Chapter VIII: Clustering

Information Retrieval & Data Mining
Universität des Saarlandes, Saarbrücken
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Chapter VIII: Clustering*

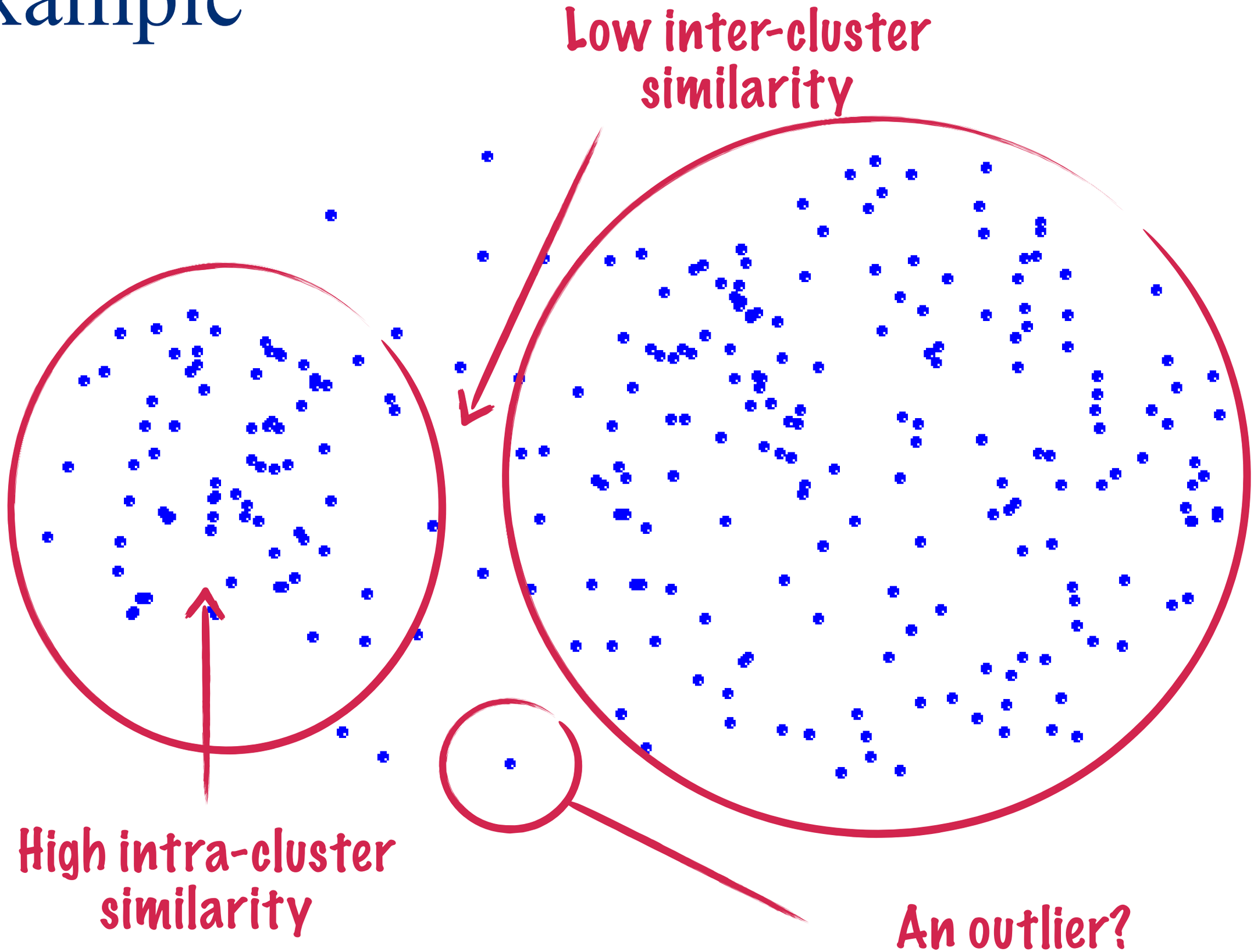
*Zaki & Meira, Chapters 13–15; Tan, Steinbach & Kumar, Chapter 8

1. Basic idea

1. Example

2. Distances between objects

Example


Low inter-cluster similarity
High intra-cluster similarity
An outlier?

The clustering task

- Given a set U of objects and a distance $d: U^2 \rightarrow R^+$ between them, group objects of U into **clusters** such that the distance between points in the same cluster is low and the distance between the points in different clusters is large
  - Small and large are not well defined
  - Clustering can be
    - **exclusive** (each point belongs to exactly one cluster)
    - **probabilistic** (each point-cluster pair is associated with a probability of the point belonging to that cluster)
    - **fuzzy** (each point can belong to multiple clusters)
  - Number of clusters can be pre-defined or not

On distances

- A function $d: U^2 \rightarrow R^+$ is a **metric** if:
  - $d(u,v) = 0$ if and only if $u = v$ — Self-similarity
  - $d(u,v) = d(v,u)$ for all $u, v \in U$ — Symmetry
  - $d(u,v) \leq d(u, w) + d(w, v)$ for all u, v, and $w \in U$ — Triangle inequality
- A metric is a **distance**; if $d: U^2 \rightarrow [0, a]$ for some positive a, then $a - d(u,v)$ is **similarity**
- Common metrics:
  - L_p: $\left(\sum_{i=1}^{d} |u_i - v_i|^p\right)^{\frac{1}{p}}$ for d-dimensional space
    - L_1 = Hamming = city-block; L_2 = Euclidean
  - Correlation distance: $1 - \varphi$
  - Jaccard distance: $1 - |A \cap B| / |A \cup B|$

More on distances

- For all-numerical data, the **sum of squared errors** (SSE) is the most common one
  - SSE: $\sum_{i=1}^{d} |u_i - v_i|^2$
- For all-binary data, either Hamming or Jaccard is used
- For categorical data either
  - first convert the data to binary by adding one binary variable per category label and then use Hamming; or
  - count the agreements and disagreements of category labels with Jaccard
- For mixed data, some combination must be used

Implicit distance and distance matrix

$$\begin{pmatrix} 0 & d_{1,2} & d_{1,3} & & d_{1,n} \\ d_{1,2} & 0 & d_{2,3} & \cdots & d_{2,n} \\ d_{1,3} & d_{2,3} & 0 & & d_{3,n} \\ & \vdots & & \ddots & \vdots \\ d_{1,n} & d_{2,n} & d_{3,n} & \cdots & 0 \end{pmatrix}$$

A **distance** (or **dissimilarity**) **matrix** is

- n-by-n for n objects
- non-negative ($d_{i,j} \geq 0$)
- symmetric ($d_{i,j} = d_{j,i}$)
- zero on diagonal ($d_{i,i} = 0$)

2. Representative-based clustering

1. Partitions and prototypes
2. The *k*-means algorithm
   - 2.1. Basic algorithm
   - 2.2. Analysis
   - 2.3. The *k*-means++ algorithm
3. The EM clustering algorithm
   - 3.1. 1-D Gaussian
   - 3.2. General Gaussian
   - 3.3. The *k*-means as EM
4. How to select the *k*

Partitions and prototypes

- Exclusive representative-based clustering:
  - The set of objects U is partitioned into k clusters $C_1, C_2, ..., C_k$
    - $\cup_i C_i = U$ and $C_i \cap C_j = \emptyset$ for $i \neq j$
  - Each cluster is represented by a prototype (also called centroid or mean) $\boldsymbol{\mu}_i$
    - Prototype does not have to be (and usually is not) one of the objects
  - Clustering quality is based on sum of squared errors between objects in cluster and cluster prototype

$$\sum_{i=1}^{k} \sum_{x_j \in C_i} \|\mathbf{x}_j - \boldsymbol{\mu}_i\|_2^2 = \sum_{i=1}^{k} \sum_{x_j \in C_i} \sum_{l=1}^{d} (x_{jl} - \mu_{il})^2$$

Over all clusters

Over all objects in this cluster

Over all dimensions

The naïve algorithm

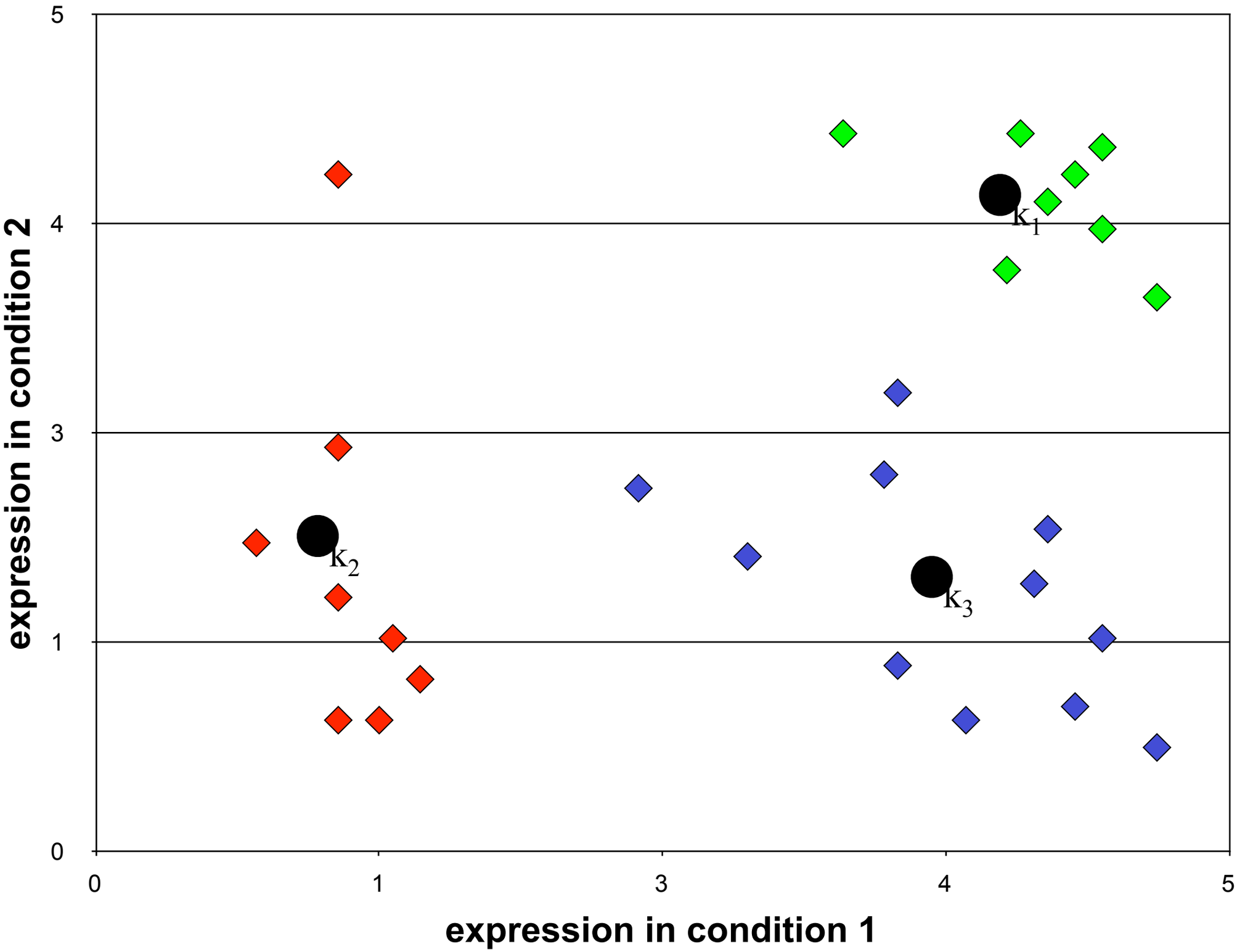
- The naïve algorithm:
  - Generate all possible clusterings one-by-one
  - Compute the squared error
  - Select the best
- But this approach is infeasible
  - There are too many possible clusterings to try
    - k^n different clusterings to k clusters (some possibly empty)
    - The number of ways to cluster n points in k nonempty clusters is the Stirling number of the second kind, $S(n, k)$,

$$S(n,k) = \left\{ {n \atop k} \right\} = \frac{1}{k!} \sum_{j=0}^{k} (-1)^j \binom{k}{j} (k-j)^n$$

An iterative ***k*-means** algorithm

1. select k random cluster centroids
2. assign each point to its closest centroid and compute the error
3. **do**
   - 3.1. **for each** cluster C_i
     - 3.1.1. compute new centroid as $\boldsymbol{\mu}_i = \frac{1}{|C_i|} \sum_{x_j \in C_i} \mathbf{x}_j$
   - 3.2. **for each** element $x_j \in U$
     - 3.2.1. assign x_j to its closest cluster centroid
4. **while** error decreases

k-means example



Some notes on the algorithm

- Always converges eventually
  - On each step the error decreases
  - Only finite number of possible clusterings
  - Convergence to local optimum
- At some point a cluster can become empty
  - All points are closer to some other centroid
  - Some options:
    - Split the biggest cluster
    - Take the furthest point as a singleton cluster
- Outliers can yield bad clusterings

Computational complexity

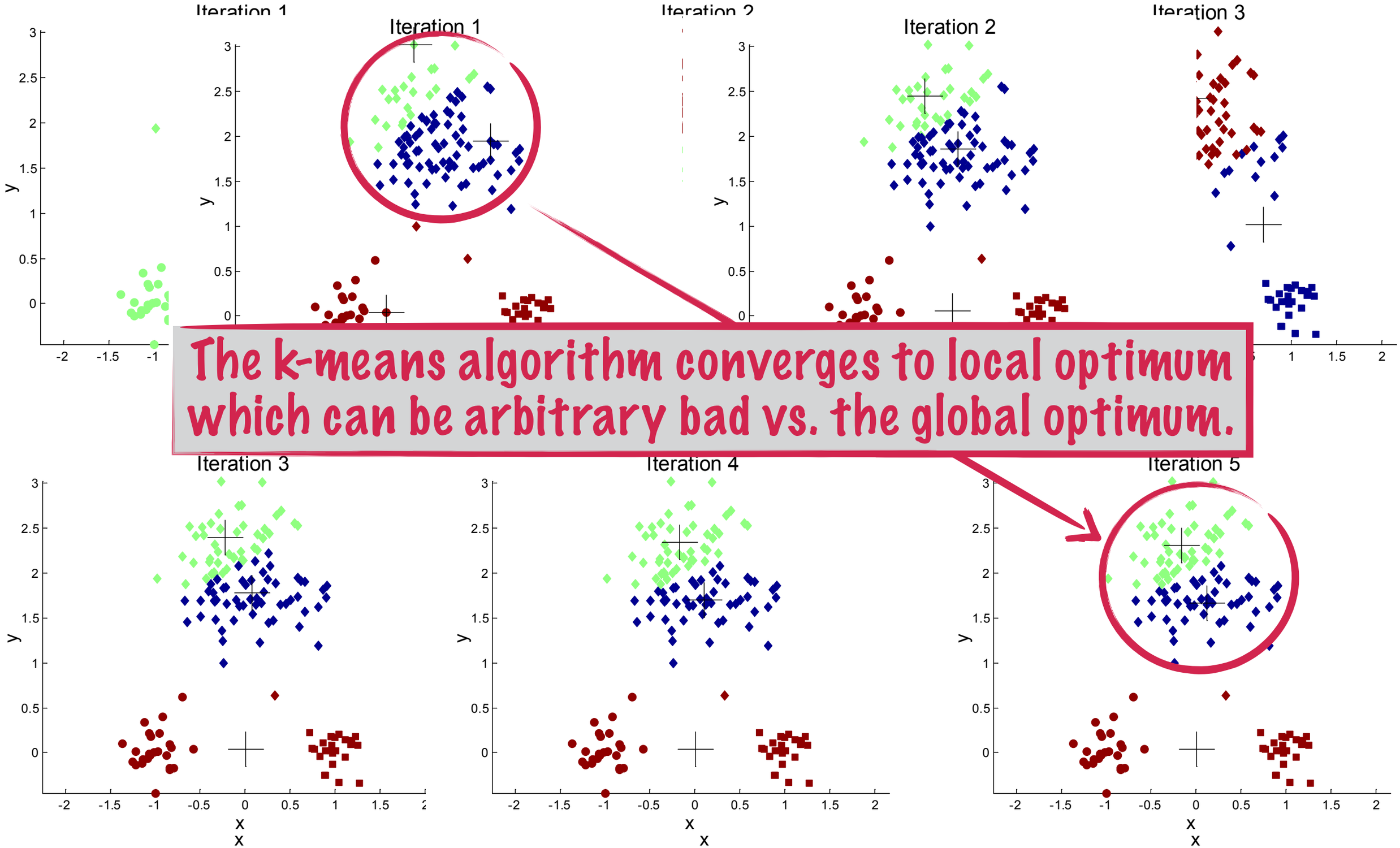
- How long does the iterative *k*-means algorithm take?
  - Computing the centroid takes O(*nd*) time
    - Averages over total of *n* points in *d*-dimensional space
  - Computing the cluster assignment takes O(*nkd*) time
    - For each *n* points we have to compute the distance to all *k* clusters in *d*-dimensional space
  - If the algorithm takes *t* iterations, the total running time is O(*tnkd*)
  - But how many iterations we need?

How many iterations?

- In practice the algorithm doesn't usually take many iterations
  - Some hundred iterations is usually enough
- Worst-case upper bound is $O(n^{dk})$
- Worst-case lower bound is superpolynomial: $2^{\Omega(\sqrt{n})}$

- The discrepancy between practice and worst-case analysis can be (somewhat) explained with smoothed analysis [Arthur & Vassilvitskii '06]:
  - If the data is sampled from independent d-dimensional normal distributions with same variance, iterative k-means algorithm will terminate in time $O(n^k)$ with high probability.

On the importance of initial centroids



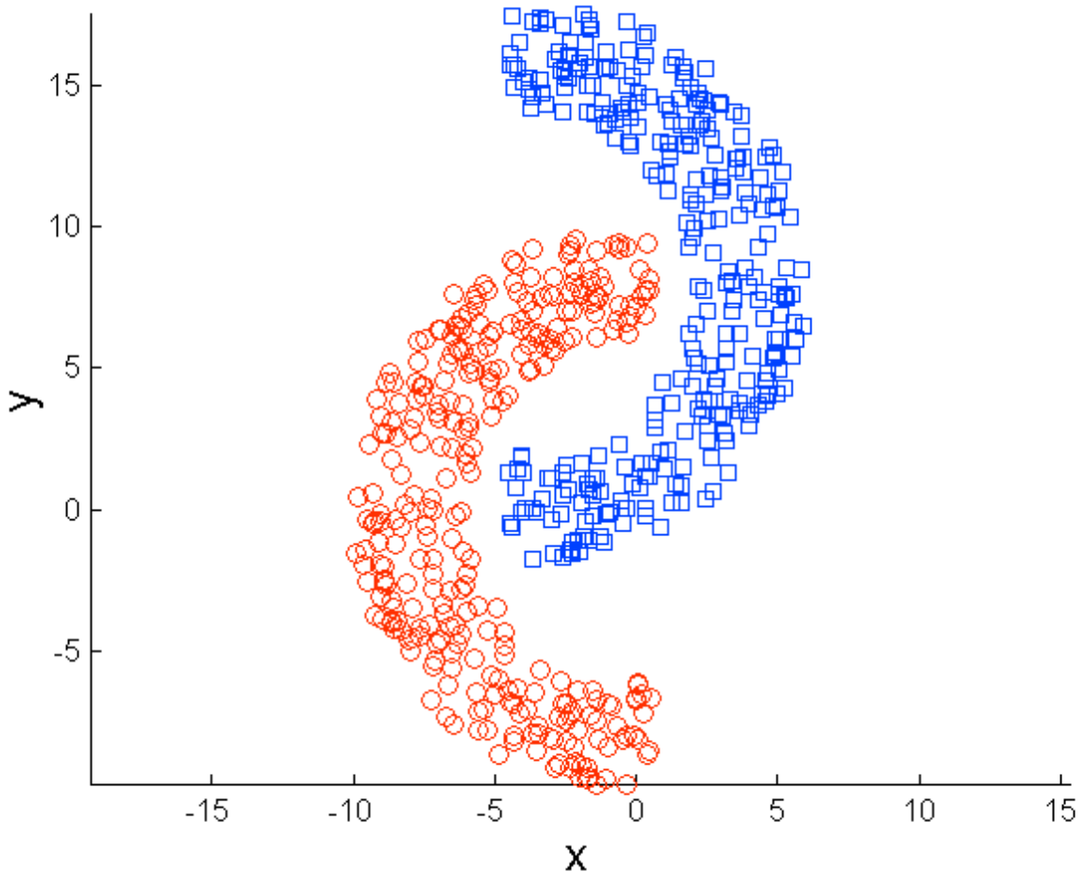
The k-means algorithm converges to local optimum which can be arbitrary bad vs. the global optimum.

The k-means++ algorithm

- Careful initial seeding [Arthur & Vassilvitskii '07]:
  - Choose first centroid u.a.r. from data points
  - Let $D(x)$ be the shortest distance from x to any already-selected centroid
  - Choose next centroid to be x' with probability $\frac{D(x')^2}{\sum_{x \in X} D(x)^2}$
    - Points that are further away are selected more probably
  - Repeat until k centroids have been selected and continue as normal iterative k-means algorithm
- The k-means++ algorithm achieves $O(\log k)$ approximation ratio on expectation
  - $E[\text{cost}] \leq 8(\ln k + 2)\text{OPT}$
- The k-means++ algorithm converges fast in practice

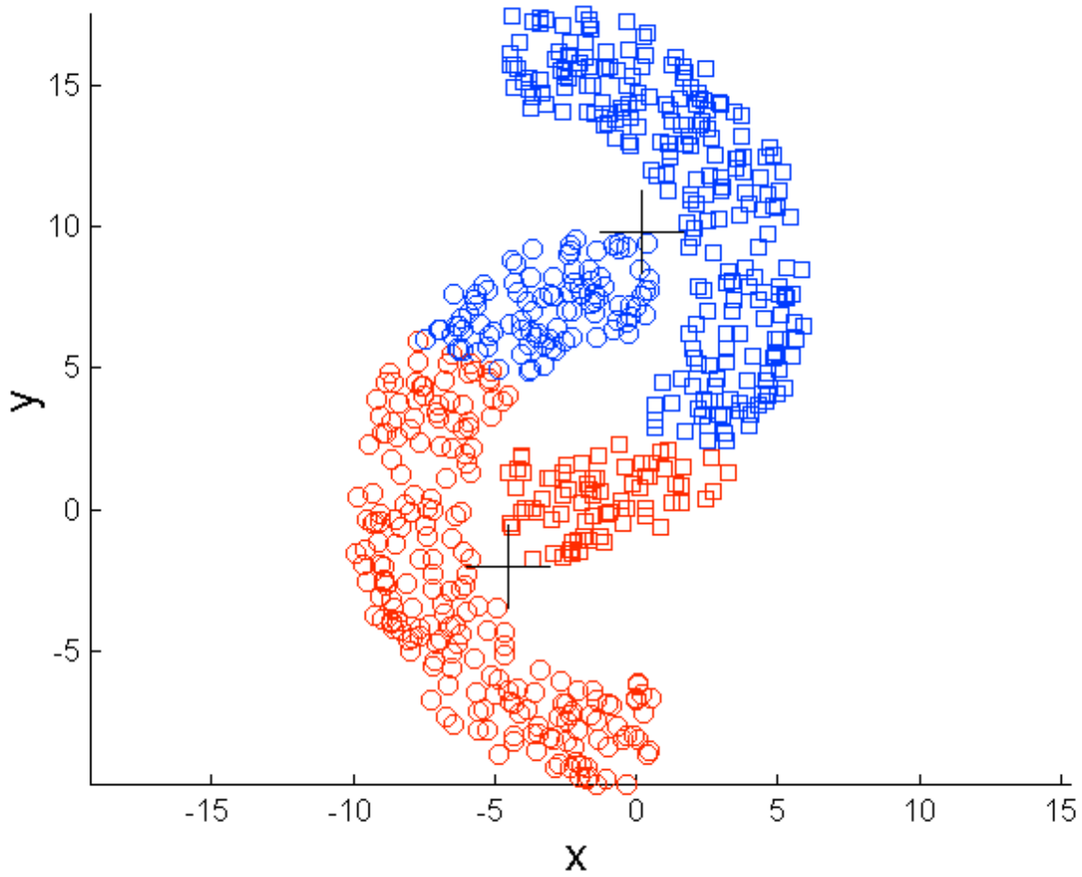
Limitations of cluster types for k-means

- The clusters have to be of roughly equal size
- The clusters have to be of roughly equal density
- The clusters have to be of roughly spherical shape



Original Points

Original Points



K-means (3 Clusters)

K-means (2 Clusters)

The EM clustering algorithm

- Probabilistic clustering
  - I.e. not exclusive
- Representative in a way
  - Each cluster is represented by some parameters
  - The parameters can include cluster centroid
- Requires us to assume something about the distribution of the points
  - For now, each cluster is independent Gaussian
- We use the expectation-maximization approach

The basics

- We aim at finding parameters μ_i and Σ_i for each Gaussian cluster plus k mixture parameters $P(C_i)$ (all together denoted by θ)
  - pdf of point x in cluster i is

$$f_i(\mathbf{x}) = f(\mathbf{x} \mid \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) = (2\pi)^{-\frac{d}{2}} |\boldsymbol{\Sigma}_i|^{-\frac{1}{2}} \exp\left\{ -\frac{(\mathbf{x} - \boldsymbol{\mu}_i)^T \boldsymbol{\Sigma}_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i)}{2} \right\}$$

  - Total pdf of x is a mixture model of the k cluster Gaussians:

$$f(\mathbf{x}) = \sum_{i=1}^{k} f_i(\mathbf{x}) P(C_i) = \sum_{i=1}^{k} f(\mathbf{x} \mid \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) P(C_i)$$

  - The log-likelihood of the data D given parameters θ is then

$$\ln P(D \mid \theta) = \sum_{j=1}^{n} \ln \left(\sum_{i=1}^{k} f(\mathbf{x}_j \mid \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) P(C_i) \right)$$

The general EM clustering algorithm

- Initialization
  - Initialize parameters θ randomly
- Expectation step
  - Compute the posterior probability $P(C_i \mid x_j)$
  - Per Bayes's theorem

$$P(C_i \mid x_j) = \frac{P(x_j \mid C_i)P(C_i)}{\sum_{a=1}^{k} P(x_j \mid C_a)P(C_a)}$$

- Maximization step
  - Re-estimate θ given $P(C_i \mid x_j)$
- Repeat *E* and *M* steps until convergence

EM with Gaussians in 1-D

- Now pdf is $f(x \mid \mu_i, \sigma_i^2) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left\{-\frac{(x-\mu_i)^2}{2\sigma_i^2}\right\}$
- Initialization step
  - Mean μ is sampled u.a.r. from possible values, $\sigma^2 = 1$, and $P(C_i) = 1/k$ (each cluster is equiprobable)
- Expectation step

$$w_{ij} = P(C_i \mid x_j) = \frac{f(x_j \mid \mu_i, \sigma_i^2)P(C_i)}{\sum_{a=1}^{k} f(x_j \mid \mu_a, \sigma_a^2)P(C_a)}$$

- Maximization step

Weighted variance

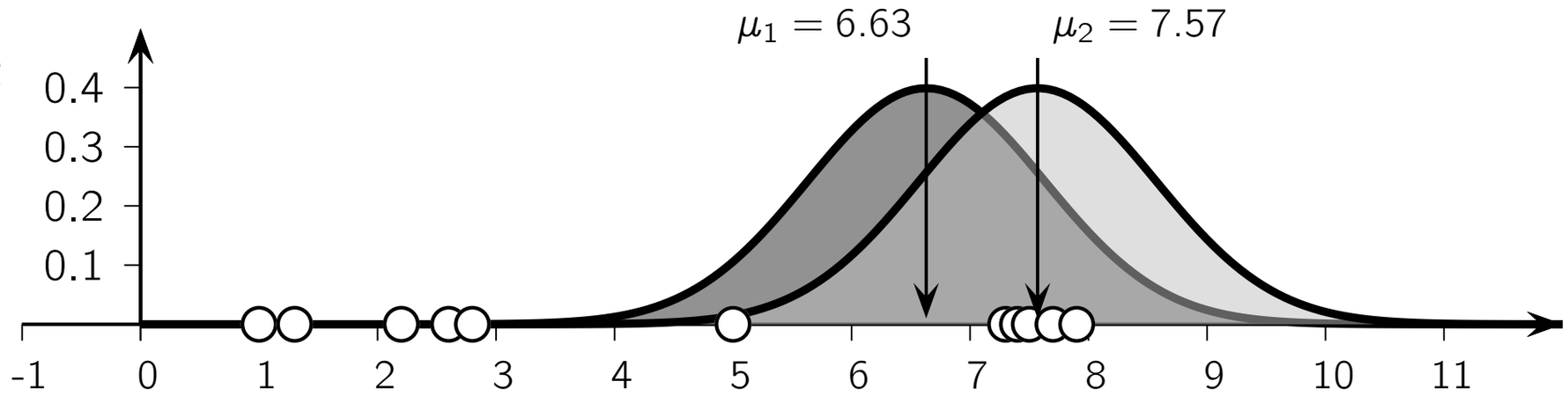
Fraction of weight in cluster i

$$\mu_i = \frac{\sum_{j=1}^{n} w_{ij} x_j}{\sum_{j=1}^{n} w_{ij}} \qquad \sigma_i^2 = \frac{\sum_{j=1}^{n} w_{ij}(x_j - \mu_i)^2}{\sum_{j=1}^{n} w_{ij}} \qquad P(C_i) = \frac{\sum_{j=1}^{n} w_{ij}}{n}$$

Weighted mean

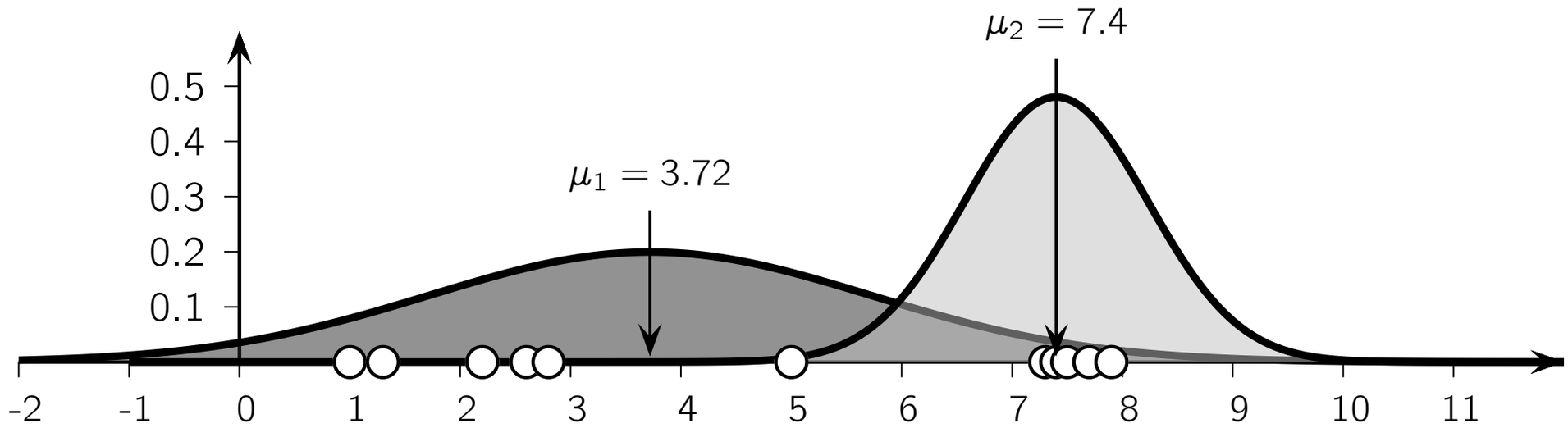
Example

Initialization



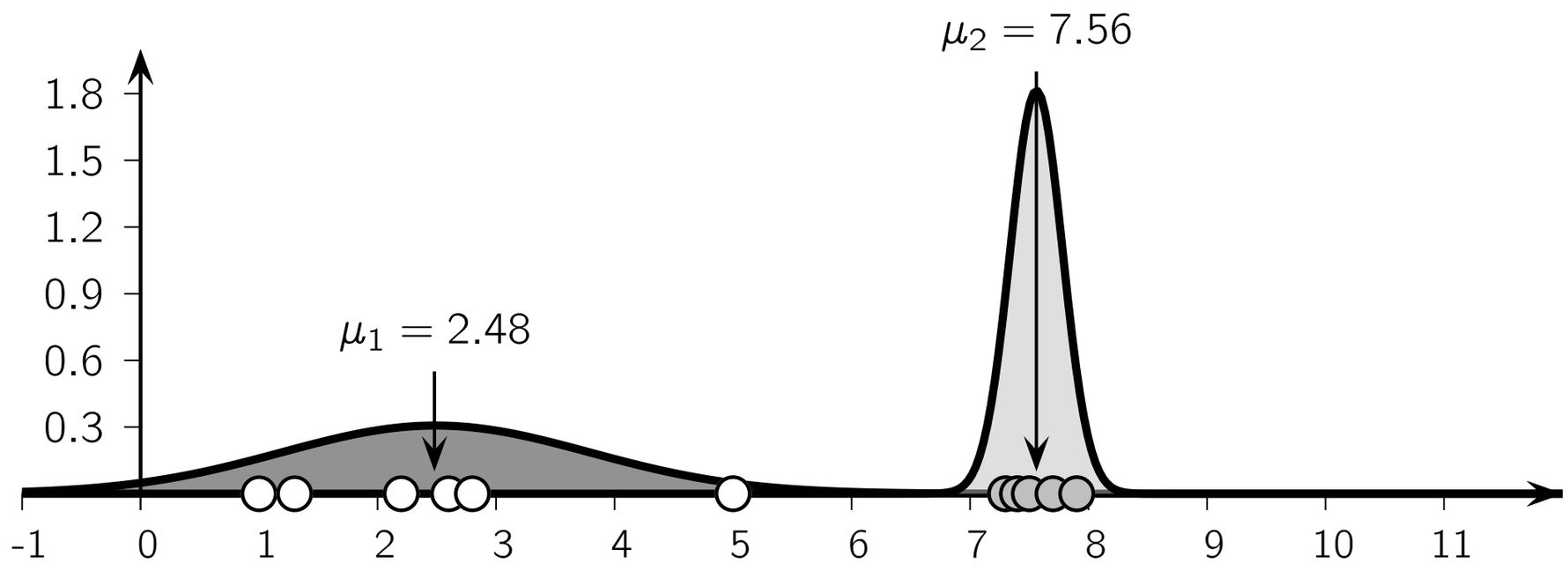
(a) Initialization: $t = 0$

Iteration 1



(b) Iteration: $t = 1$

Iteration 5



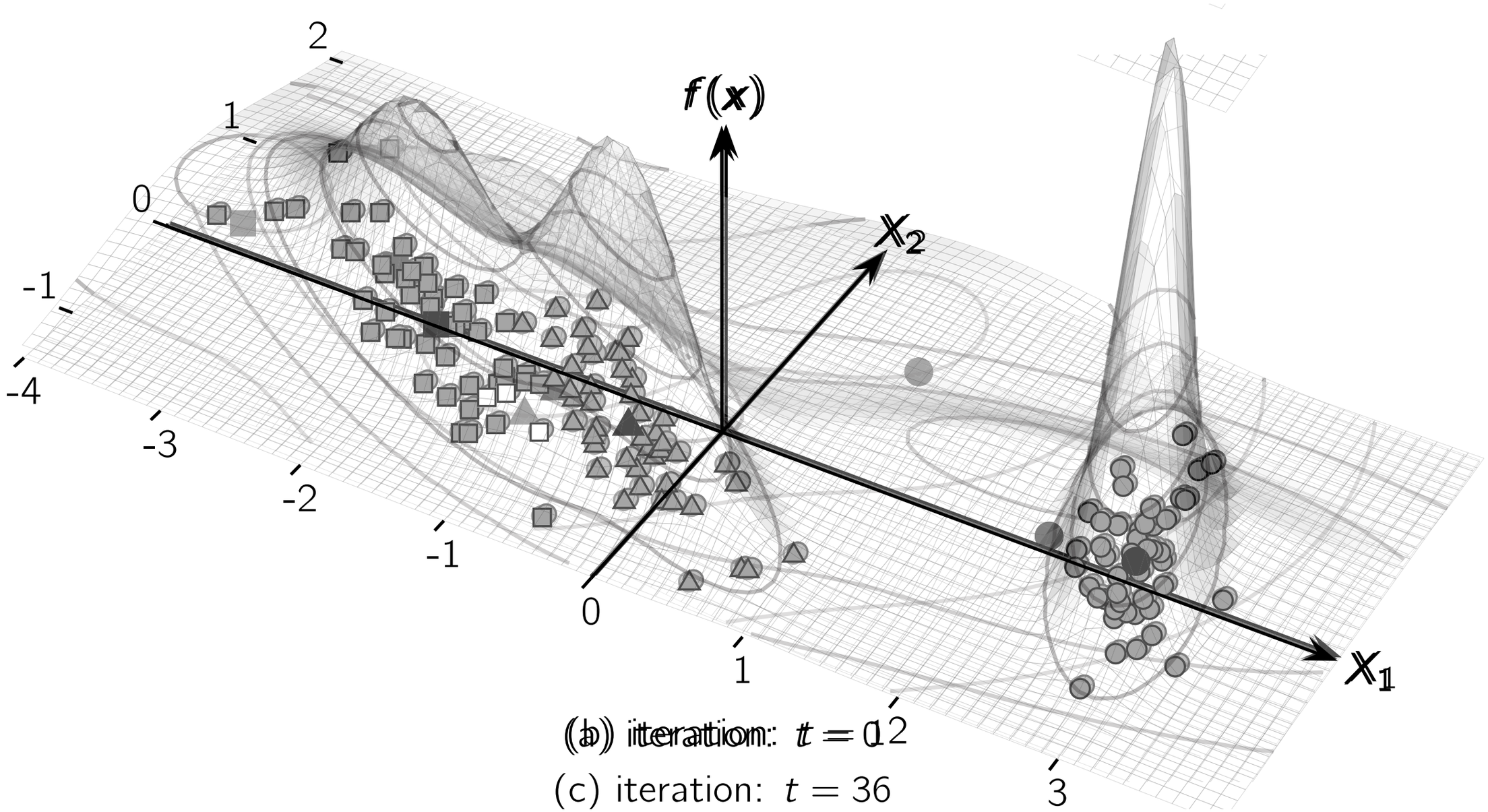
(c) Iteration: $t = 5$ (converged)

EM in *d* dimensions

- The covariance matrix requires $d(d + 1)/2$ parameters to be estimated
  - Often all dimensions are assumed to be independent, yielding d parameters
- The expectation step is as in 1-D
- The mean and prior $P(C_i)$ are estimated as in 1-D
- The variance of cluster i in dimension a is

$$(\sigma_{aa}^{i})^2 = \frac{\sum_{j=1}^{n} w_{ij}(x_{ja} - \mu_{ia})^2}{\sum_{j=1}^{n} w_{ij}}$$

Example



(b) iteration: $t = 12$

(c) iteration: $t = 36$

k-means as EM

- The iterative k-means algorithm can be seen as a special case of EM algorithm using different cluster density function
  - $P(x_j \mid C_i) = 1$ iff centroid i is the closest to point x_j
- The posterior probability is then
  - $P(C_i \mid x_j) = 1$ iff point x_j belongs to cluster i
- The parameters are the centroids and $P(C_i)$
  - The covariance matrix can be ignored

How to select *k*

- Both *k*-means and EM require user to define *k* before the algorithm is run
  - But what if we don't know the *k*?
- The larger the *k*,
  - the smaller the error
  - the more complex the model
  - the higher the risk for over-fitting

Cross-validation

- As with regression:
  - Hold out some random points (test set)
  - Run clustering on the remaining points (training set)
  - Compute the error with test set included
  - Re-iterate with different values of k and select the one with least overall error
- Normally N-fold cross validation
  - Typically $N = 10$
  - Data is divided in N even sized sets
  - Cross-validation is run N times, each time keeping one set as the test set and rest $N - 1$ sets together as the training set

AIC and BIC

- Let ln(L) be the maximized log-likelihood of the clustering (obtained e.g. via EM algorithm)
- Let $p(k)$ be the number of parameters we need for k clusters
  - For Gaussian with independent dimensions, p(k) = $k(d+2)$
    - k clusters, d variances, mean, and mixture parameter $P(C_i)$
- Idea: We need to pay for each new parameter in our model
- In **Akaike Information Criterion** (AIC) we select k that minimizes AIC = $2p(k) - 2\ln(L)$
- In **Bayesian Information Criterion** (BIC) we select k that minimizes BIC = $p(k)\ln(n) - 2\ln(L)$