machine learning

03 - k-means

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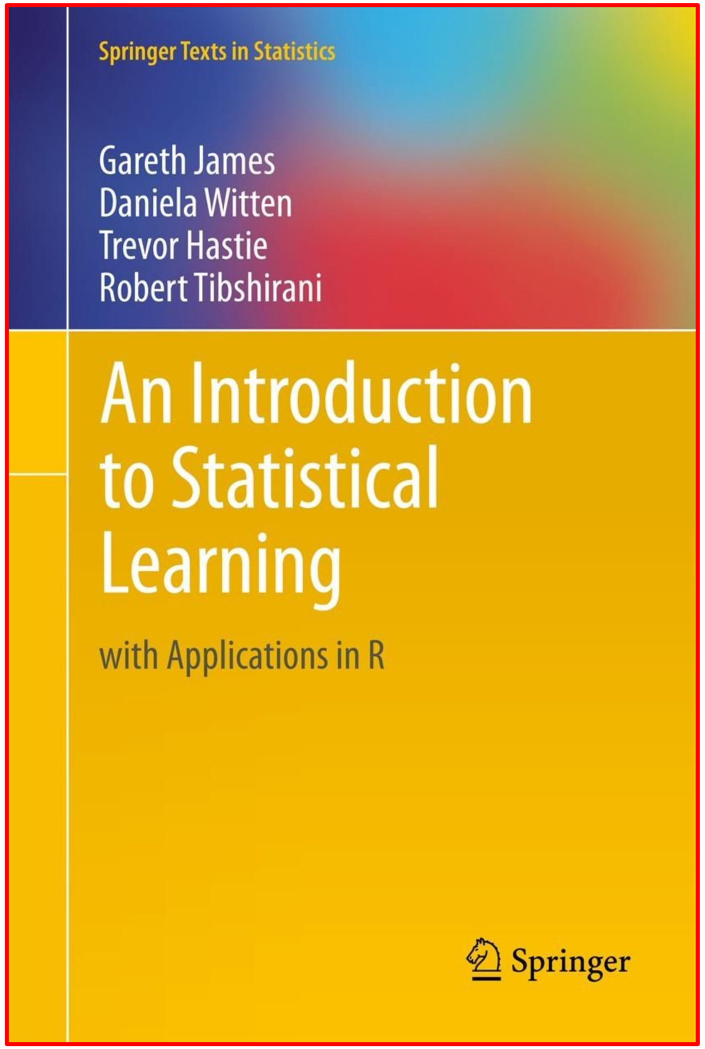
k-means theory

Chapter 10
An Introduction to Statistical Learning
by Gareth James, et al.

https://www-bcf.usc.edu/~gareth/ISL/ISLR%20Seventh%20Printing.pdf



k-means theory

- **Unsupervised** learning algorithm
- It is one of the simplest way to solve a **clustering** problem
- typical clustering problems:
    - cluster similar documents
    - custer customers
    - market segmentation
    - identify similar physical groups

k-means theory

- what is a cluster?
  A cluster refers to a collection of data points aggregated together because of certain similarities.

k-means theory

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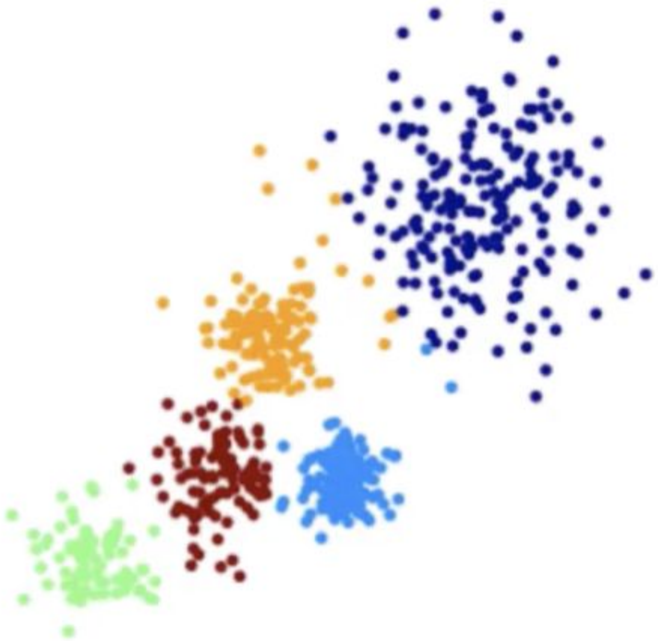
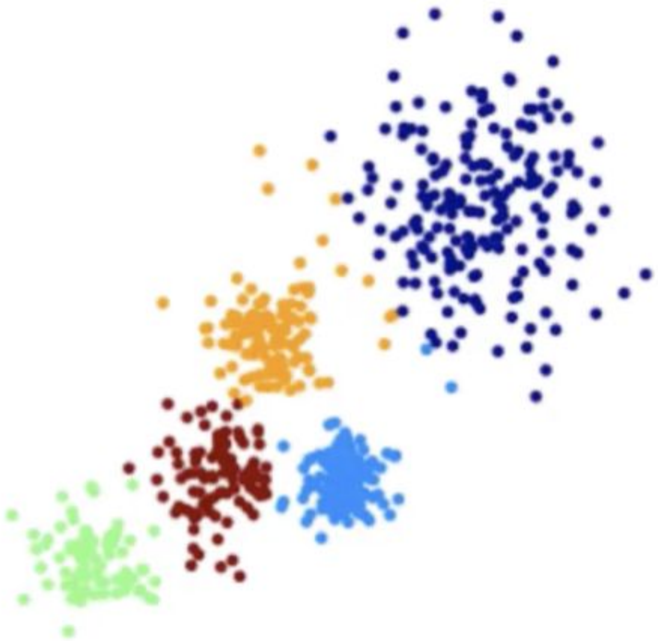


k-means theory

- The objective of K-means is simple: group similar data points together and discover underlying patterns. To achieve this objective, K-means looks for a fixed number (k) of clusters in a dataset.

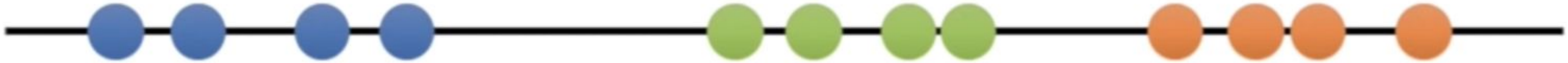


k-means theory

- Imagine you have some data you can plot in a line
- You already know the data is grouped in 3 clusters

k-means theory

- Imagine you have some data you can plot in a line
- You already know the data is grouped in 3 clusters
- In this case, the clusters are easy to see



k-means theory

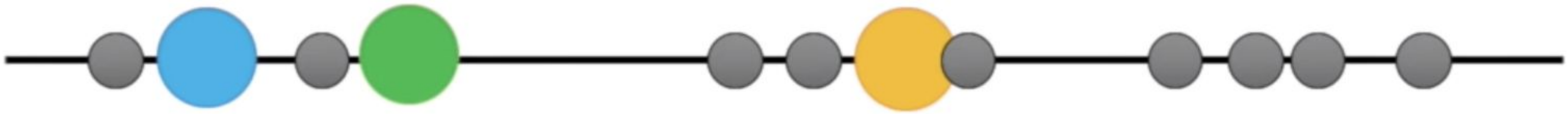
0. Let’s start with the raw data

k-means theory

1. Select the number of clusters you want to identify.
   This is the "K" in K-Means clustering
   Let's select k = 3

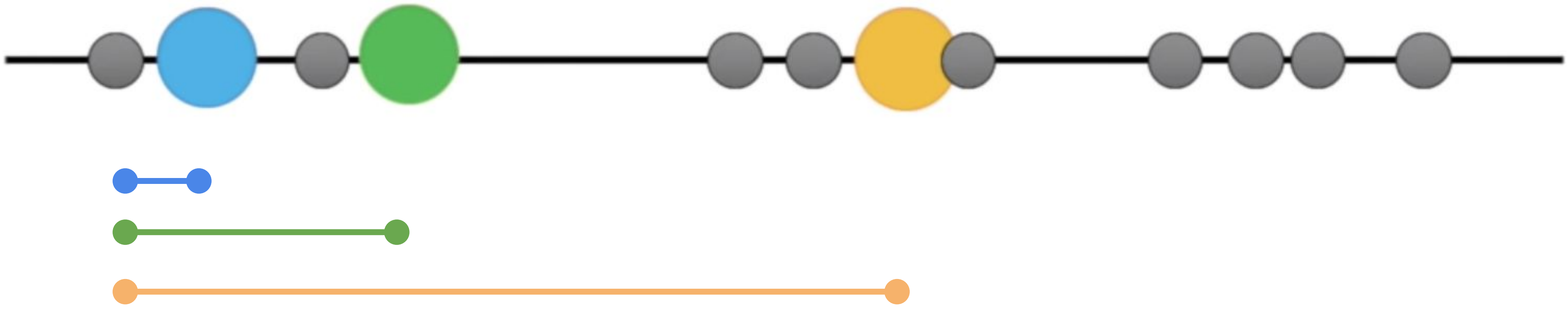
k-means theory

2. Randomly select 3 distinct data points
These are the initial clusters centroids



k-means theory

3. Measure the distance between the first point and the three centroids



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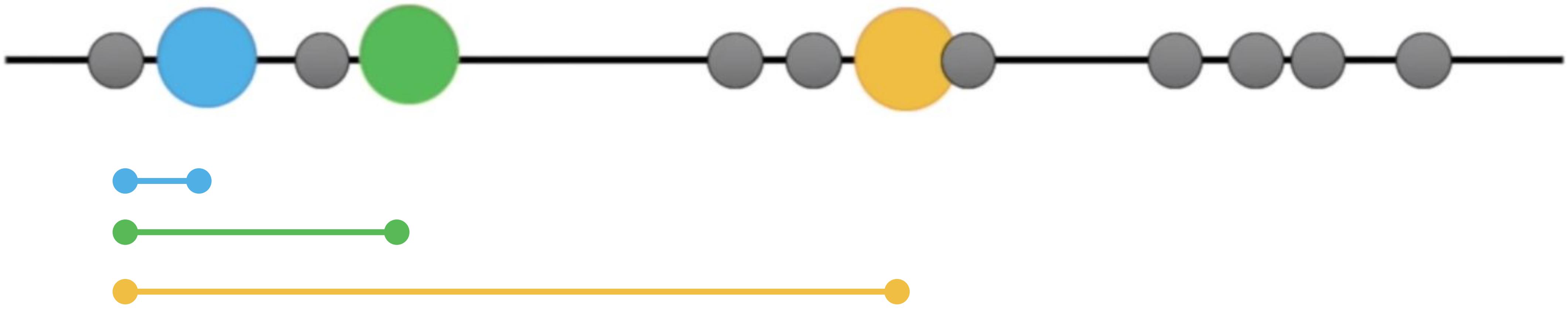
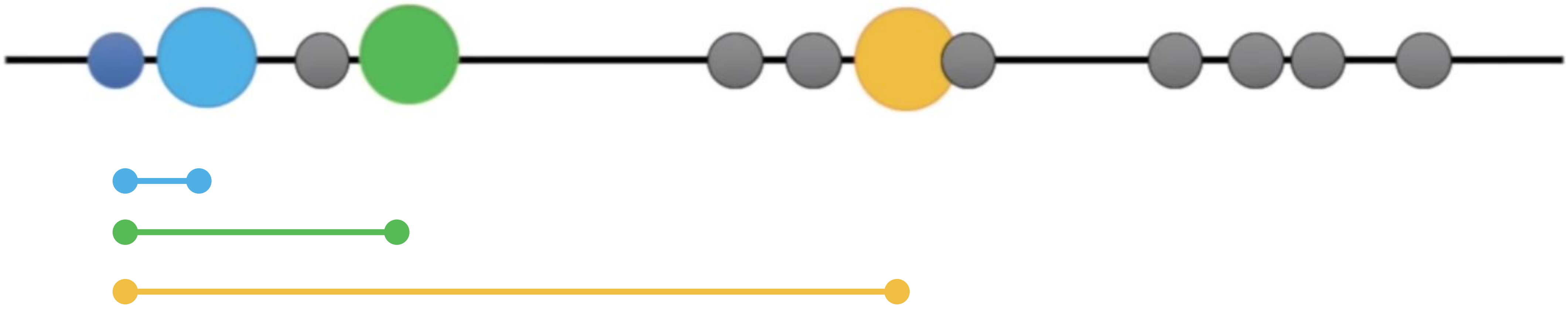
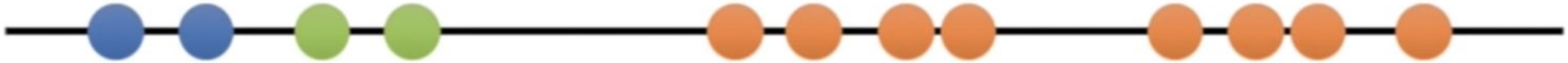


4. Assigns the point to the cluster to which the centroid is closest



k-means theory

4. Assigns the point to the cluster to which the centroid is closest
Do the same thing for the rest of points



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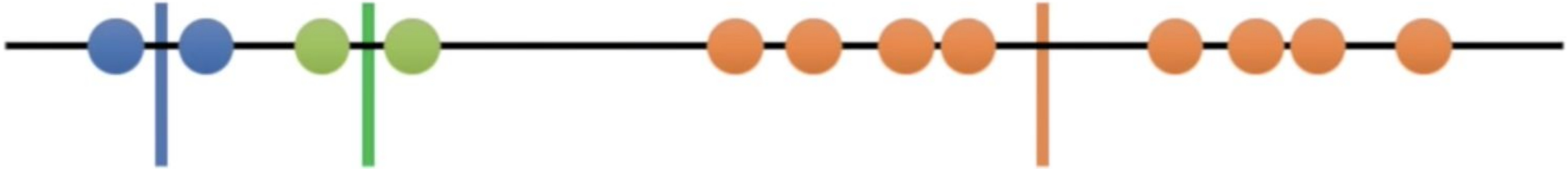
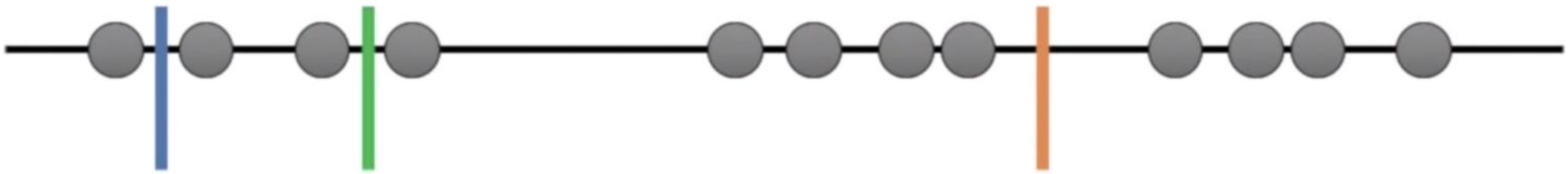
5. Calculate the mean of each cluster



k-means theory

6. Repeat the process but using the mean instead of the centroids



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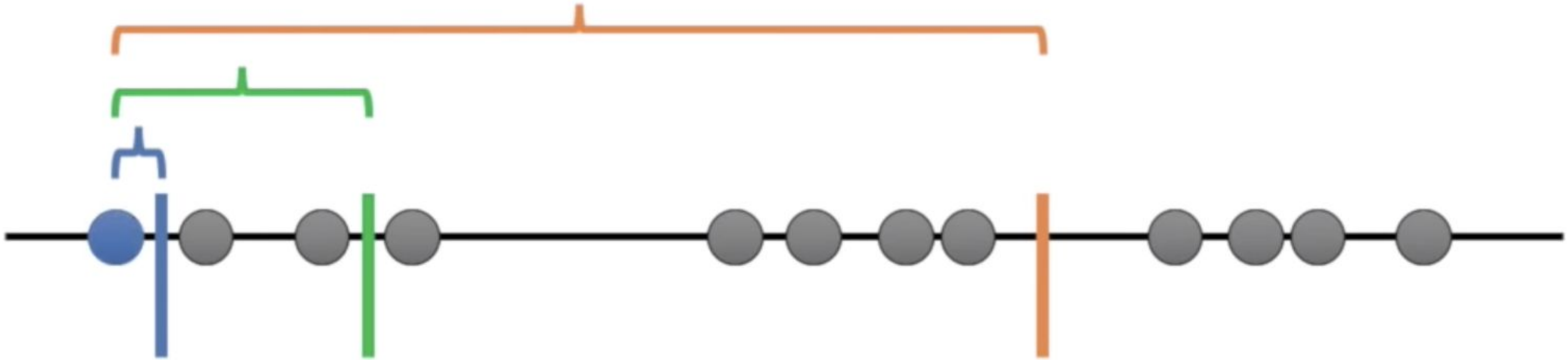

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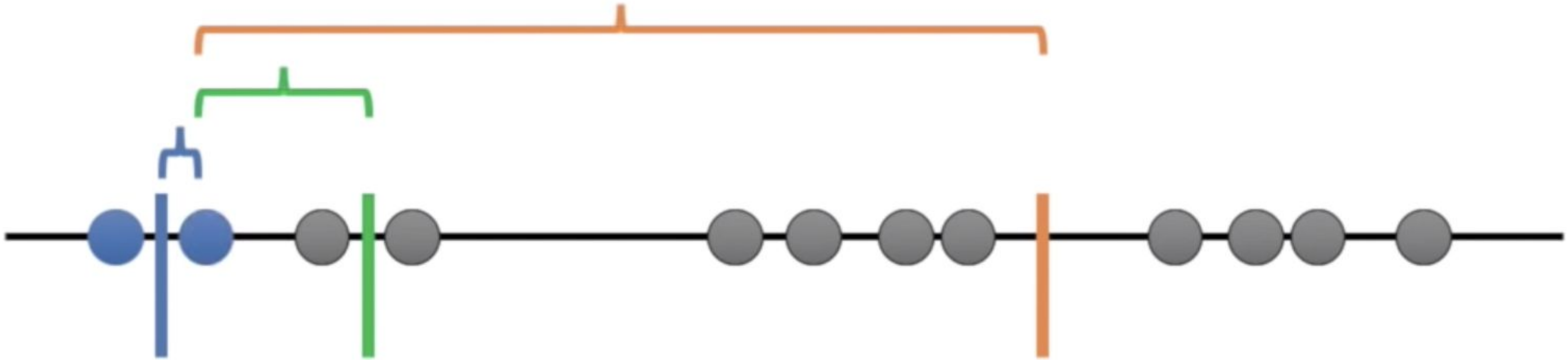

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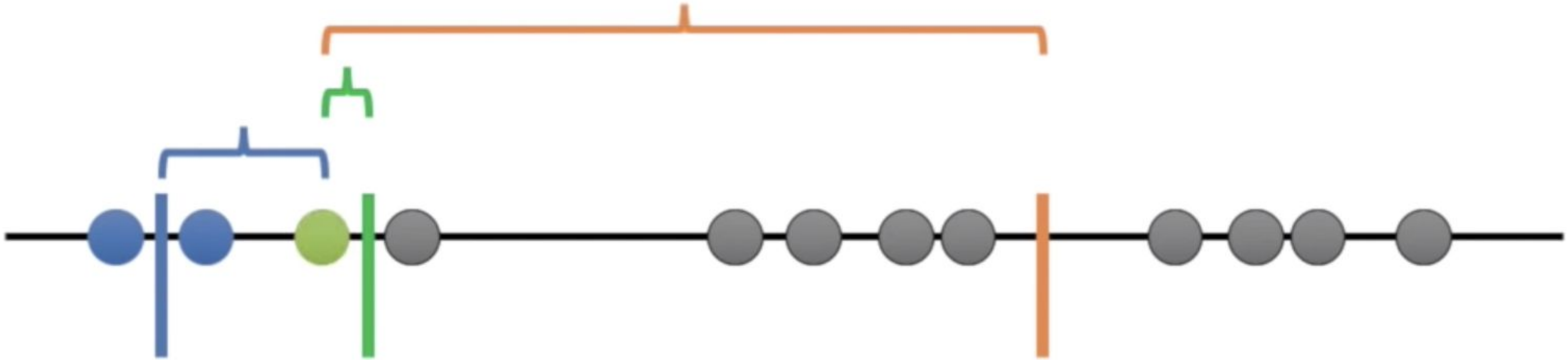

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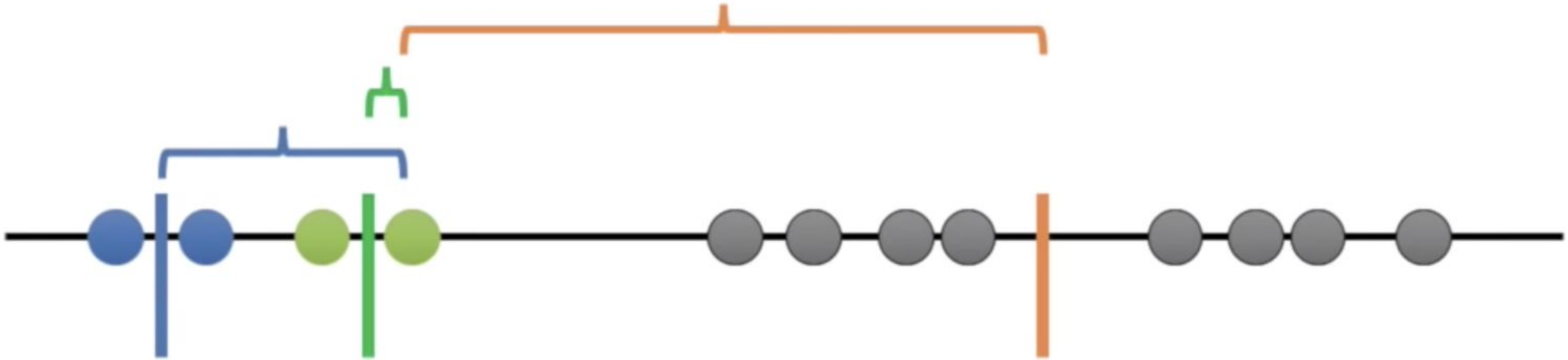

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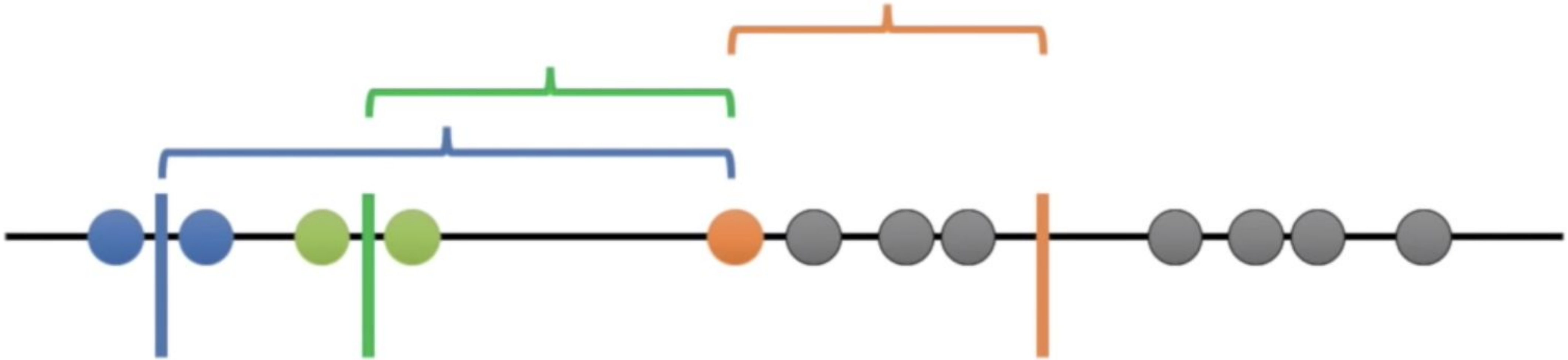

k-means theory

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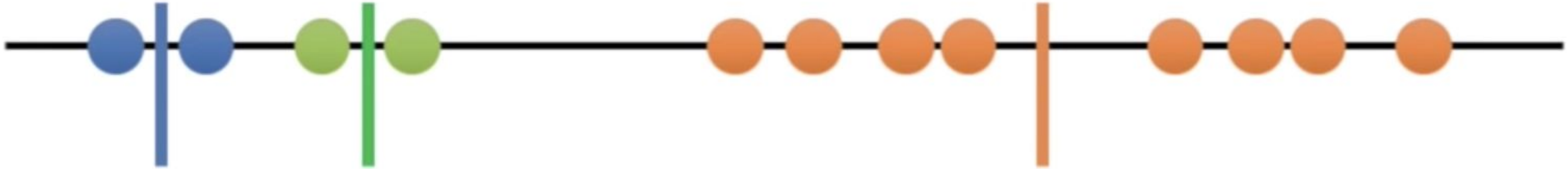
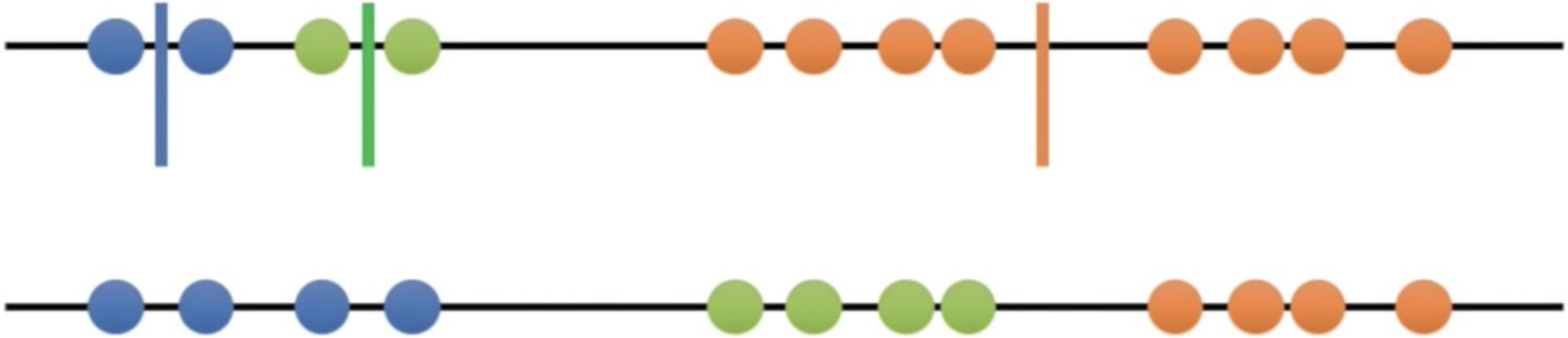
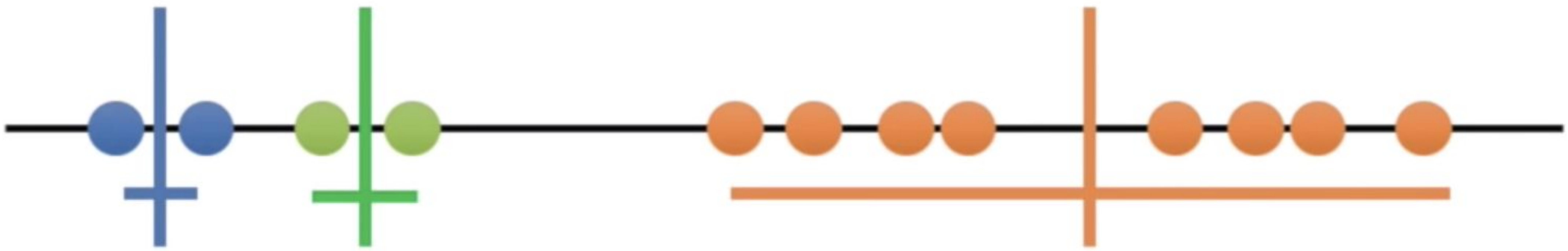


But this is not what we expected to have!



k-means theory

7. Add the variation within cluster



k-means theory

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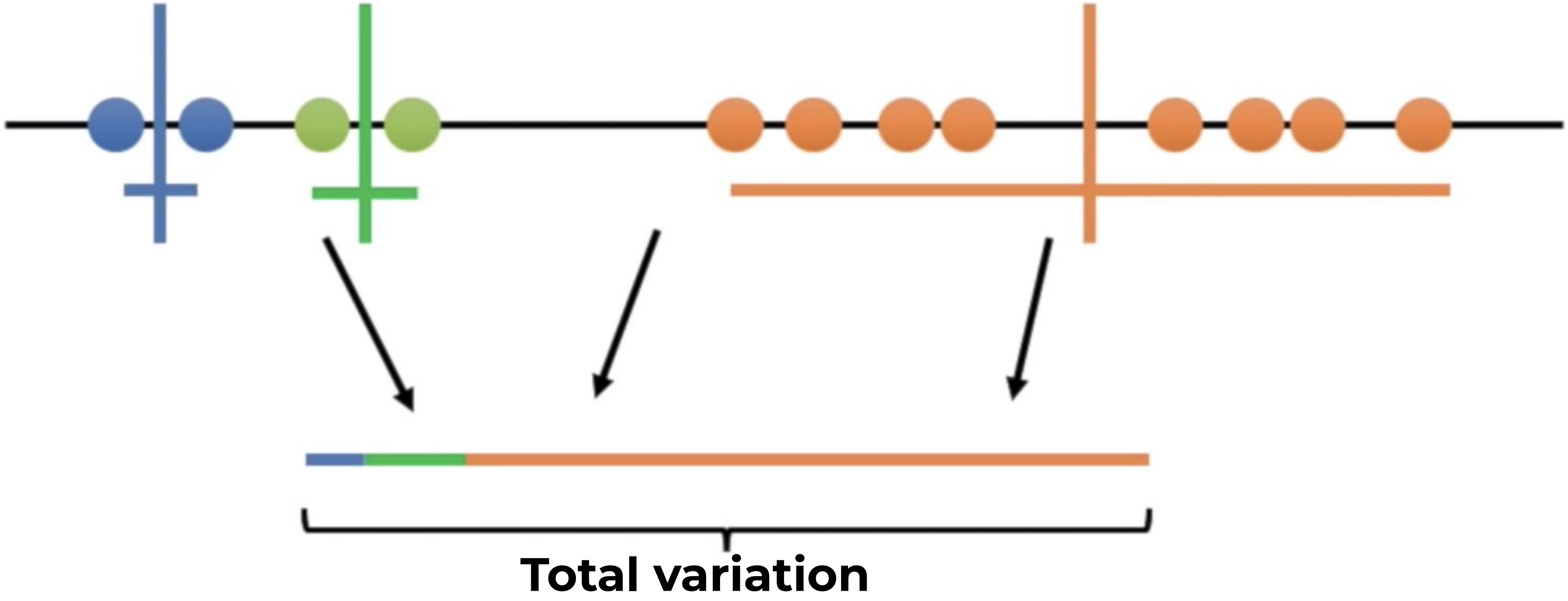

k-means theory

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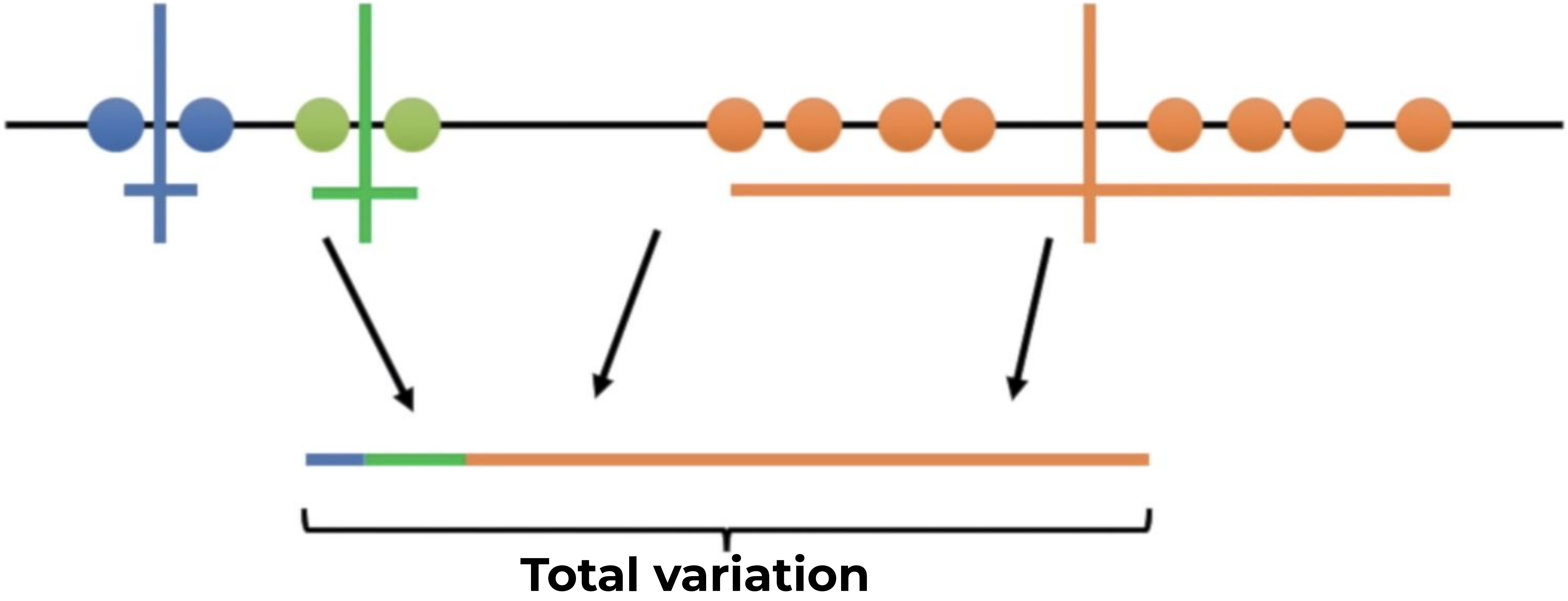
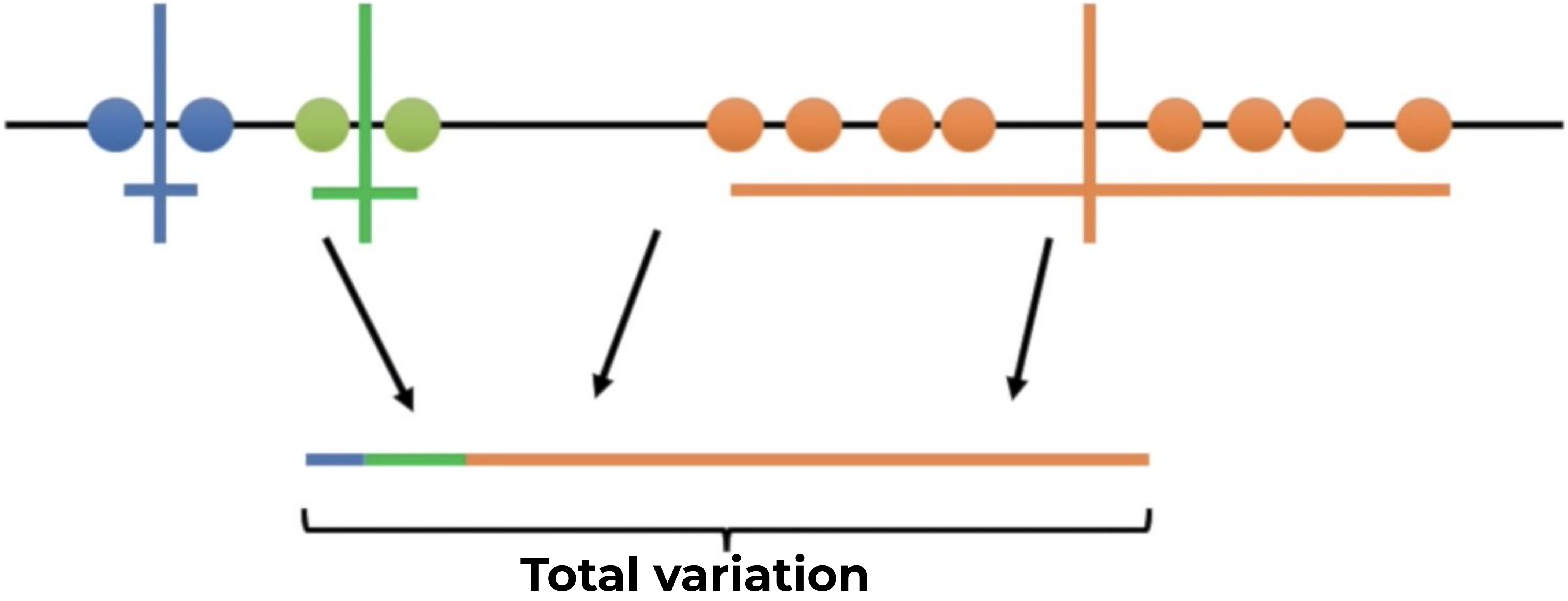


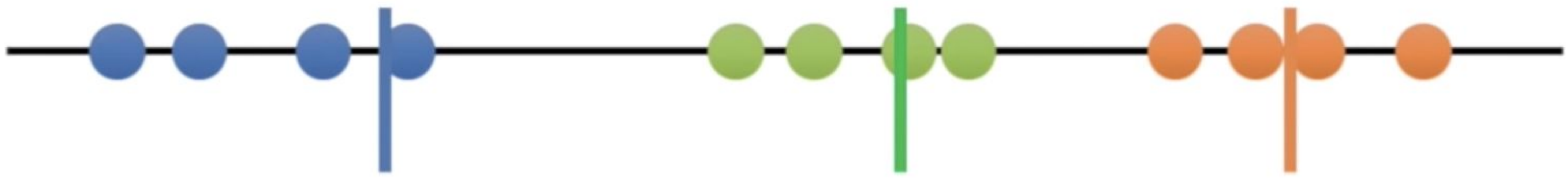
7. Add the variation within cluster

The goal now is to minimize the total variation. How?? -> **Iterate**



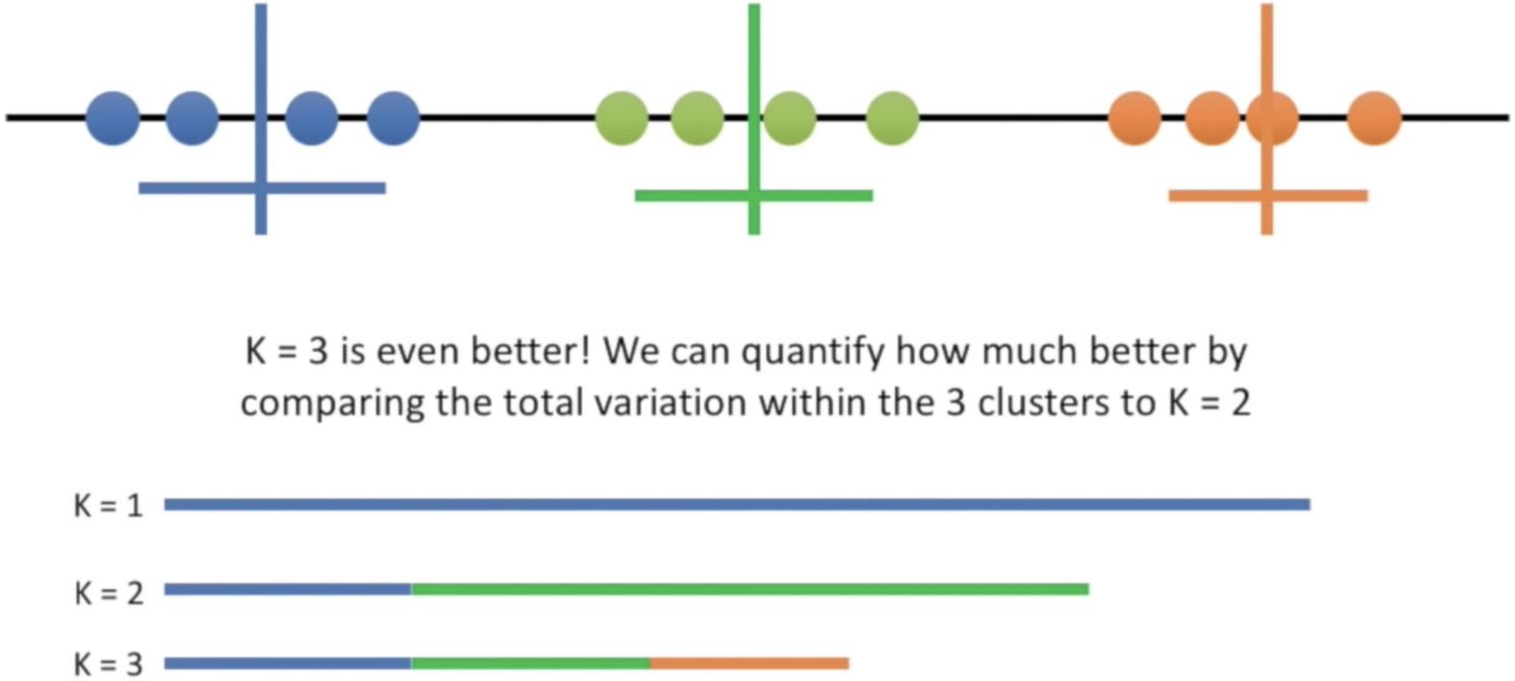
k-means theory

We have finally reach the cluster that minimize the total variation



k-means theory

What is the best K? The one that minimize the variation



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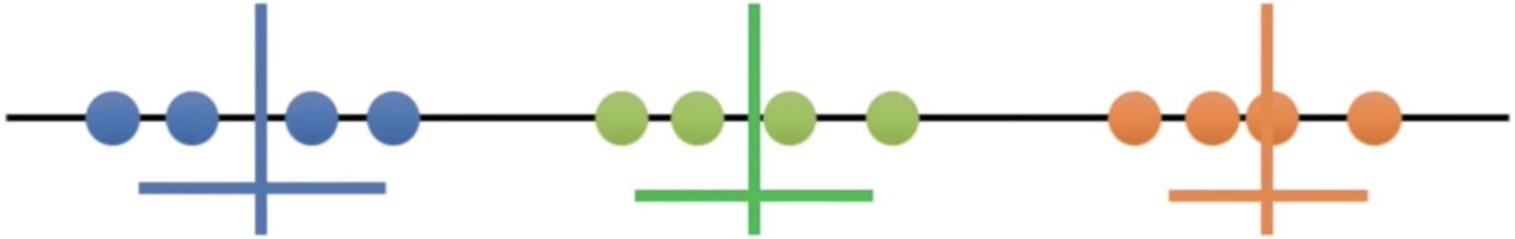
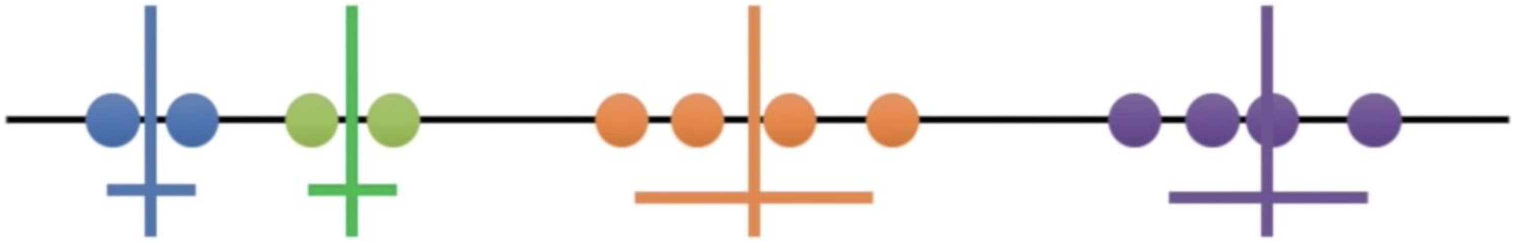
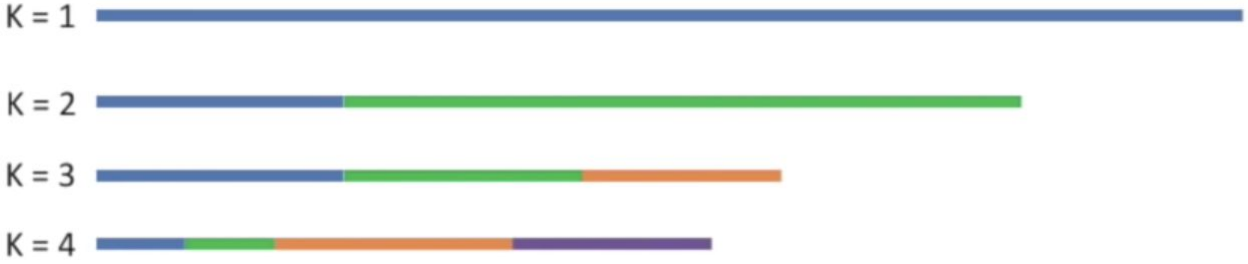


What if we try k = 4?





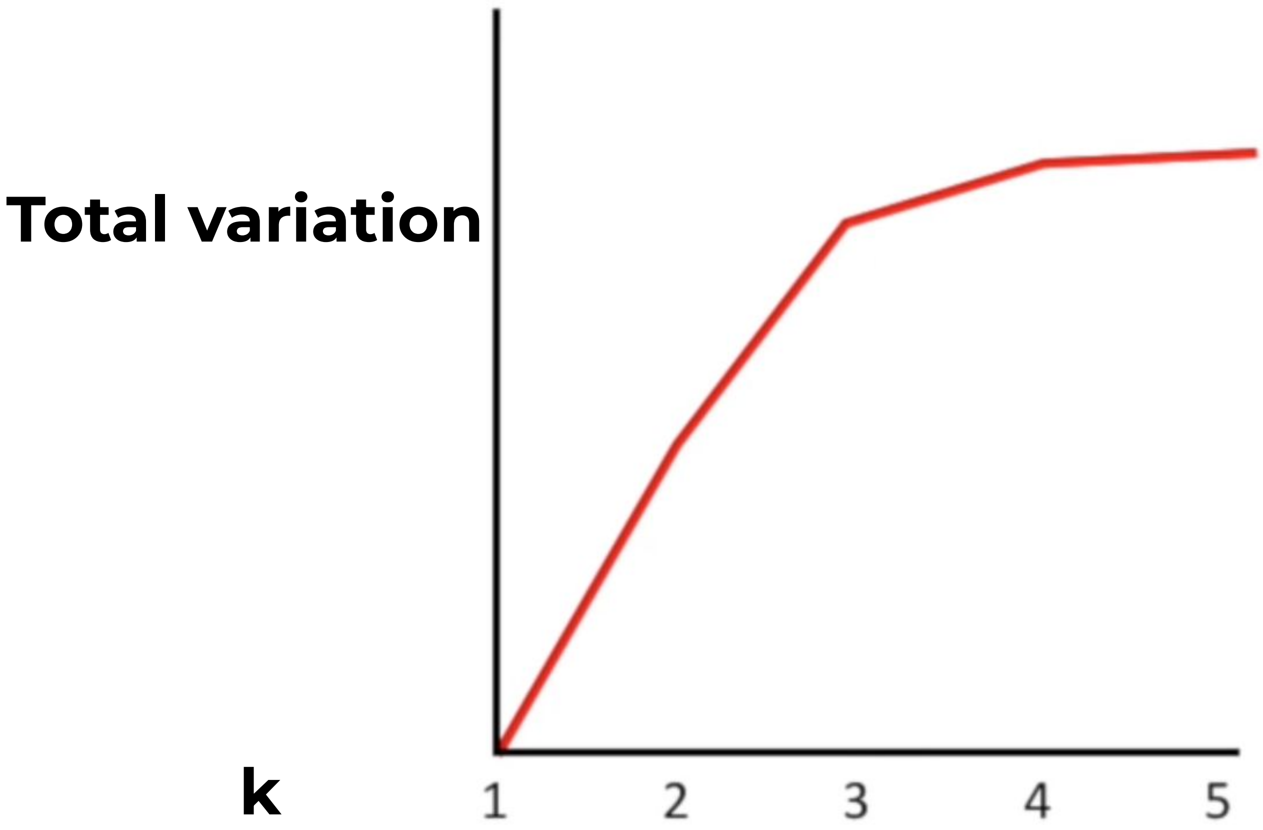
k-means theory

Each time we add a cluster (increases k by 1) the total variation is smaller.

So the best solution is when there is only one cluster per data point, innit??

If K=N then the variation is 0

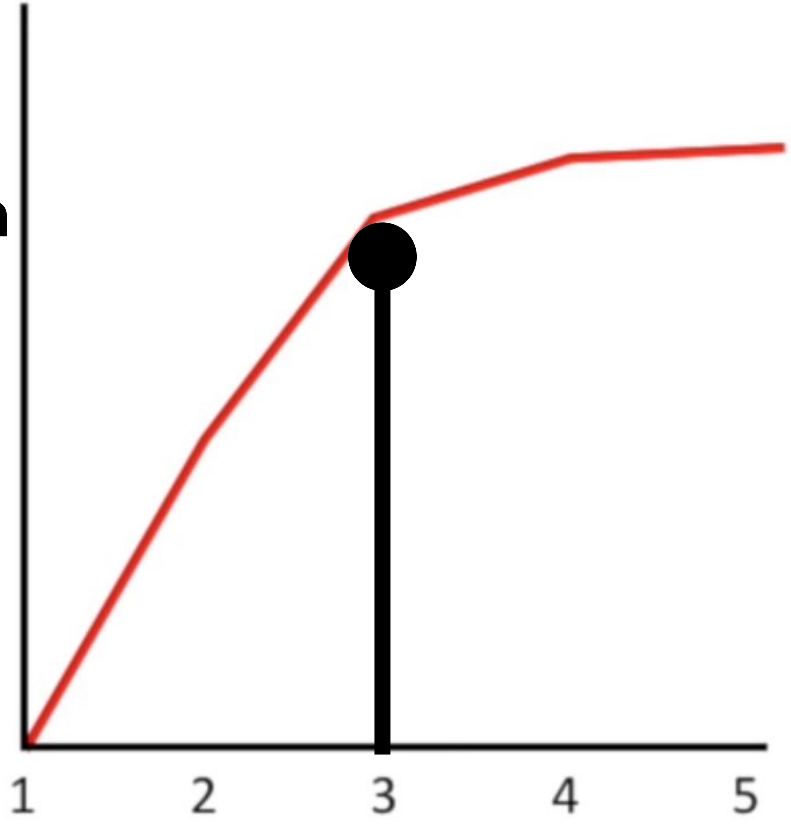
Solution : The elbow method



k-means theory

Solution : The elbow method

Total variation



k

k-means theory

- The objective of K-means is simple: group similar data points together and discover underlying patterns. To achieve this objective, K-means looks for a fixed number (k) of clusters in a dataset.

k-means theory

1. Initialize **cluster centroids** $\mu_1, \mu_2, \ldots, \mu_k \in \mathbb{R}^n$ randomly.

2. Repeat until convergence: {

   For every i, set
   $$c^{(i)} := \arg\min_j ||x^{(i)} - \mu_j||^2.$$

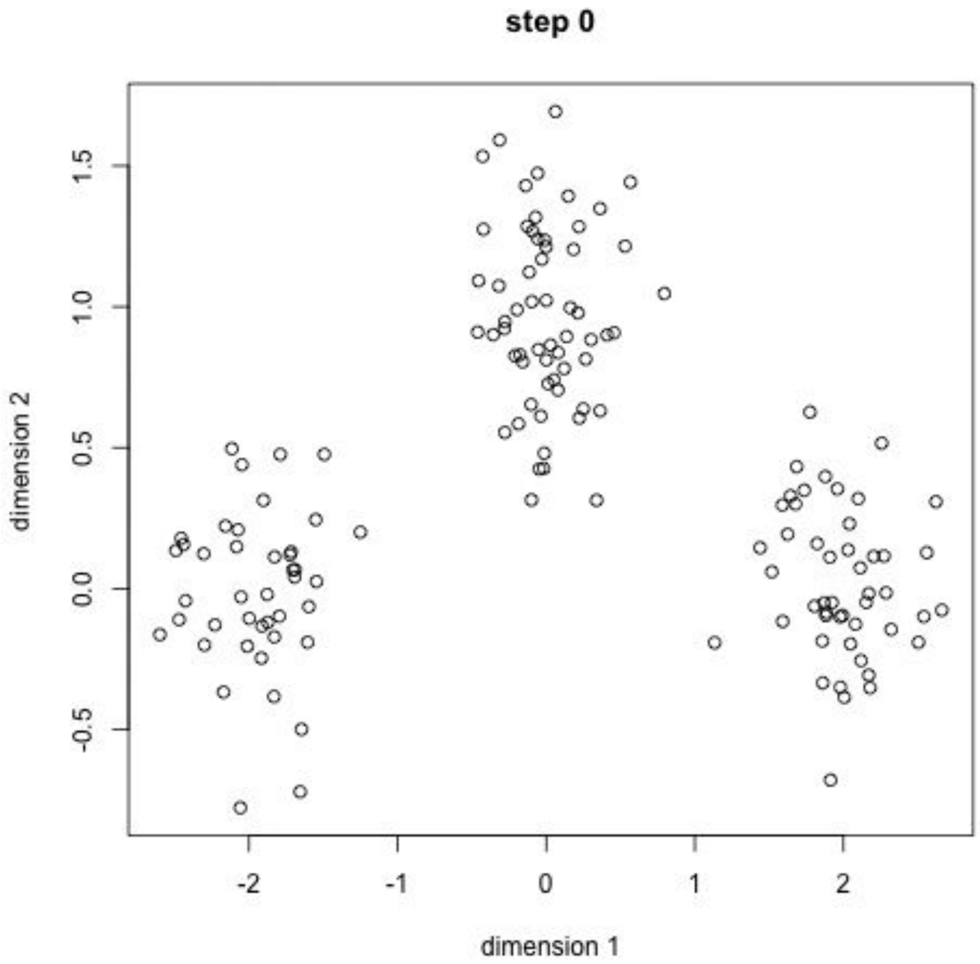
   For each j, set
   $$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

   }

k-means theory

1. **you** choose a number of clusters **K**
2. kmeans randomly create K centroids (which are the imaginary data point that represent the cluster) and assign each data point to the cluster which centroid is closest
3. Until convergence repeat:
    a. for each cluster, compute the cluster centroid by taking the **mean** vector of data points in the cluster
    b. assign each data point to the cluster for which the centroid is the closest.

k-means theory



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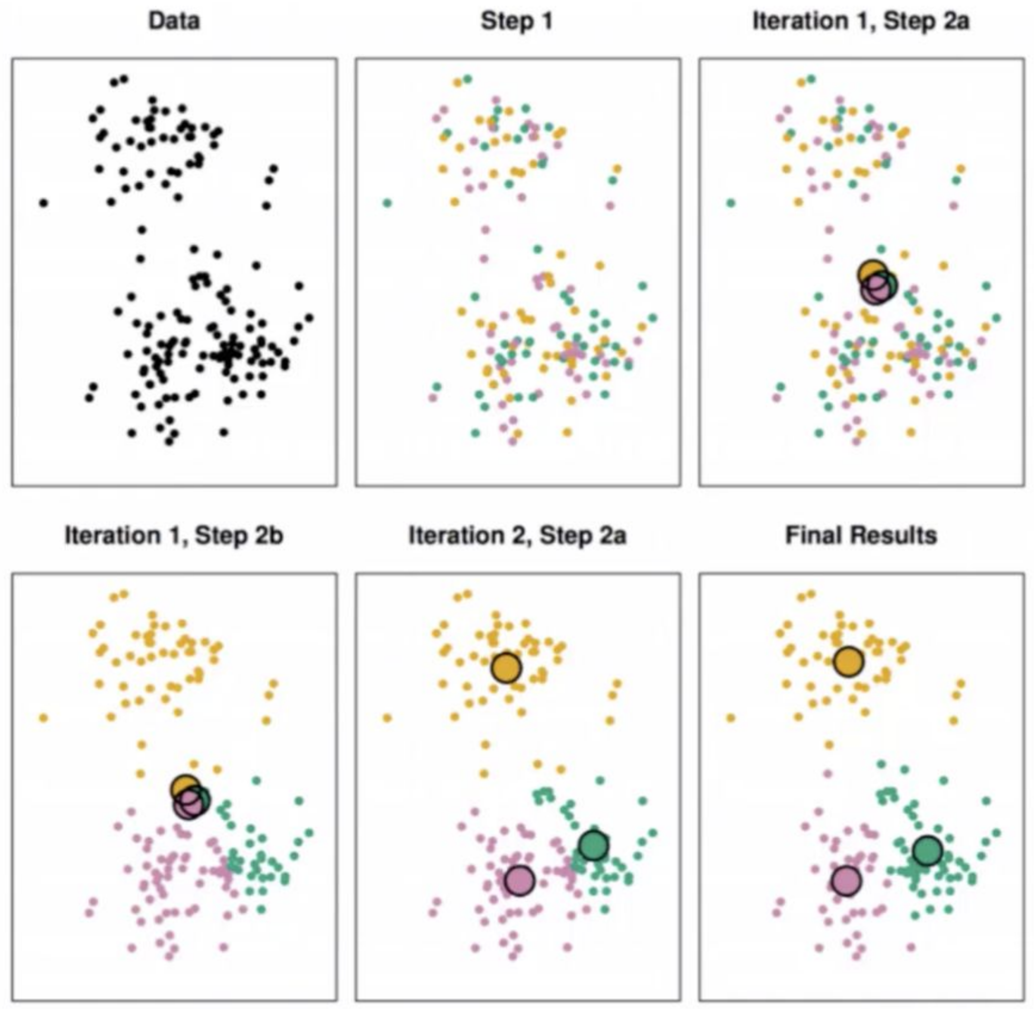

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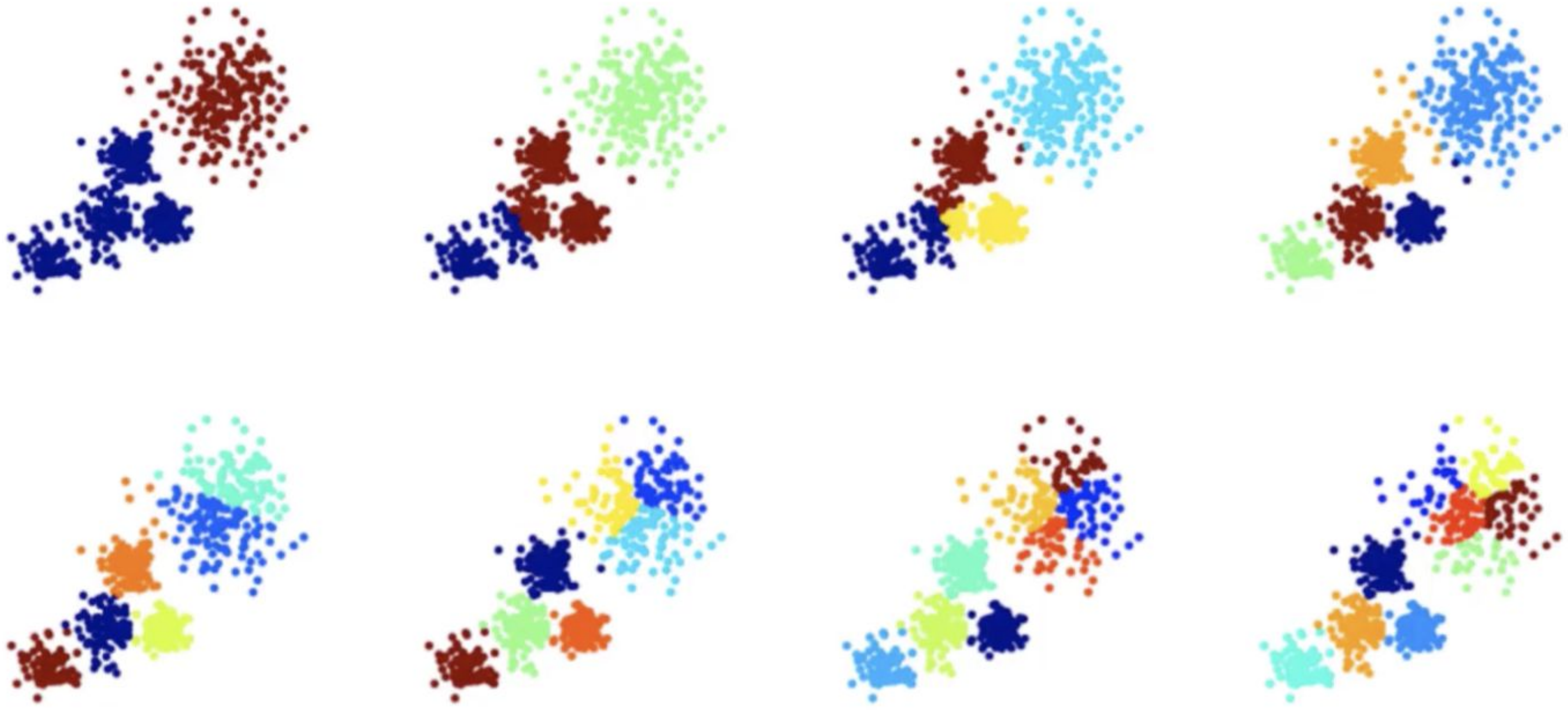

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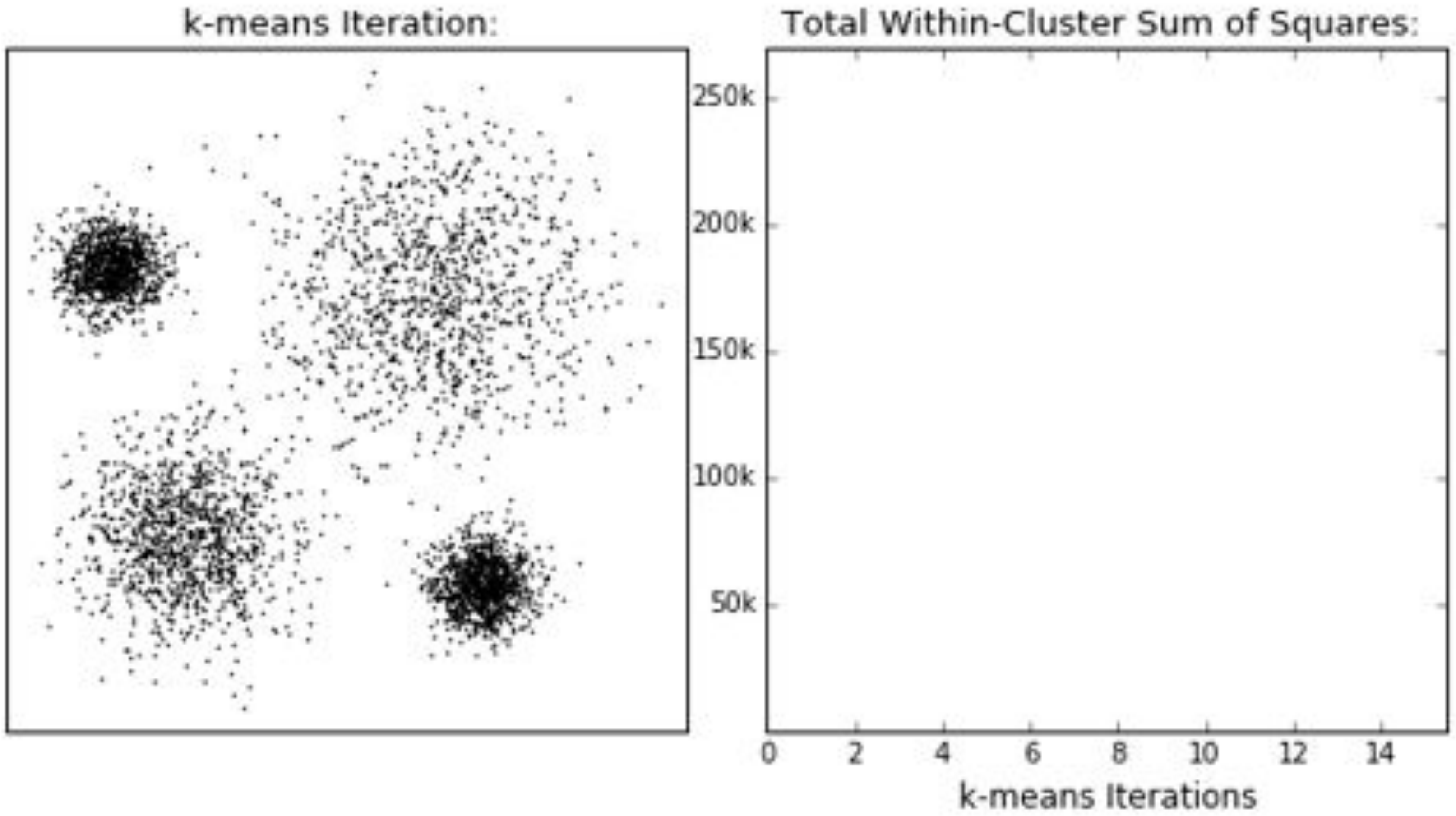

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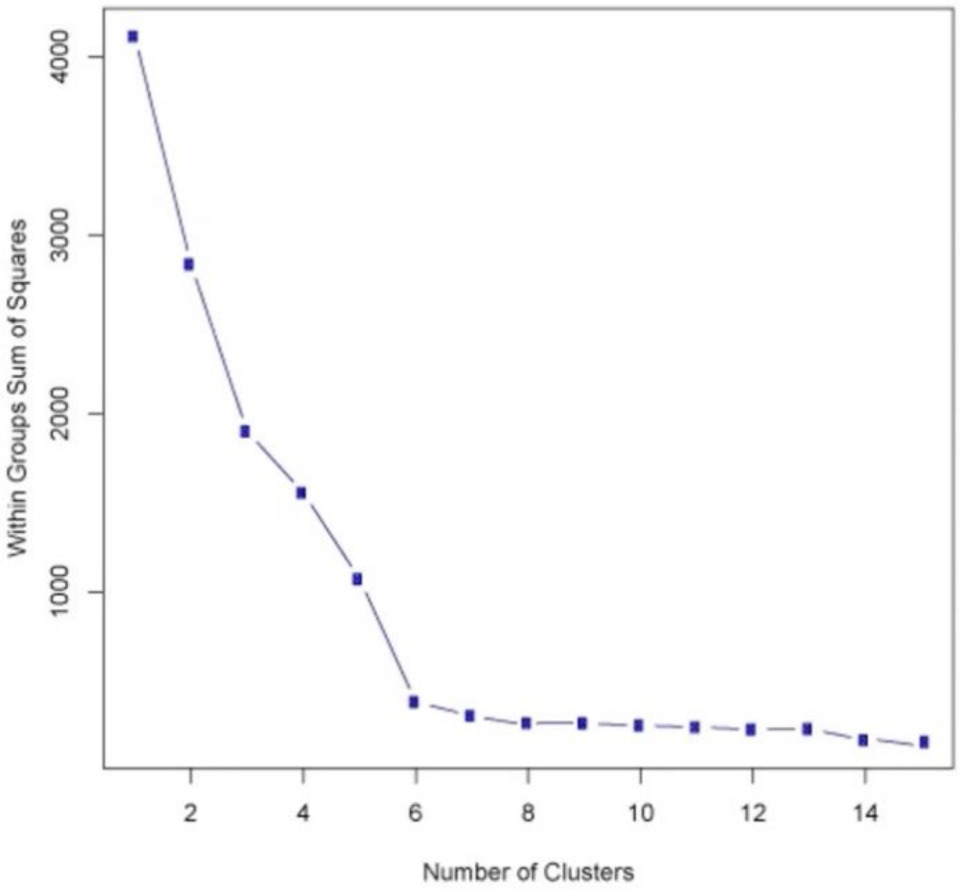

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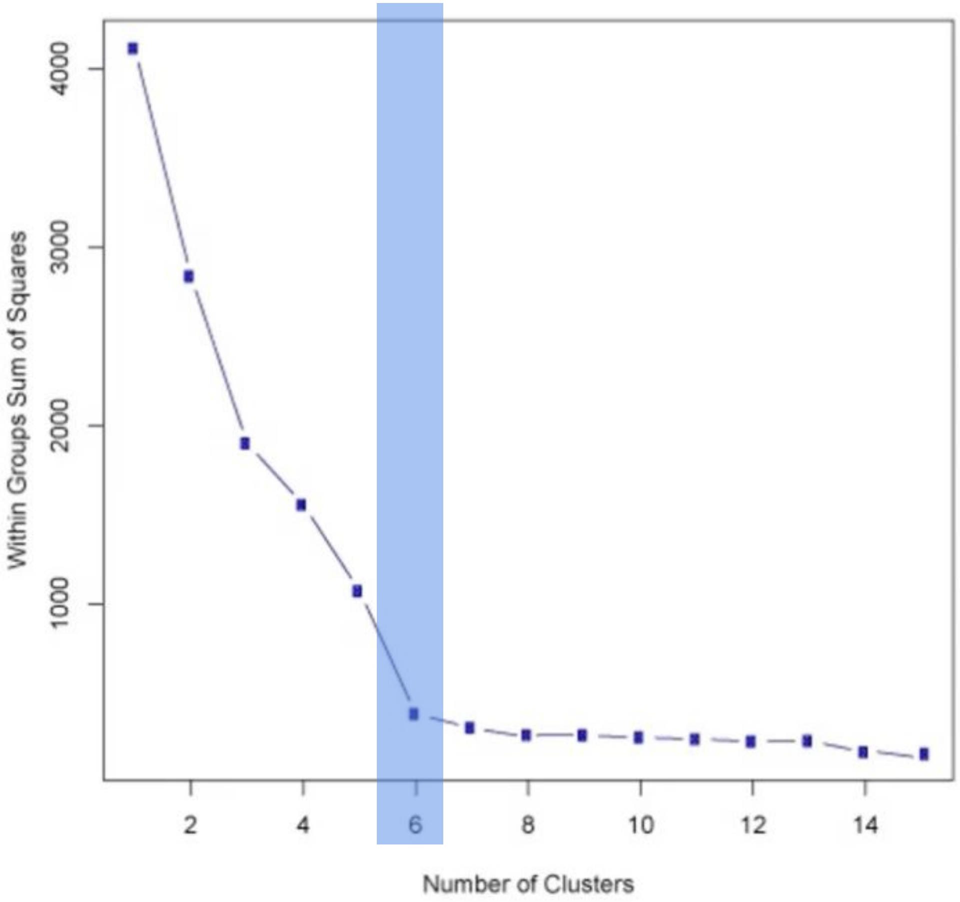

k-means theory