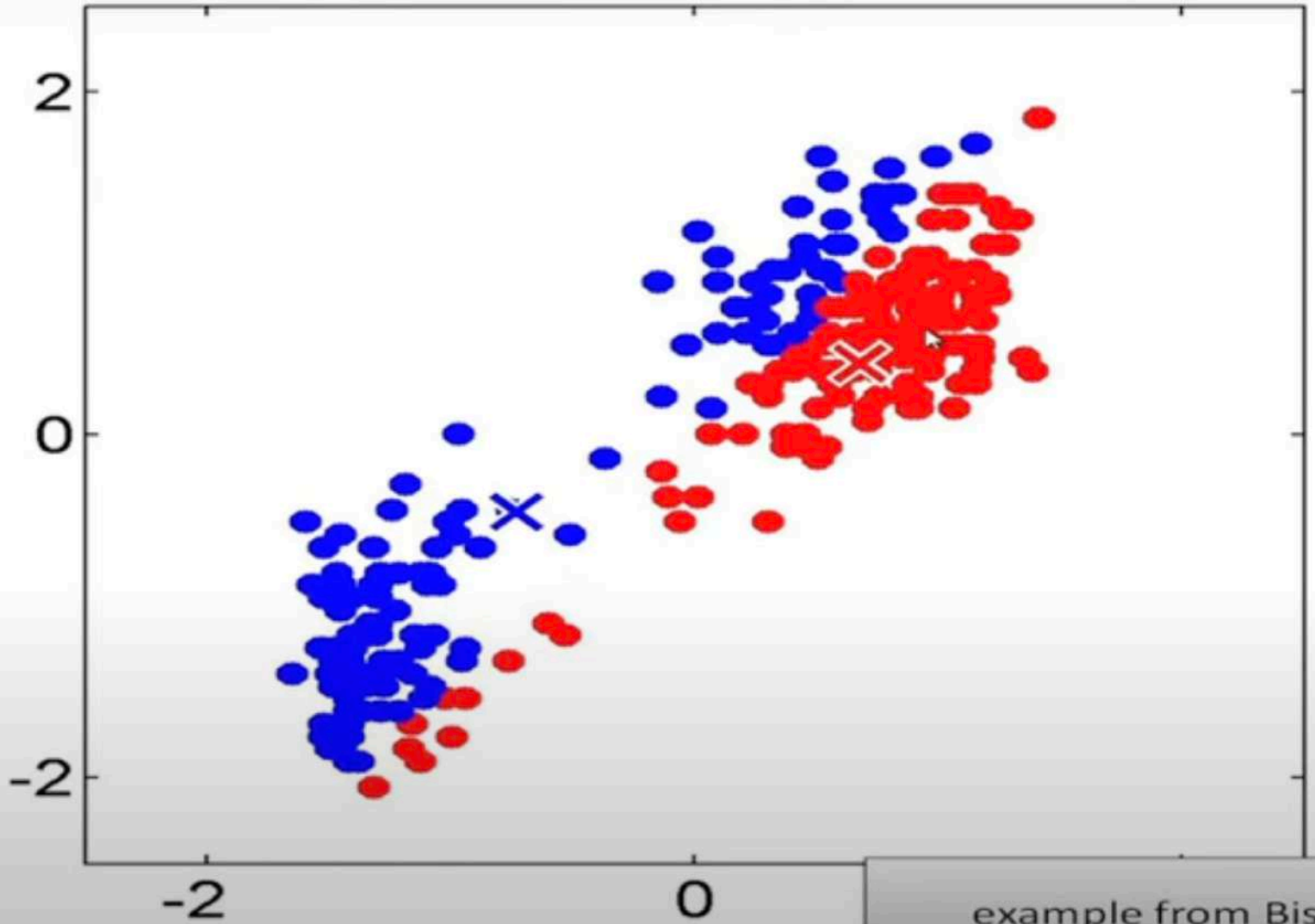

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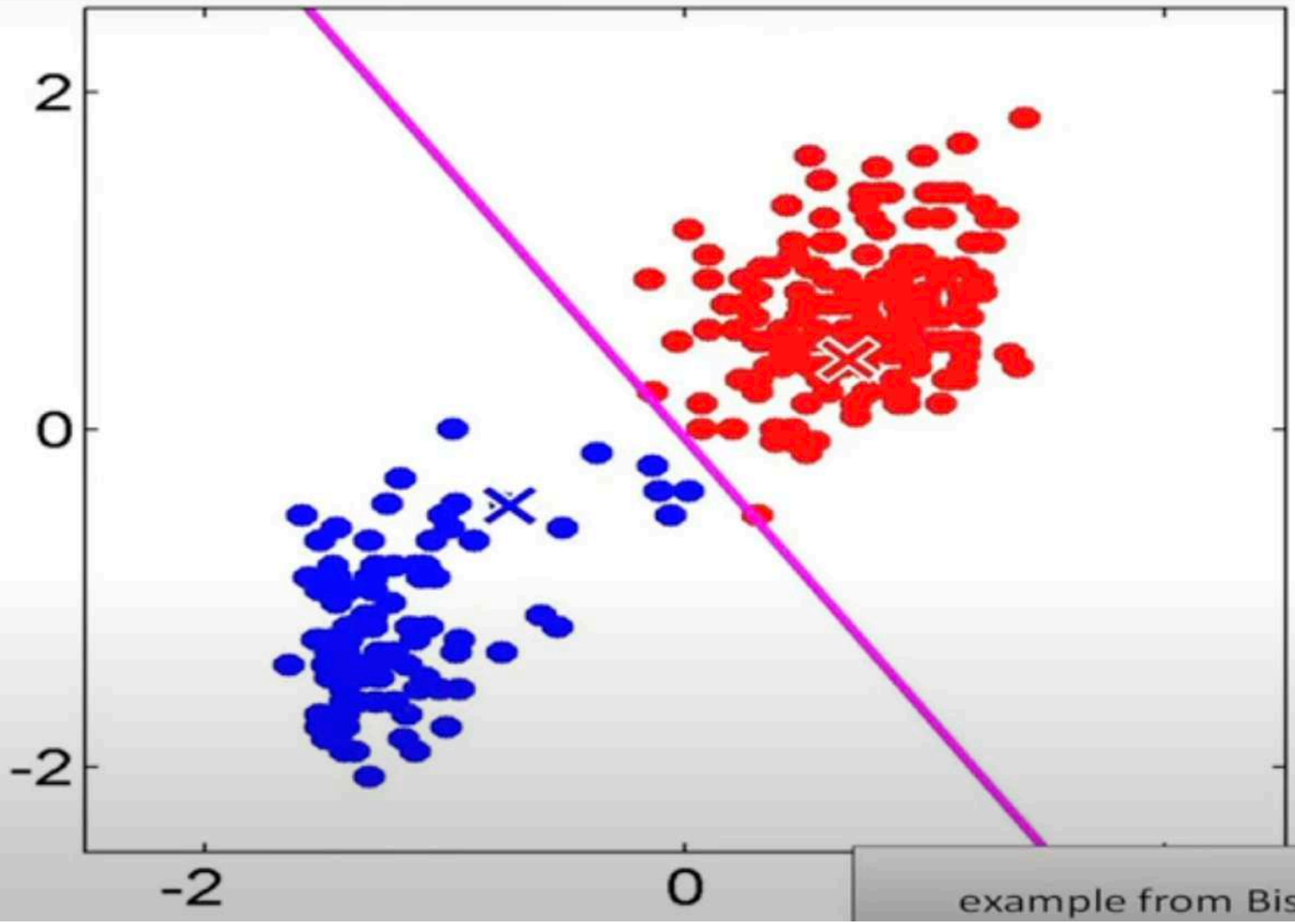
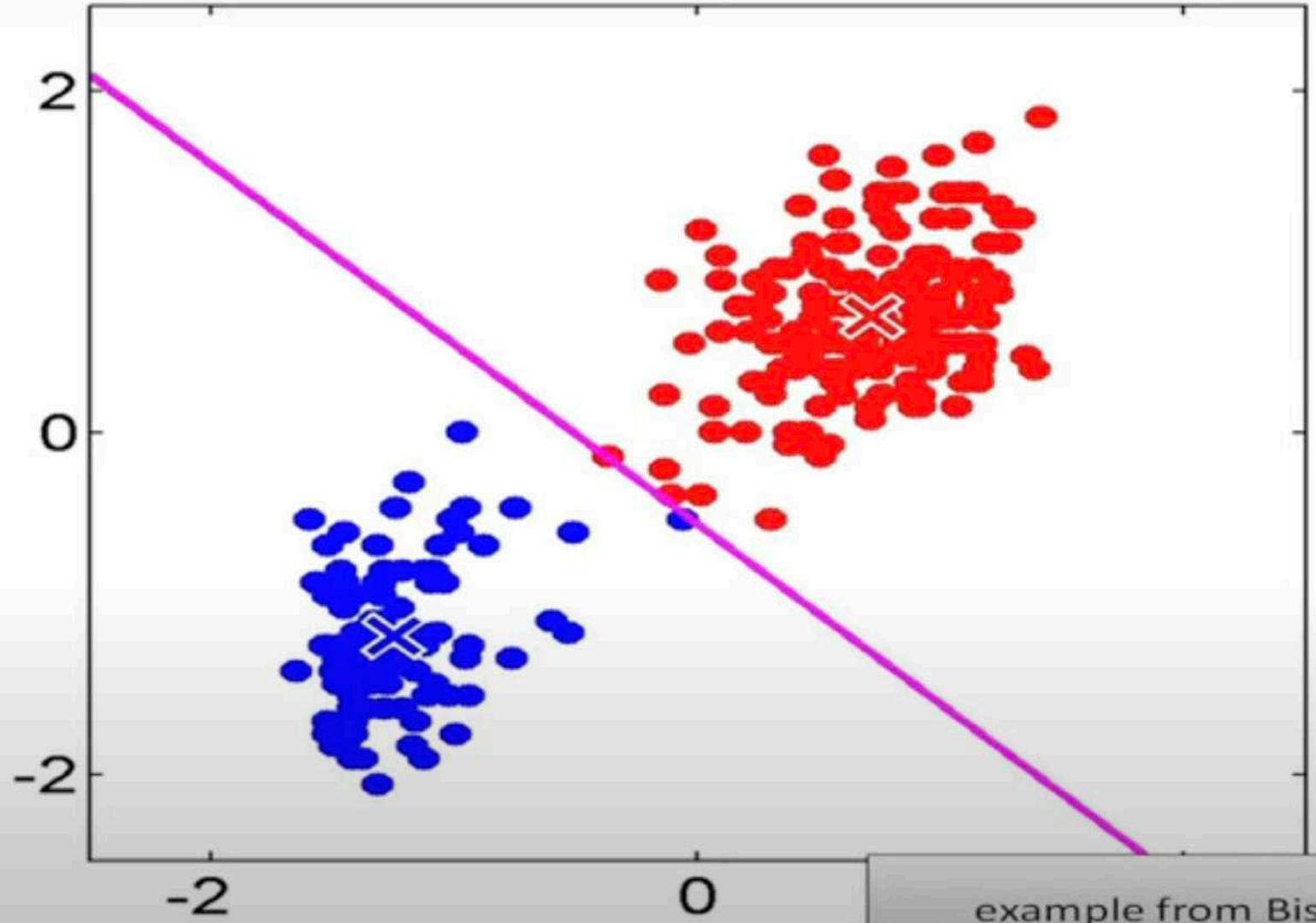


example from Bishop's Book



example from Bishop's Book

Model-based clustering

- Assume k probability distributions with parameters $\theta_1, \theta_2, \ldots, \theta_k$
- Given data X, compute $\theta_1, \theta_2, \ldots, \theta_k$ such that

  $Pr(X|\theta_1, \theta_2, \ldots, \theta_k)$ [likelihood] or

  $\ln Pr(X|\theta_1, \theta_2, \ldots, \theta_k)$ [log likelihood]

is maximized.

- Every point $x \epsilon X$ may be generated by multiple distributions with some probability

EM Algorithm

- Initialize the parameters $\theta_1, \theta_2, \ldots, \theta_k$ randomly
- Let each parameter corresponds to a cluster center (mean)
- Iterate between two steps
  - Expectation step: (probabilistically) assign points to clusters
  - Maximation step: estimate model parameters that maximize the likelihood for the given assignment of points

EM Algorithm

Expectation step: (probabilistically) assign points to clusters

compute Prob(point | mean)

Prob(mean | point) =
Prob(mean) Prob(point | mean) / Prob(point)

Maximation step: estimate model parameters that maximize the likelihood for the given assignment of points

Each mean = Weighted avg. of points

Weight = Prob(mean | point)

EM Algorithm

- Initialize k cluster centers
- Iterate between two steps
  - **E**xpectation step: assign points to clusters

$$\Pr(x_i \in C_k) = \frac{\Pr(x_i | C_k)}{\sum_j \Pr(x_i | C_j)}$$

$$w_k = \frac{\sum_i \Pr(x_i \in C_k)}{n}$$

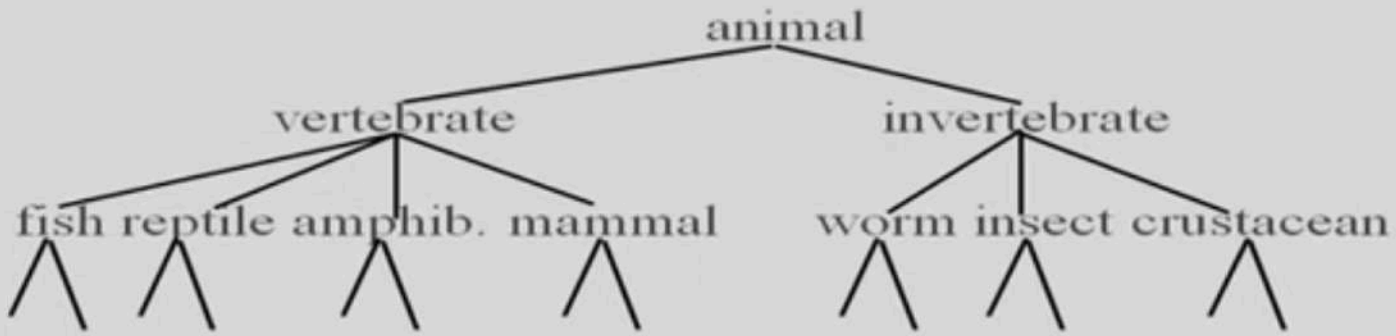
  - **M**aximization step: estimate model parameters

$$r_k = \frac{1}{n} \sum_{i=1}^{n} \frac{\Pr(x_i \in C_k)}{\sum_j \Pr(x_i \in C_j)}$$

K-means Algorithm

- Goal: represent a data set in terms of K clusters each of which is summarized by a prototype μ_k
- Initialize prototypes, then iterate between two phases:
  - E-step: assign each data point to nearest prototype
  - M-step: update prototypes to be the cluster means

Hierarchical Clustering

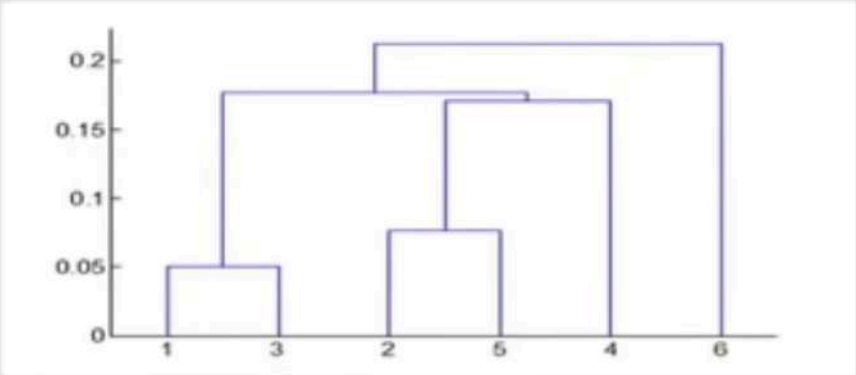


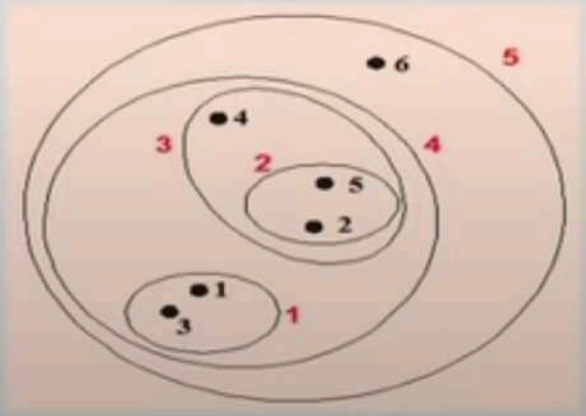
- Produce a nested sequence of clusters.
- One approach: recursive application of a partitional clustering algorithm.

Types of hierarchical clustering

- Agglomerative (bottom up) clustering: It builds the dendrogram (tree) from the bottom level, and
  - merges the most similar (or nearest) pair of clusters
  - stops when all the data points are merged into a single cluster (i.e., the root cluster).
- Divisive (top down) clustering: It starts with all data points in one cluster, the root.
  - Splits the root into a set of child clusters. Each child cluster is recursively divided further
  - stops when only singleton clusters of individual data points remain, i.e., each cluster with only a single point

Dendrogram: Hierarchical Clustering

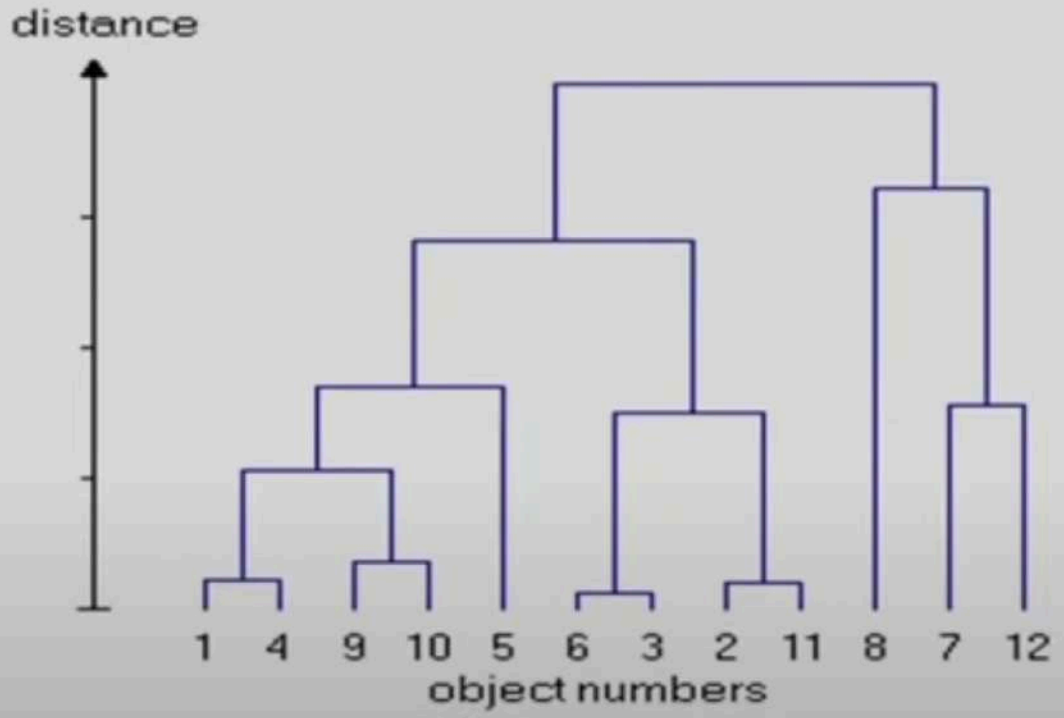




Dendrogram

- Given an input set S
- nodes represent subsets of S
- Features of the tree:
- The root is the whole input set S.
- The leaves are the individual elements of S.
- The internal nodes are defined as the union of their children.

Dendrogram: Hierarchical Clustering



Dendrogram

- Each level of the tree represents a partition of the input data into several (nested) clusters or groups.
- May be cut at any level: Each connected component forms a cluster.

Hierrarchical Agglomerative clustering

- Initially each data point forms a cluster.
- Compute the distance matrix between the clusters.
- Repeat
  - Merge the two closest clusters
  - Update the distance matrix
- Until only a single cluster remains.

Different definitions of the distance leads to different algorithms.

Initialization

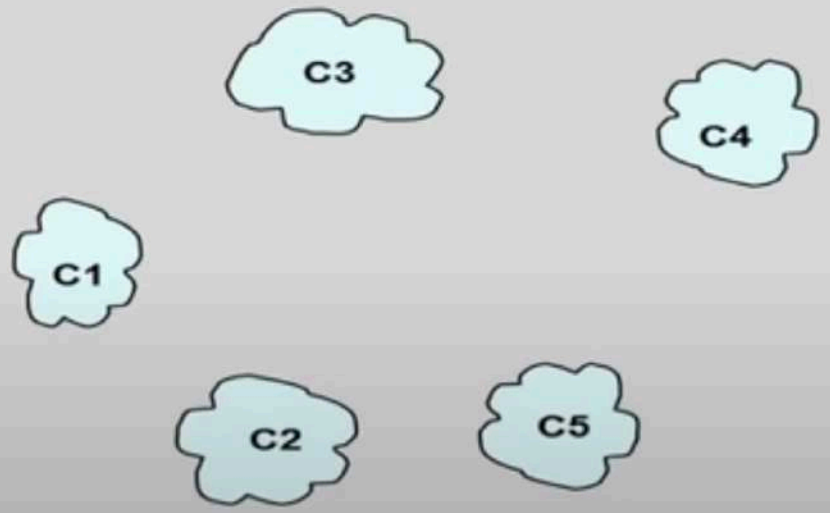
- Each individual point is taken as a cluster
- Construct distance/proximity matrix

	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
. .						

Distance/Proximity Matrix

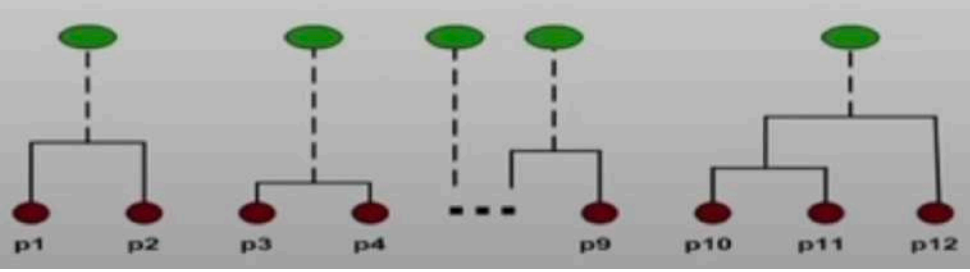
Intermediate State

- After some merging steps, we have some clusters



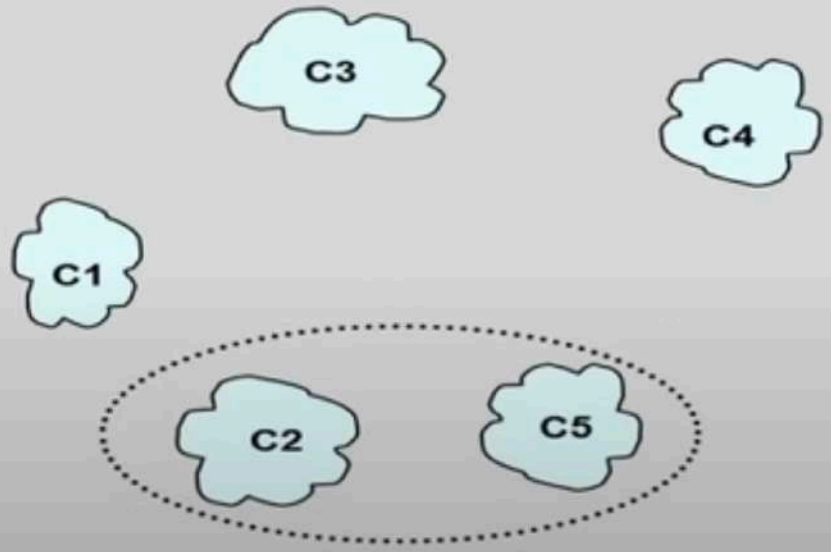
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance/Proximity Matrix



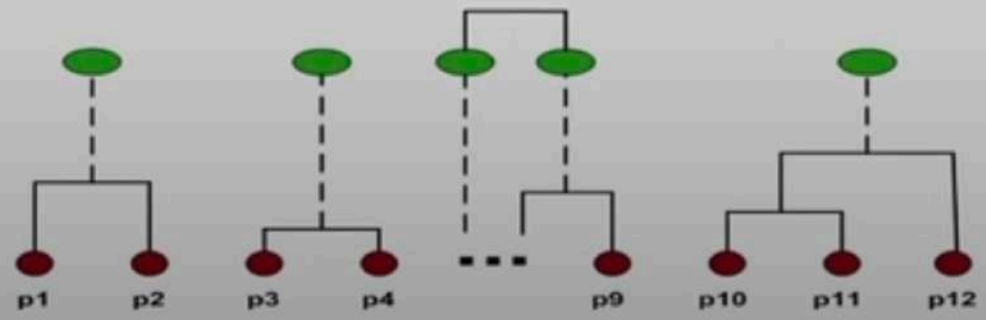
Intermediate State

Merge the two closest clusters (C2 and C5) and update the distance matrix.



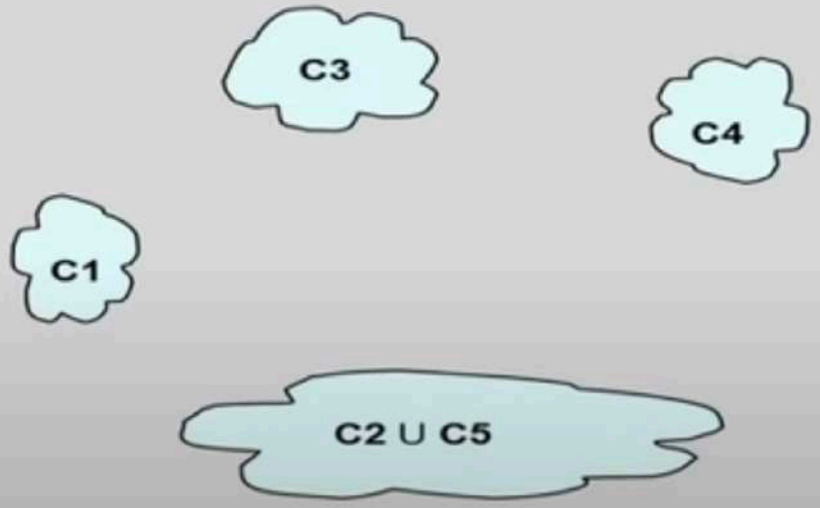
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance/Proximity Matrix

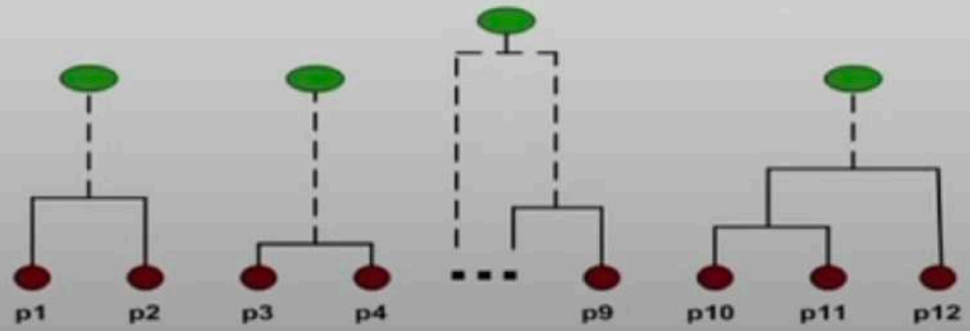


After Merging

- Update the distance matrix



	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		



Closest Pair

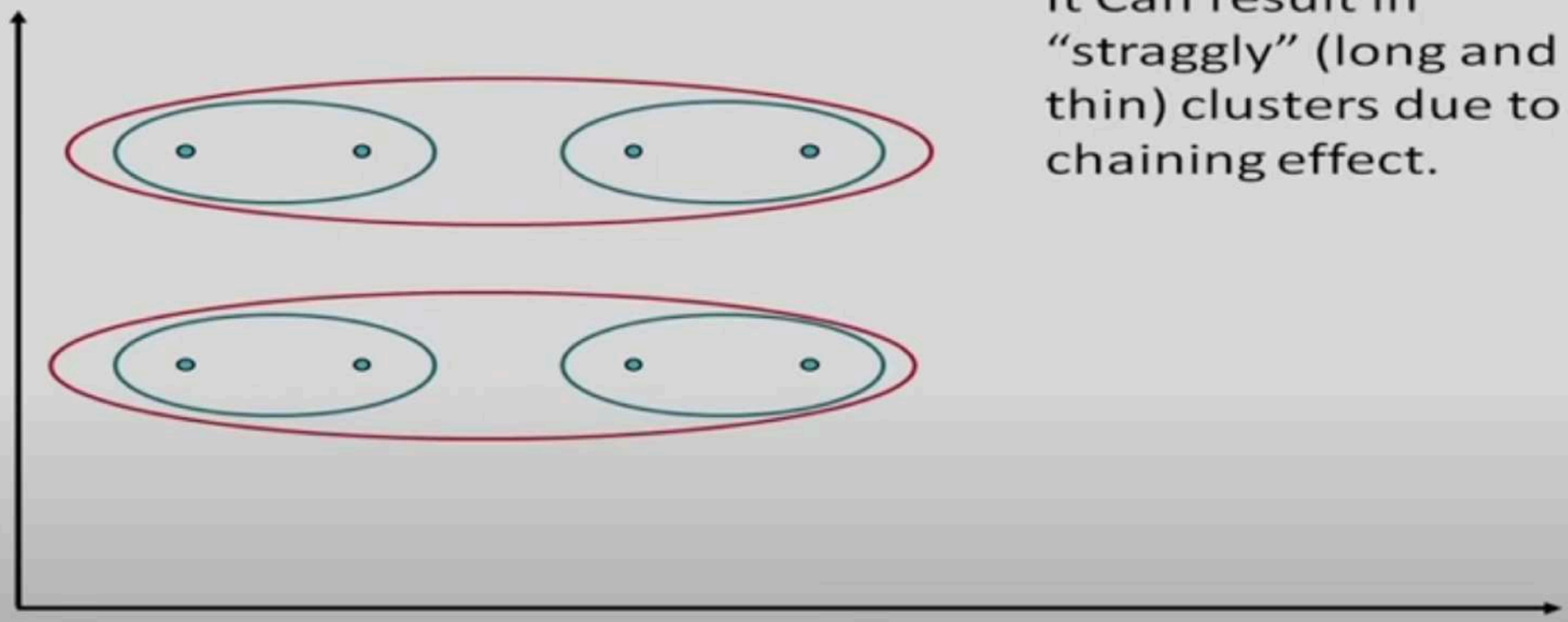
- A few ways to measure distances of two clusters.
- **Single-link**
  - Similarity of the *most* similar (single-link)
- **Complete-link**
  - Similarity of the *least* similar points
- **Centroid**
  - Clusters whose centroids (centers of gravity) are the most similar
- **Average-link**
  - Average cosine between pairs of elements

Distance between two clusters

- Single-link distance between clusters C_i and C_j is the *minimum distance* between any object in C_i and any object in C_j

$$sim(C_i, C_j) = \max_{x \in C_i, y \in C_j} sim(x, y)$$

Single Link Example



It Can result in "straggly" (long and thin) clusters due to chaining effect.

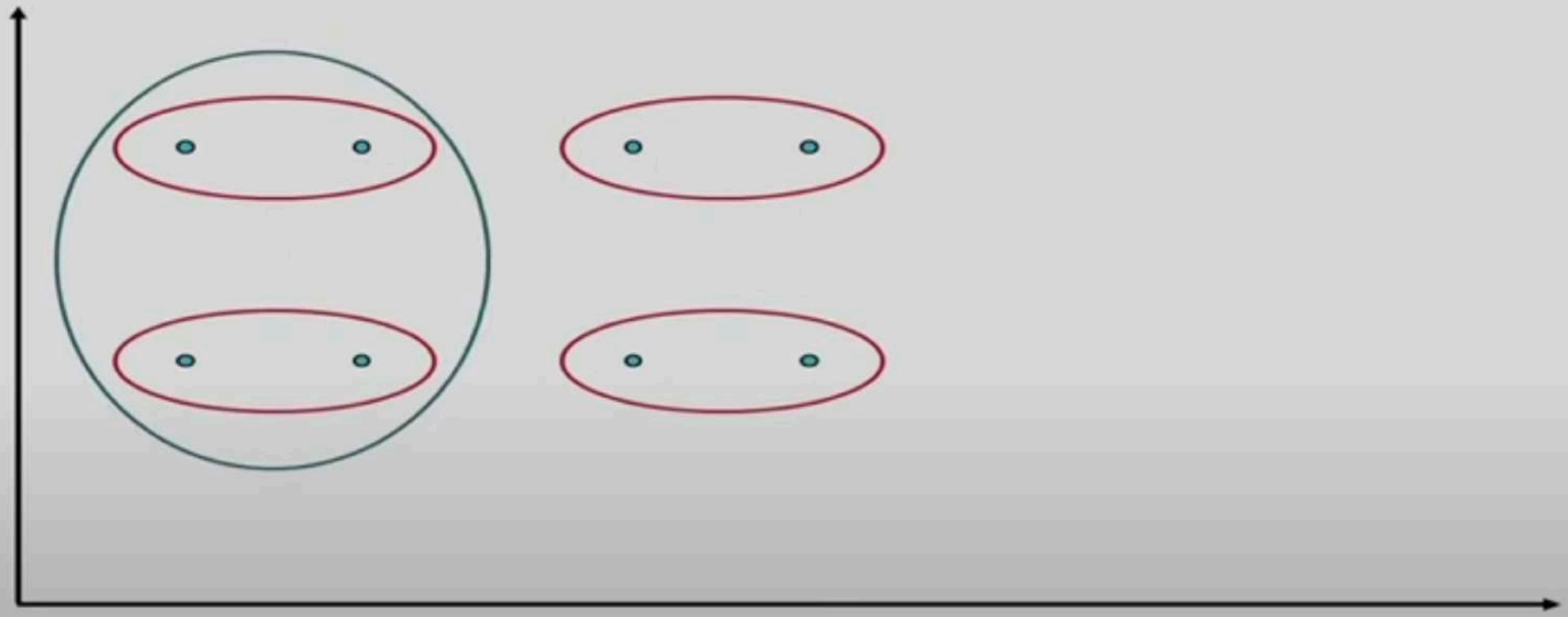
Complete link method

- The distance between two clusters is the distance of two furthest data points in the two clusters.

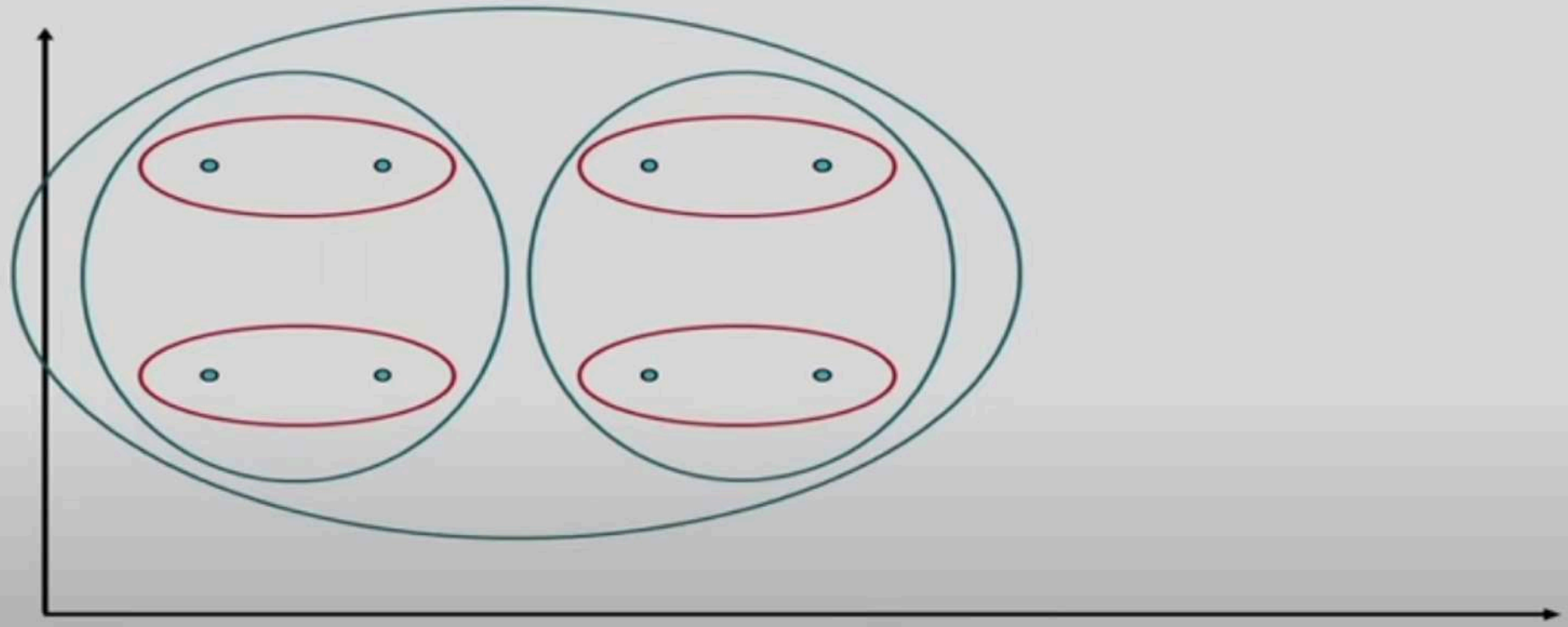
$$sim(c_i, c_j) = \min_{x \in c_i, y \in c_j} sim(x, y)$$

- Makes "tighter," spherical clusters that are typically preferable.
- It is sensitive to outliers because they are far away

Complete Link Example



Complete Link Example



Computational Complexity

- In the first iteration, all HAC methods need to compute similarity of all pairs of N initial instances, which is $O(N^2)$.
- In each of the subsequent $N-2$ merging iterations, compute the distance between the most recently created cluster and all other existing clusters.
- In order to maintain an overall $O(N^2)$ performance, computing similarity to each other cluster must be done in constant time.
  - Often $O(N^3)$ if done naively or $O(N^2 \log N)$ if done more cleverly

Average Link Clustering

- Similarity of two clusters = average similarity between any object in Ci and any object in Cj

$$sim(c_i, c_j) = \frac{1}{|C_i||C_j|} \sum_{\vec{x} \in C_i} \sum_{\vec{y} \in C_j} sim(\vec{x}, \vec{y})$$

- Compromise between single and complete link. Less susceptible to noise and outliers.
- Two options:
  - Averaged across all ordered pairs in the merged cluster
  - Averaged over all pairs *between* the two original clusters

The complexity

- All the algorithms are at least $O(n^2)$. n is the number of data points.
- Single link can be done in $O(n^2)$.
- Complete and average links can be done in $O(n^2 \log n)$.
- Due the complexity, hard to use for large data sets.