Clustering
k-mean clustering

Genome 373

Genomic Informatics

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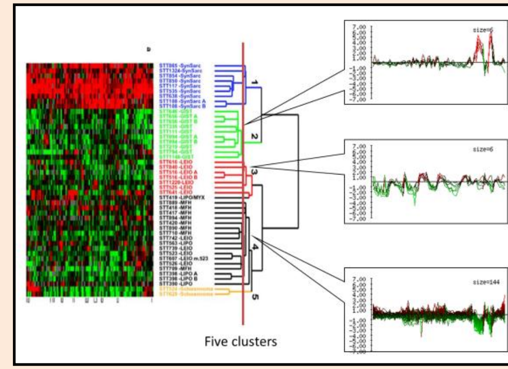
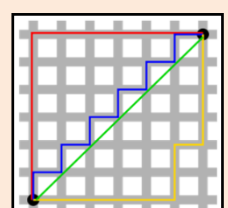
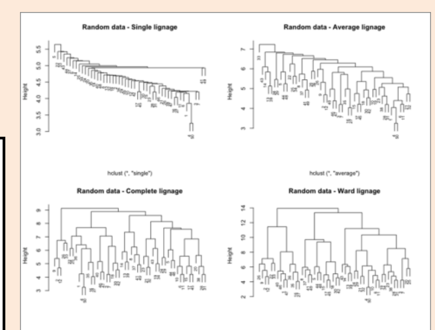
A quick review

- The clustering problem:
  - partition genes into distinct sets with high homogeneity and high separation
  - Clustering (unsupervised) vs. classification



- Clustering methods:
  - Agglomerative vs. divisive; hierarchical vs. non-hierarchical
- **Hierarchical clustering algorithm:**
  1. Assign each object to a separate cluster.
  2. Find the pair of clusters with the shortest distance, and regroup them into a single cluster.
  3. Repeat 2 until there is a single cluster.
- Many possible distance metrics
- **Metric matters**





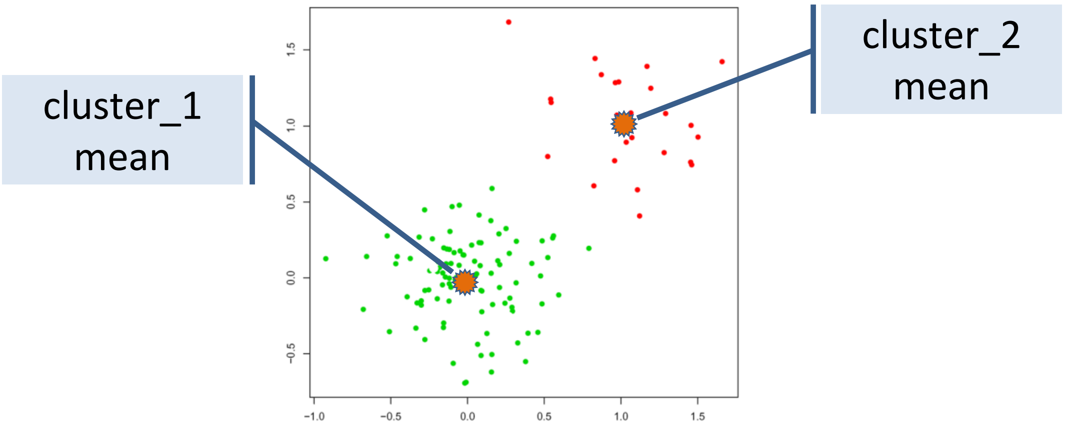
K-mean clustering

Divisive

Non-hierarchical

K-mean clustering

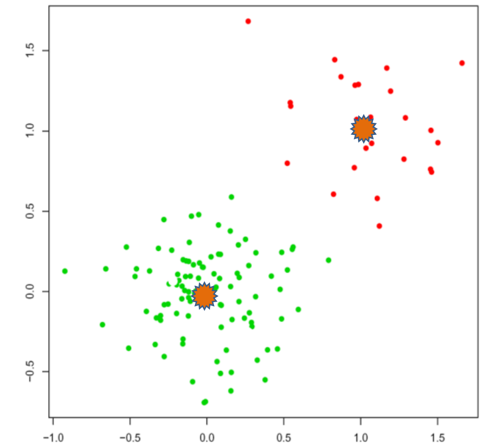
- **An algorithm for partitioning *n* observations/points into *k* clusters such that each observation belongs to the cluster with the nearest mean/center**



- Isn't this a somewhat circular definition?
  - Assignment of a point to a cluster is based on the proximity of the point to the cluster mean
  - But the cluster mean is calculated based on all the points assigned to the cluster.

K-mean clustering: Chicken and egg

- An algorithm for partitioning *n* observations/points into *k* clusters such that each observation belongs to the cluster with the nearest mean/center



- **The chicken and egg problem:**
  I do not know the means before I determine the partitioning into clusters
  I do not know the partitioning into clusters before I determine the means

- **Key principle - cluster around <u>mobile</u> centers:**
  - Start with some **random** locations of means/centers, partition into clusters according to these centers, and then correct the centers according to the clusters (somewhat similar to expectation-maximization algorithm)

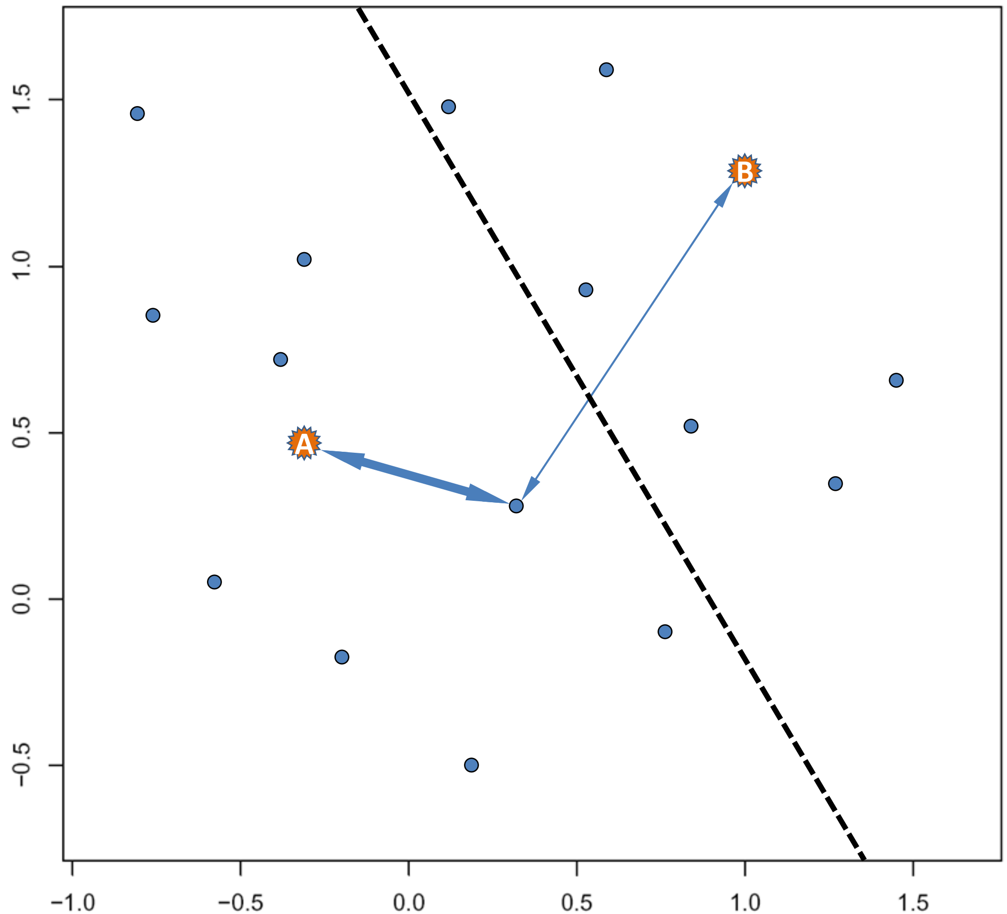
K-mean clustering algorithm

- The number of centers, ***k***, has to be specified a-priori
- **Algorithm:**
  1. Arbitrarily select *k* initial centers
  2. Assign each element to the closest center
  3. Re-calculate centers (mean position of the assigned elements)
  4. Repeat 2 and 3 until one of the following termination conditions is reached:
     i. The clusters are the same as in the previous iteration
     ii. The difference between two iterations is smaller than a specified threshold
     iii. The maximum number of iterations has been reached

How can we do this efficiently?

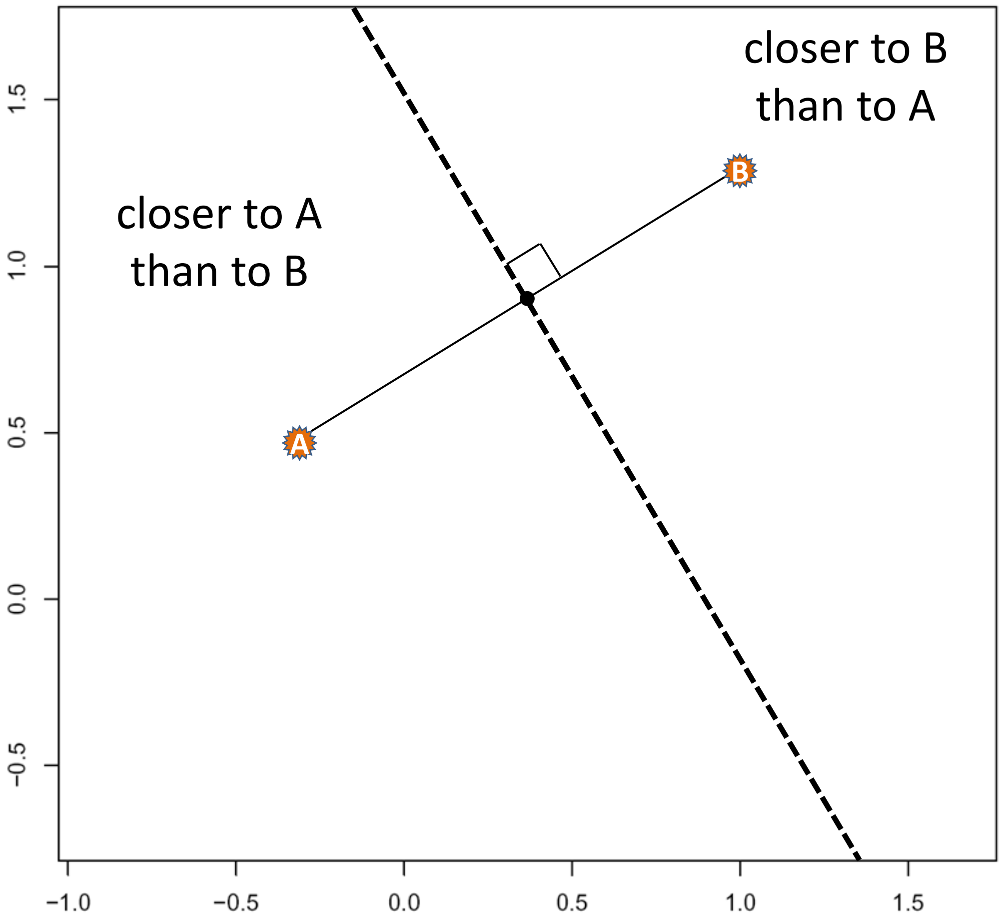
Partitioning the space

- Assigning elements to the closest center



Partitioning the space

- Assigning elements to the closest center



Partitioning the space

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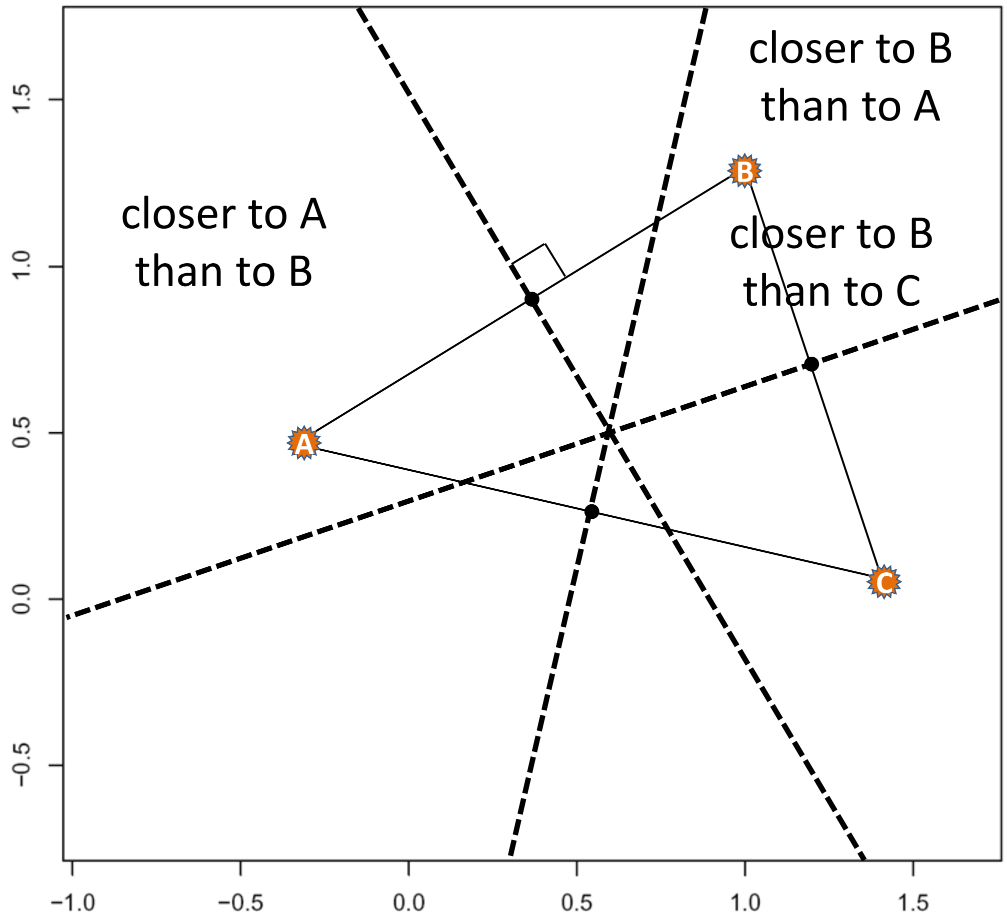
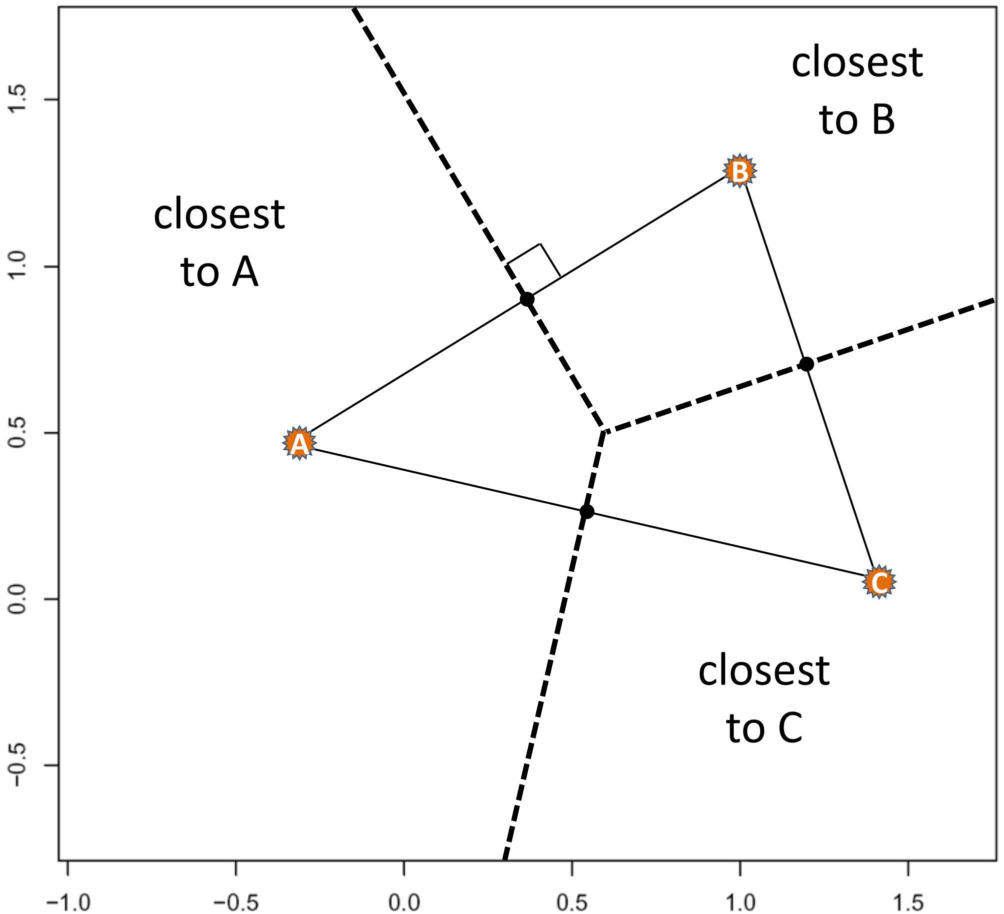


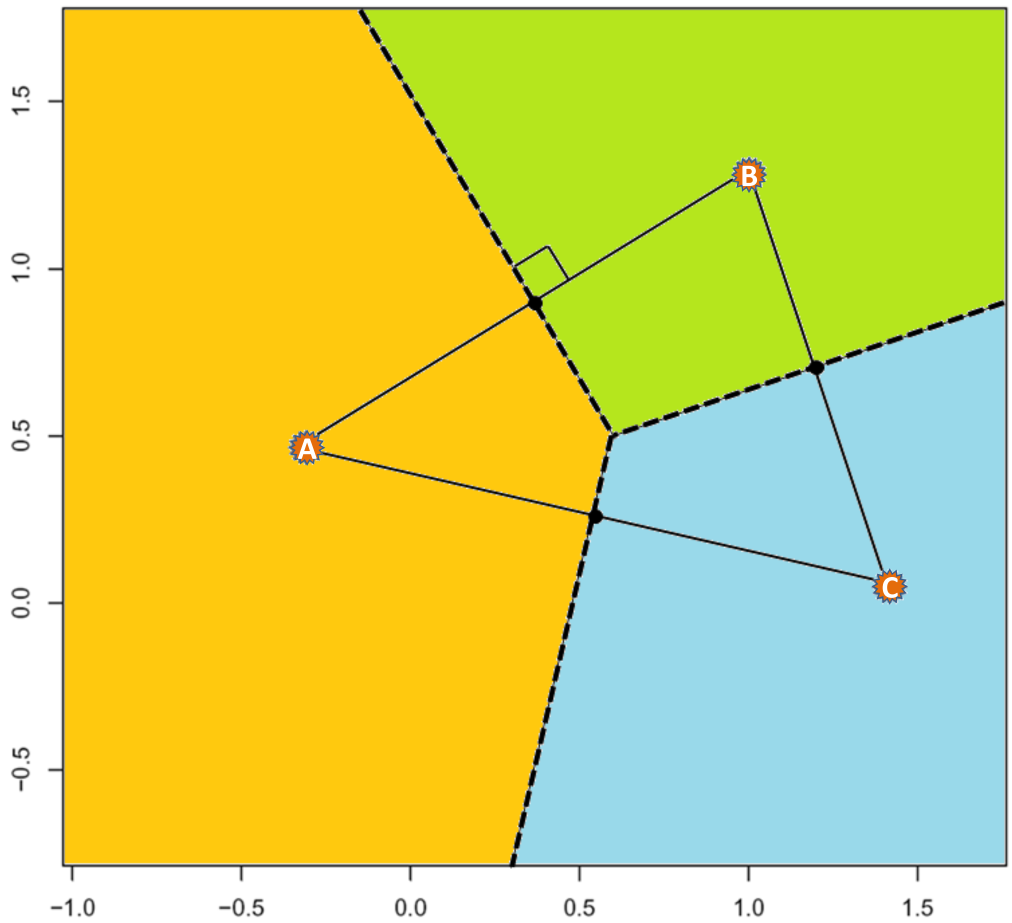
Partitioning the space

- Assigning elements to the closest center



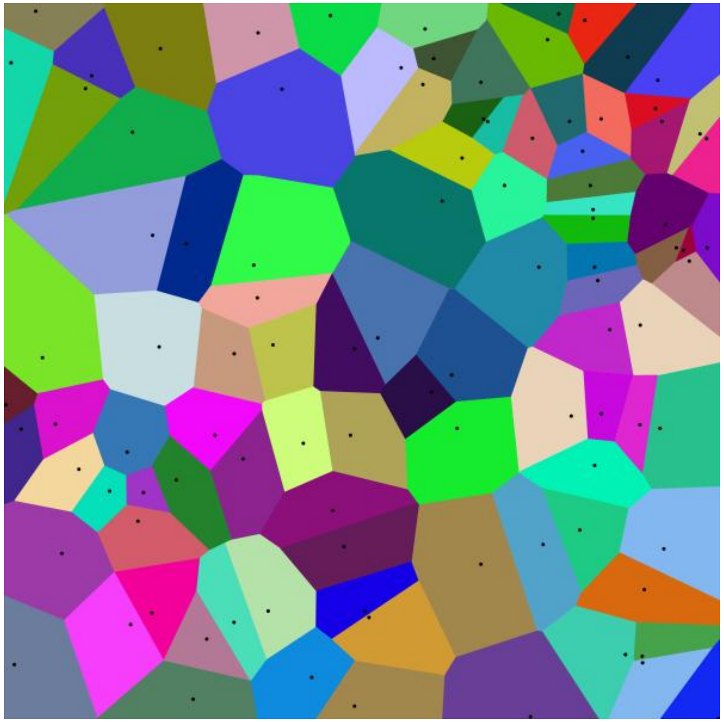
Partitioning the space

- Assigning elements to the closest center



Voronoi diagram

- Decomposition of a metric space determined by distances to a specified discrete set of “centers” in the space
- Each colored cell represents the collection of all points in this space that are closer to a specific center *s* than to any other center
- Several algorithms exist to find the Voronoi diagram.



K-mean clustering algorithm

- The number of centers, ***k***, has to be specified a priori

- **Algorithm:**
  1. Arbitrarily select *k* initial centers
  2. Assign each element to the closest center **(Voronoi)**
  3. Re-calculate centers (mean position of the assigned elements)
  4. Repeat 2 and 3 until one of the following termination conditions is reached:
     1. The clusters are the same as in the previous iteration
     2. The difference between two iterations is smaller than a specified threshold
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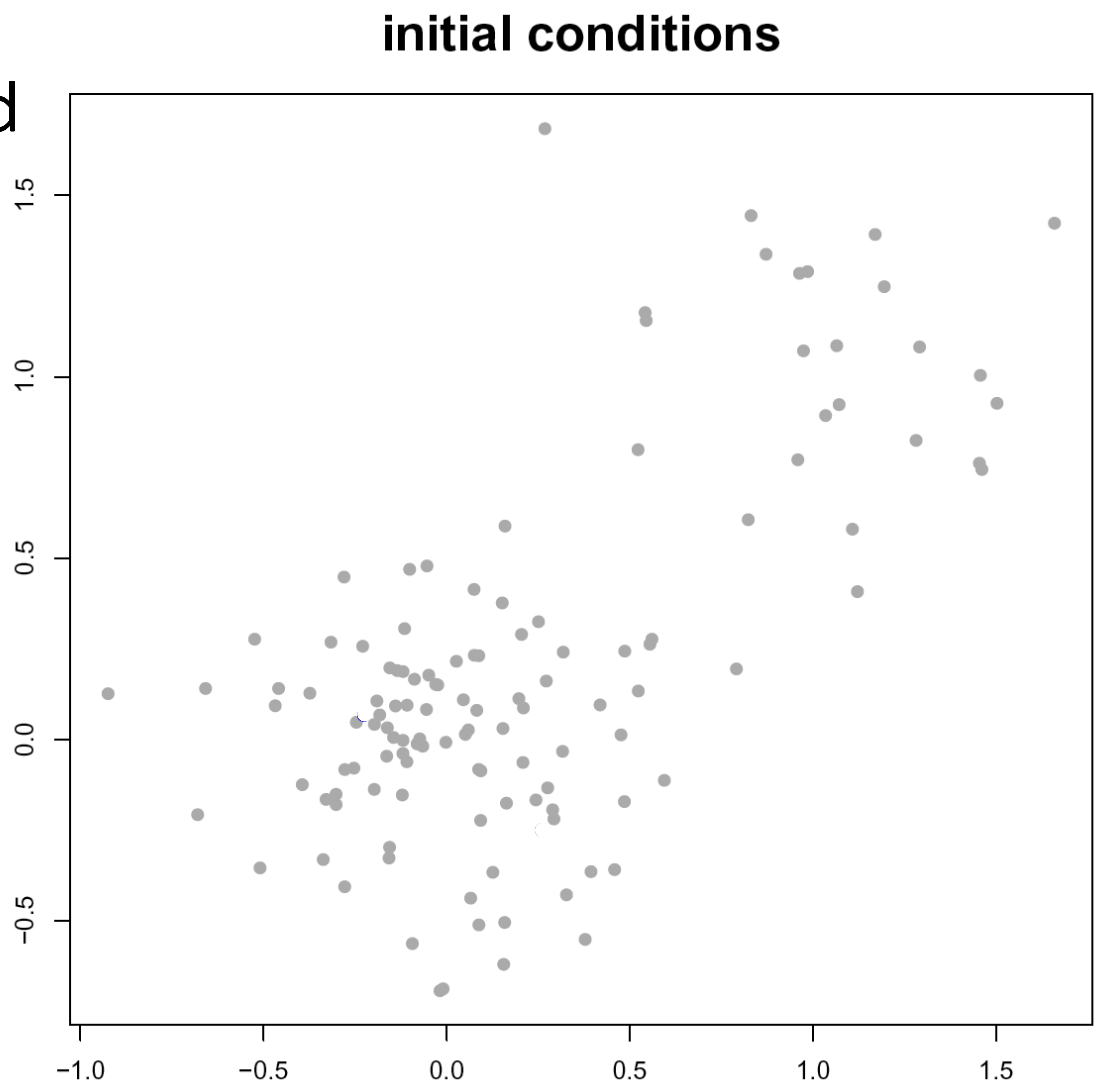
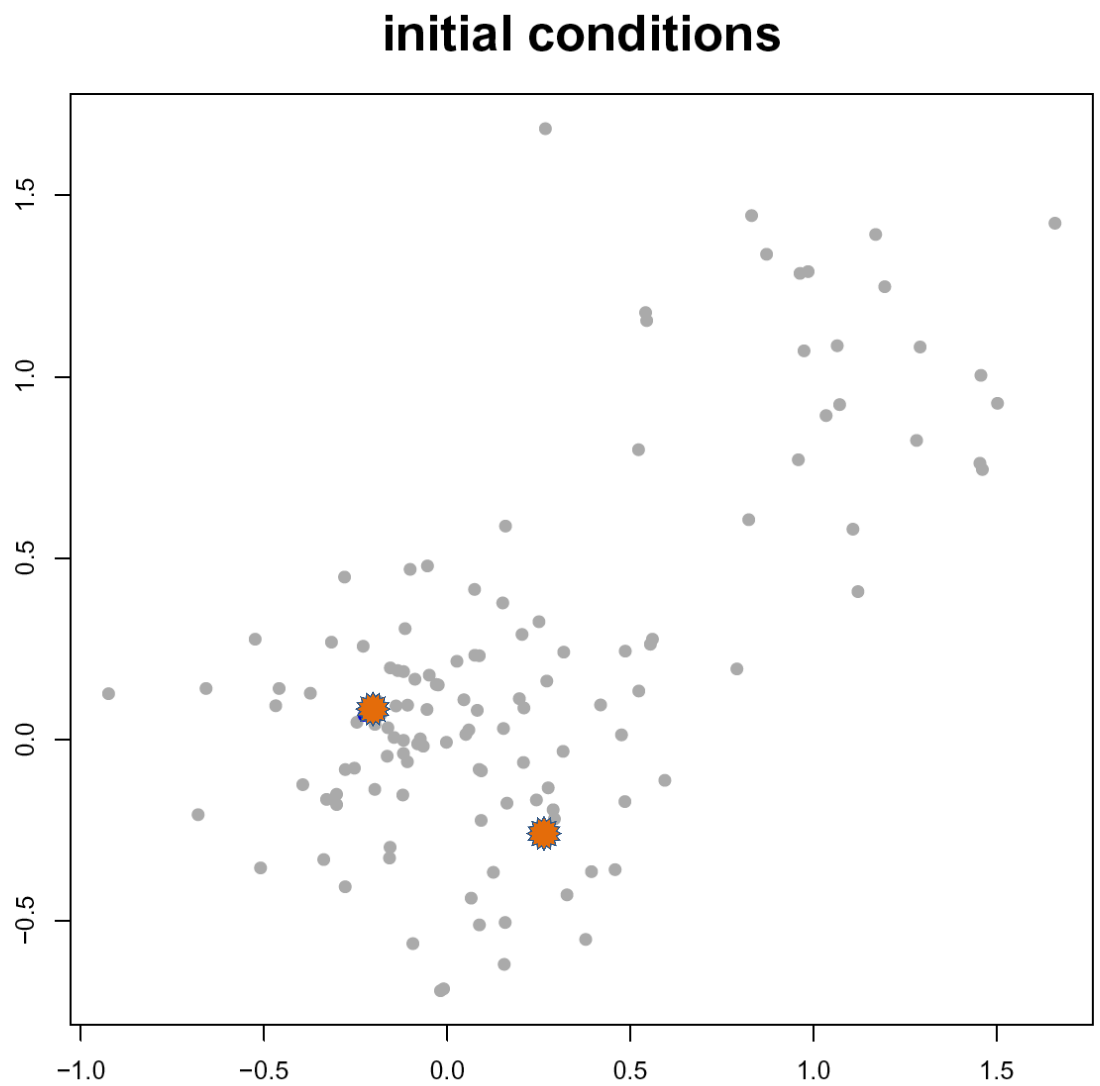
K-mean clustering example

- Two sets of points randomly generated
  - 200 centered on (0,0)
  - 50 centered on (1,1)



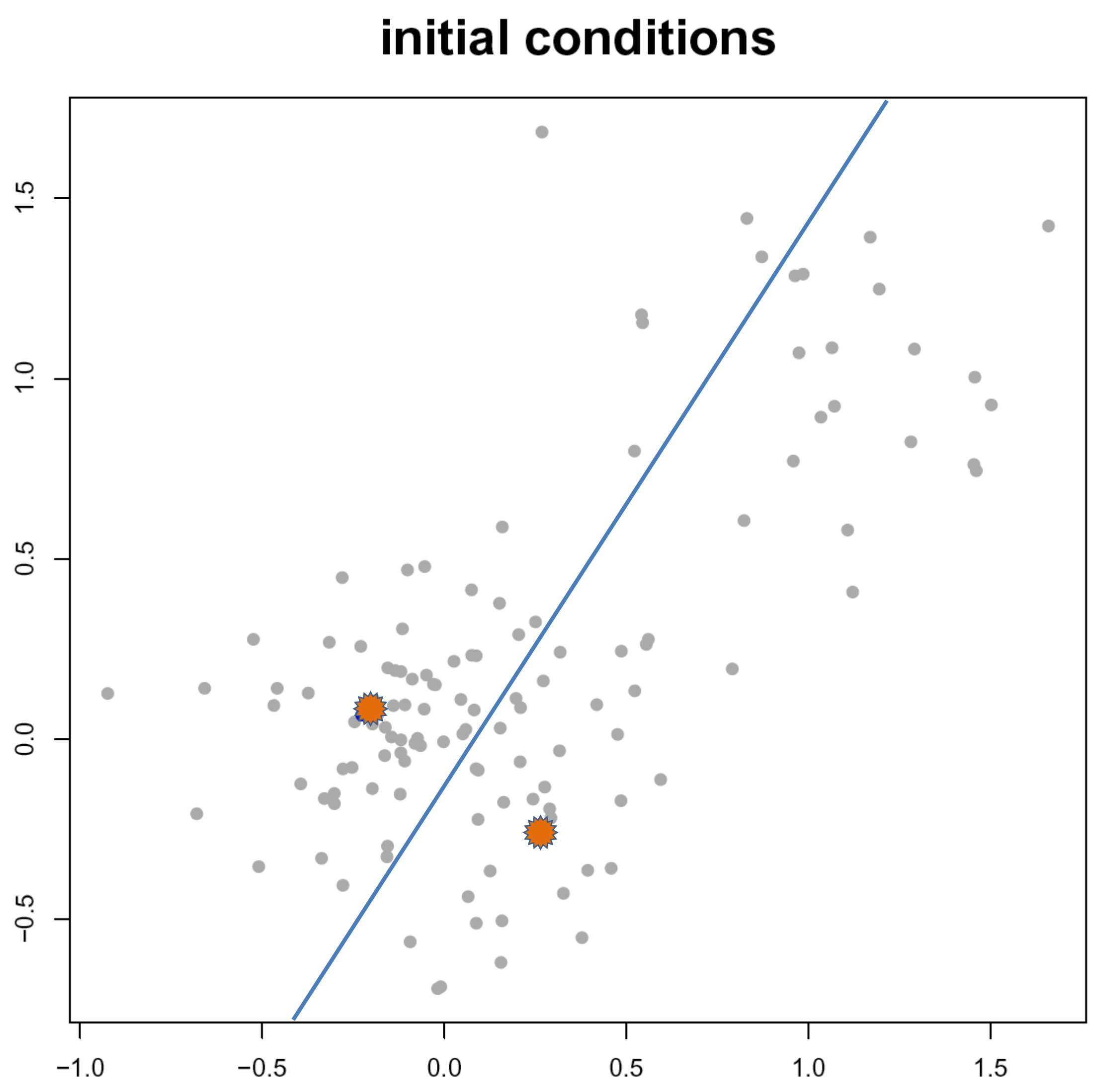
K-mean clustering example

- Two points are randomly chosen as centers (stars)



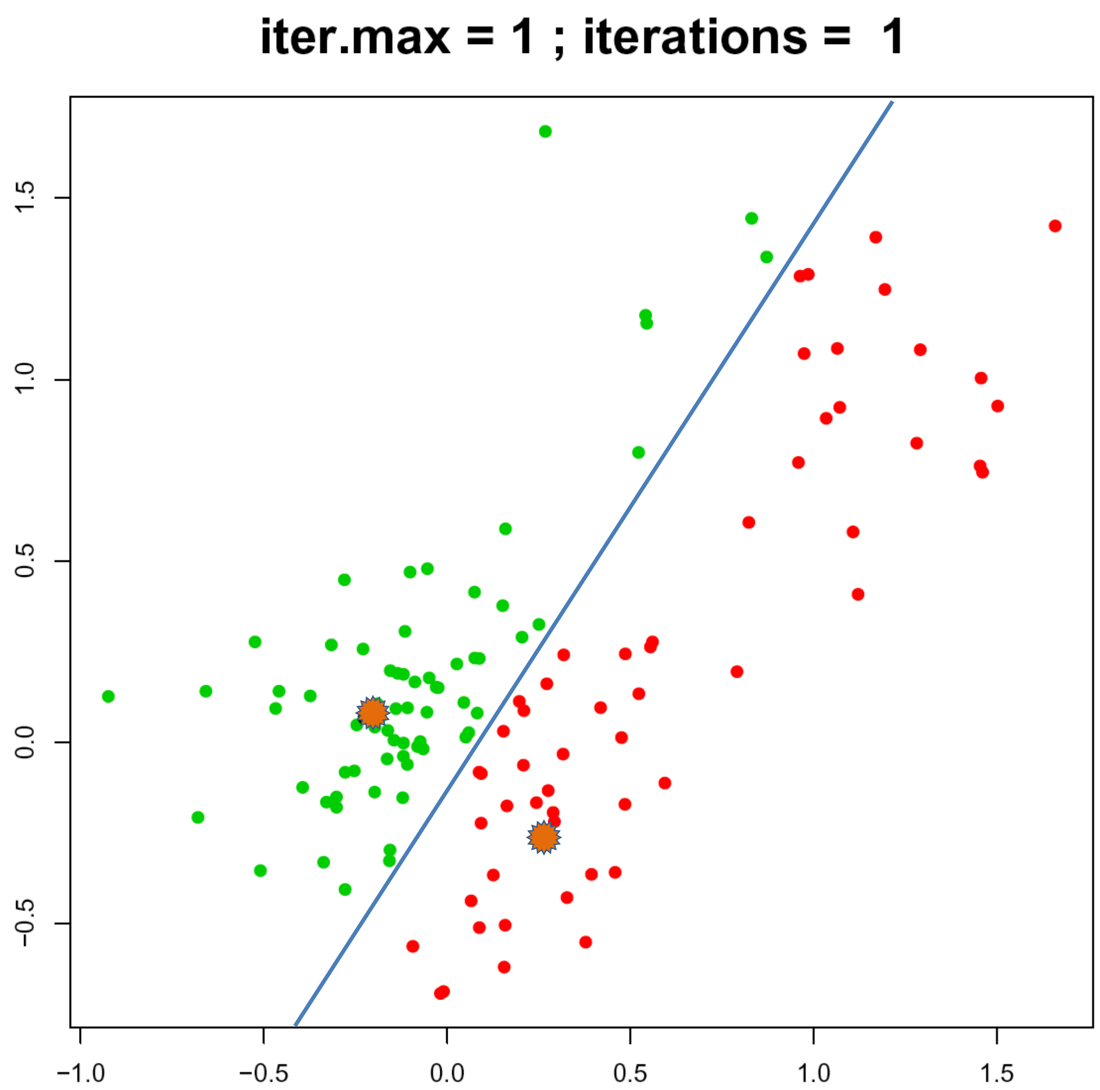
K-mean clustering example

- Each dot can now be assigned to the cluster with the closest center



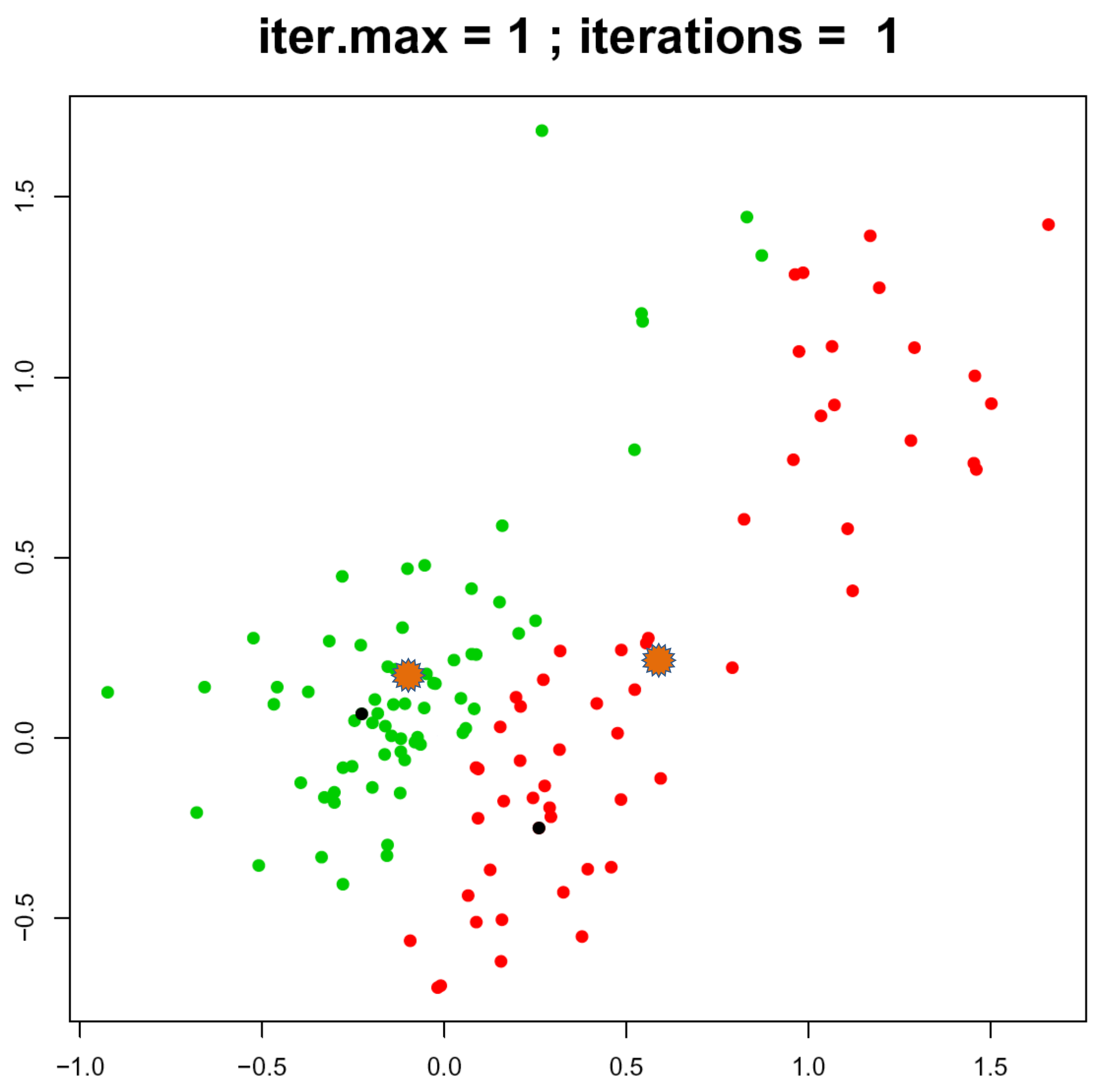
K-mean clustering example

- First partition into clusters



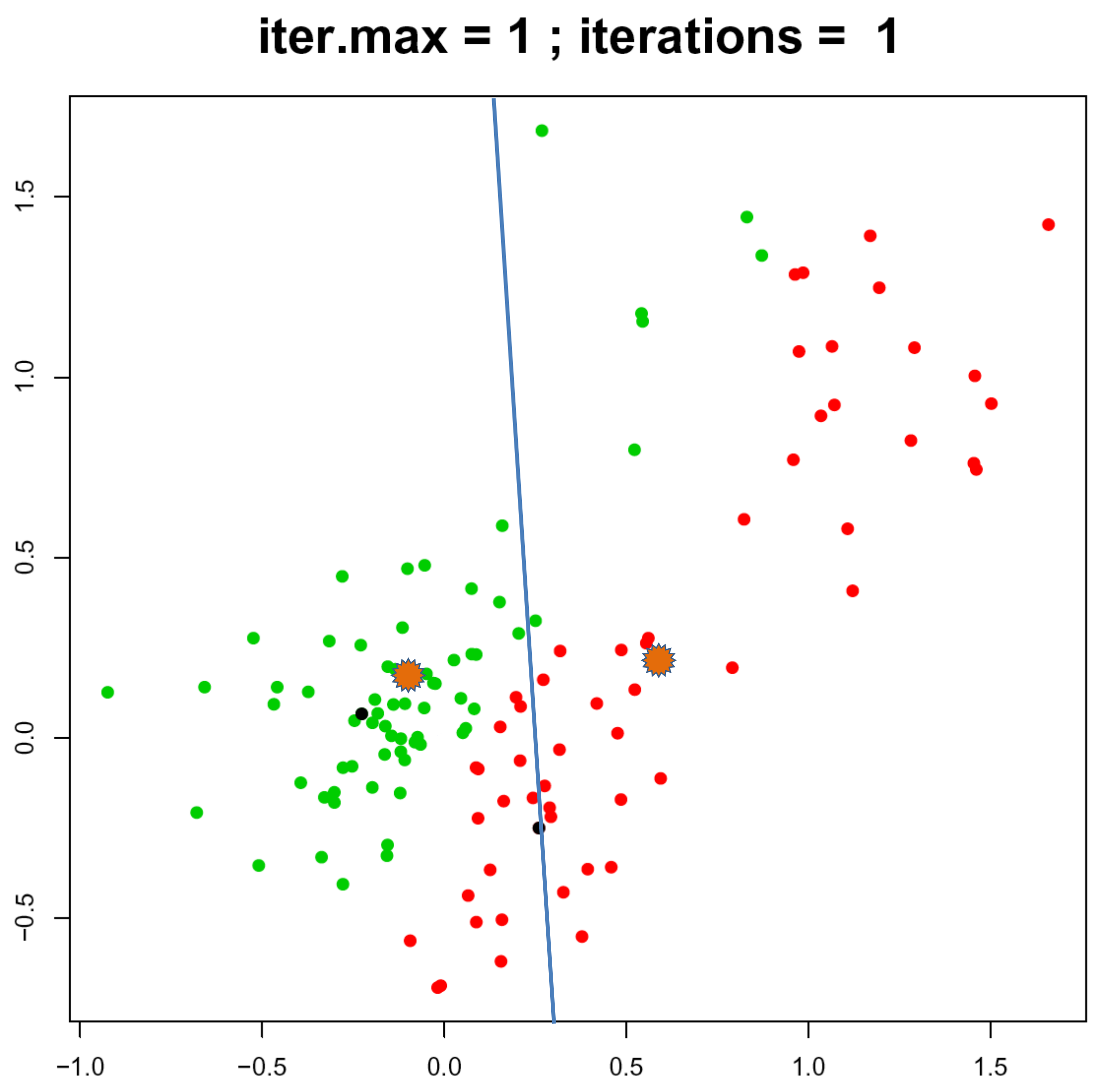
K-mean clustering example

- Centers are re-calculated



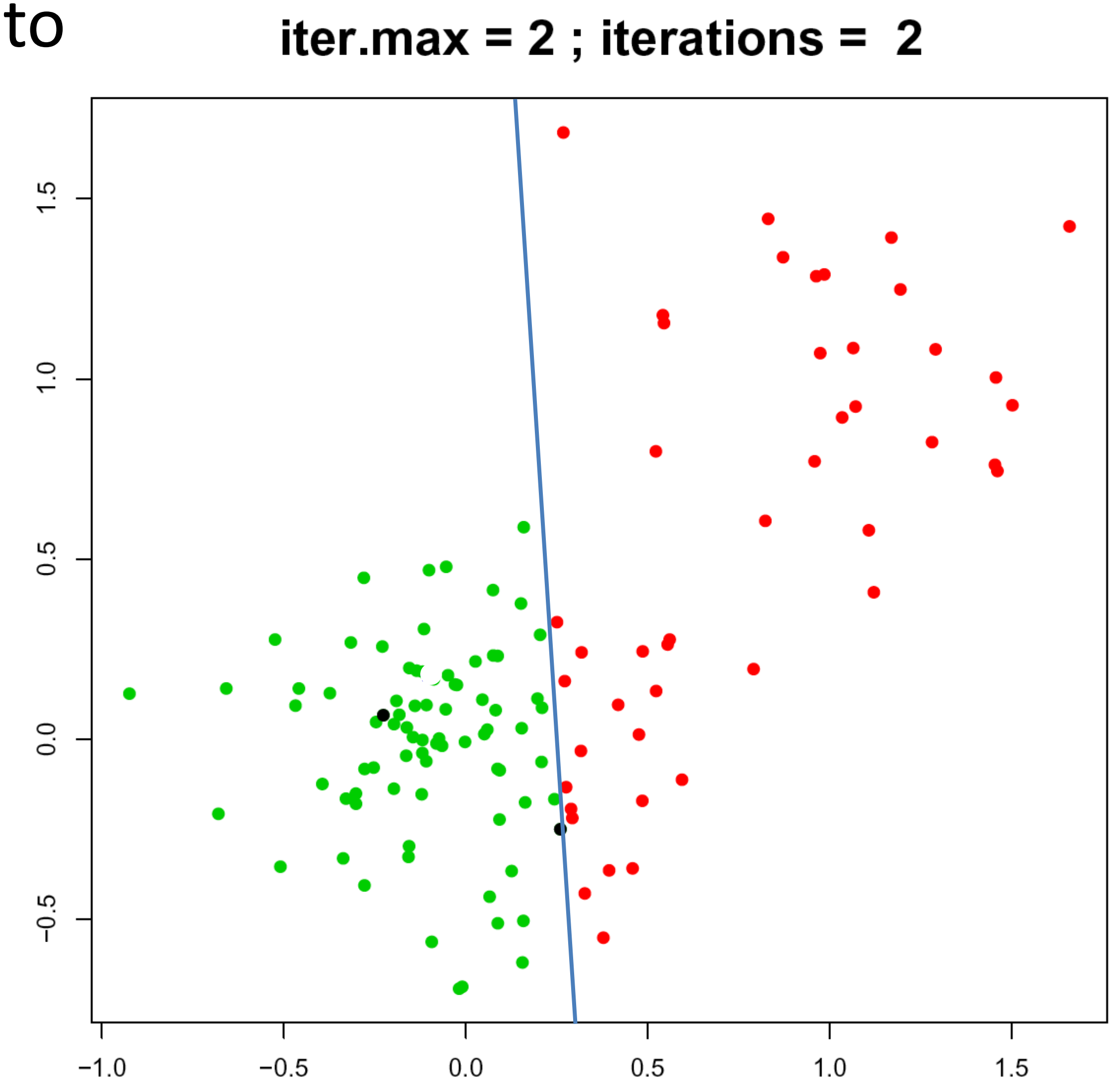
K-mean clustering example

- And are again used to partition the points



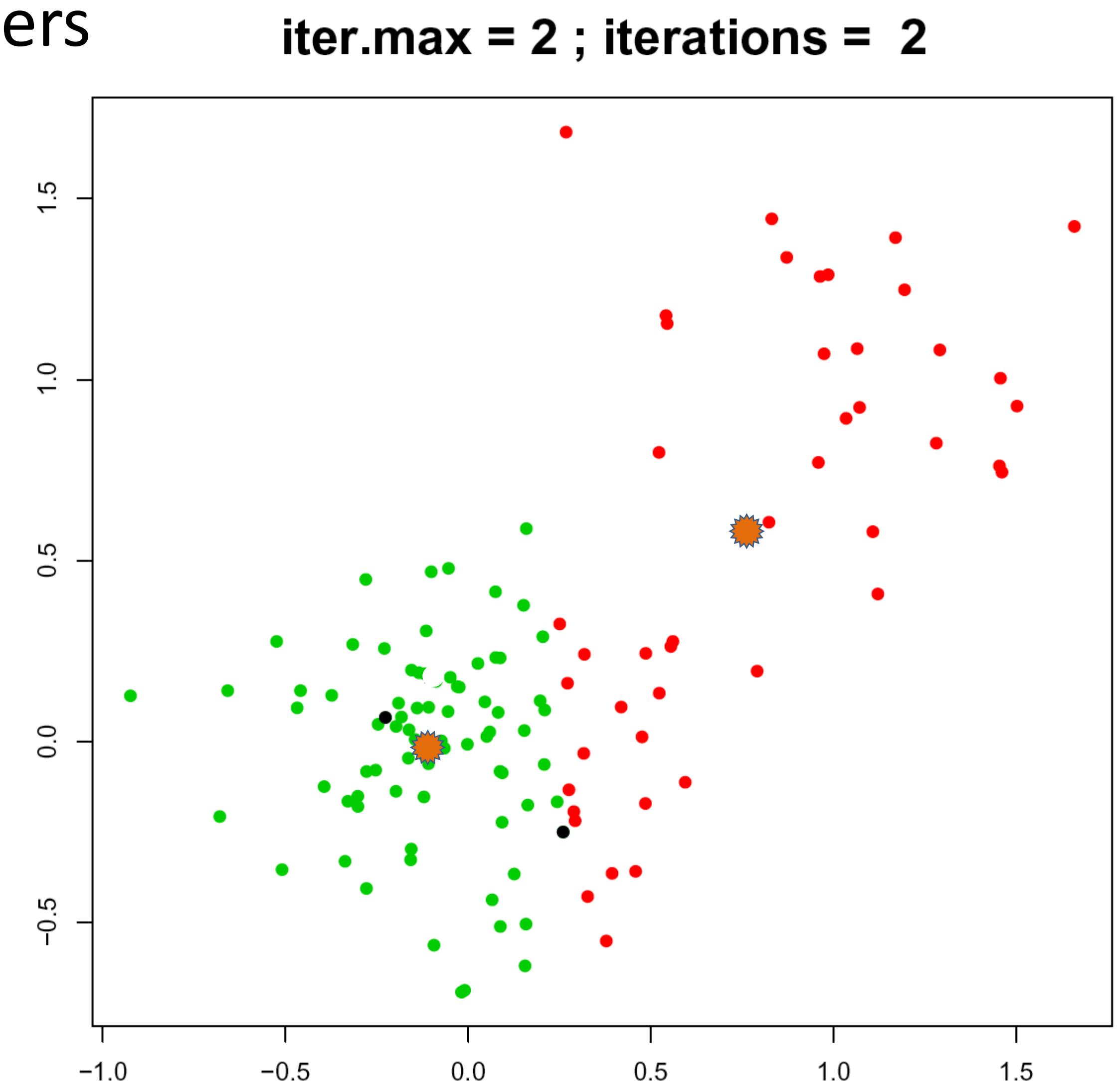
K-mean clustering example

- Second partition into clusters



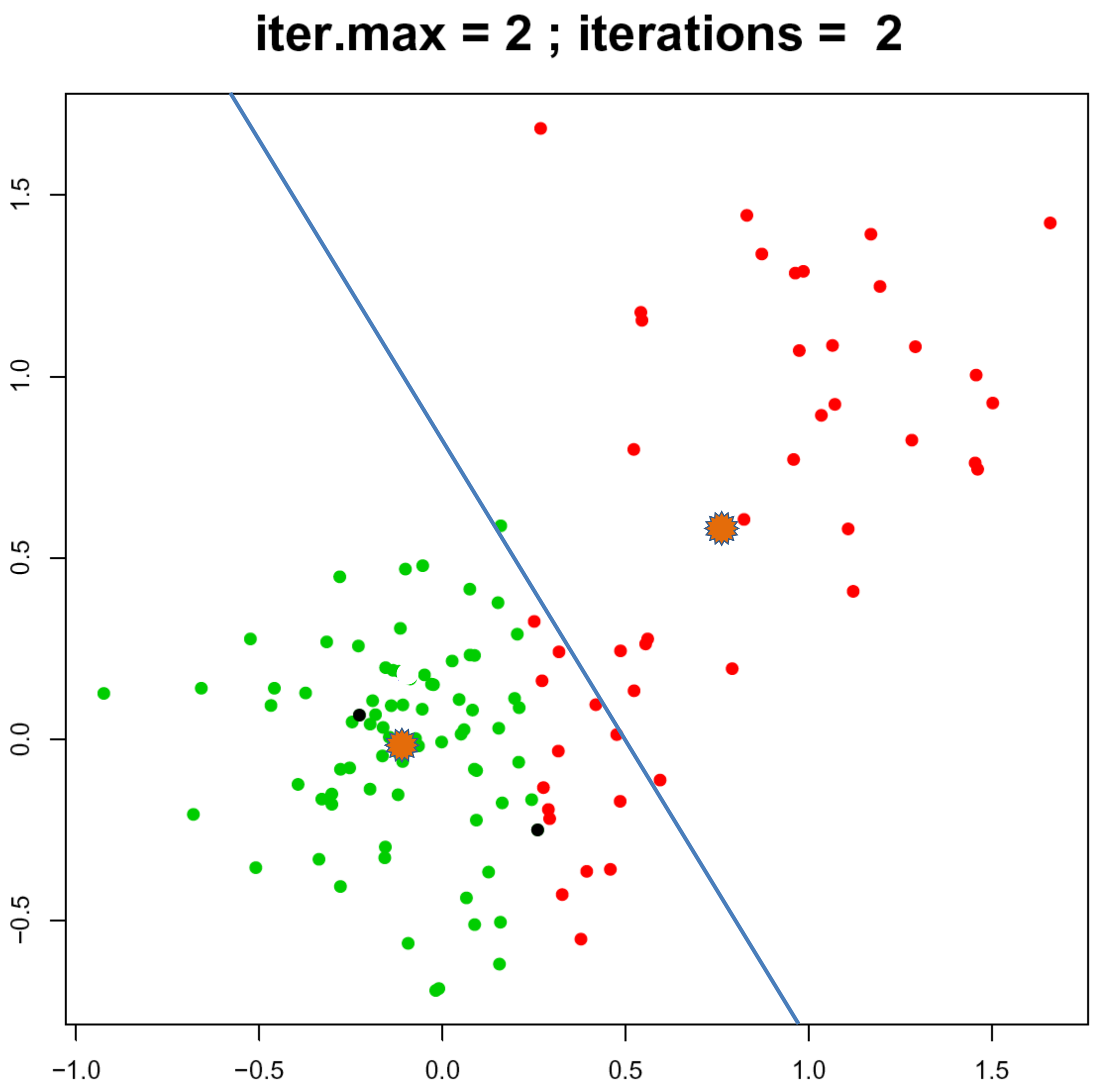
K-mean clustering example

- Re-calculating centers again



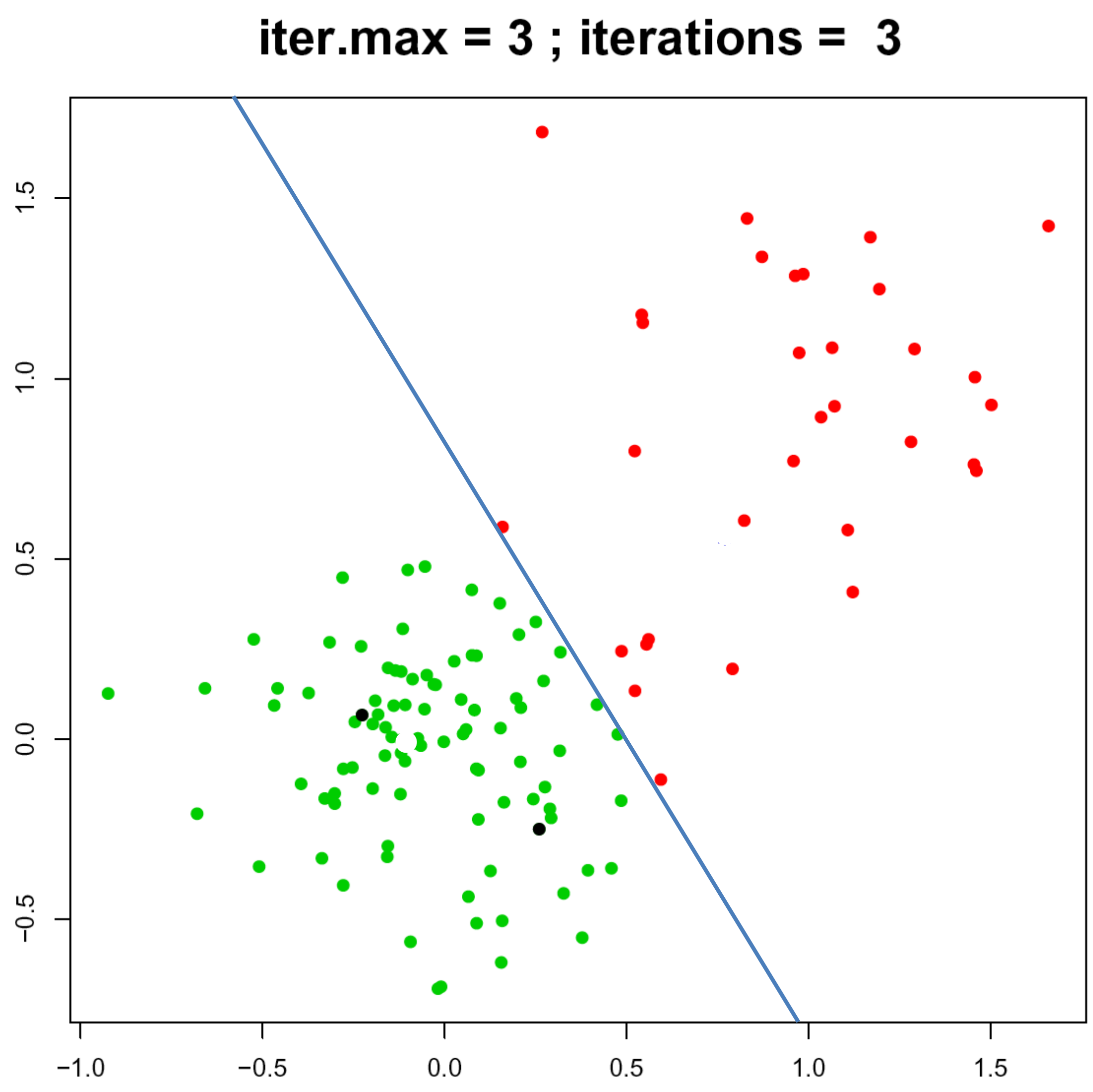
K-mean clustering example

- And we can again partition the points



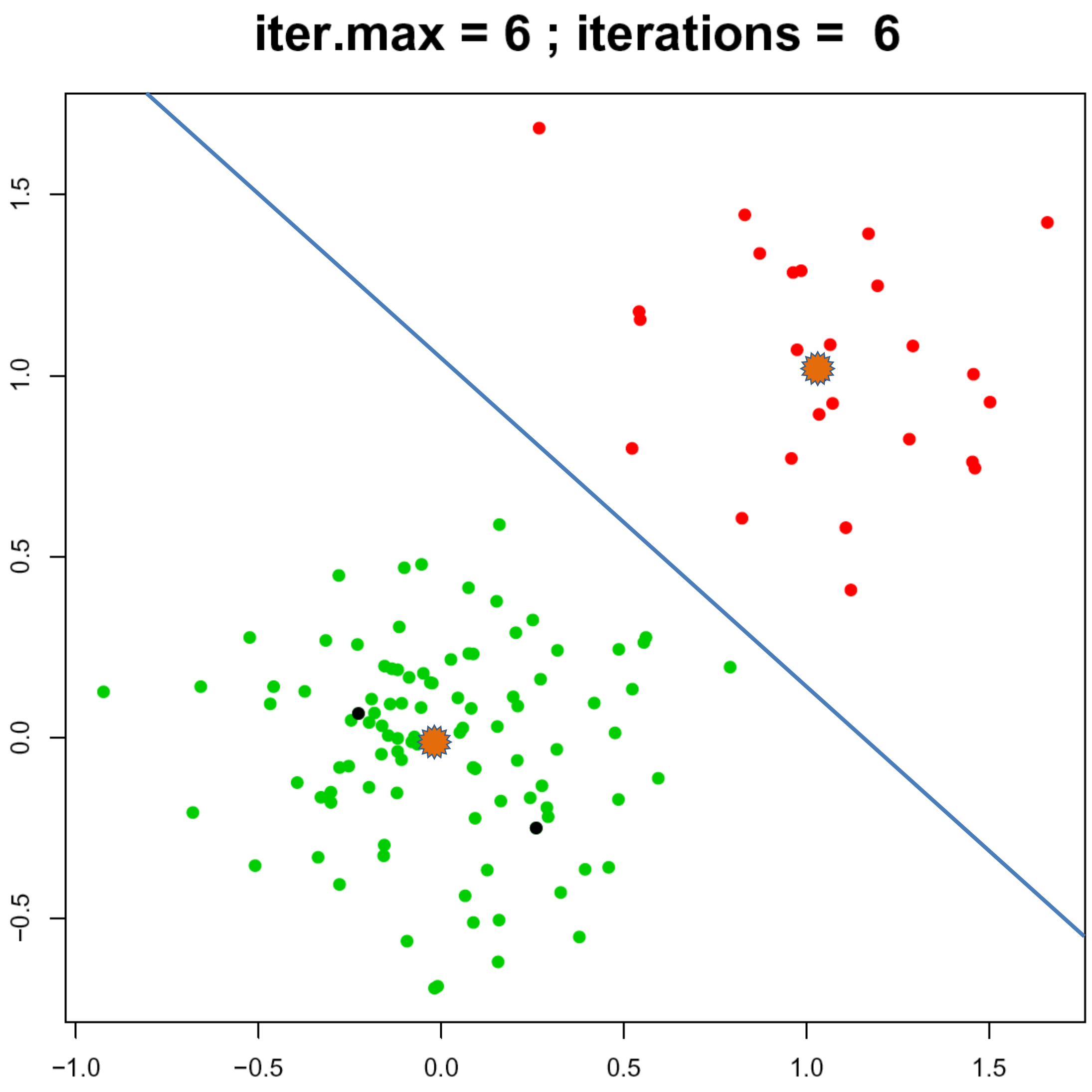
K-mean clustering example

- Third partition into clusters



K-mean clustering example

- After 6 iterations:
- The calculated centers remains stable



K-mean clustering: Summary

- The convergence of k-mean is usually quite fast (sometimes 1 iteration results in a stable solution)
- K-means is time- and memory-efficient
- **Strengths:**
  - Simple to use
  - Fast
  - Can be used with very large data sets
- **Weaknesses:**
  - **The number of clusters has to be predetermined**
  - The results may vary depending on the initial choice of centers

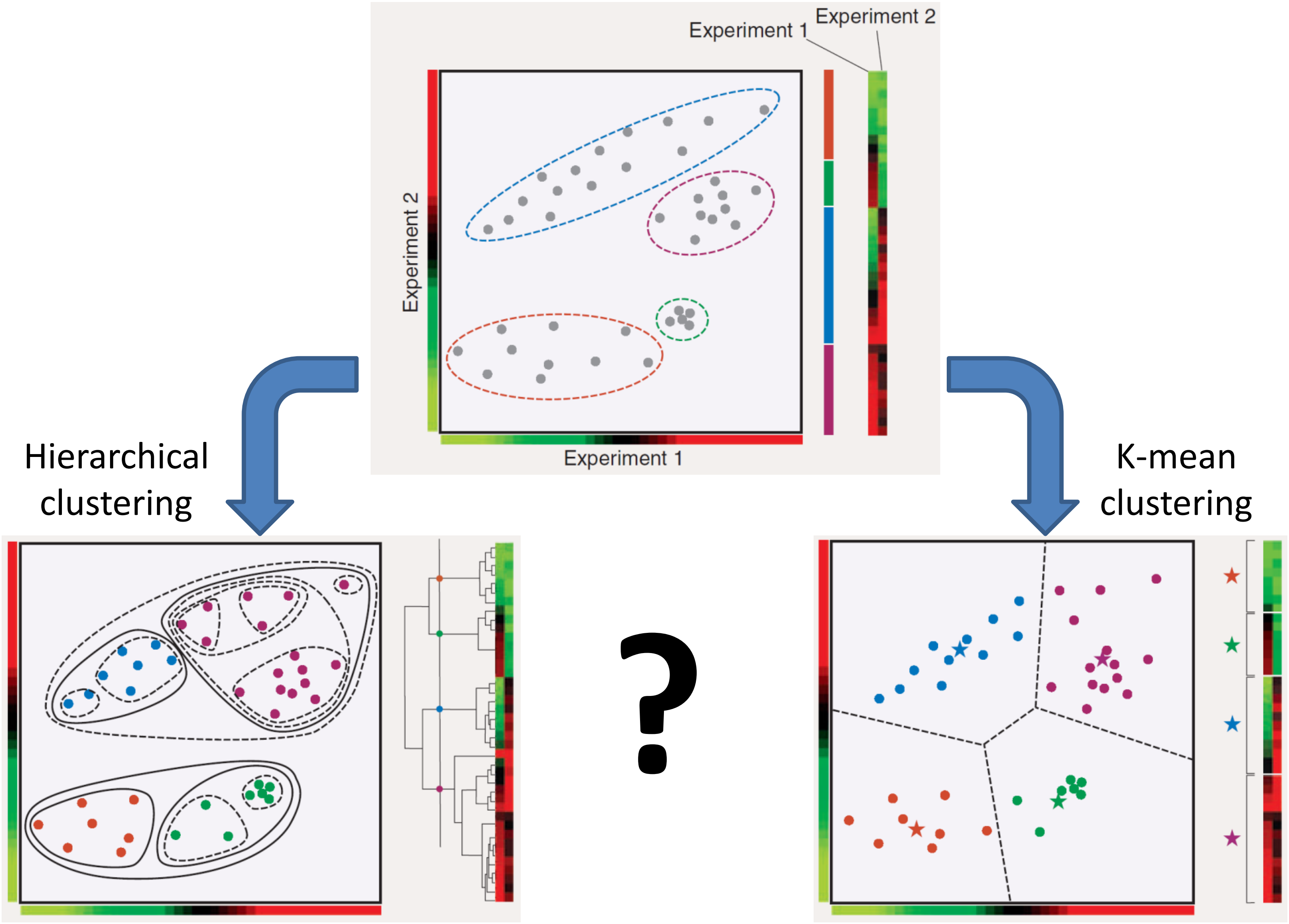
K-mean clustering: Variations

- Expectation-maximization (**EM**):
  maintains **probabilistic** assignments to clusters, instead of deterministic assignments, and multivariate Gaussian distributions instead of means.

- k-means++: attempts to choose better starting points.

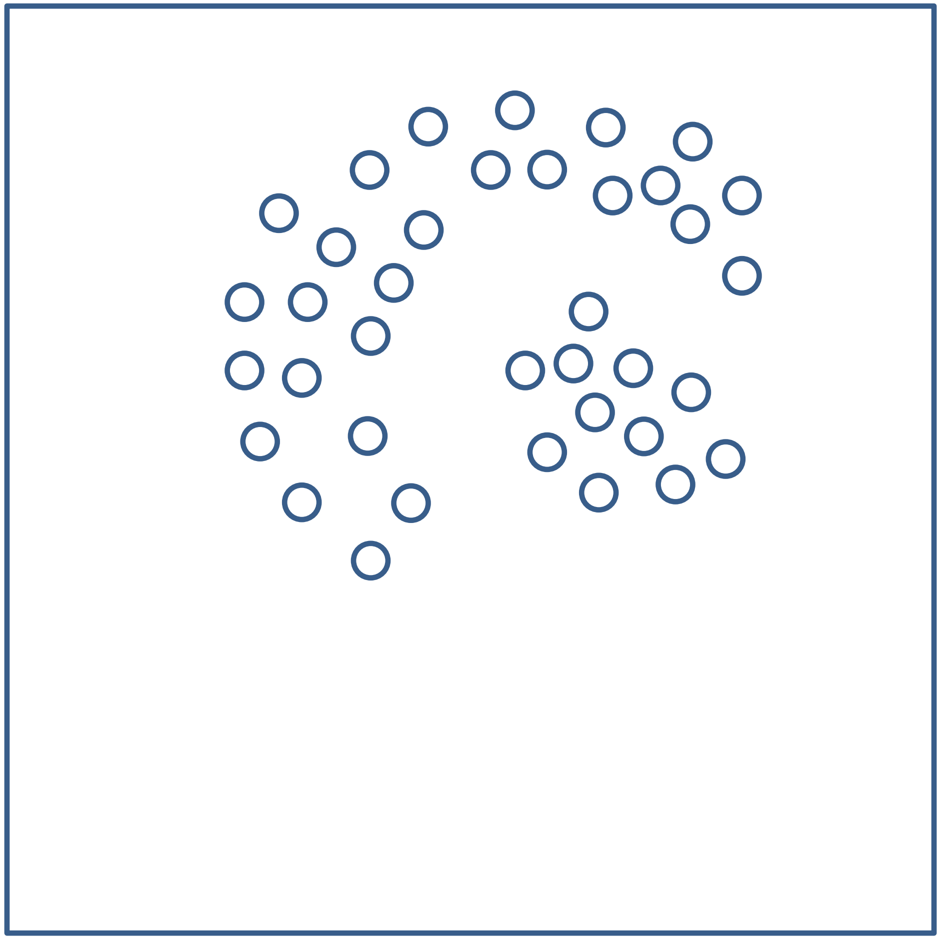
- Some variations attempt to escape local optima by swapping points between clusters

The take-home message



D'haeseleer, 2005

What else are we missing?



What else are we missing?

- What if the clusters are not "linearly separable"?