Partitionnement de données

Sergey Kirgizov, avec Maximilien Danisch de Sorbonne Université

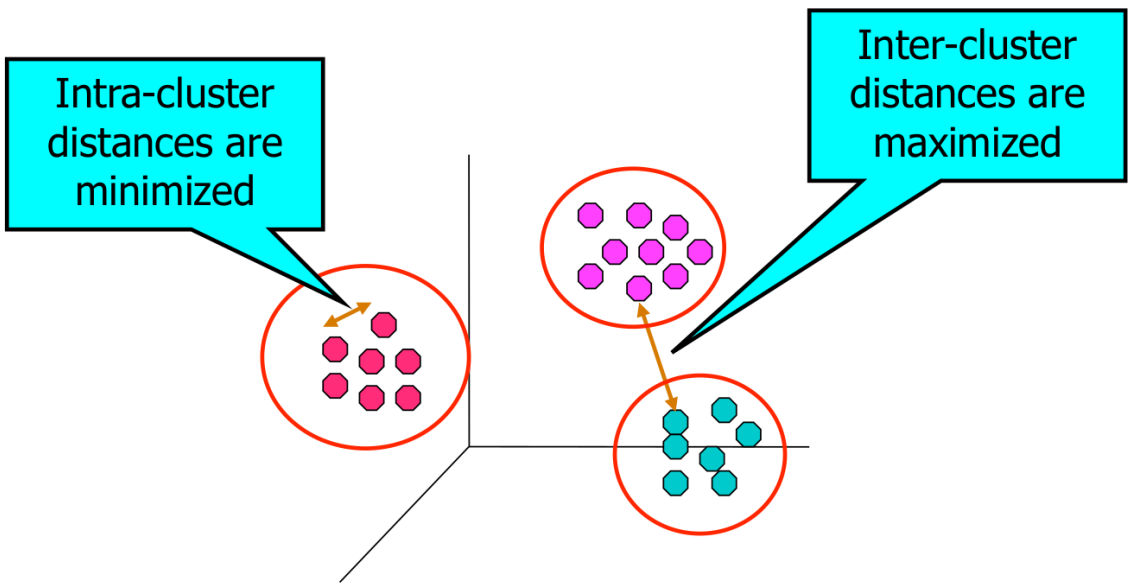
Partitionnement, qu'est-ce que c'est ?

Partitionnement

Trouver des groupes d'objets tels que

- les objets d'un groupe sont similaires dans un certain sens.
- les objets de différents groupes sont différents

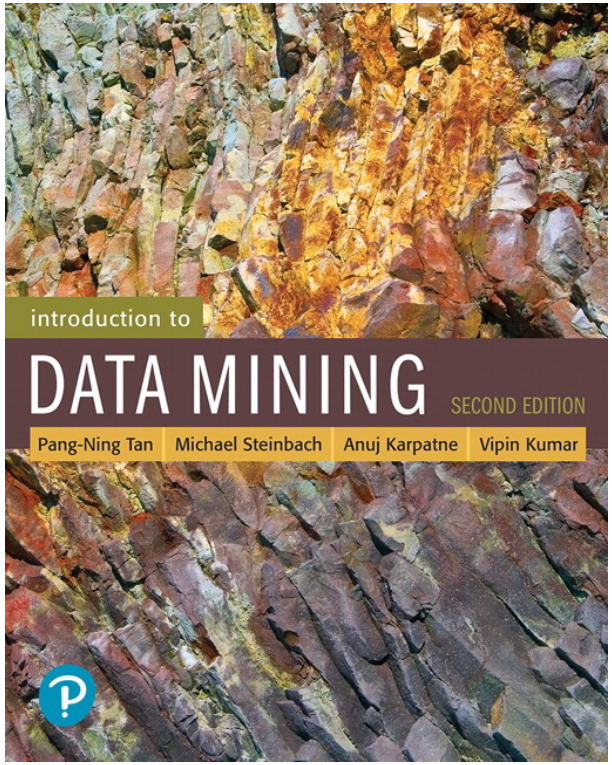
Les similarités sont souvent traduits par les distances



Pourquoi faire ?

- Compréhension : par exemple regrouper les gènes et les protéines qui ont les fonctionnalités similaires
- Faire un résumé : réduire la taille de grands ensembles de données.
- Visualiser les groupes de données
- Autres applications :
  `https://en.wikipedia.org/wiki/Cluster_analysis#Applications`

Livre



Introduction to Data Mining, (2nd edition), Chapter 7
Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, Vipin Kumar

`https://www-users.cs.umn.edu/~kumar001/dmbook/index.php`
`https://www-users.cs.umn.edu/~kumar001/dmbook/ch7_clustering.pdf`

Partitionnement de données

Types de partitionnement

- Classique, non-chevauchant
- Chevauchant
- Hiérarchique
- “Fuzzy clustering”
- etc...

Algorithmes :

- **K-Means**
- Mean-shift
- DBSCAN
- GMM : Gaussian Mixture Model
- etc...

k-means : SSE (a.k.a. distortion)

k-means can be seen as a heuristic to minimize the Sum of Squared Errors (SSE) :

$$SSE = \sum_{i=1}^{n} \sum_{j=1}^{k} w_{i,j} ||x_i - \mu_j||_2^2$$

with

- μ_j the vector of centroid j and
- $w_{i,j} = 1$ if the sample x_i is in cluster j and 0 otherwise.

Optimisation

Étant donné n points, trouvez une partition en k clusters qui minimise la somme des carrés des distances entre chaque point et le centre de gravité de son cluster.

Décision

Étant donné n points et un nombre d, existe-t-il une partition en k clusters telle que la somme des carrés des distances entre chaque point et le centre de gravité de son cluster soit d'au plus d ?

Le problème de décision correspondant est NP-complete !

`https://cs.stackexchange.com/questions/153074/is-k-means-clustering-strictly-np-hard`

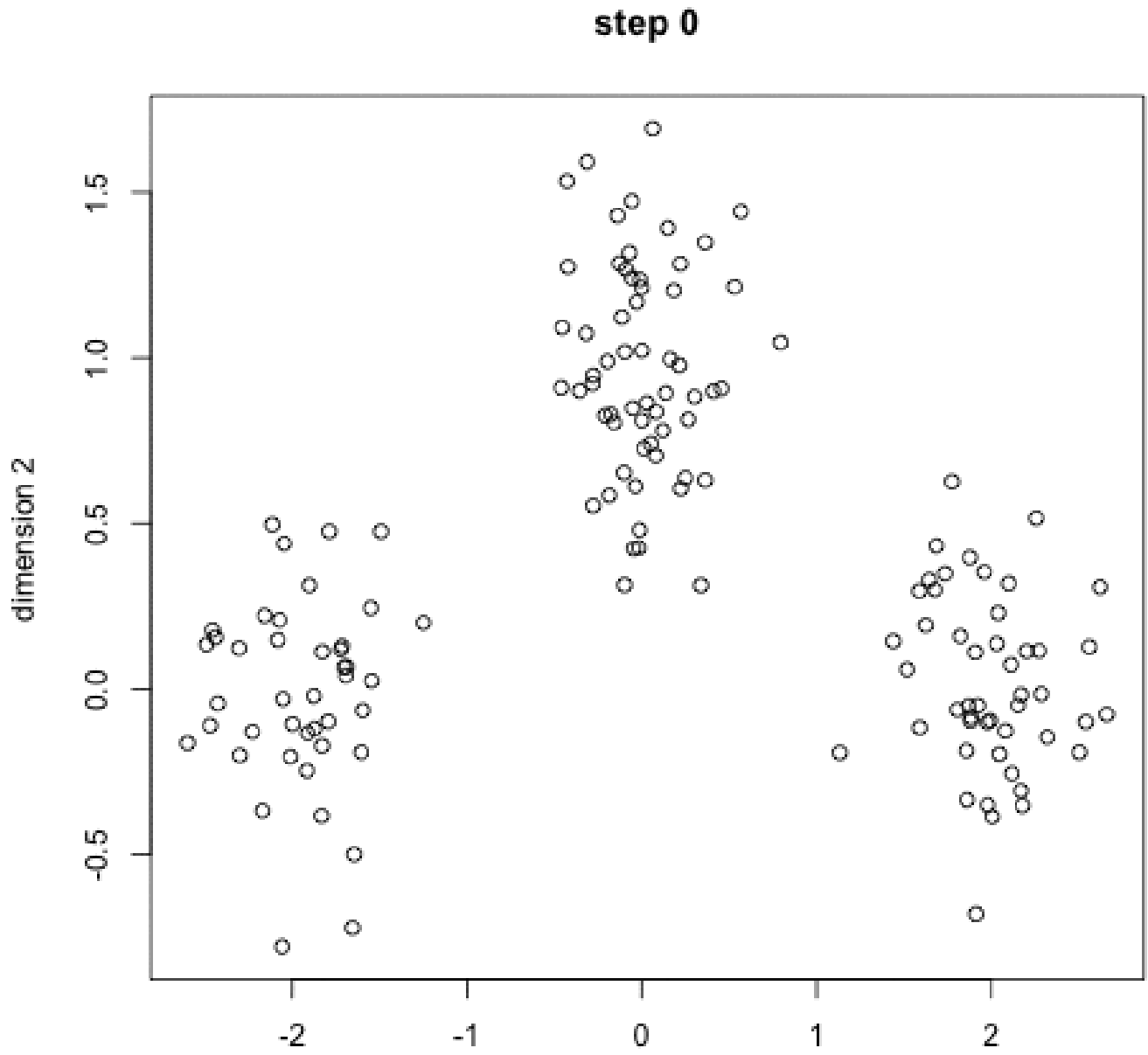
k-means by Lloyd-Max Algorithm

- Stuart P. Lloyd, 1957
- Joel Max, 1960

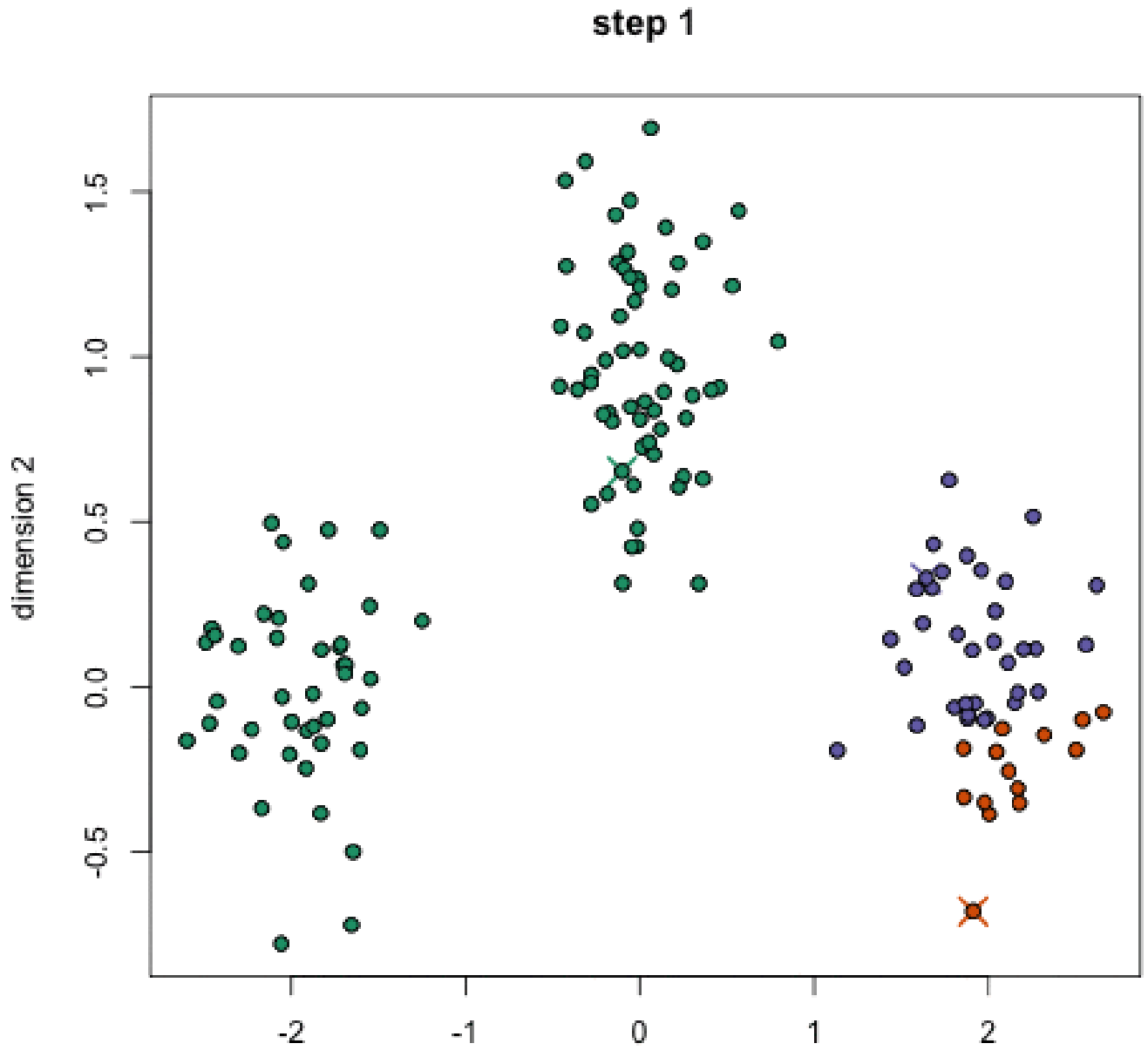
Algorithm

- Randomly chose k initial centroids
- While True :
  - Create k clusters by assigning each example to closest centroid
  - Compute k new centroids by averaging examples in each clustering
  - If centroids don't change :
    - Break

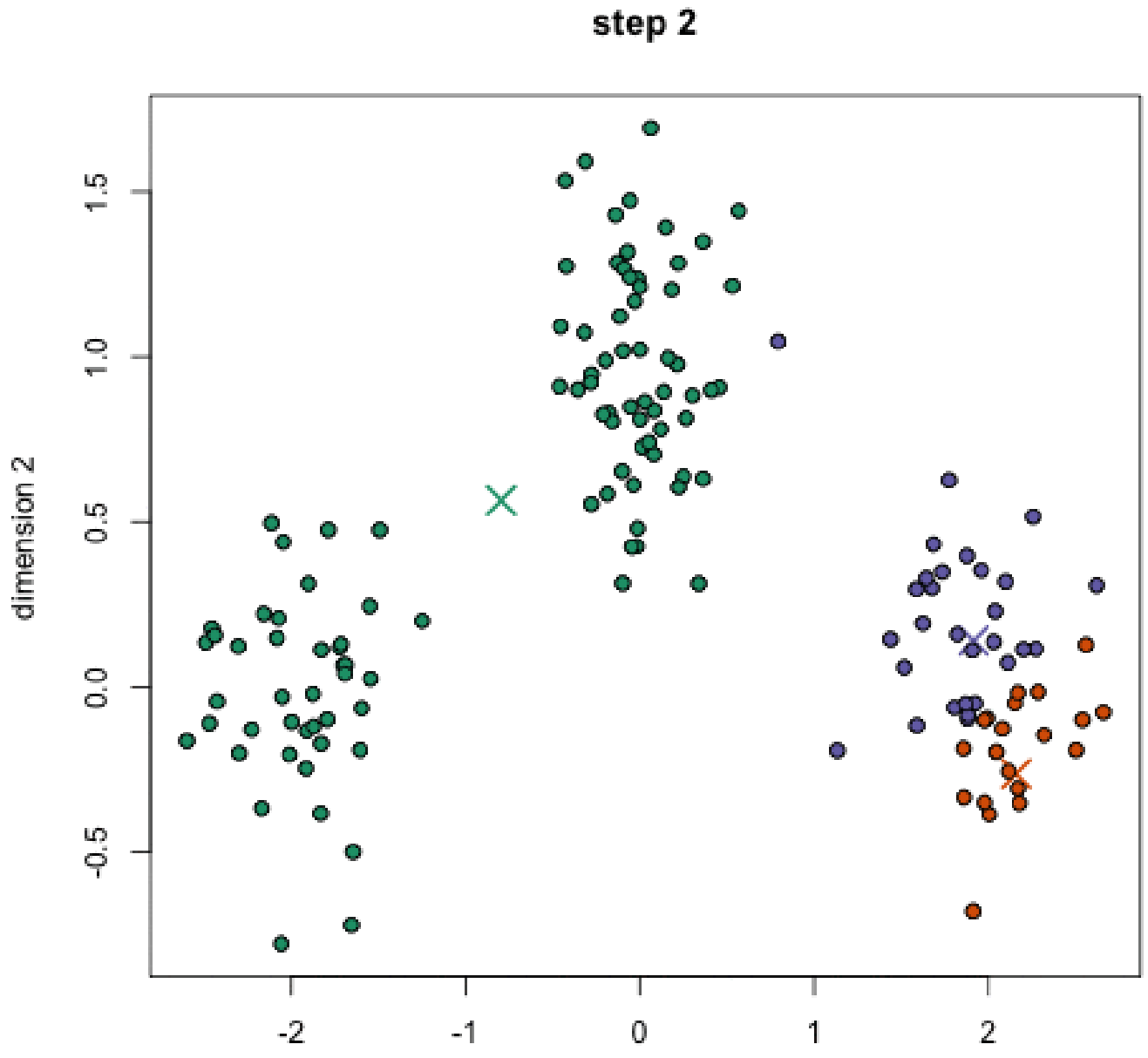
k-means exemple



k-means exemple



k-means exemple



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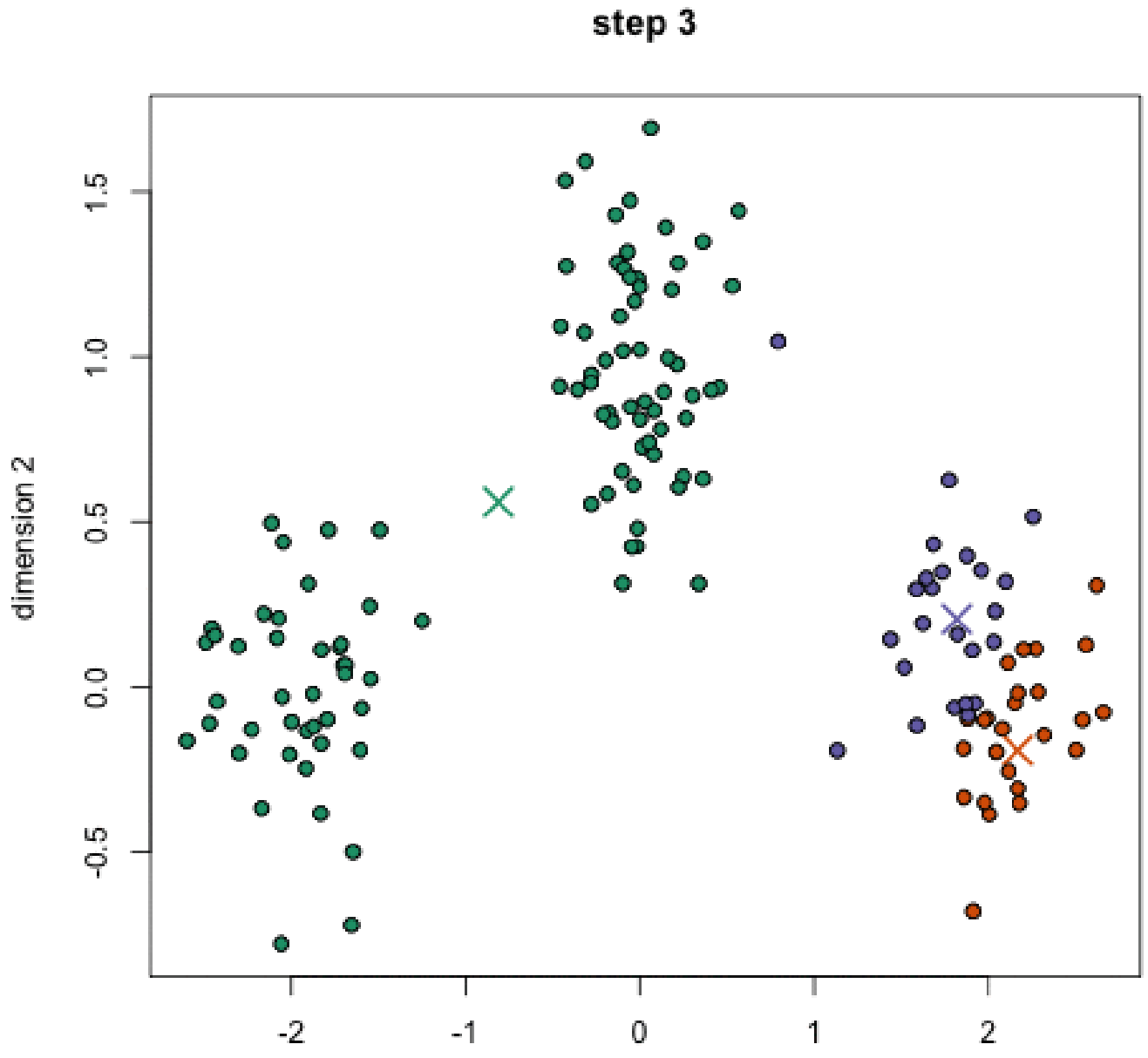
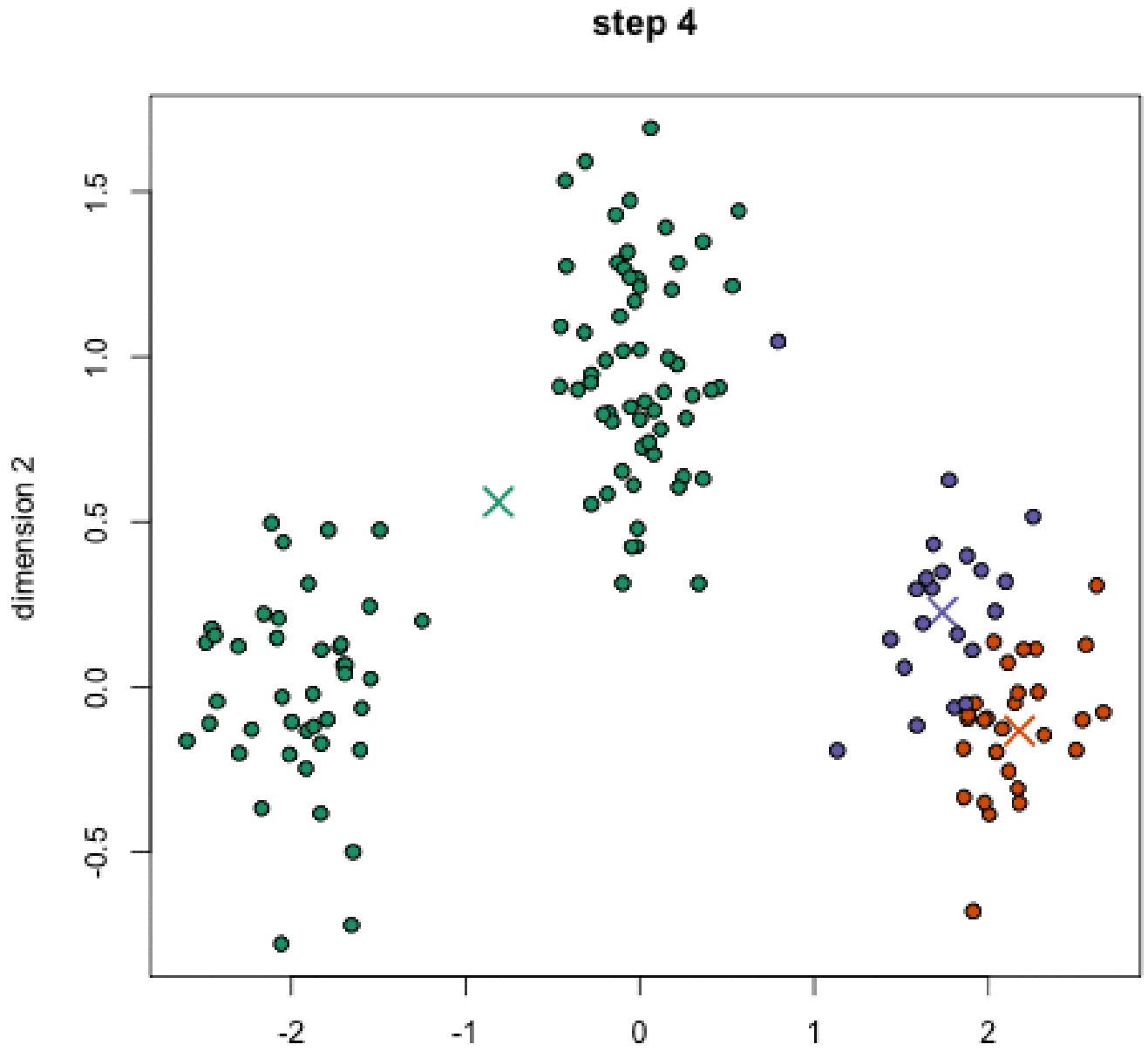
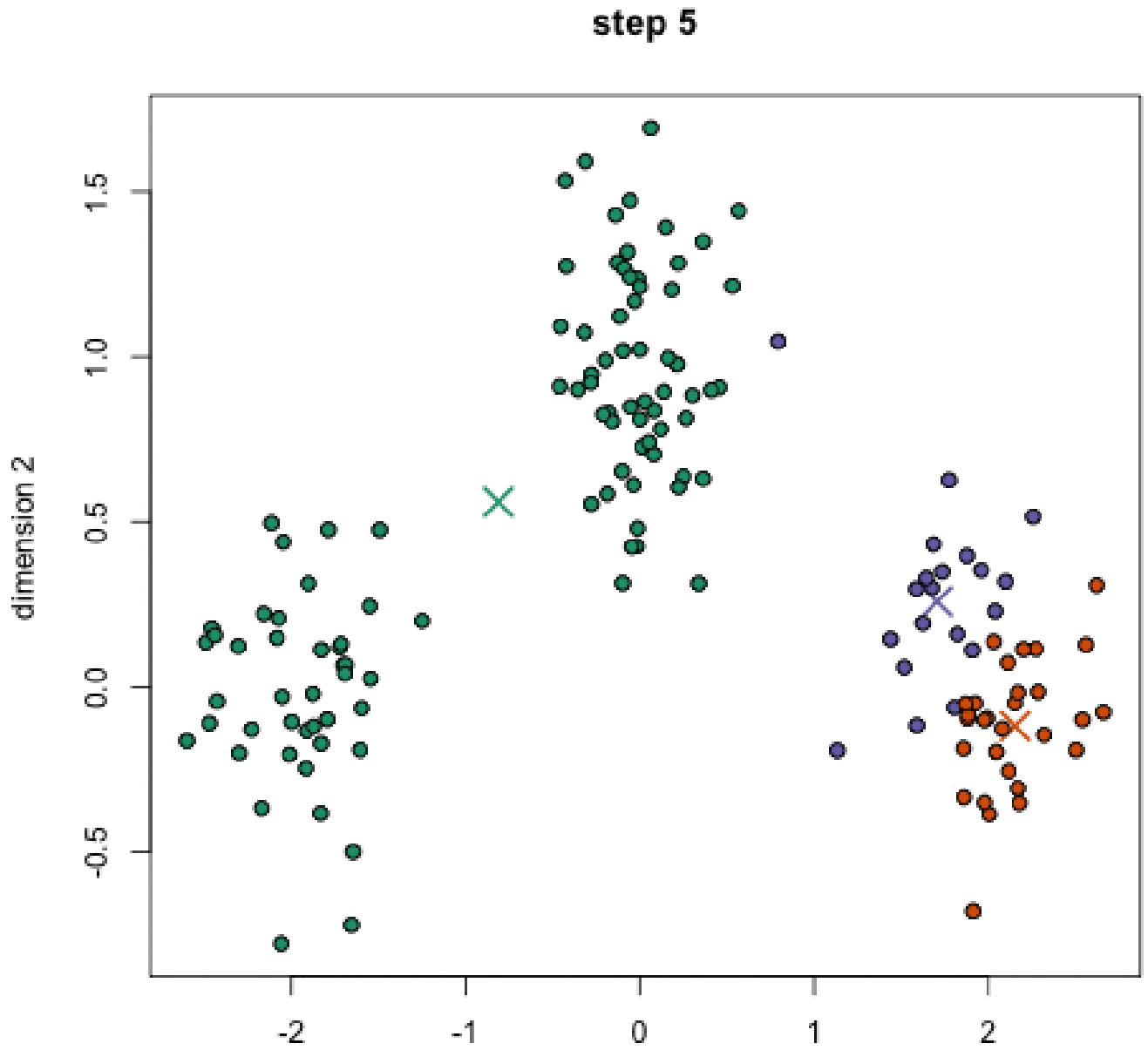


k-means exemple



k-means exemple



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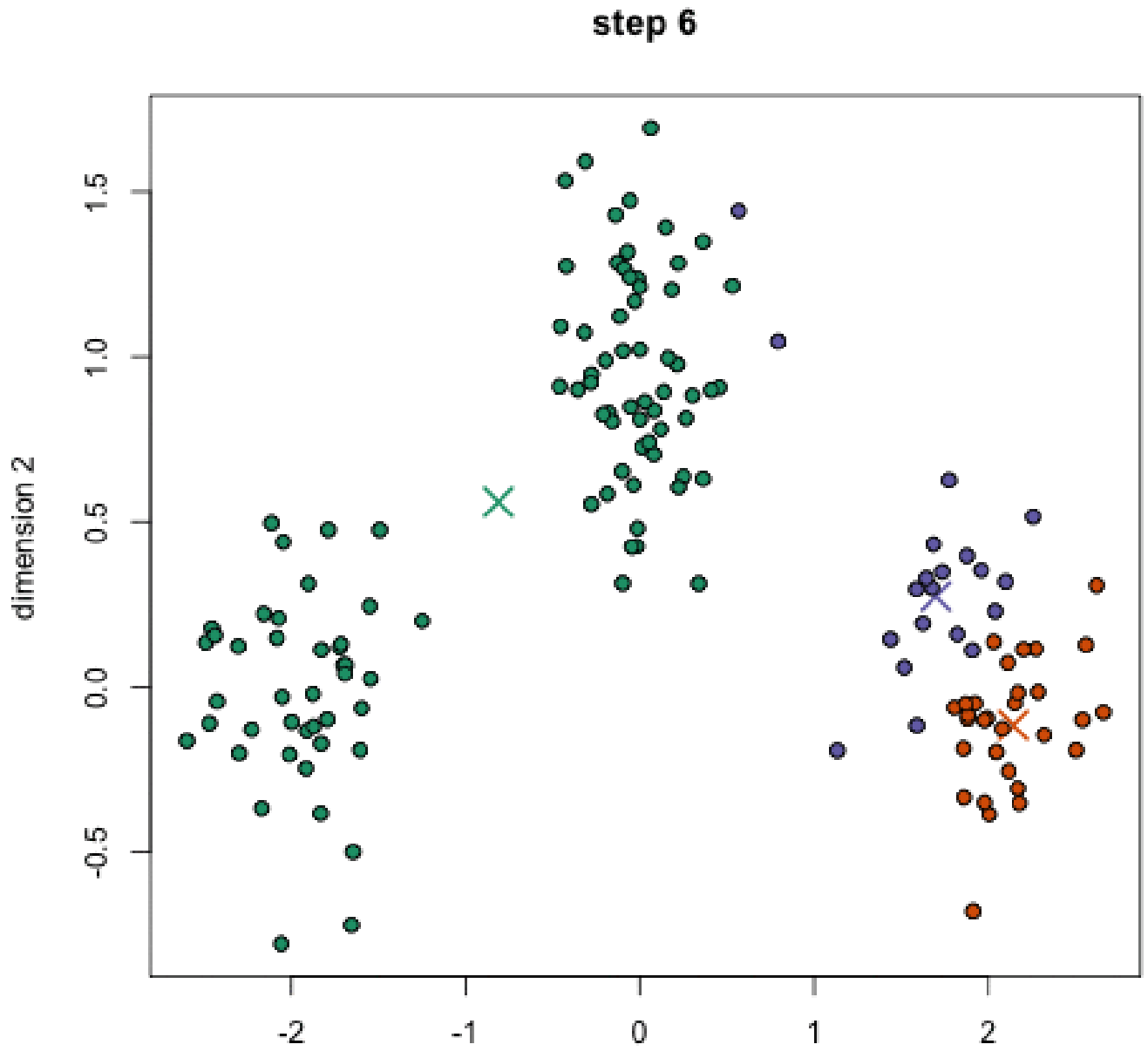

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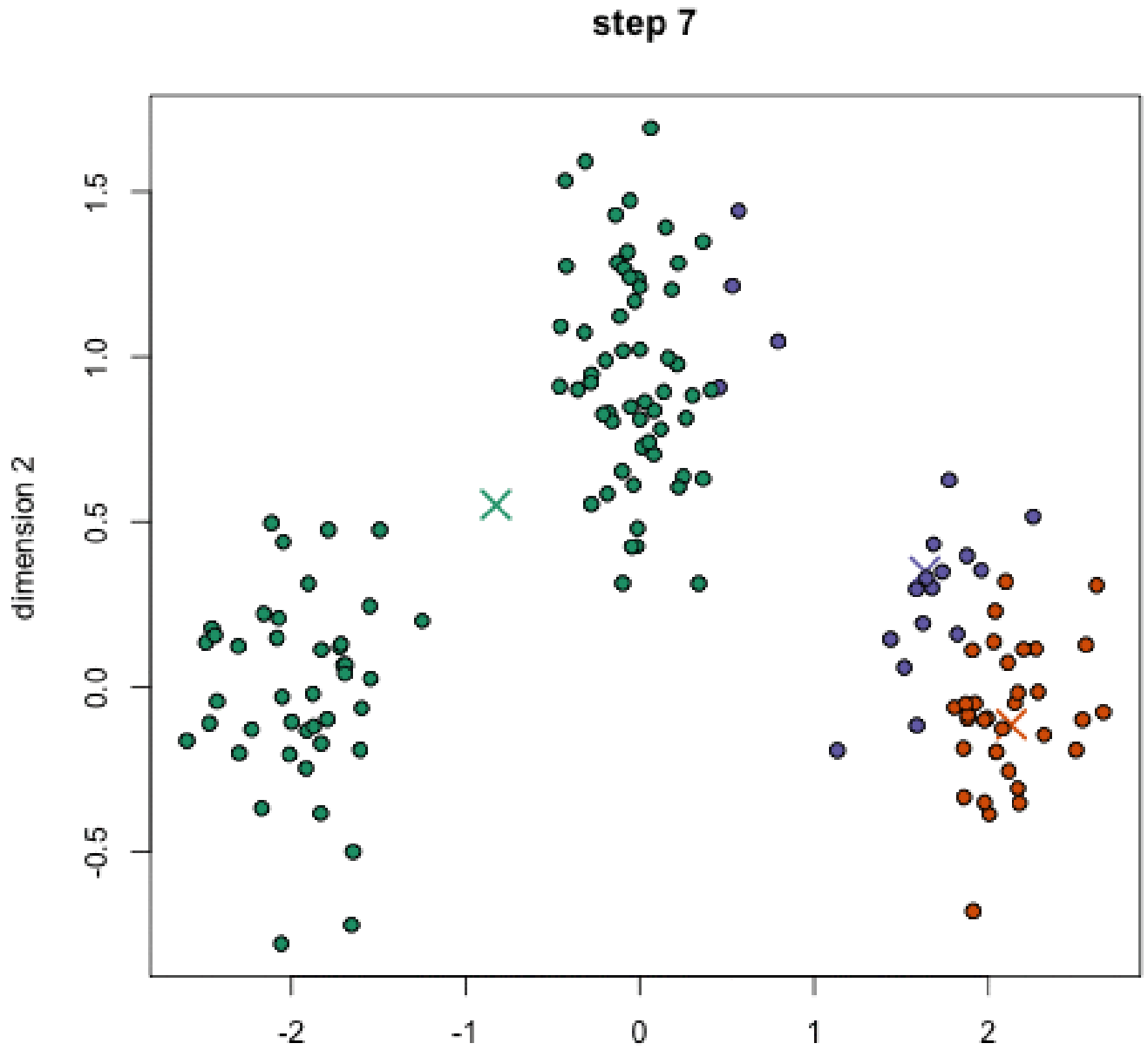

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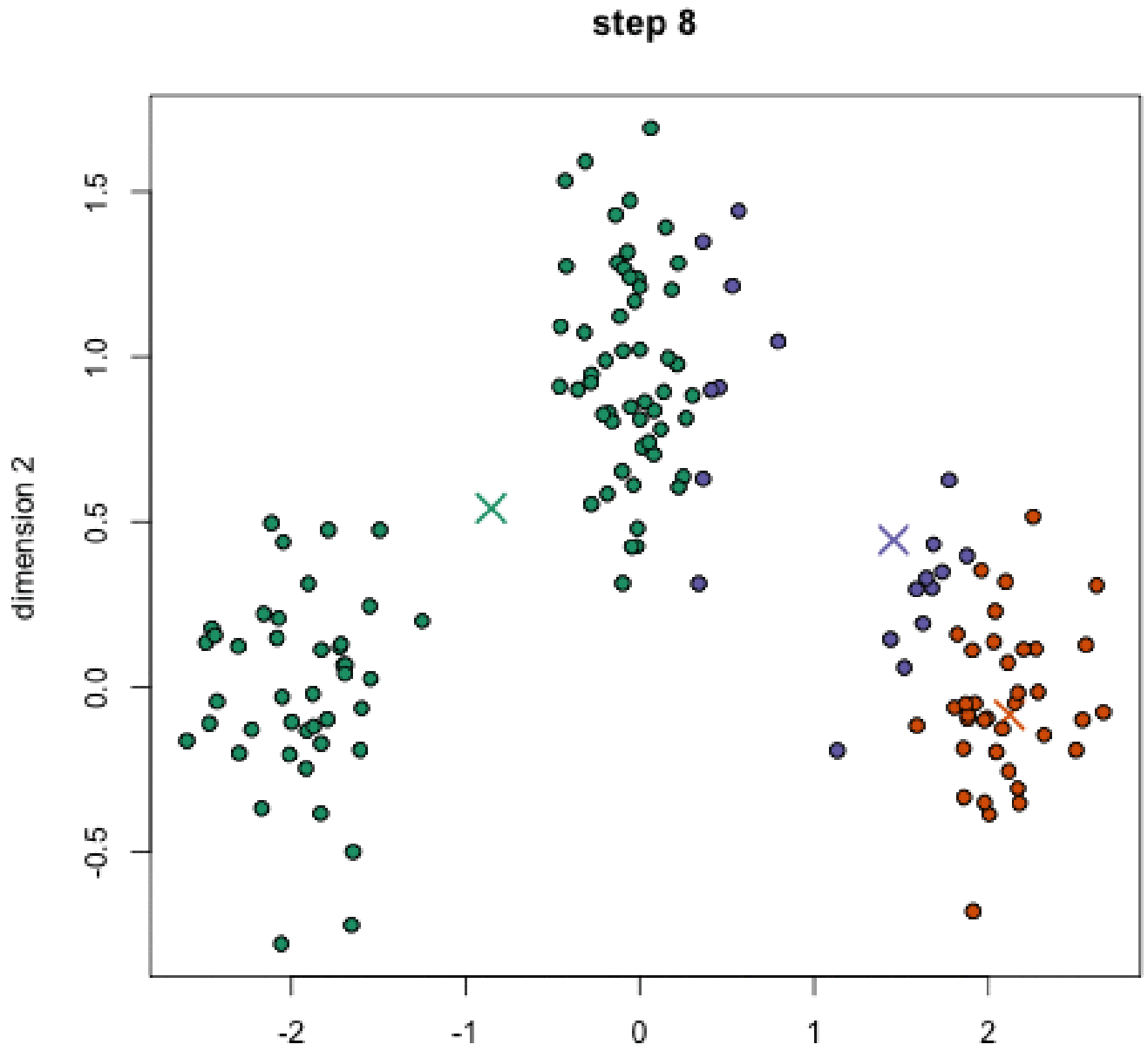
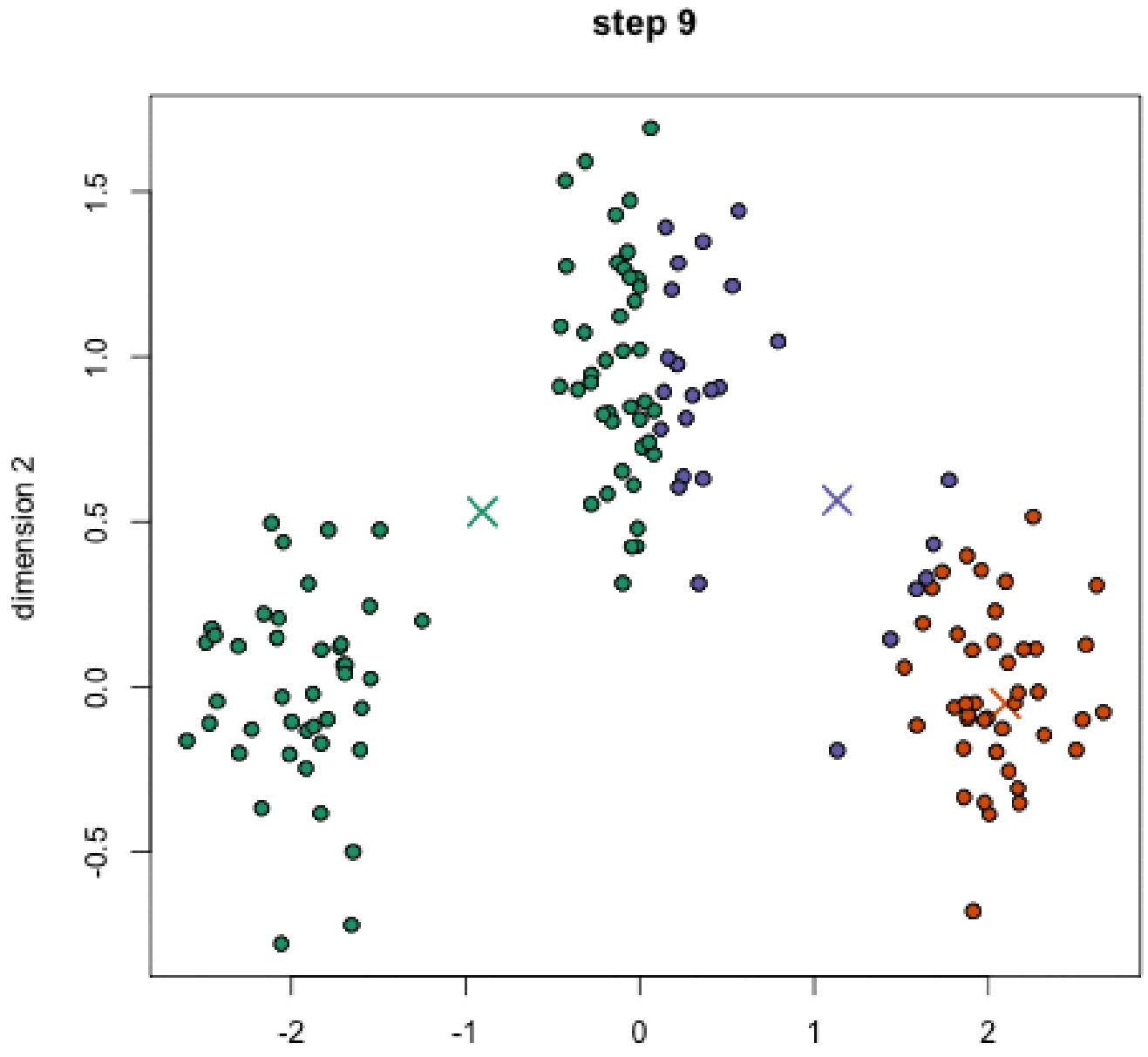


k-means exemple



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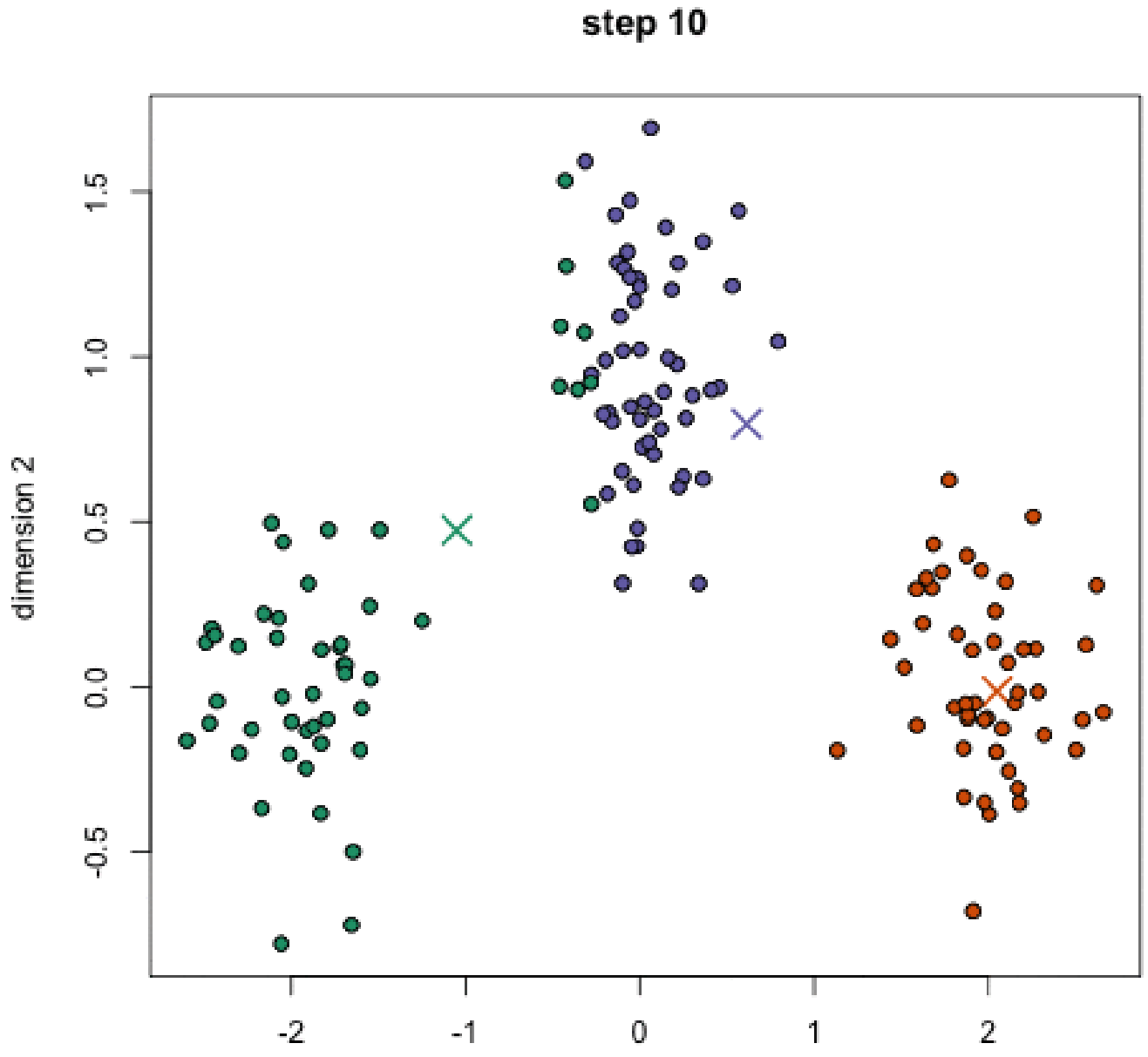

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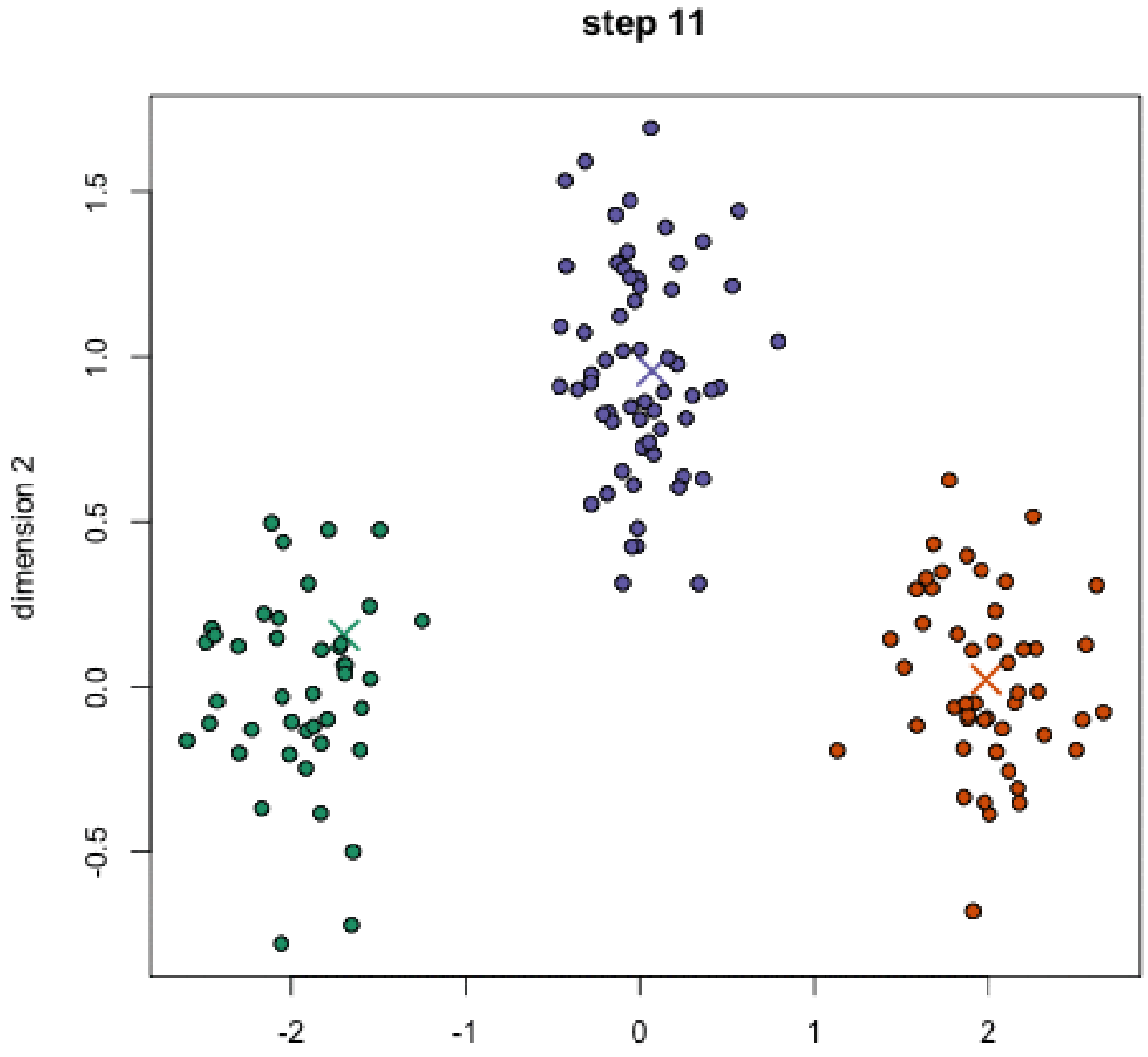
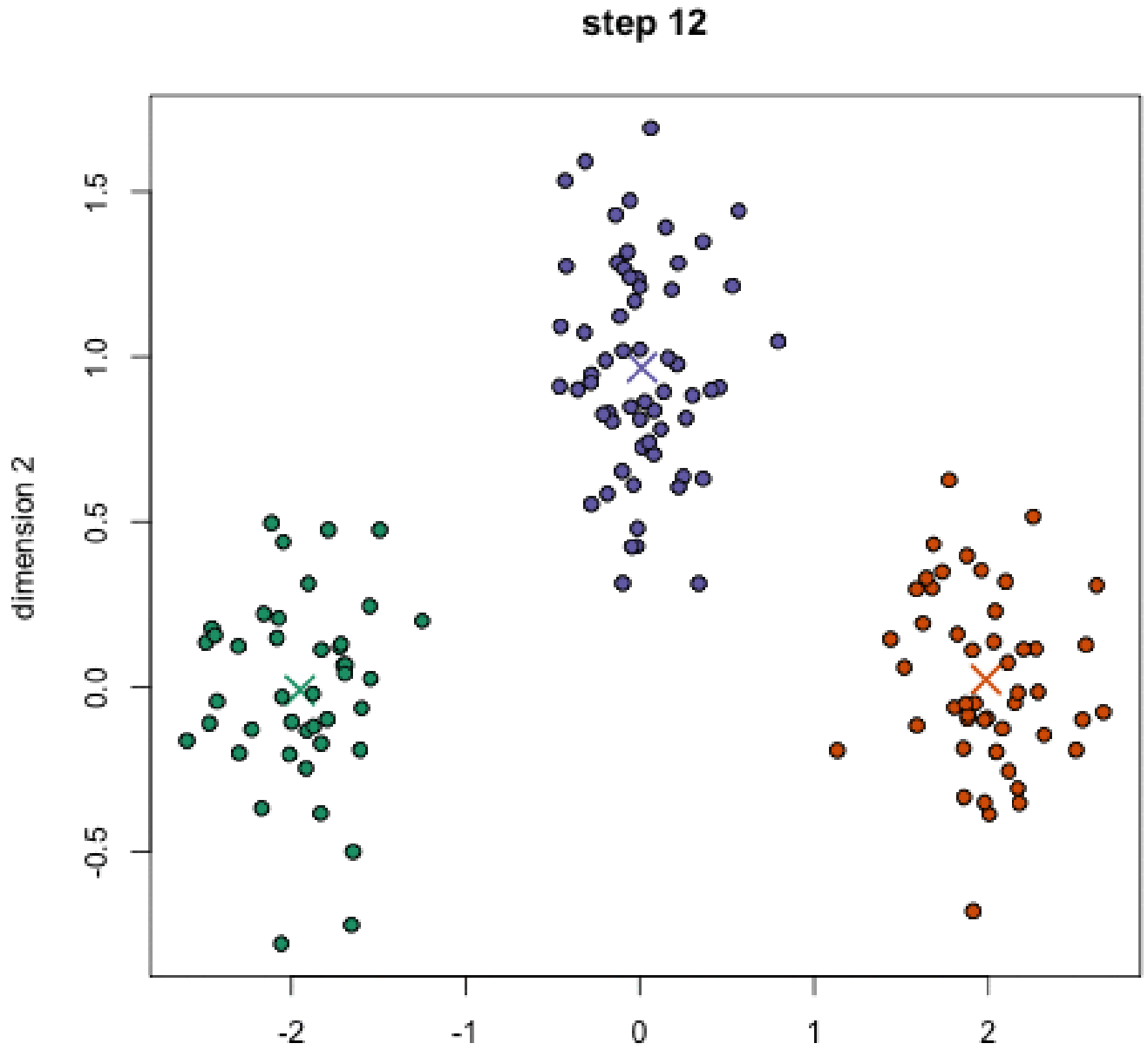


k-means exemple

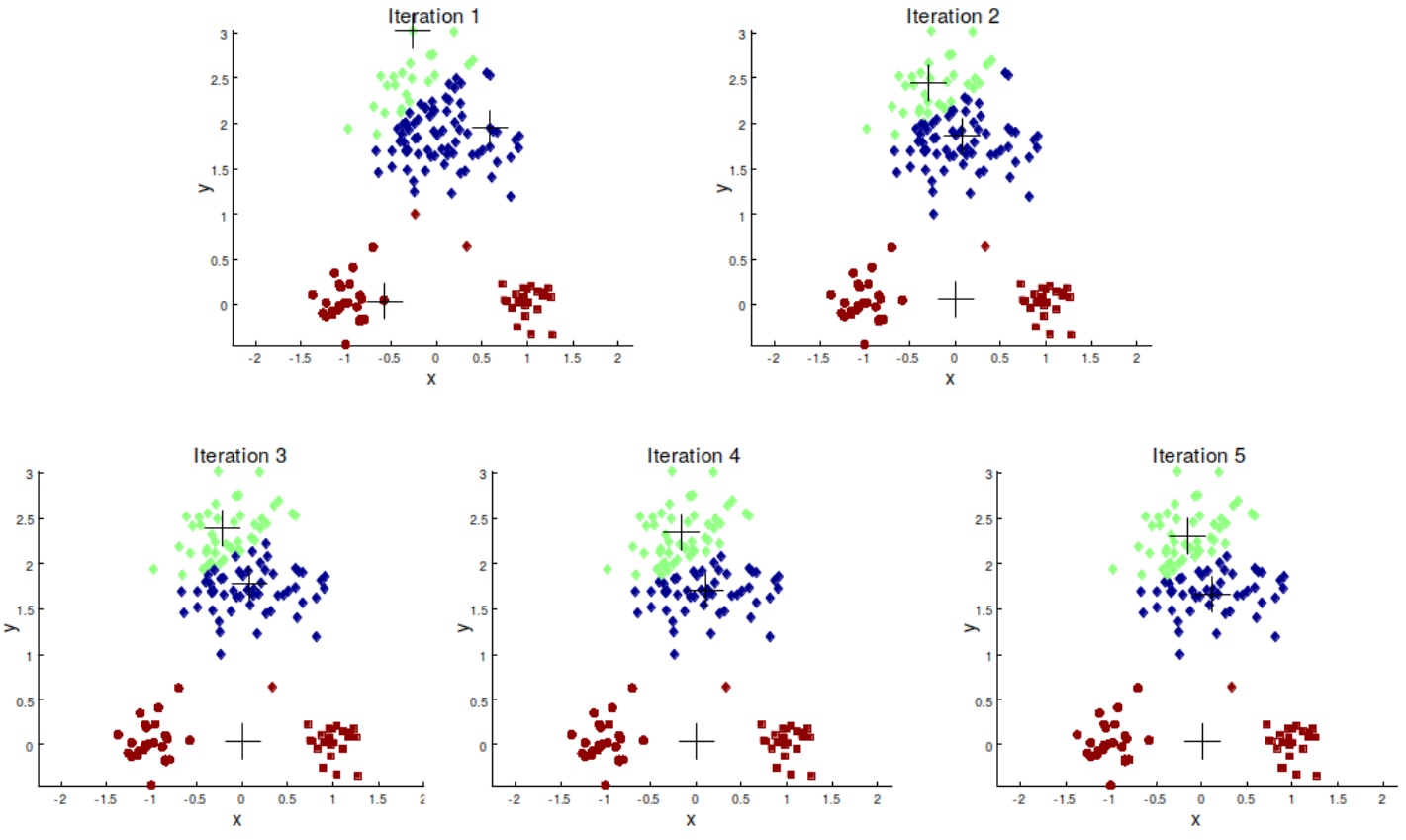


Limitation of k-means : clusters

- k-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes
- k-means has problems when the data contains outliers.

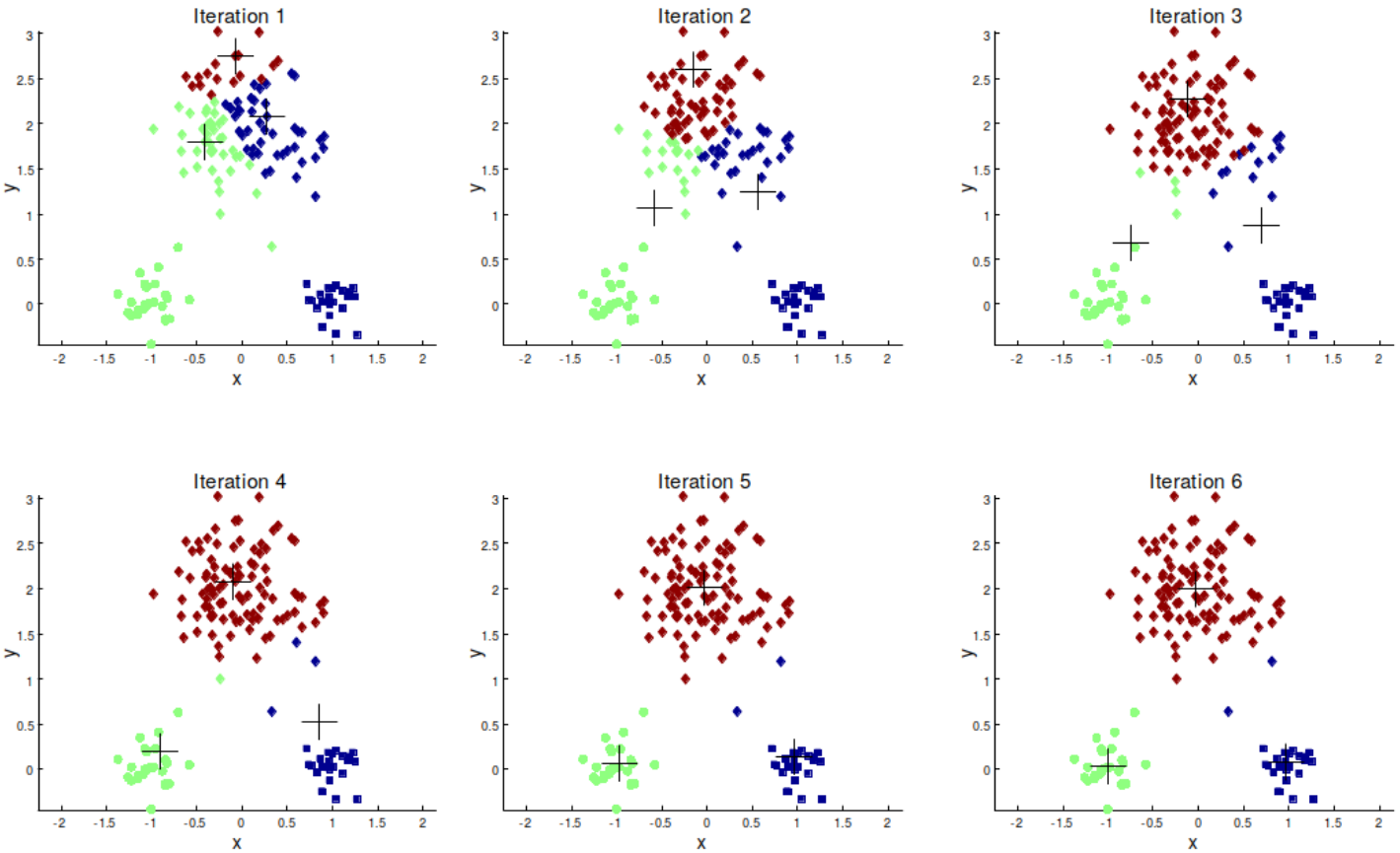
Normalising the data and removing outliers can help !

Limitation of k-means : initialisation



Using multiple runs or kmeans++ can help !

Limitation of k-means : initialisation



Using multiple runs or kmeans++ can help !

La sélection aléatoire de points de départ ne garantit rien sur la qualité de la solution finale.

k-means++

Un algorithme $O(\log k)$-approché. Une bonne sélection de points de départ.

k-means++ : The Advantages of Careful Seeding David Arthur et Sergei Vassilvitskii
`http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf`

En spark : `https://spark.apache.org/docs/latest/ml-clustering.html#k-means`

3 k-means++ is $O(\log k)$-Competitive

In this section, we show the following theorem.

Theorem 3.1. *If $\mathcal{C}$ is constructed with k-means++, then the corresponding potential function ϕ satisfies, $E[\phi] \leq 8(\ln k + 2)\phi_{\text{OPT}}$.*

In fact, we prove this holds after only Step 1 of the algorithm above. As noted above, Steps 2-4 can only decrease ϕ.

Our analysis consists of two parts. First, we show that k-means++ is competitive in those clusters of $\mathcal{C}_{\text{OPT}}$ from which it chooses a center. This is easiest in the case of our first center, which is chosen uniformly at random.

Lemma 3.2. *Let A be an arbitrary cluster in $\mathcal{C}_{\text{OPT}}$, and let $\mathcal{C}$ be the clustering with just one center, which is chosen uniformly at random from A. Then, $E[\phi(A)] = 2\phi_{\text{OPT}}(A)$.*

Proof. Let $c(A)$ denote the center of mass of A. By Lemma 2.1, we know that since $\mathcal{C}_{\text{OPT}}$ is optimal, $c(A)$ must be the center corresponding to the cluster A. By the same Lemma, we also have,

$$\begin{aligned} E[\phi(A)] &= \frac{1}{|A|}\sum_{a_0 \in A}\sum_{a \in A}\|a - a_0\|^2 \\ &= \frac{1}{|A|}\sum_{a_0 \in A}\left(\sum_{a \in A}\|a - c(A)\|^2 + |A| \cdot \|a_0 - c(A)\|^2\right) \\ &= 2\sum_{a \in A}\|a - c(A)\|^2, \end{aligned}$$

and the result follows. □

Our next step is to prove an analog of Lemma 3.2 for the remaining centers, which are chosen with D^2 weighting.

Streaming k-means

Streaming k-means

When data arrive in a stream, we may want to estimate clusters dynamically, updating them as new data arrive. `spark.mllib` provides support for streaming k-means clustering, with parameters to control the decay (or "forgetfulness") of the estimates. The algorithm uses a generalization of the mini-batch k-means update rule. For each batch of data, we assign all points to their nearest cluster, compute new cluster centers, then update each cluster using:

$$c_{t+1} = \frac{c_t n_t \alpha + x_t m_t}{n_t \alpha + m_t} \tag{1}$$

$$n_{t+1} = n_t + m_t \tag{2}$$

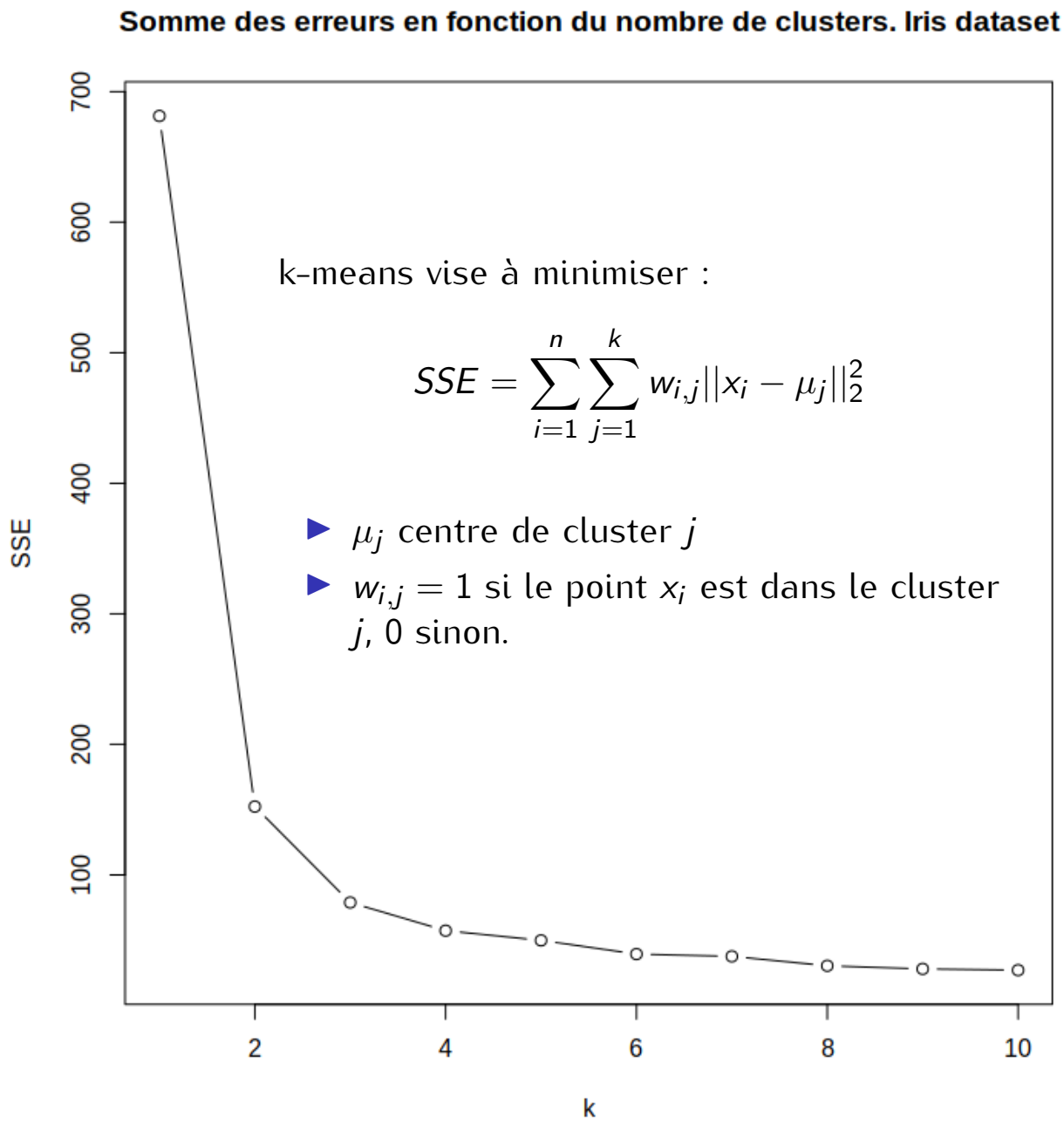
Where c_t is the previous center for the cluster, n_t is the number of points assigned to the cluster thus far, x_t is the new cluster center from the current batch, and m_t is the number of points added to the cluster in the current batch. The decay factor α can be used to ignore the past: with α=`1` all data will be used from the beginning; with α=`0` only the most recent data will be used. This is analogous to an exponentially-weighted moving average.

The decay can be specified using a `halfLife` parameter, which determines the correct decay factor `a` such that, for data acquired at time `t`, its contribution by time `t + halfLife` will have dropped to 0.5. The unit of time can be specified either as `batches` or `points` and the update rule will be adjusted accordingly.

> En spark :
> `https://spark.apache.org/docs/latest/mllib-clustering.html#streaming-k-means`

Comment choisir le nombre de clusters k ?

Coude-critère (elbow method)

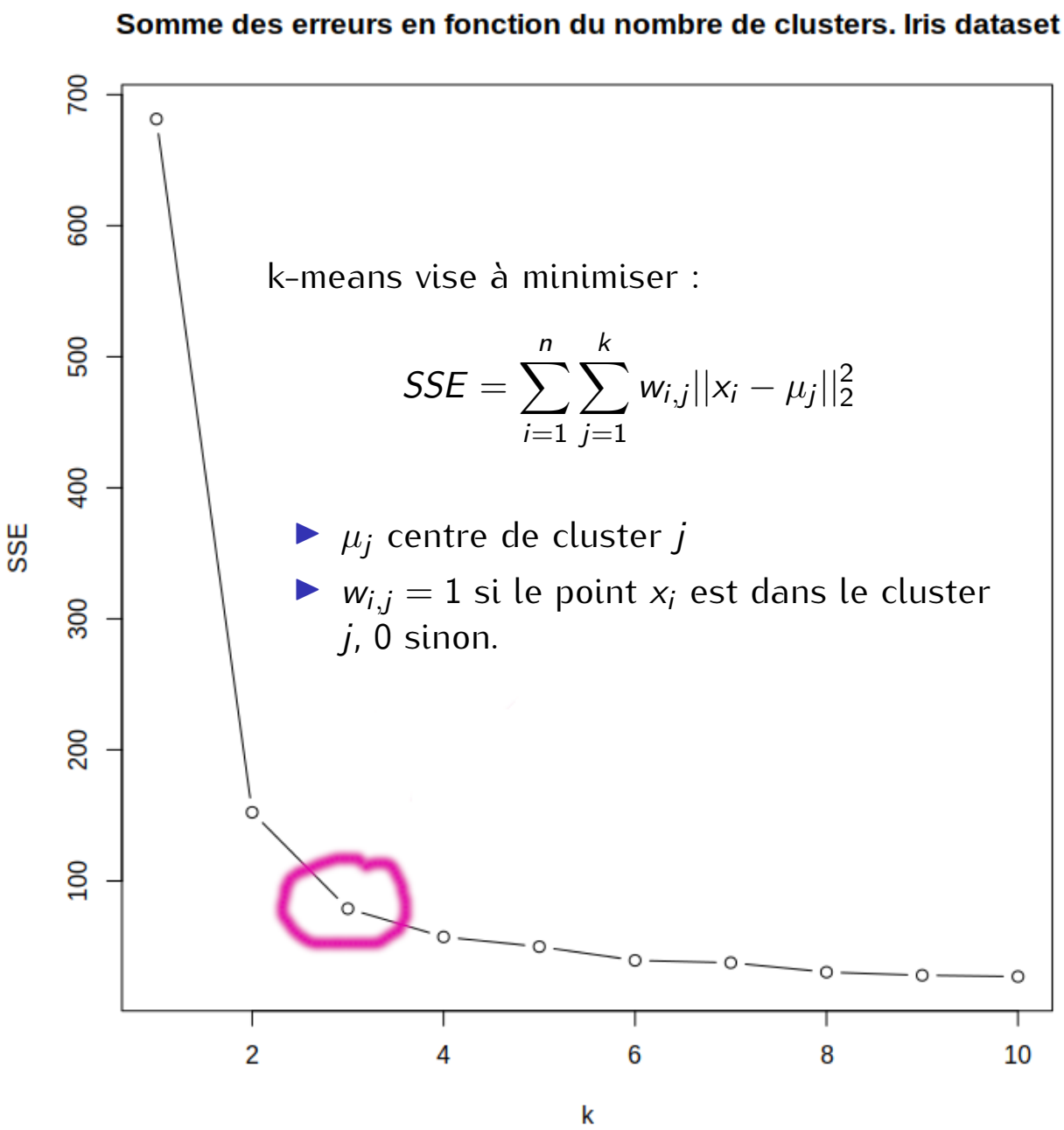


k-means vise à minimiser :

$$SSE = \sum_{i=1}^{n} \sum_{j=1}^{k} w_{i,j} ||x_i - \mu_j||_2^2$$

- μ_j centre de cluster j
- $w_{i,j} = 1$ si le point x_i est dans le cluster j, 0 sinon.

Coude-critère (elbow method)



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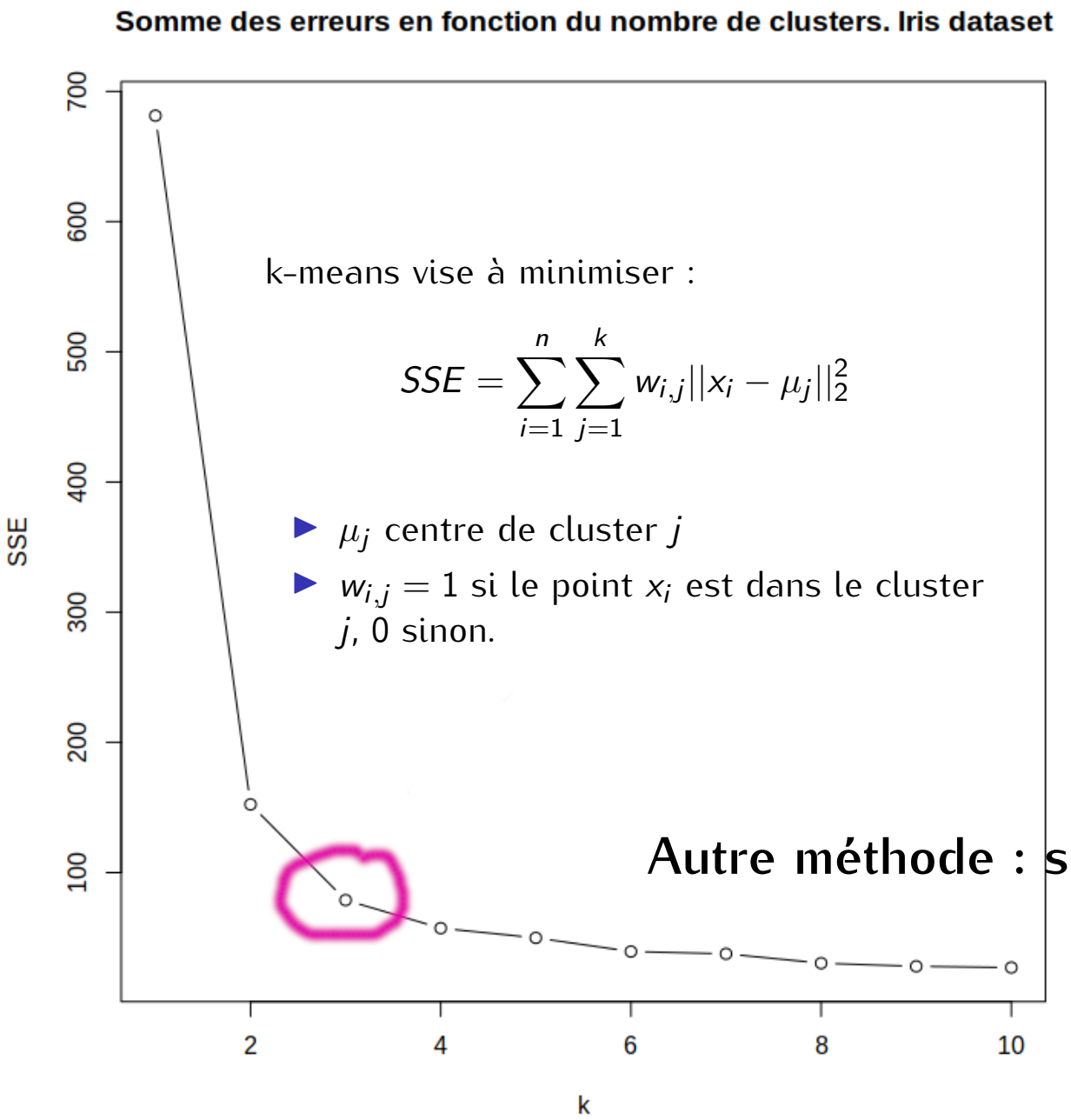

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Autre méthode : silhouette

Questions ?