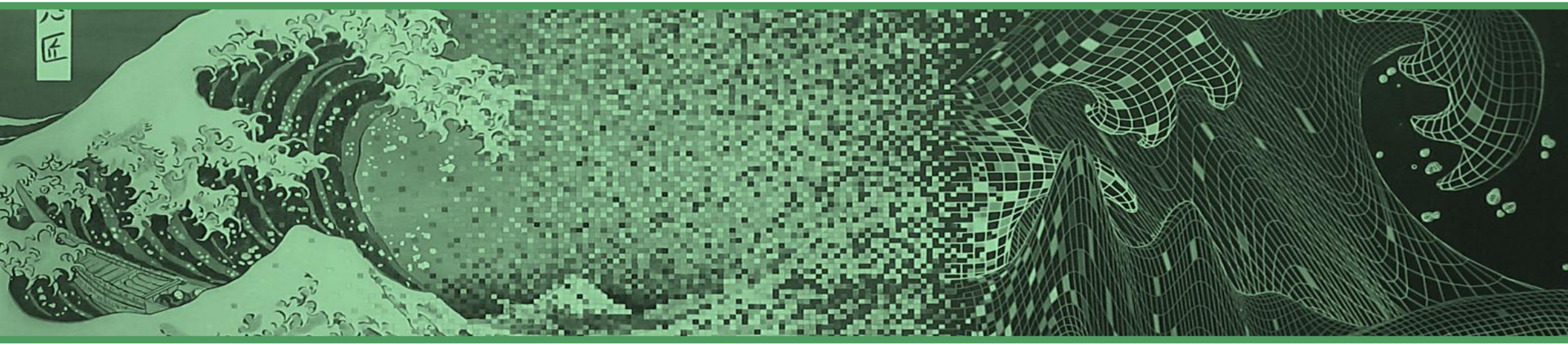
TÉCNICO LISBOA

Clustering

Clustering approaches and evaluation



Aprendizagem 2023

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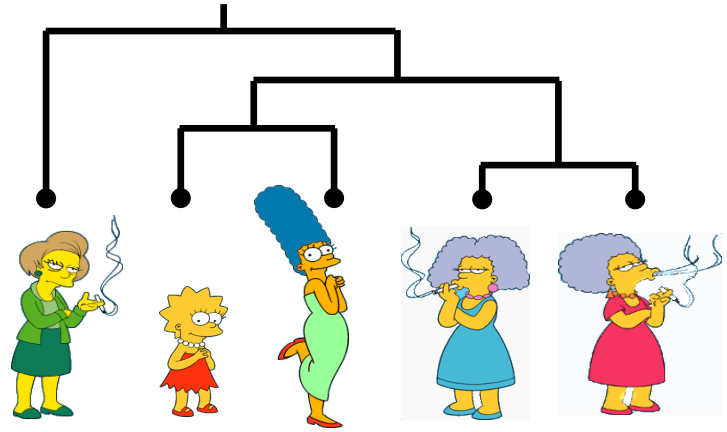
Outline

- **Introduction to clustering**
- **Partition-based clustering: *k*-means**
- **Model-based clustering: EM**
- **Evaluation**
  - external measures: purity
  - internal measures: silhouette
- **Advanced aspects**

Motivation

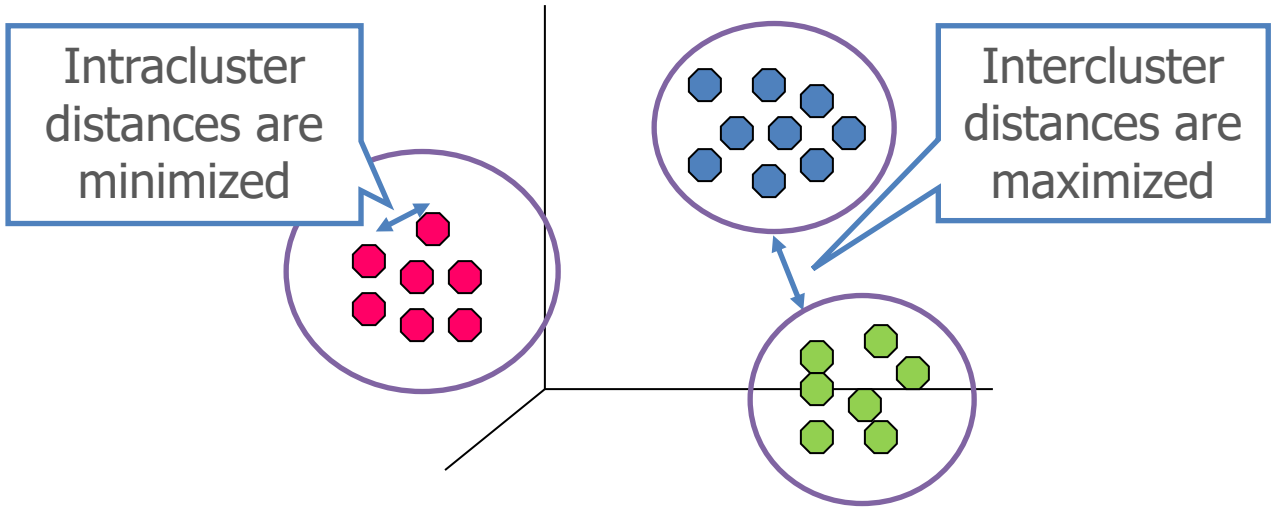


- **Patients** with a shared clinical condition: how to **understand disease**?
  - stratified diagnostics and therapeutics
  - cancer types, dementia progression, risk groups
- **Customers**: how to segment their profile for **personalized marketing**?
- **Webpages**, shopping products, **media**, **documents**: how to categorize them for **recommendations**?
- **Genes**, proteins and metabolites with different expression and concentration profile: how to understand their correlated behavior (biological functions)?
- **Students**, researchers, professors: how to improve science and **education**?

Clustering

Cluster: group of data observations

Cluster analysis: group observations into clusters according to their (dis)similarity: observations in the same cluster are more similar than those in different clusters



Notes on notation: when all attributes are numeric: data observations = data point

ML applications

- Stand-alone tool to get **insight into data structure**
- **Unsupervised data labeling**
- **Preprocessing step** to facilitate other tasks
  - **prediction**: e.g. learn one predictor per cluster to mitigate challenges arising from data heterogeneity
  - **outlier analysis**: identify observations that deviate from expectations
- **Data compression**
  - reduce the number of data points: centers of the clusters seen as the reference/prototype observations
  - highly common when handling very large data (e.g. webpage retrieval, e-commerce)

Clustering: distance and approach

Two major factors impact solutions: ***distance* + *approach***

- **Distance metrics** depend on the:
  - input variables:
    - *numeric* distances, e.g. Euclidean $\left(d(\mathbf{a},\mathbf{b}) = \sqrt{\sum_{j=1}^{m}(a_j - b_j)^2}\right)$
    - *nominal* distances, e.g. Hamming
    - *ordinal* encodings
    - *non-iid attributes*
  - data structure: multivariate, time series, image, spatiotemporal data, events…
- **Clustering approach:** partitioning, hierarchical, density-based, model-based

Recall the distances introduced for kNN!

Distances in clustering

- Given a cluster of observations C_j
  - **mean center** of a cluster: $\mathbf{c}_j = \frac{1}{|\mathrm{C}_j|} \sum_{\mathbf{x} \in \mathrm{C}_j} \mathbf{x}$
  - **cluster**: $\mathrm{C}_j = \{\mathbf{x} \mid d(\mathbf{x}, \mathbf{c}_j) = \min_i d(\mathbf{x}, \mathbf{c}_i)\}$

- Distances can be applied between:
  - two observations $d(\mathbf{x}_i, \mathbf{x}_j)$
  - one observation and a cluster $d(\mathbf{x}_i, \mathbf{c}_j)$
  - two clusters $d(\mathbf{c}_i, \mathbf{c}_j)$

- (Squared) **error** of **clustering solution**: $E = \sum_{k=1}^{K} \sum_{\mathbf{x} \in \mathrm{C}_k} d(\mathbf{x}, \mathbf{c}_k)^2$

Approaches

Partitioning: ⇐

– Create partitions and iteratively update them (e.g. *k*-means, *k*-modes, *k*-medoids)

Hierarchical:

– Create hierarchical decomposition of data points

Density-based:

– Group points based on connectivity and density functions

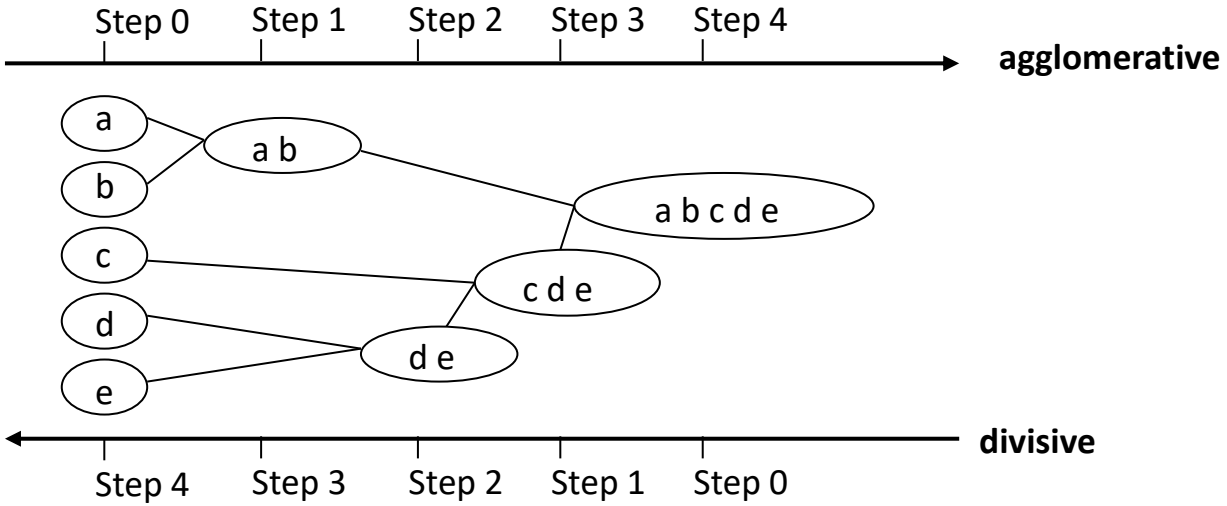
Model-based: ⇐

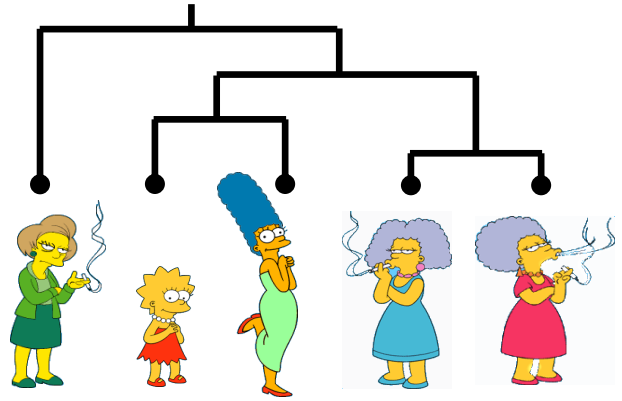
– Data are seen as a mixture of distributions (e.g. EM)

Tree/hierarchical clustering

- Tree clustering algorithm allow us to reveal the internal similarities of a given pattern set
  - similarities structured hierarchically
  - for n patterns these algorithm generates a sequence of 1 to n clusters

- Tree (dendrogram) can be structured bottom up or top down





Goal for today

- **Goal**
  - given a set of n observations (sample) $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$
  - partition the data set into K clusters (we can assume for now that K is given) where $K \ll n$

- First, we approach clustering with a non-probabilistic technique called ***k*-means** [Lloyd, 1982]
- Then, we introduce the latent variable view of mixture distributions
  - discrete latent variables defining assignments of data points to specific components of the mixture
  - a general technique to find maximum likelihood estimators in latent variable models is the **expectation-maximization** (EM) algorithm

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Centers and distances

- Custer as a group of data points with…
  - small inter-point distances when compared with the distances to points outside of the cluster

- The cluster centers (also called **centroids**) represent the compressed data set
  - **mean center** of a cluster: $\boldsymbol{c}_k = \frac{1}{|\mathrm{C}_k|} \sum_{\mathbf{x} \in \mathrm{C}_k} \mathbf{x}$

- Data points are grouped into clusters according to a distance function, applicable to…
  - two observations $d(\mathbf{x}_i, \mathbf{x}_j)$
  - one observation and a cluster $d(\mathbf{x}_i, \boldsymbol{c}_k)$

Clustering objective function

- In this context, a cluster is defined as

$$\mathrm{C}_k = \{\mathbf{x} \mid d(\mathbf{x}, \boldsymbol{c}_k) = \min_i d(\mathbf{x}, \boldsymbol{c}_i)\}$$

- We can then define an objective function to assess the error of a clustering solution
  - squared **error**

$$E = \sum_{k=1}^{K} \sum_{\mathbf{x} \in \mathrm{C}_k} \|\mathbf{x} - \boldsymbol{c}_k\|^2 = \sum_{k=1}^{K} \sum_{\mathbf{x} \in \mathrm{C}_k} d(\mathbf{x}, \boldsymbol{c}_k)^2$$

Partitioning algorithms

Given *k* clusters:

1. partition objects into *k* non-empty subsets
2. compute the centroid $\boldsymbol{c}_k$ of each subset
   – centroid is the center of mass: e.g. mean or median centers
3. reassign each observation to the cluster with the nearest centroid
4. goto *step 2, stop* when:
   i) assignment does not change, *ii*) $|E^{new} - E^{old}| < \varepsilon$, or *iii*) max iterations is reached

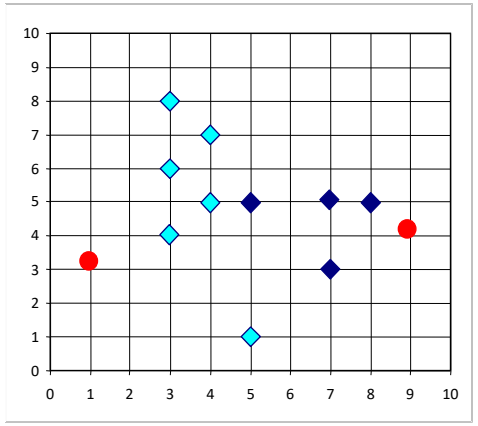
Variants

– centroid calculus

– selection of the initial seeds

– adjustments for **batches** of observations (instead of all) for very large datasets

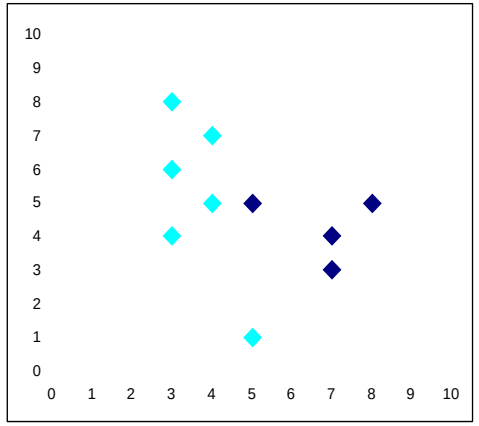
k-means



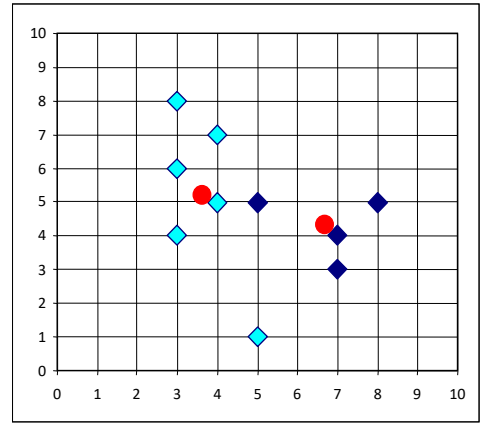
k=2

Arbitrarily choose k object as initial cluster center

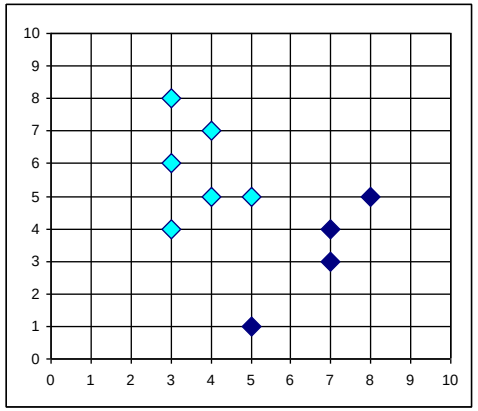
Assign each objects to most similar center



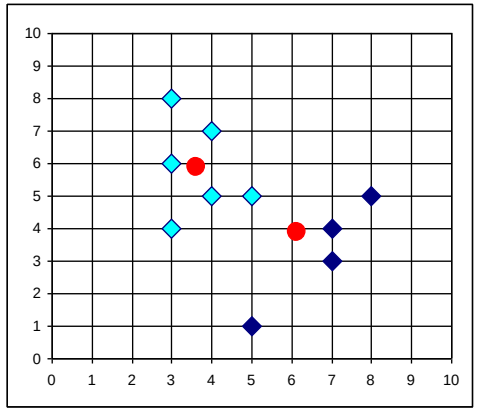
Update the cluster means



reassign



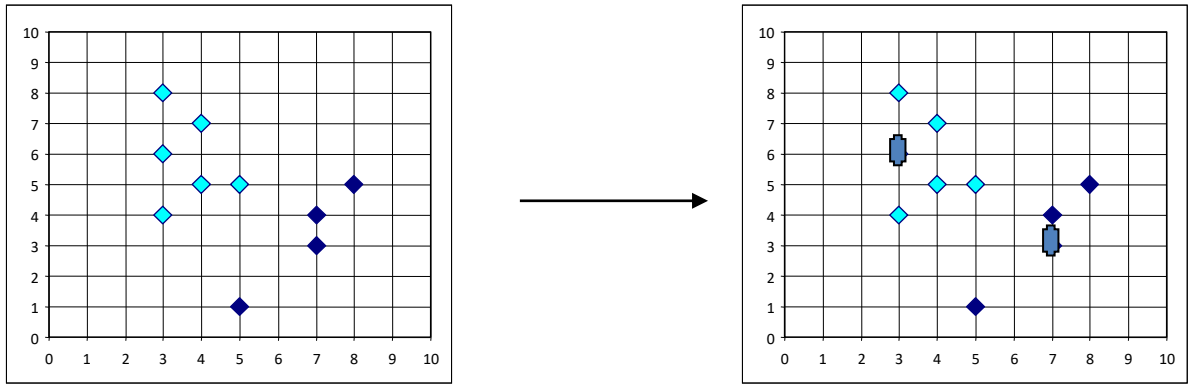
Update the cluster means



k-medoids

1. **numeric** data: centroid as the mean or median
2. **categoric** data: centroid as the mode – *k*-modes [Huang'98]
   - frequency-based procedure to update modes of clusters
3. **mixed** data: centroid combining mean and modes (***k*-prototype**)

- ***k*-medoids**: the **most centrally located observation** in a cluster is the centroid
  - observation with minimum average distance to all observations in the cluster
- What is the algorithm most robust to outliers: *k*-means or *k*-medoids?

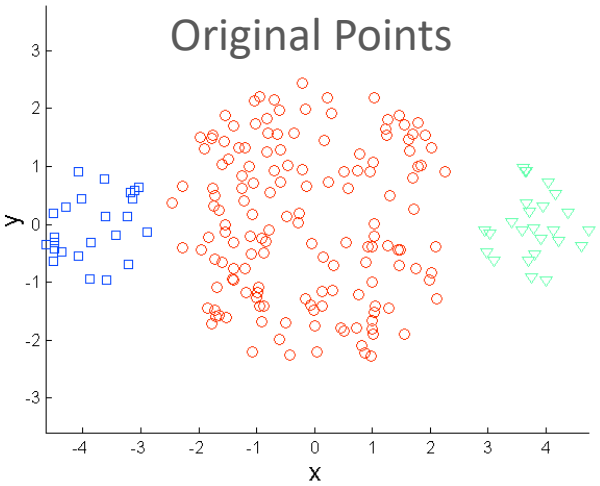


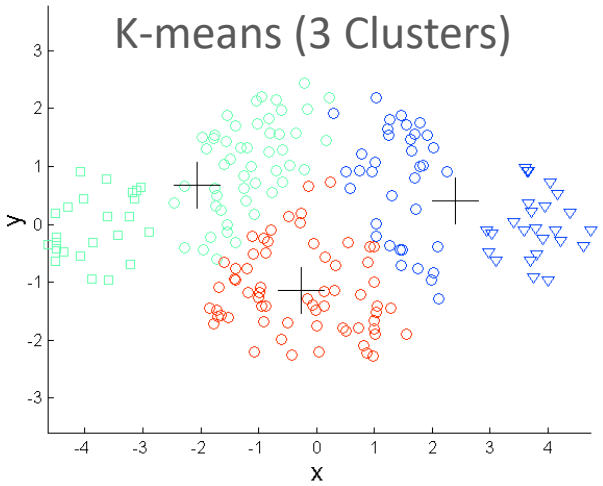
k-means: challenges

- **Efficiency**: $O(tkn)$ n=#observation, k=#clusters, t=#iterations, usually $k, t \ll n$
- **Problems**
  - dependent on initialization
  - sensitive to outliers
  - sensitive noisy data
    - noise can substantially distort centroids
  - not suitable to discover clusters with *non-convex shapes*
    - deal only with clusters with spherical symmetrical point distribution
  - need to specify k, the *number* of clusters, in advance
  - convergence?

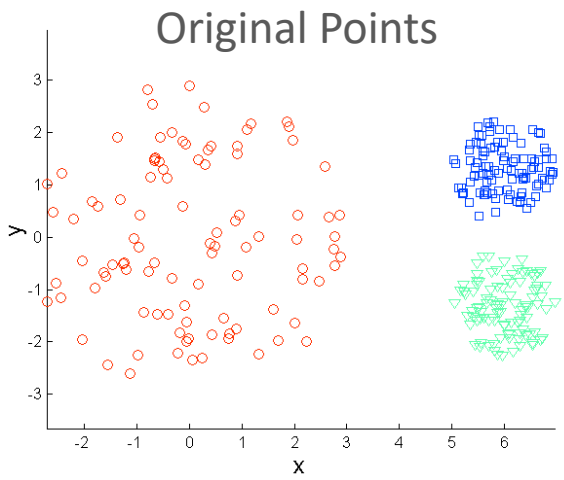
Limitations of k-means

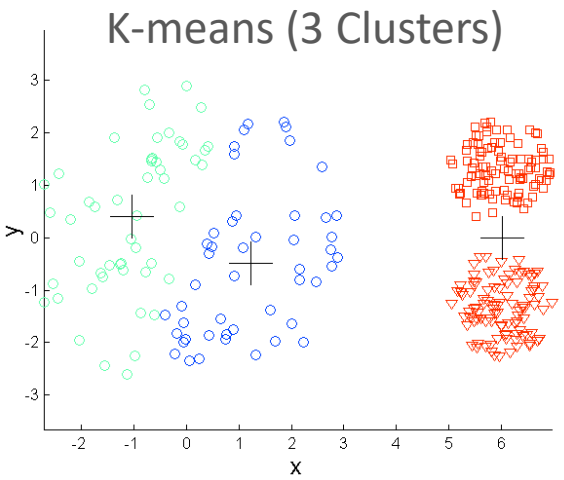
Different sizes





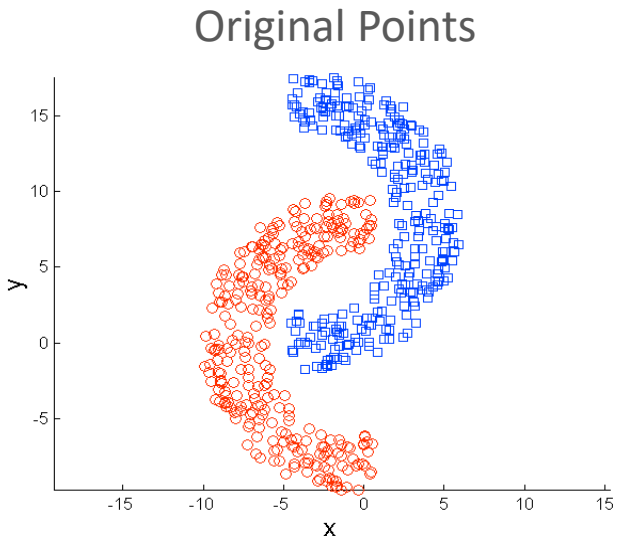
Different densities

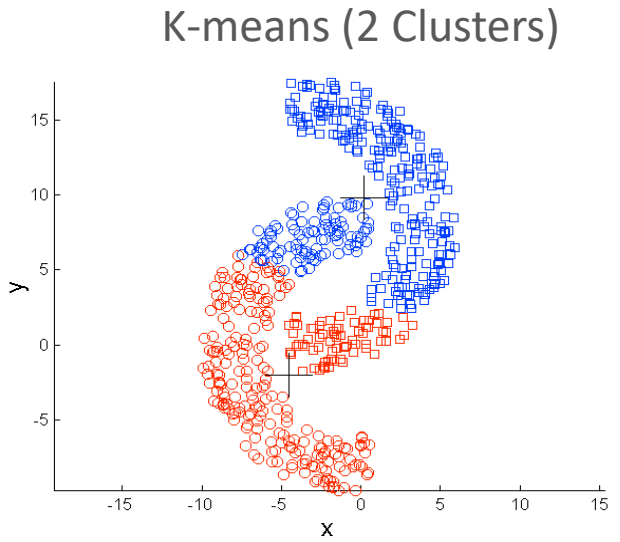




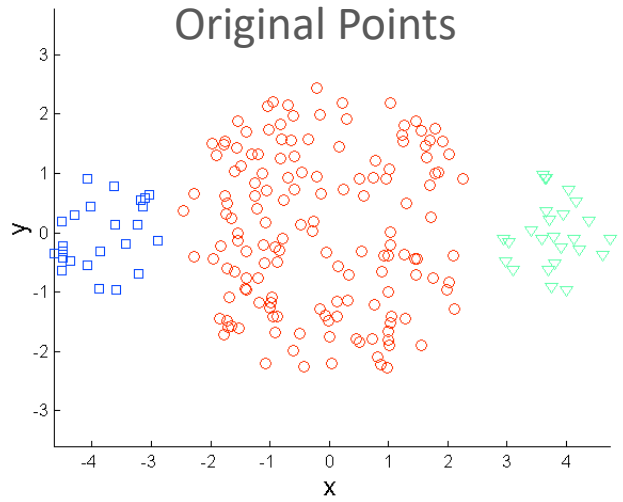
Limitations of k-means

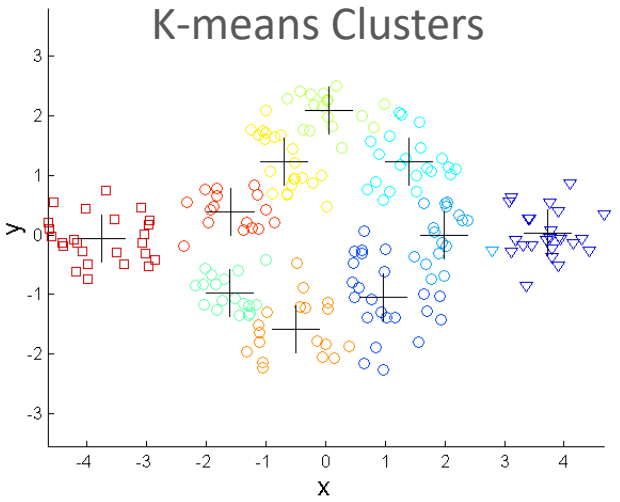
Non-globular shapes



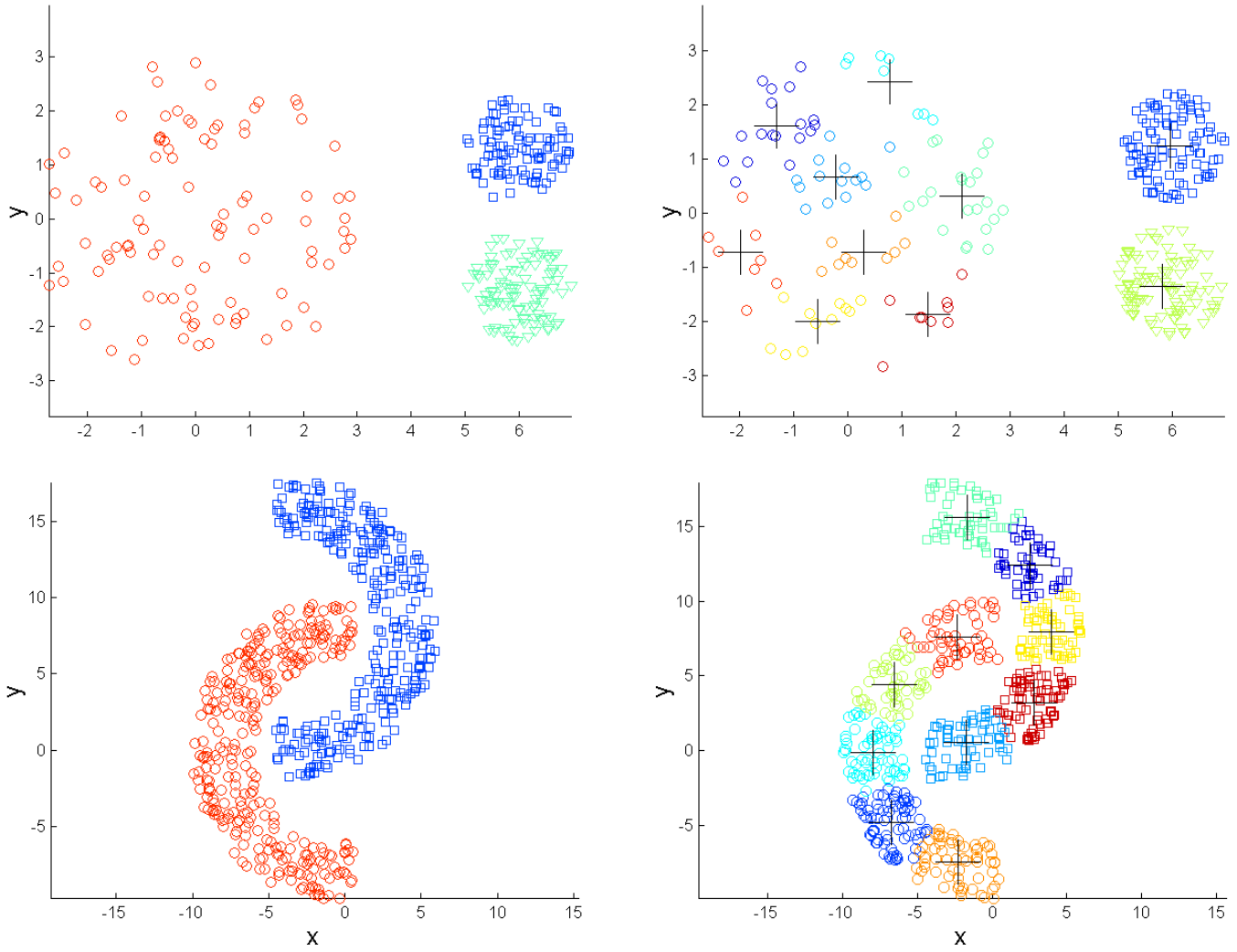


Fixed number of clusters





Overcoming k-means limitations



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EM clustering

- **Expectation maximization** (EM) clustering
  - cluster described by a multivariate distribution
  - observations have a probability of belonging to each cluster
    - **soft** clustering (in contrast with hard clustering)

- Recovering **essentials**
  - **posterior** probability (after the evidence is obtained): $P(cluster = k \mid \mathbf{x})$
  - **Baye's rule** $P(cluster = k|\mathbf{x}) = \frac{P(\mathbf{x}|cluster=k)P(cluster=k)}{P(\mathbf{x})}$
  - **covariance**: direction and strength on how two variables y_i and y_j vary
  - **univariate Gaussian** probability density function, $p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-u}{\sigma}\right)^2}$

Multivariate Gaussian

- A Gaussian distribution in a m-dimensional space is defined as:

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{m/2}|\Sigma|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\mathbf{u})^T \Sigma^{-1}(\mathbf{x}-\mathbf{u})}$$

  - where $\mathbf{u}$ is the m-dimensional mean vector
  - Σ is the $m \times m$ covariance matrix
  - $|\Sigma|$ is the determinant of Σ

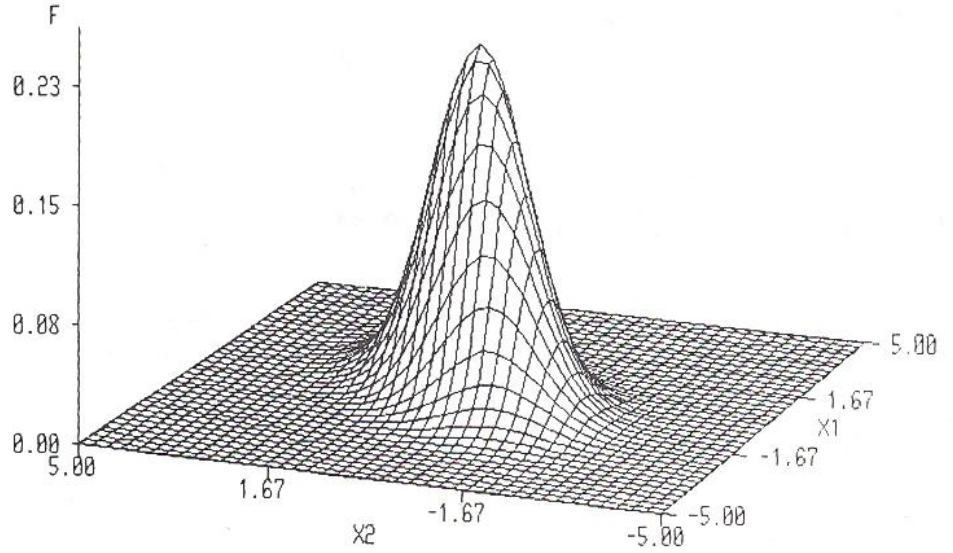
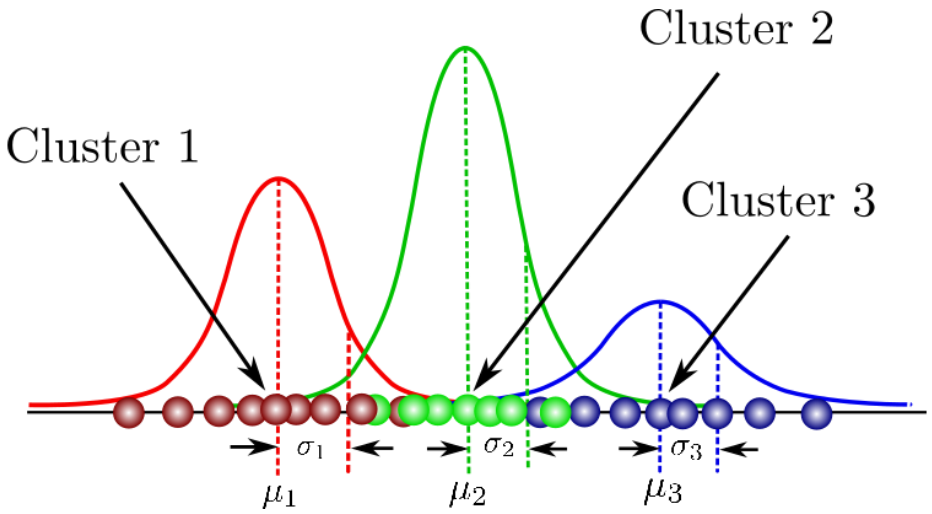
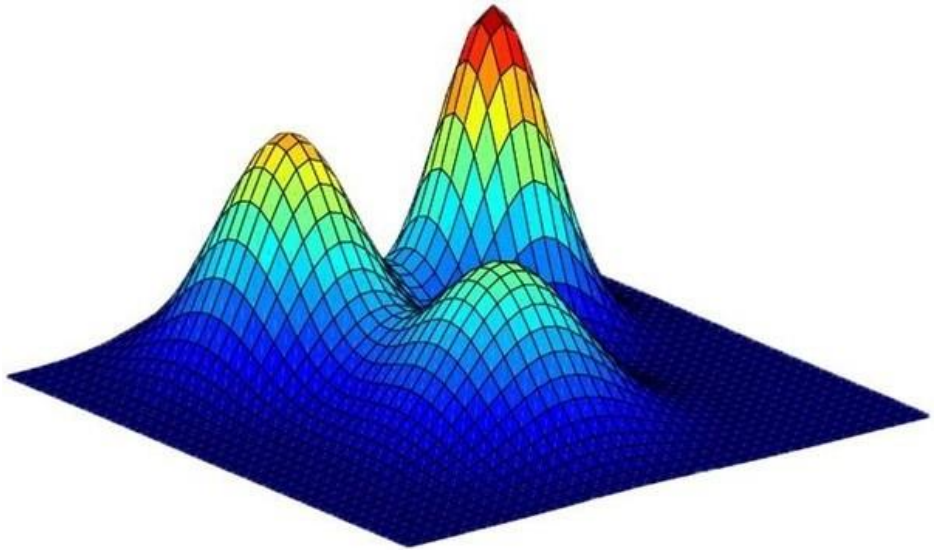


FIG. 7.3. The bivariate normal distribution.

Gaussian mixture

- What kind of probability distribution might have generated the data?
  - clustering presumes that the data are generated from a mixture of distributions





$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \cdot N(\mathbf{x}|\mathbf{u}_k, \Sigma_k) \quad \text{with} \quad \sum_{k=1}^{K} \pi_k = 1$$

Gaussian of cluster c_k

- Univariate density
  - cluster c_k generates x

$$p(x|c_k) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}\left(\frac{x-u_k}{\sigma_k}\right)^2}$$

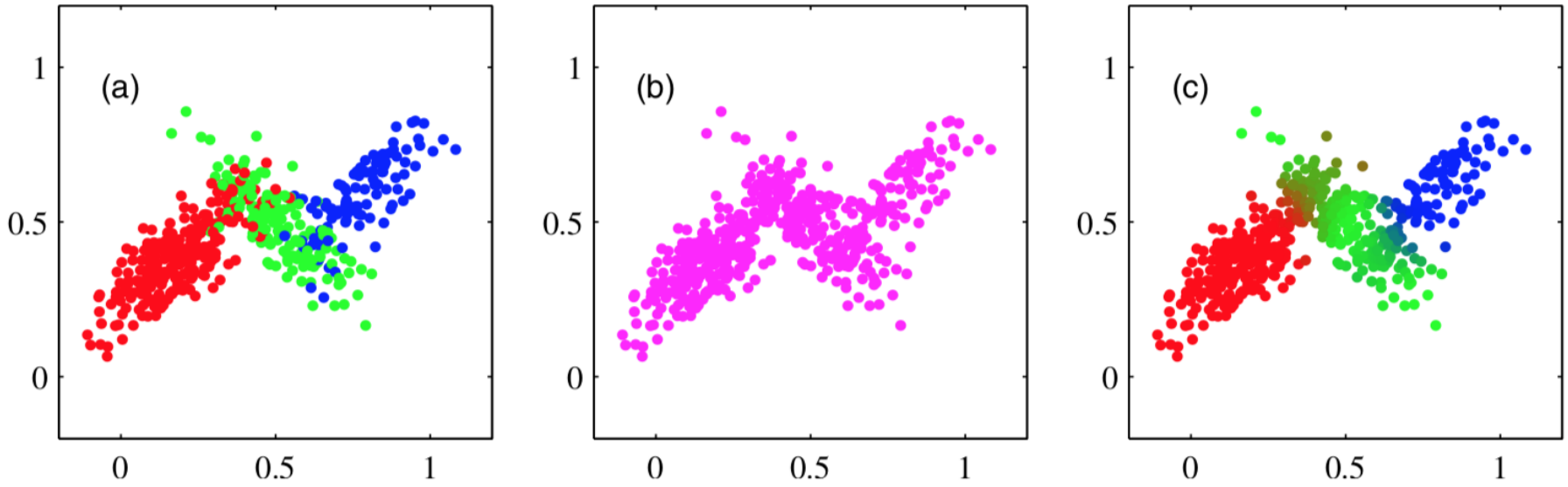
    - where u_k and σ_k are the mean and standard deviation of component c_k

- Multivariate density
  - $\mathbf{x}$ generated by cluster c_k

$$p(\mathbf{x}|c_k) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\mathbf{u}_k)^T \Sigma_k^{-1} (\mathbf{x}-\mathbf{u}_k)}$$

    - where $\mathbf{u}_k$ and Σ_k are the mean vector and covariance matrix of component c_k

Example



(a) three components of the mixture depicted in red, green, and blue

(b) the corresponding samples from the marginal distribution $p(\mathbf{x})$

(c) the same samples in which the colors represent the value of the responsibilities

$$p(c_k \mid \mathbf{x}) = \frac{p(\mathbf{x}|c_k)p(c_k)}{p(\mathbf{x})}$$

Maximum likelihood

- Training set consists on n observations (sample)

$$X = (\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_n)$$

- We can represent the dataset as a design matrix X of size $n \times m$ as before

- The log of the likelihood function is given by

$$\log p(X|\boldsymbol{\pi}, \mathbf{u}, \boldsymbol{\Sigma}) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \pi_k \cdot N(\mathbf{x}|\mathbf{u}_k, \Sigma_k) \right)$$

EM algorithm

- Given a Gaussian mixture model, the goal is to maximize the likelihood function
  - … with respect to the parameters: means, covariances and the mixing coefficients

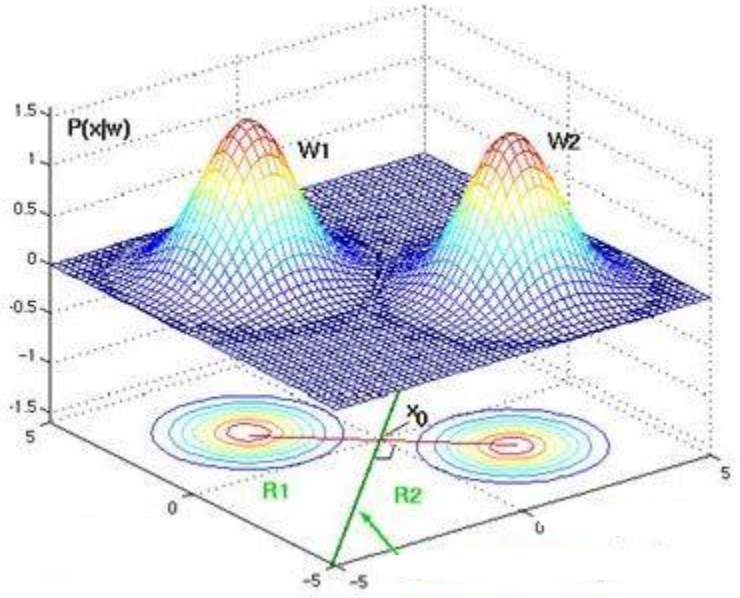
- Four major steps
  - 1. **Initialization**
  - 2. **Expectation**
  - 3. **Maximization**
  - 4. **Evaluate** the log likelihood

$$\log p(X|\boldsymbol{\pi}, \mathbf{u}, \boldsymbol{\Sigma}) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \pi_k \cdot N(\mathbf{x}|\mathbf{u}_k, \Sigma_k) \right)$$

  - if convergence criterion is not satisfied return to step 2

1. Initialization

- We initialize the mixture parameters arbitrarily
  - mean vectors, usually correspond to random points
  - covariance matrices, generally correspond to identity matrix
  - π_k mixing coefficients, generally initialized as $1/K$ (equiprobability)



2. Expectation (E-step)

- Compute for each data point $\mathbf{x}_i$ and each cluster c_k

$$\gamma_{ki} = p(c_k \mid \mathbf{x}_i) = \frac{p(\mathbf{x}_i|c_k)p(c_k)}{p(\mathbf{x}_i)} = \frac{N(\mathbf{x}_i|\mathbf{u}_k, \Sigma_k) \cdot \pi_k}{\sum_k \pi_k N(\mathbf{x}_i|\mathbf{u}_k, \Sigma_k)}$$

- As $p(\mathbf{x}_i)$ is invariant to the components, we can compute…

$$p(c_k, \mathbf{x}_i) = p(\mathbf{x}_i|c_k)p(c_k) = N(\mathbf{x}_i|\mathbf{u}_k, \Sigma_k) \cdot \pi_k$$

and then normalize, $\gamma_{ki} = p(c_k \mid \mathbf{x}_i) = \frac{p(c_k, \mathbf{x}_i)}{\sum_j p(c_j, \mathbf{x}_i)}$

3. Maximization (M-step)

- Each observation $\mathbf{x}_i$ will contribute to update cluster $\mathbf{c}_k$ with weight γ_{ki}
- Accordingly, recalculate the components of the mixture. For each $\mathbf{c}_k$:

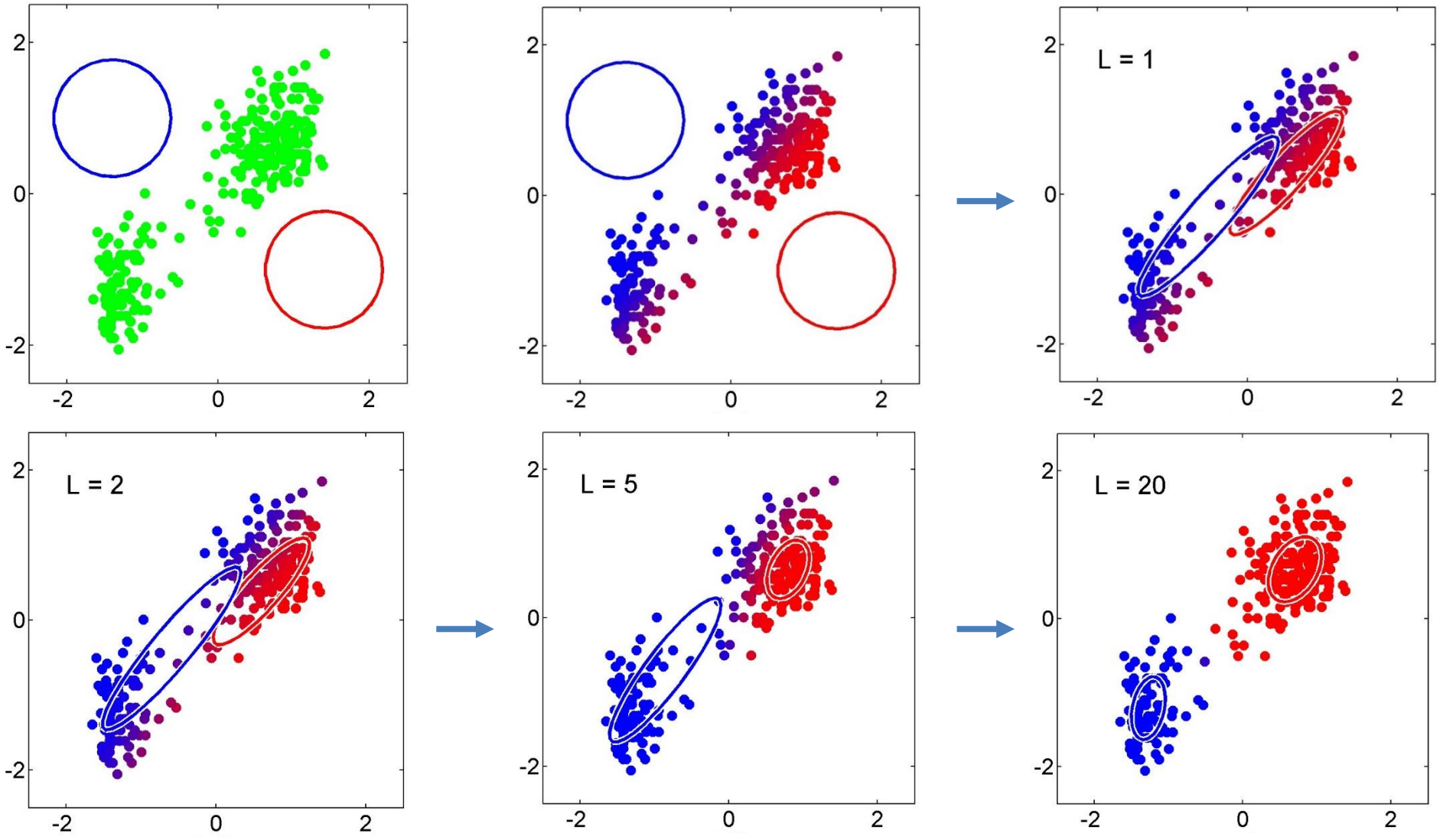
$$N_k = \sum_{i=1}^{n} \gamma_{ki}$$

$$\mathbf{u}_k = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ki} \cdot \mathbf{x}_i$$

$$\Sigma_k = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ki} \cdot (\mathbf{x}_i - \mathbf{u}_k) \cdot (\mathbf{x}_i - \mathbf{u}_k)^T$$

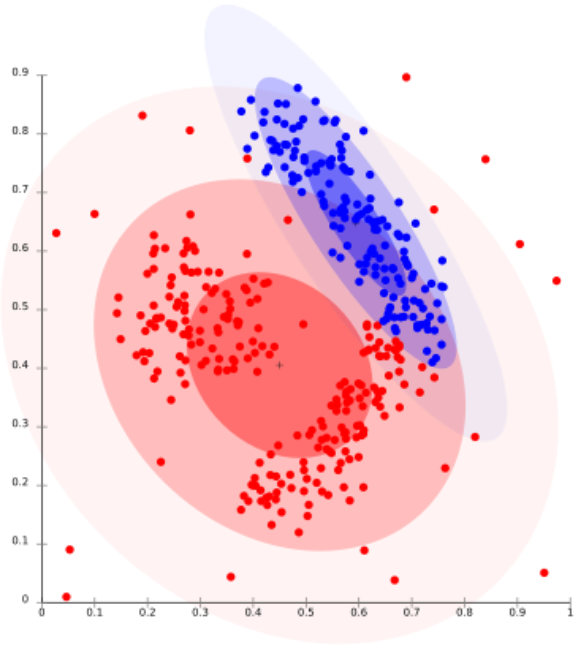
$$\pi_k = p(\mathrm{c}_k) = \frac{N_k}{N}$$

EM example



Challenges

- Gaussian components can shrink to covers just a single point
- When variance goes to zero, likelihood will go to infinity
- Two components can “merge” acquiring identical means and variances and sharing their data points
- Other serious problems, especially in high dimensions



- Extension of EM **beyond Gaussian mixture** assumptions
  - <u>exactly as we work with Bayesian approaches</u>:

    replacing $p(c_k, \mathbf{x}_i)$ by alternative probabilistic views

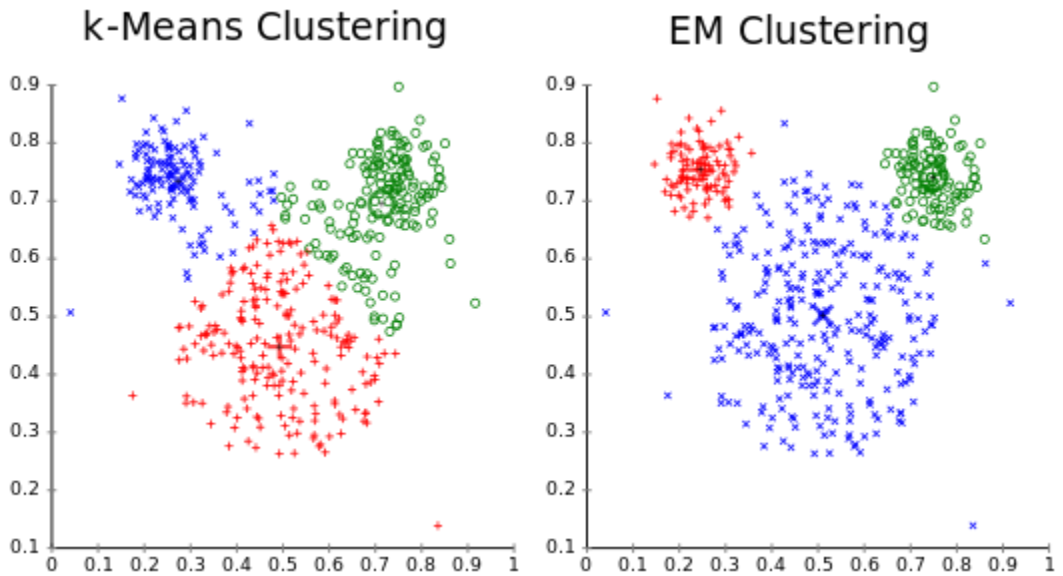
EM exercise

- Given:
  - data $\mathbf{x} = \left\{\begin{pmatrix}2\\2\end{pmatrix}, \begin{pmatrix}0\\2\end{pmatrix}, \begin{pmatrix}0\\0\end{pmatrix}\right\}$
  - two clusters with priors $p(c_k) = \frac{1}{2}$

- *Exercise*: perform one step of the EM under the following assumptions:
  - real-valued data given by **Gaussian mixture** $\mathbf{u}_1 = \begin{pmatrix}2\\2\end{pmatrix}, \mathbf{u}_2 = \begin{pmatrix}0\\0\end{pmatrix}, \Sigma_1 = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}, \Sigma_2 = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$
  - independent $\{0,1,2\}$-ordinal variables with **multinomial distribution** $\mathbf{u}_1 = \begin{pmatrix}0.1\\0.2\\0.7\end{pmatrix}, \mathbf{u}_2 = \begin{pmatrix}0.5\\0.3\\0.2\end{pmatrix}$

EM and K-means Clustering

- Practical comparison shows close similarity, yet…
  - *k*-means algorithm performs a **hard assignment** of data points to clusters, in which each data point is associated uniquely with one cluster
    - in *k*-means the shape of the cluster is described by Euclidean distance function…
  - EM algorithm makes a **soft assignment** based on the posterior probabilities



Outline

- Introduction to clustering
- Partition-based clustering: *k*-means
- Model-based clustering: EM
- **Evaluation**
  - **external measures: purity**
  - **internal measures: silhouette**
- Advanced aspects

Evaluation: clustering validation

- 3 kinds of validity measures: external, internal and relative indexes
- **External criteria** (supervised): extent to which cluster labels match **pre-specified structure**
  - requires prior or expert knowledge
- **Internal criteria** (unsupervised): goodness without external information
  - how well they are separated (e.g. silhouette)
  - should be independent from algorithm-specific functions (unbiased)
- **Relative**: compare different cluster structures (different parameters or algorithms)

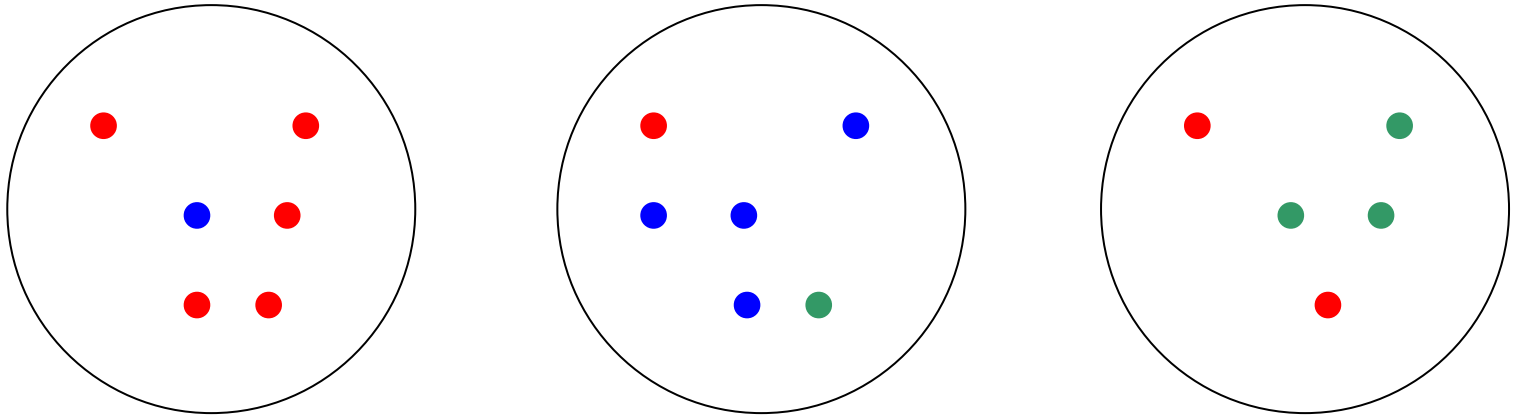
External measures: purity

- $\{C_1, C_2, \ldots, C_K\}$ is the set of clusters
  $\{L_1, L_2, \ldots, L_G\}$ is the set of reference classes

$$purity = \frac{1}{n}\sum_{k=1}^{K} \max_j(|C_k \cap L_j|)$$

- **Problem**: biased $\Rightarrow K = n$ clusters minimize error
- **Alternative**: entropy of classes in clusters (or mutual information between classes and clusters)

External measures: purity



cluster I *cluster II* *cluster III*

$$purity = \frac{1}{17}(max(1,0,5) + max(4,1,1) + max(0,3,2)) = \frac{12}{17}$$

$$purity(C_1) = \frac{5}{6}, \qquad purity(C_2) = \frac{4}{6}, \qquad purity(C_3) = \frac{3}{5}$$

Internal criteria

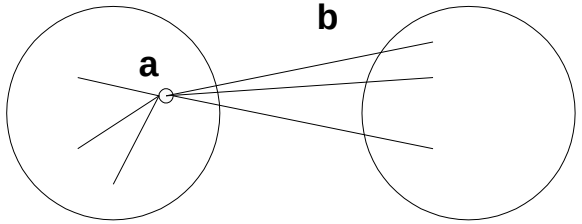
- There are two major internal criteria [Berry and Linoff, 1996]
  - **compactness** (cohesion)
    - the members of each cluster should be as close to each other as possible
    - a common measure of compactness is the variance, which should be minimized
  - **separation**
    - the clusters themselves should be widely spaced

Internal measures: silhouette

- Silhouette combines both **cohesion** and **separation**
- Calculated for a specific object $\mathbf{x}_i$
  - $a(\mathbf{x}_i)$= average distance of $\mathbf{x}_i$ to the points in its cluster
  - $b(\mathbf{x}_i)$ = min (average distance of $\mathbf{x}_i$ to points in another cluster)
  - the silhouette coefficient for a point is then given by

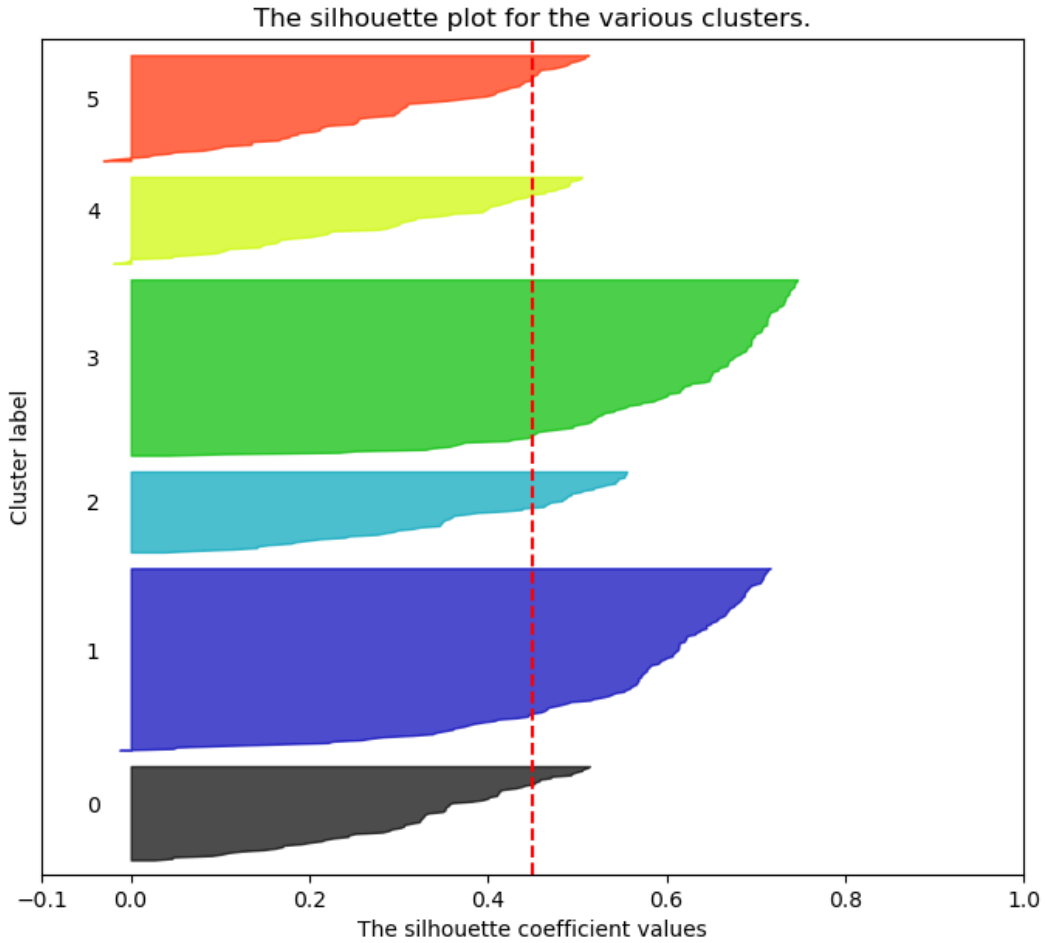
$$s(\mathbf{x}_i) = 1 - a(\mathbf{x}_i)/b(\mathbf{x}_i) \text{ if } a < b, \quad (\text{or } s = b/a - 1 \text{ if } a \geq b, \text{ not the usual case})$$

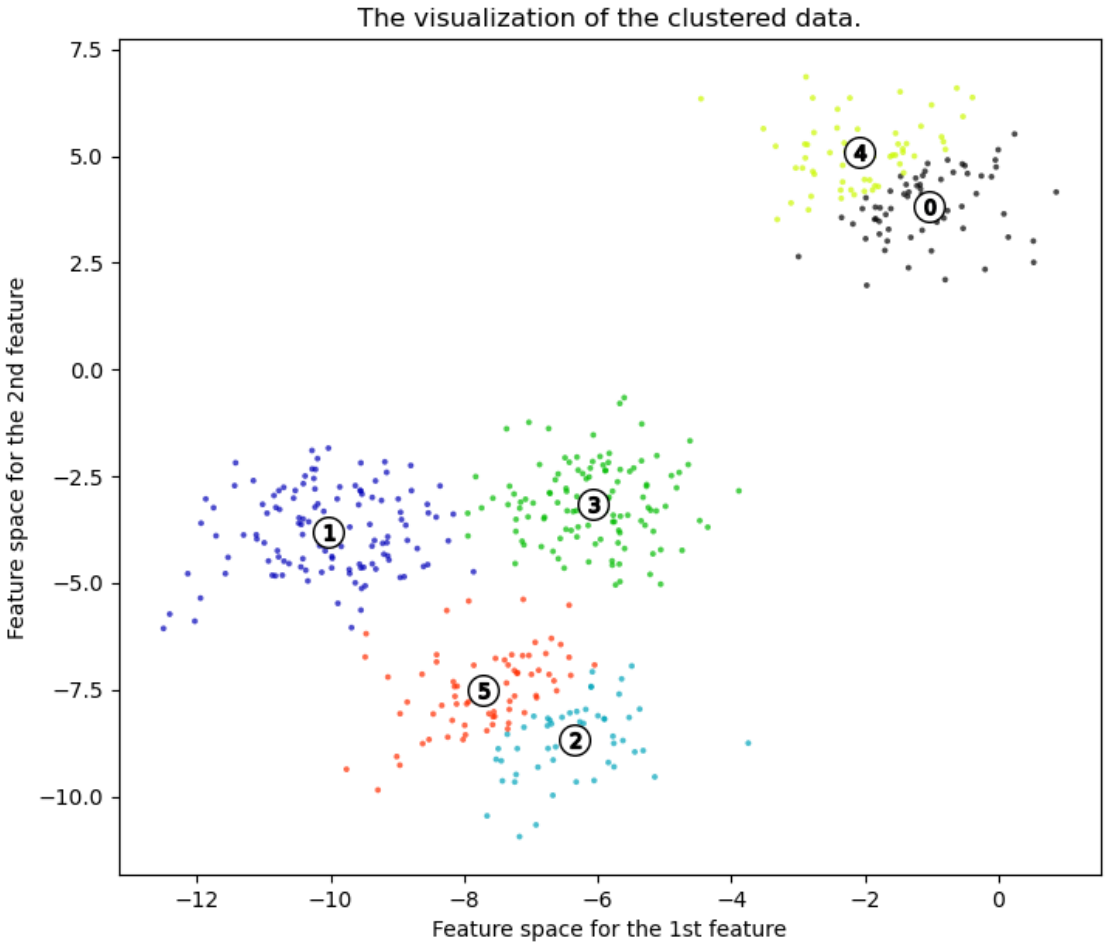
between -1 and 1 (the closer to 1 the better)



- Silhouette of **cluster**: average of observation silhouettes
- Silhouette of **clustering solution**: average of cluster silhouettes

Internal measures: silhouette





Dunn index (*optional*)

- Dunn index D_K, a cluster validity index originally proposed for *k*-means [Dunn, 1974]
  - ***compact*** and ***well-separated*** clusters

$$d(C_1, C_2) = \min_{\mathbf{x}_i \in C_1, \mathbf{x}_j \in C_2} d(\mathbf{x}_i, \mathbf{x}_j)$$

$$diam(C) = \max_{\mathbf{x}_i, \mathbf{x}_j \in C} d(\mathbf{x}_i, \mathbf{x}_j)$$

$$D_K = \frac{\min_{1 \le i < j \le K} d(C_i, C_j)}{\max_{1 \le i \le K} \{diam(C_i)\}}$$

Dunn index (*optional*)

- If the dataset contains compact and well-separated clusters:
  - the ***distance*** between the clusters is expected to be *large*
  - the ***diameter*** of the clusters is expected to be *small*
- Large values of the index indicate the presence of compact and well-separated clusters
- D_K can be **normalized** to more easily compare solutions
- Silhouette and D_k do not exhibit any trend with respect to number of clusters
  - the maximum in a plot with the indices against the number of clusters K offer an indication of the best number of clusters that fits the data

- Challenges:
  - considerable amount of time to compute silhouette and D_K
  - sensitive to the presence of noise and outliers in data

Davies-Bouldin (*optional*)

- Revision: Davies-Bouldin (DB) index (1979)

$$DB_K = \frac{1}{K}\sum_{i=1}^{K} \max_{(i,j),\, i \neq j} \left\{ \frac{diam(C_i) + diam(C_j)}{d(\boldsymbol{c}_i, \boldsymbol{c}_j)} \right\}$$

  - in contrast to D_K, small DB_K indexes correspond to good clusters, i.e. compact with centers far away
  - similarly to D_K, DB_K index exhibits no trends with respect to the number of clusters

Distances and diameters (*optional*)

- Different distances
  - **single** linkage
  - **complete** linkage
  - comparison of **centroids**
  - **average** linkage (default in silhouette)

$$d(C_1, C_2) = \min_{\mathbf{x}_i \in C_1, \mathbf{x}_j \in C_2} d(\mathbf{x}_i, \mathbf{x}_j)$$

$$d(C_1, C_2) = \max_{\mathbf{x}_i \in C_1, \mathbf{x}_j \in C_2} d(\mathbf{x}_i, \mathbf{x}_j)$$

$$d(C_1, C_1) = d(\boldsymbol{c}_1, \boldsymbol{c}_2)$$

$$d(C_1, C_2) = \frac{1}{|C_1| \times |C_2|} \sum_{\mathbf{x}_i \in C_1} \sum_{\mathbf{x}_j \in C_2} d(\mathbf{x}_i, \mathbf{x}_j)$$

- Different diameters
  - **maximum**
  - **radius**
  - **average distance**

$$diam(C) = \max_{\mathbf{x}_i, \mathbf{x}_j \in C} d(\mathbf{x}_i, \mathbf{x}_j)$$

$$diam(C) = \max_{\mathbf{x}_i \in C} d(\mathbf{x}_i, \mathbf{c})$$

$$diam(C) = \frac{1}{\frac{(|C|-1)\,|C|}{2}} \sum_{\substack{\mathbf{x}_i, \mathbf{x}_j \in C \\ i<j}} d(\mathbf{x}_i, \mathbf{x}_j)$$

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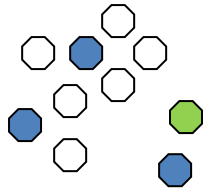
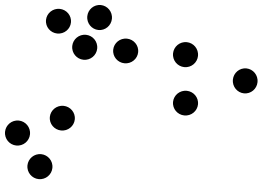
Clustering variants

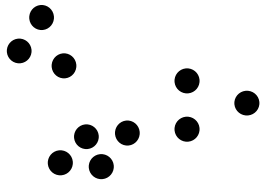
- **Semi-supervised clustering**
  - cluster observations when:
    - labels of some observations may be known **or**
    - pairs of observations are known to belong to the same cluster



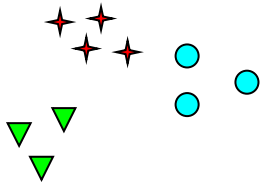
- Separation of clusters: exclusive versus **non-exclusive** (overlapping clusters)
- Hard versus **soft clustering** (each object has a membership for every cluster)
- Complete versus **partial clustering** (observations may not belong to clusters)
- Uniform versus **weighted attributes**

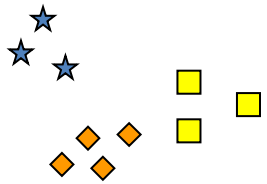
Number of clusters?



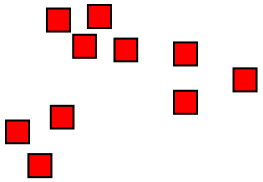


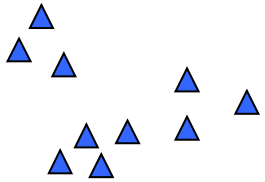
How many clusters?



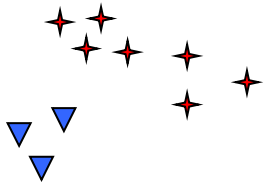


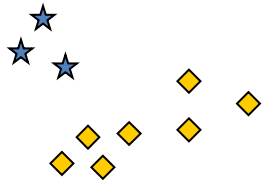
Six Clusters





Two Clusters





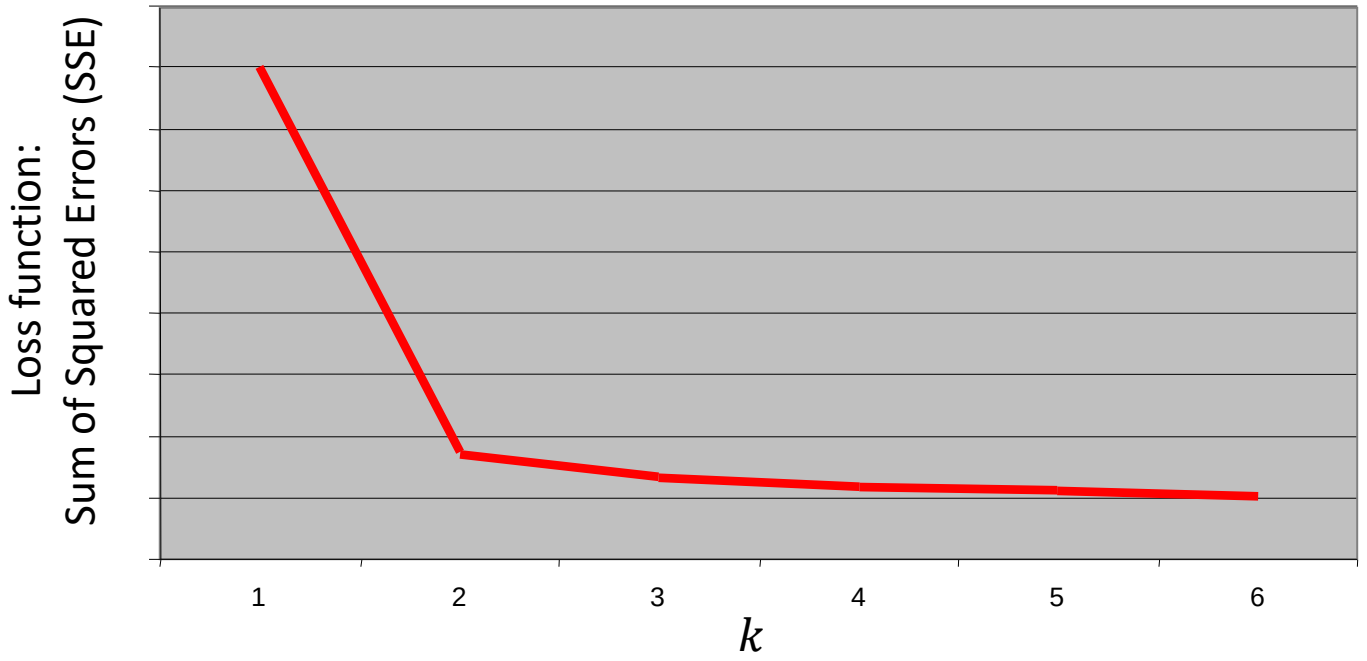
Four Clusters

Number of clusters

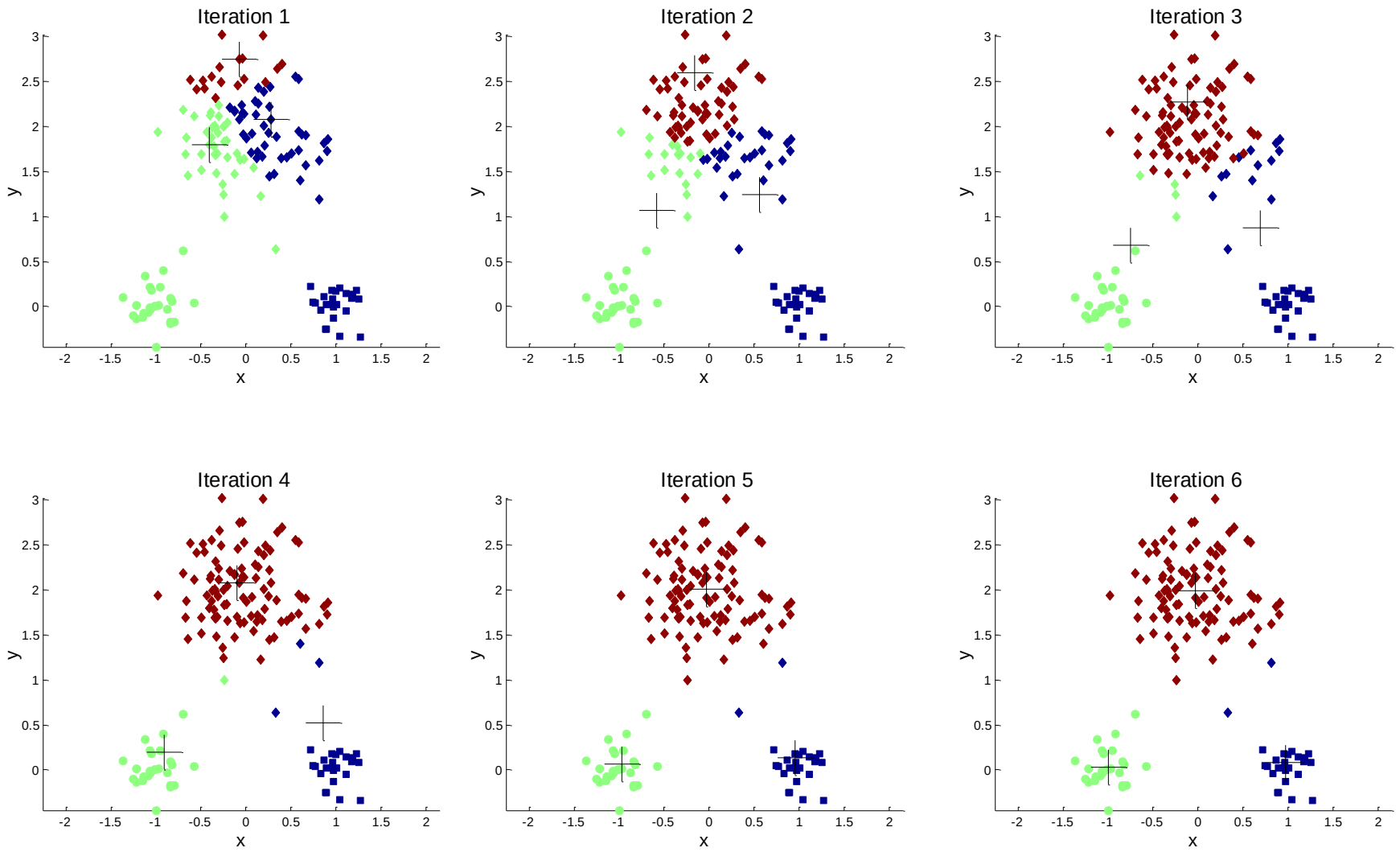
Knee/elbow finding:

- plot the squared loss function values for different k
- abrupt changes are highly suggestive => $k = 2$ clusters in the example belos

Alternatives: many others including k that maximizes internal indices (e.g. silhouette)

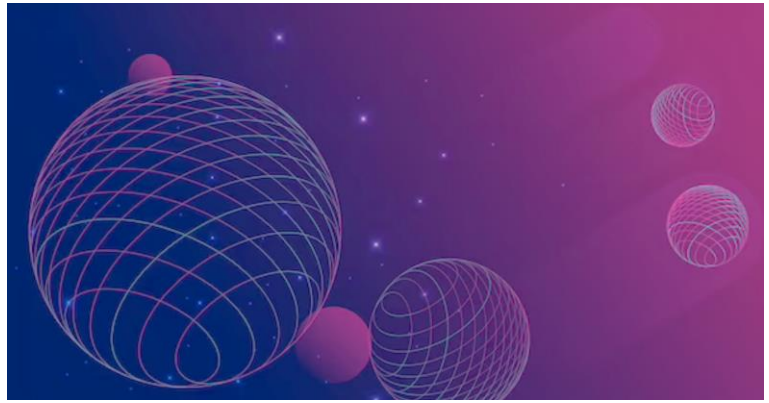


Importance of seeding initial centroids



Initialization

- Many alternatives for seeding
  - **run clustering multiple times** with varying seeds and select the best solution
  - use the **centroids** of an alternative clustering algorithm **as seeds** of the target clustering algorithm
  - **adaptive initialization**
    - choose a maximum *radius* and seed spheres (clusters) with the given radius
    - a data point becomes a new cluster seed if not covered by the existing spheres
      - K-MAI clustering (Wichert et al. 2003)
  - **alternatives**?



Pre- and post-processing

- **Pre-processing**
  - normalize data
  - data reduction and transformation
  - remove outliers

- **Post-processing**
  - eliminate small clusters that may represent outliers
  - split '*loose*' clusters (clusters with relatively high SSE)
  - merge clusters that are 'close' (clusters with relatively low SSE)
  - these steps can be integrated within the clustering process

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Thank You

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