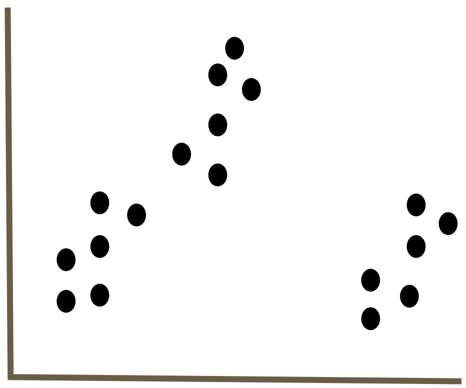
Clustering - Kmeans

Boston University CS 506 - Lance Galletti

What is a Clustering



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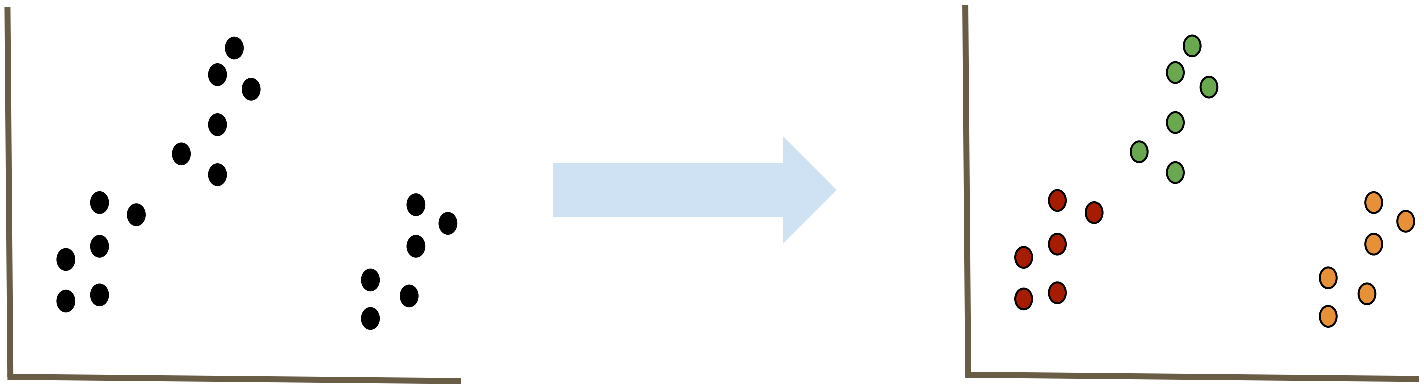
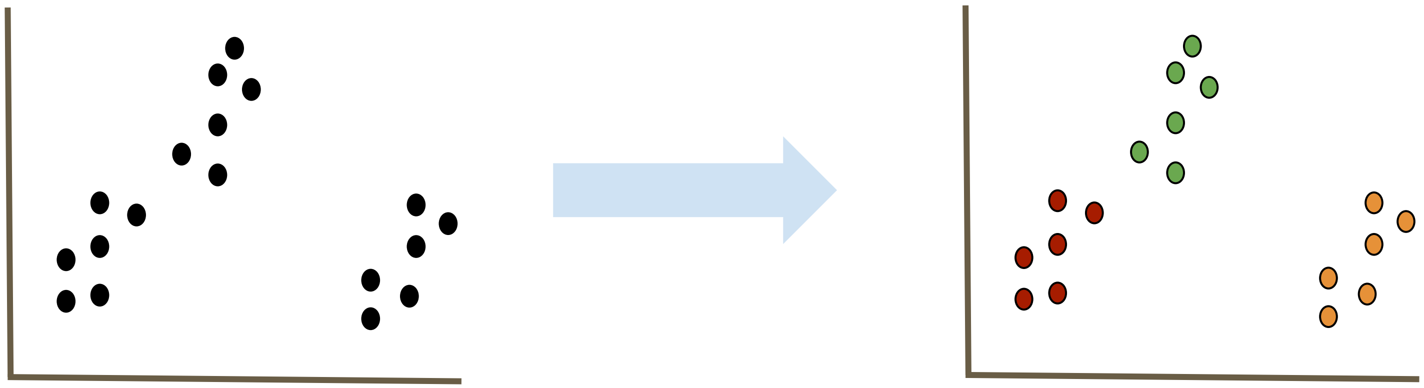


What is a Clustering

A clustering is a grouping / assignment of objects (data points) such that objects in the same group / cluster are:

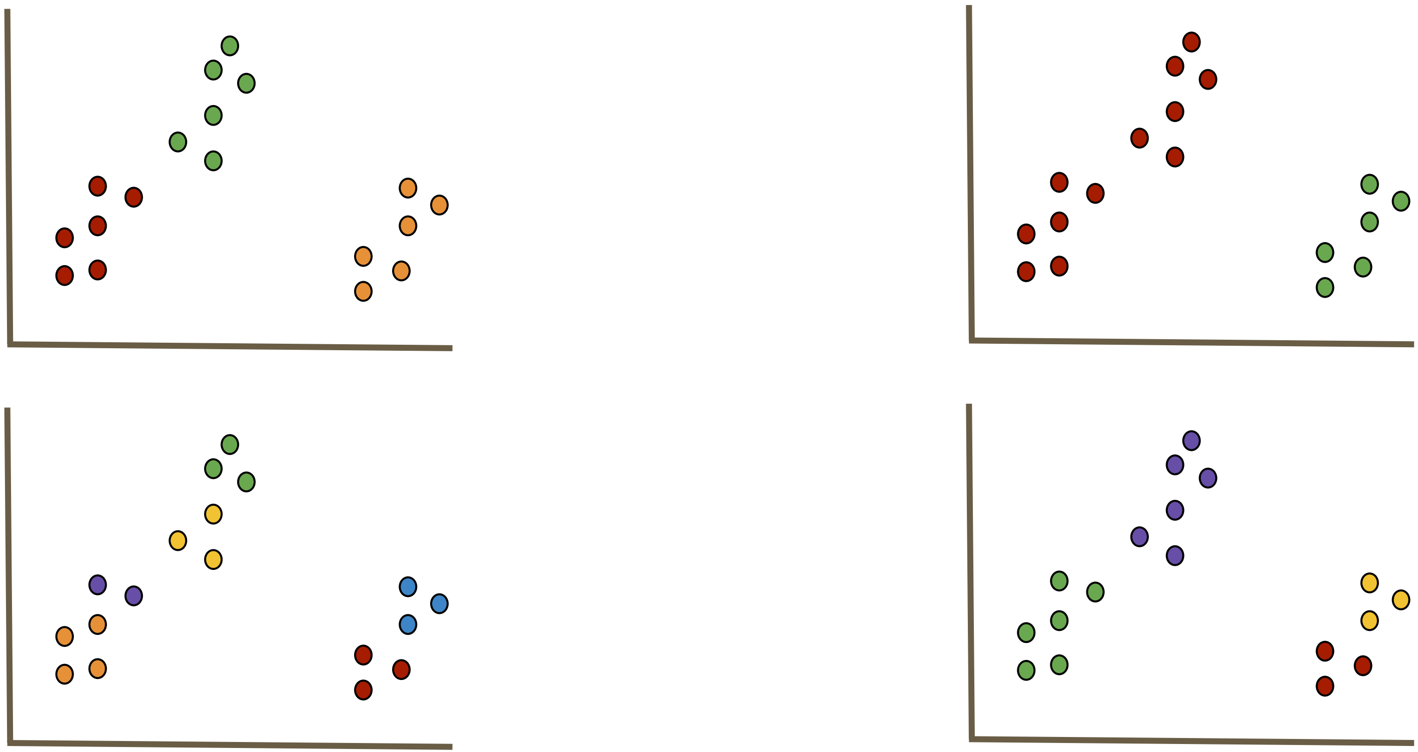
- similar to one another
- dissimilar to objects in other groups



Applications

- Outlier detection / anomaly detection
  - Data Cleaning / Processing
  - Credit card fraud, spam filter etc.
- Filling Gaps in your data
  - Using the same marketing strategy for similar people
  - Infer probable values for gaps in the data (similar users could have similar hobbies, likes / dislikes etc.)

Clusters can be Ambiguous



Types of Clusterings

Partitional

Each object belongs to exactly one cluster

Hierarchical

A set of nested clusters organized in a tree

Density-Based

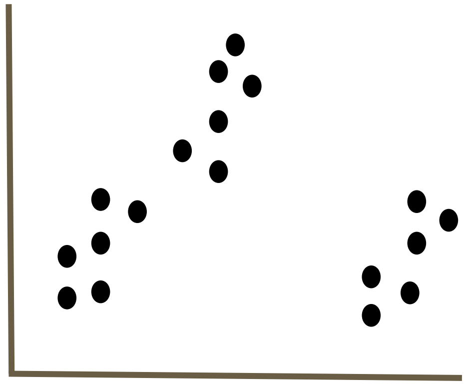
Defined based on the local density of points

Soft Clustering

Each point is assigned to every cluster with a certain probability

Partitional Clustering

Partitional Clustering



Goal: partition dataset into k partitions

Partitional Clustering

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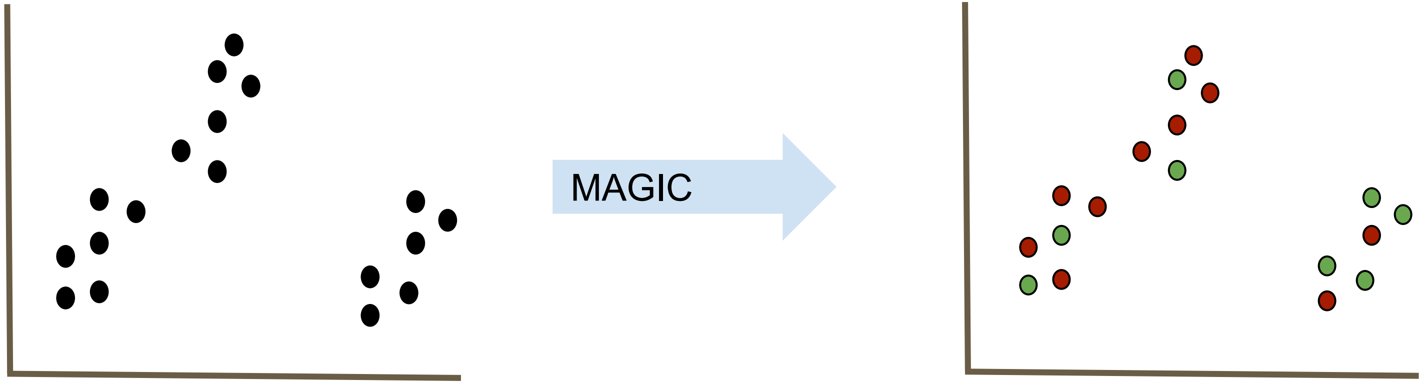

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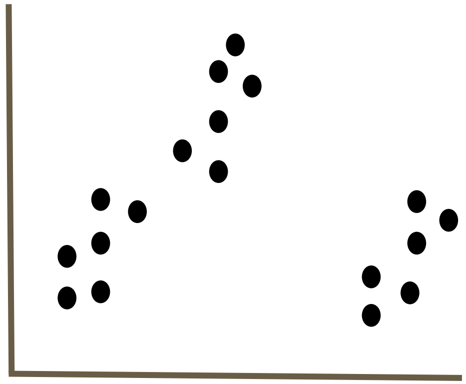

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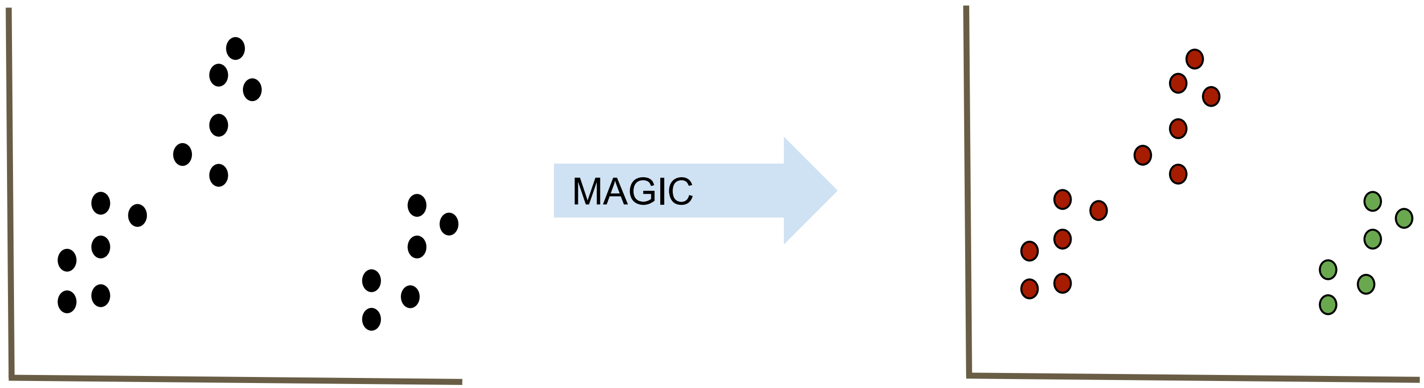

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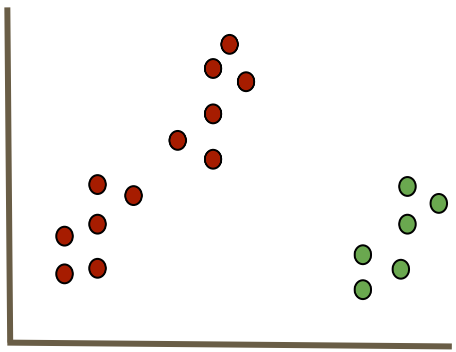
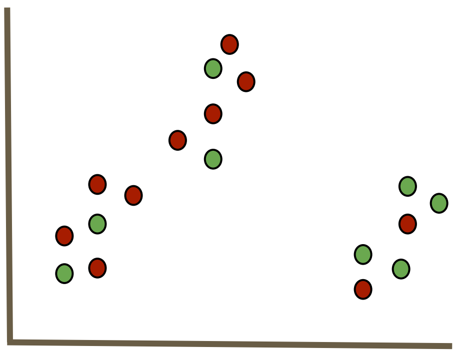
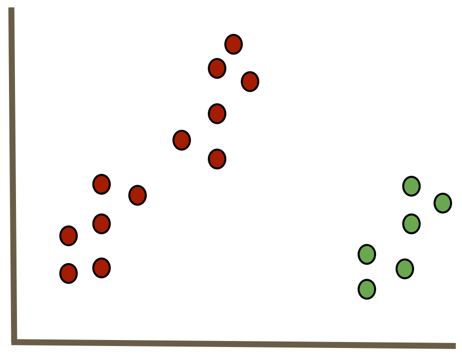
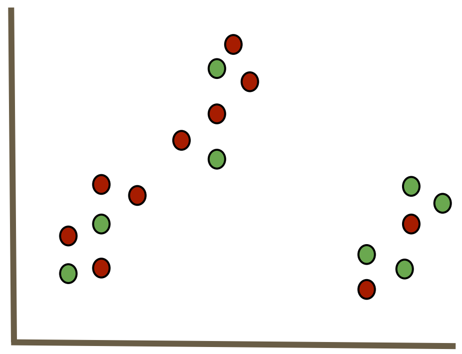




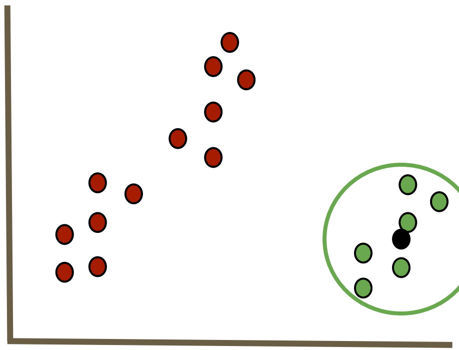
Partitional Clustering



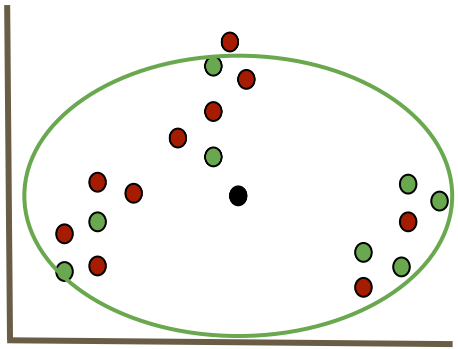
VS



Example

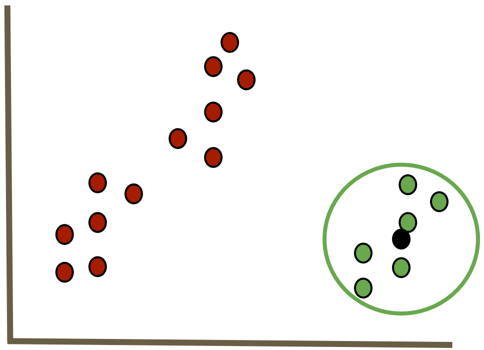


VS



Given a distance function **d**, we can find points (not necessarily part of our dataset) for each cluster called **centroids** that are at the center of each cluster.

Example



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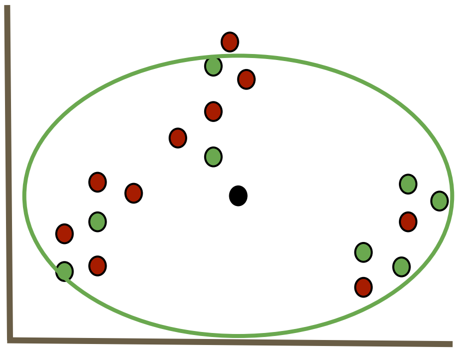
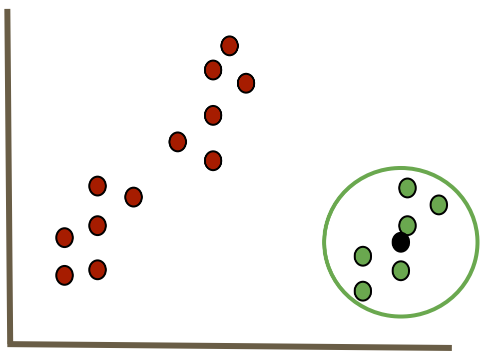


Q: When **d** is Euclidean, what is the **centroid** (also called **center of mass**) of **m** points $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$?

A: The mean / average of the points

Example



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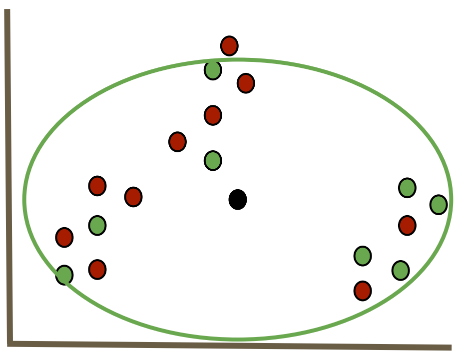


Looking at the sum of the distances of points in a cluster to its centroid also captures the "spread" (variance) of a cluster

Mean of cluster i

$$\sum_{i}^{k} \sum_{x \in C_i} d(x, \mu_i)^2$$

Cluster i

Cost Function

- Way to evaluate and compare solutions
- Hope: can find some algorithm that find solutions that make the cost small

Q: Can you suggest a cost function to use for partitional clustering?

$$\sum_{i}^{k} \sum_{x \in C_i} d(x, \mu_i)^2$$

K-means

Given $\mathbf{X} = \{\mathbf{x}_1, \ldots , \mathbf{x}_n\}$ our dataset and $\mathbf{k}$

Find $\mathbf{k}$ points $\{\boldsymbol{\mu}_1, \ldots , \boldsymbol{\mu}_k\}$ that minimize the **cost function**:

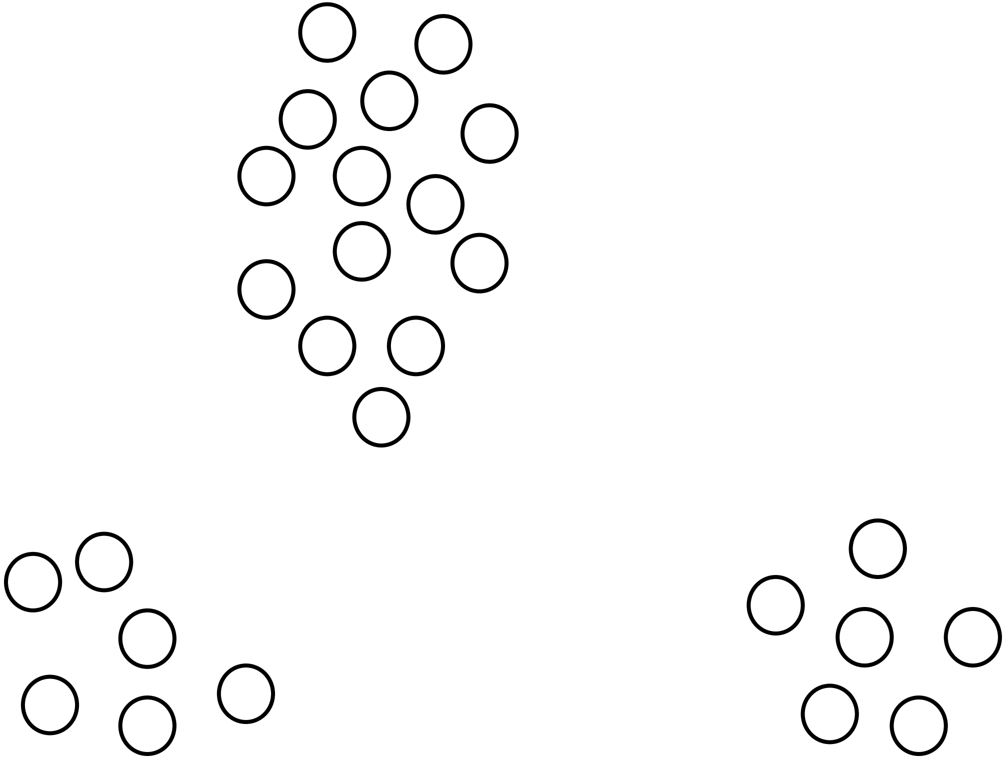
$$\sum_{i}^{k} \sum_{x \in C_i} d(x, \mu_i)^2$$

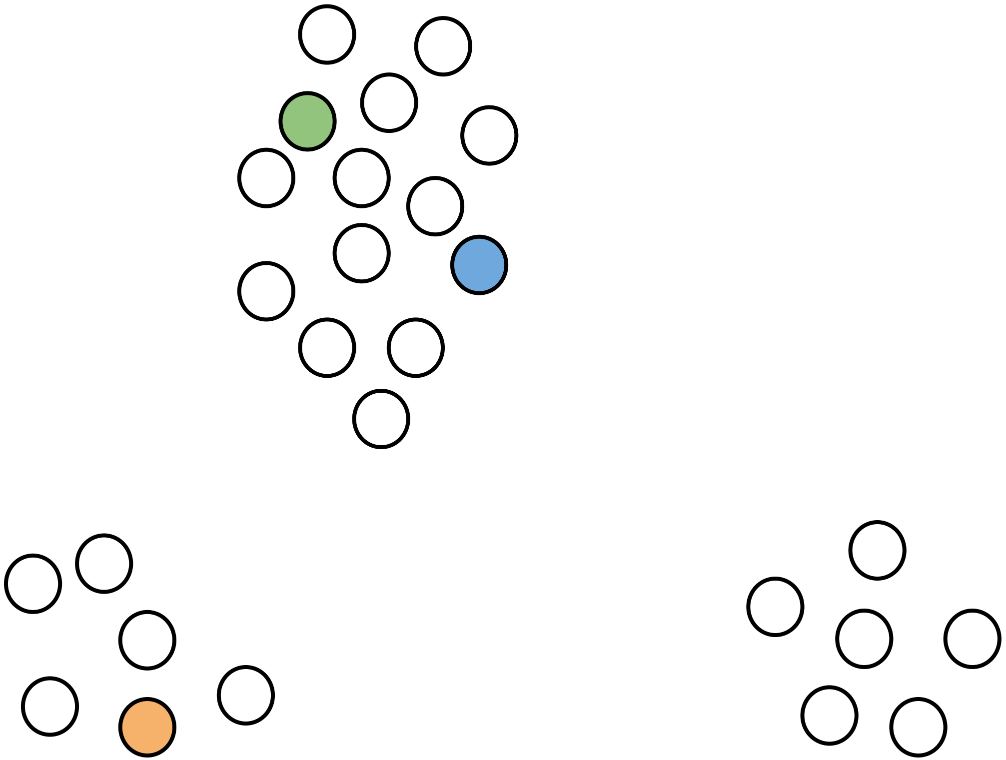
When **k=1** and **k=n** this is easy. Why?

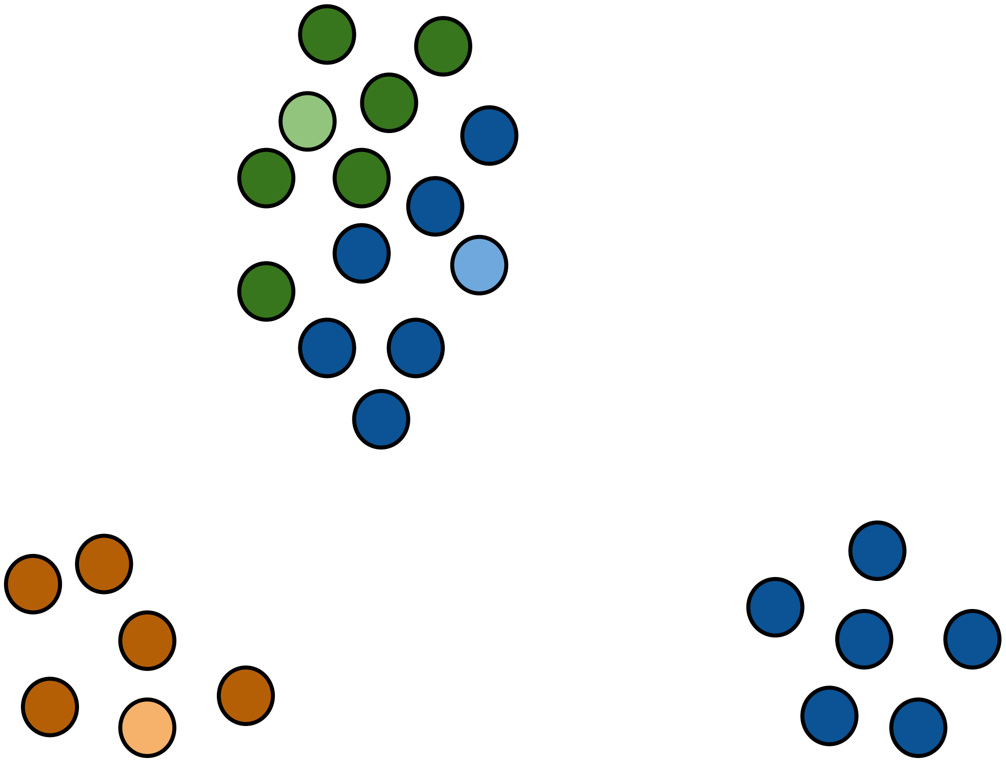
When $\mathbf{x}_i$ lives in more than 2 dimensions, this is a very difficult (**NP-hard**) problem

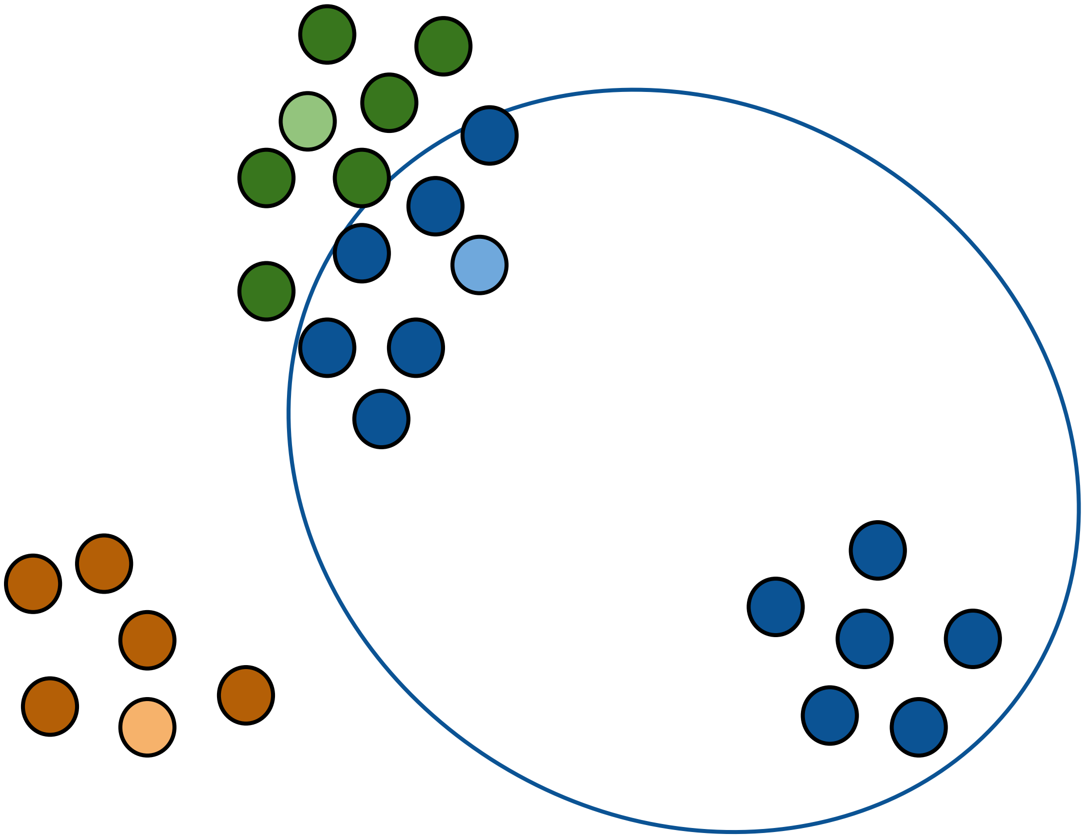
K-means - Lloyd's Algorithm

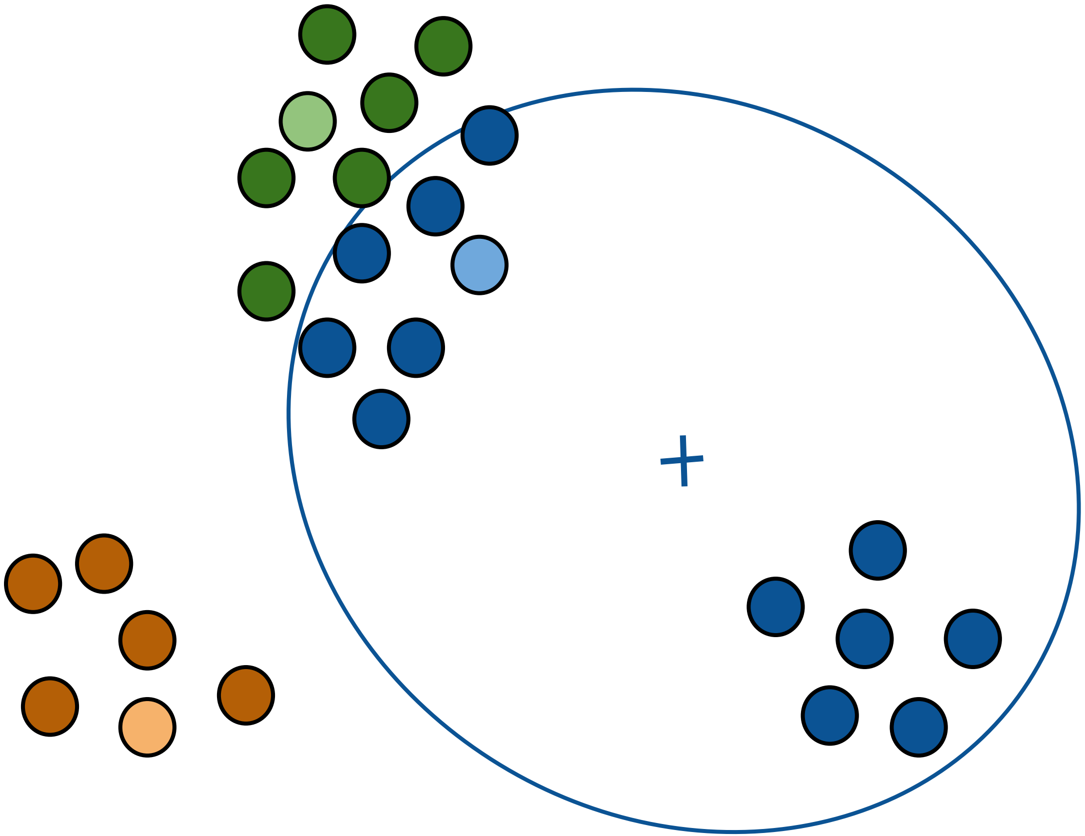
1. Randomly pick **k** centers $\{\mu_1, \dots, \mu_k\}$
2. Assign each point in the dataset to its closest center
3. Compute the new centers as the means of each cluster
4. Repeat 2 & 3 until convergence

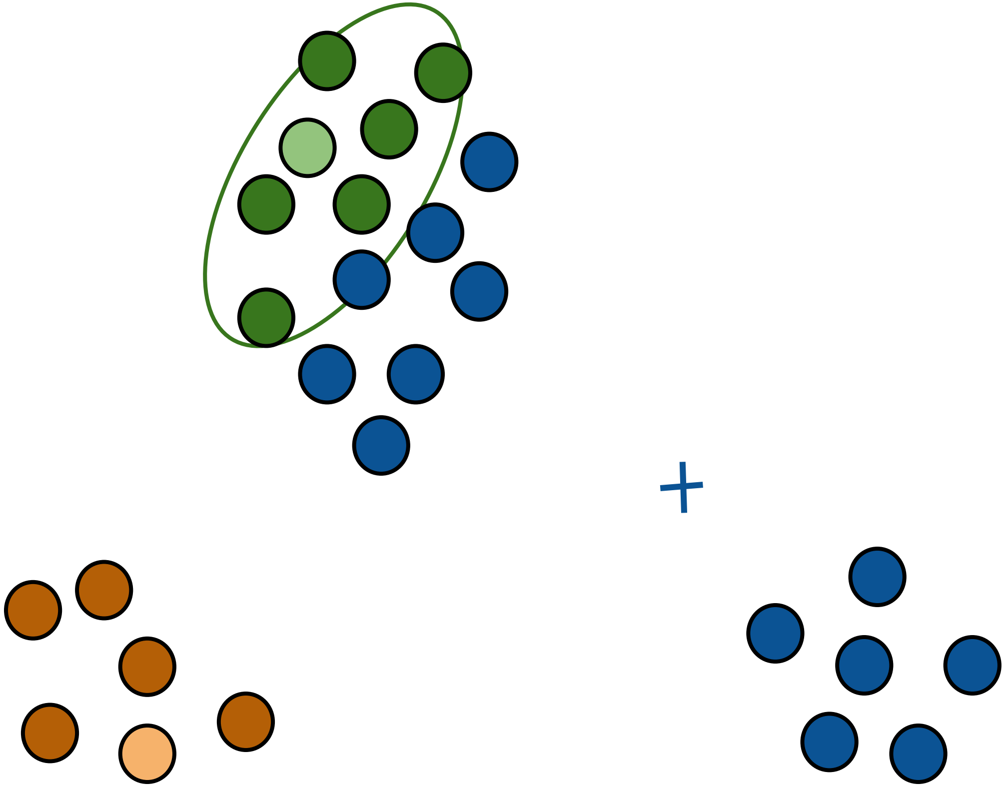


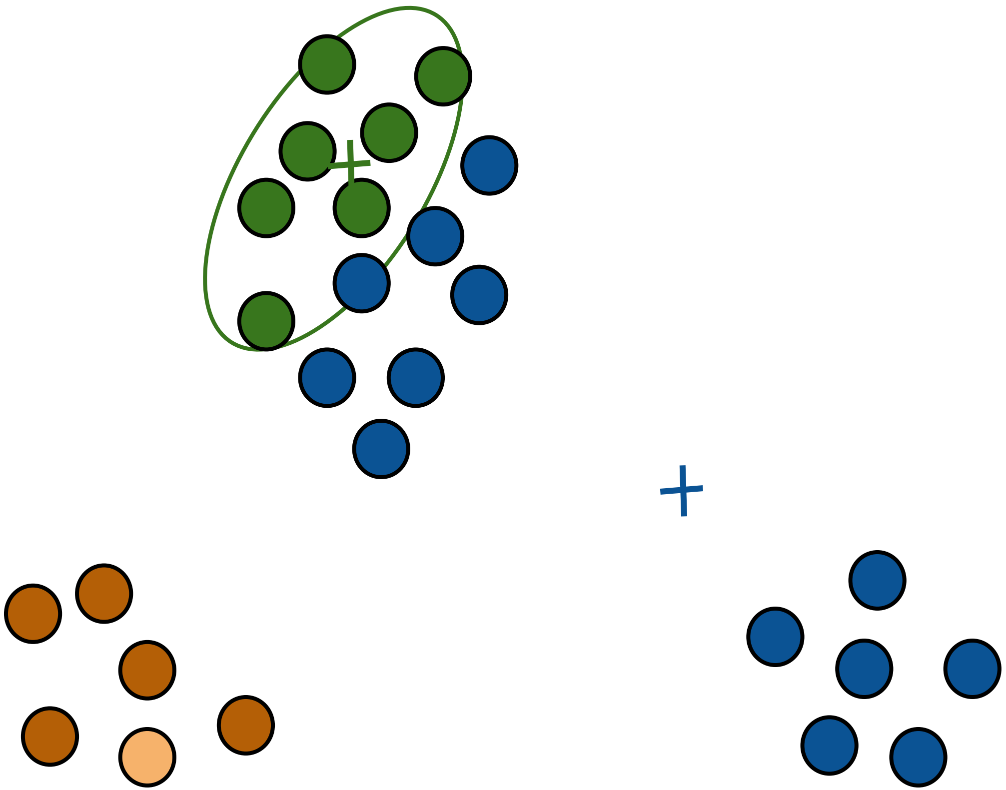


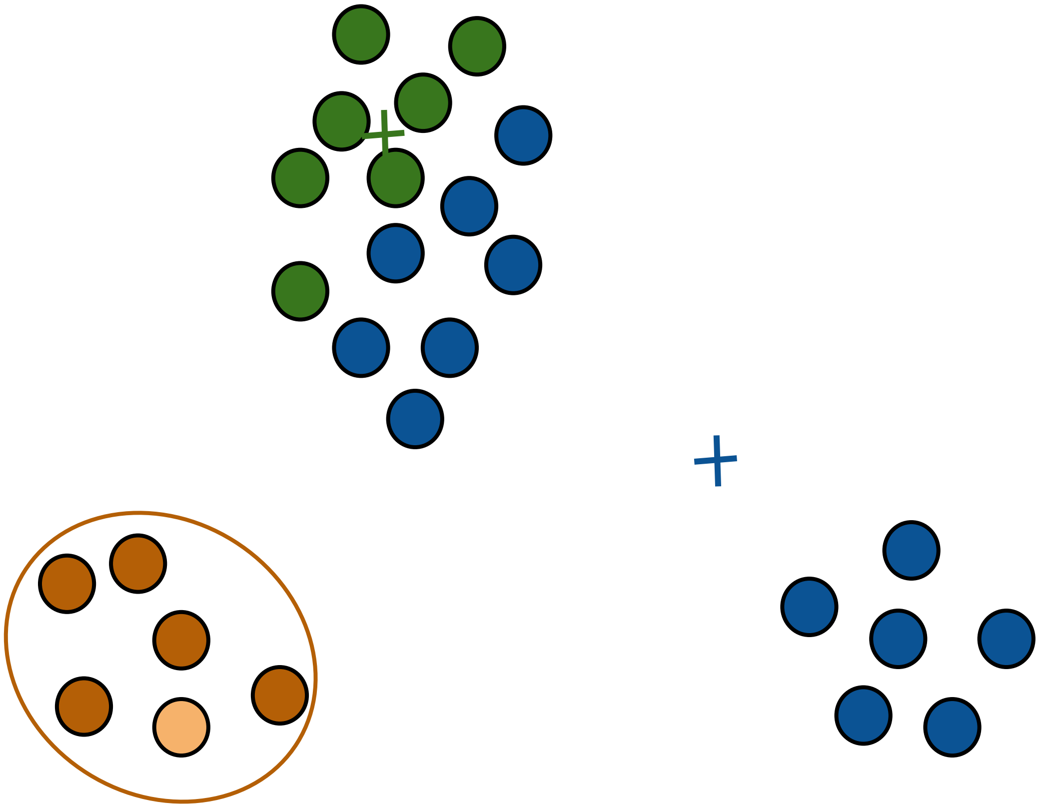


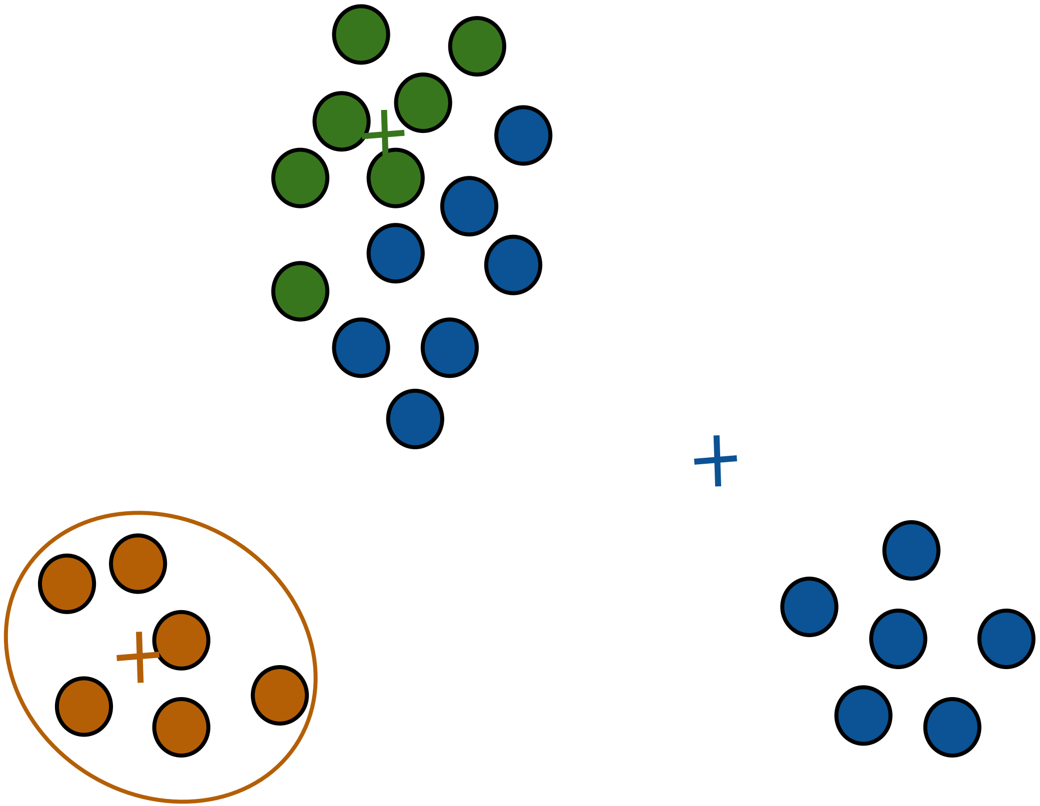


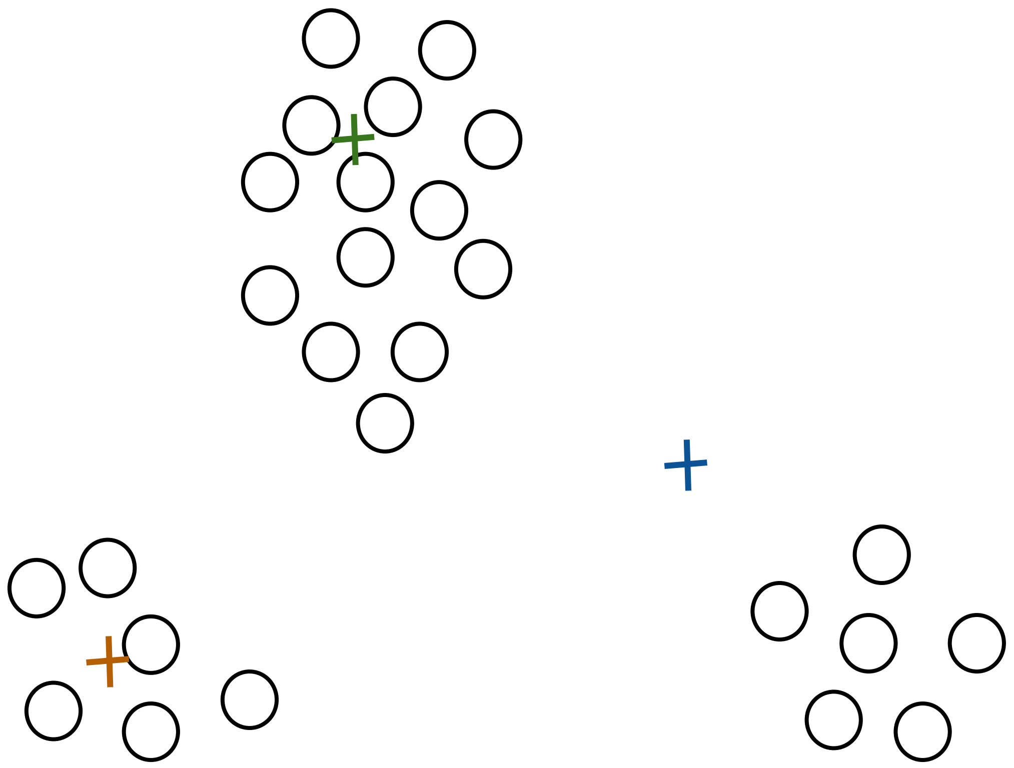


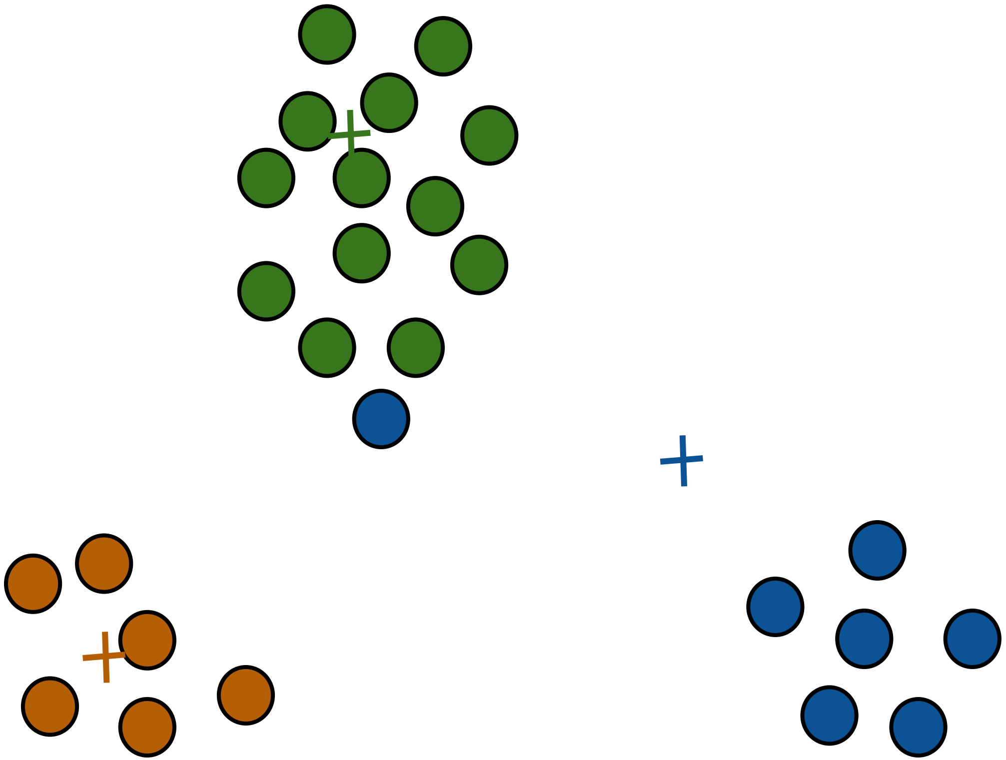


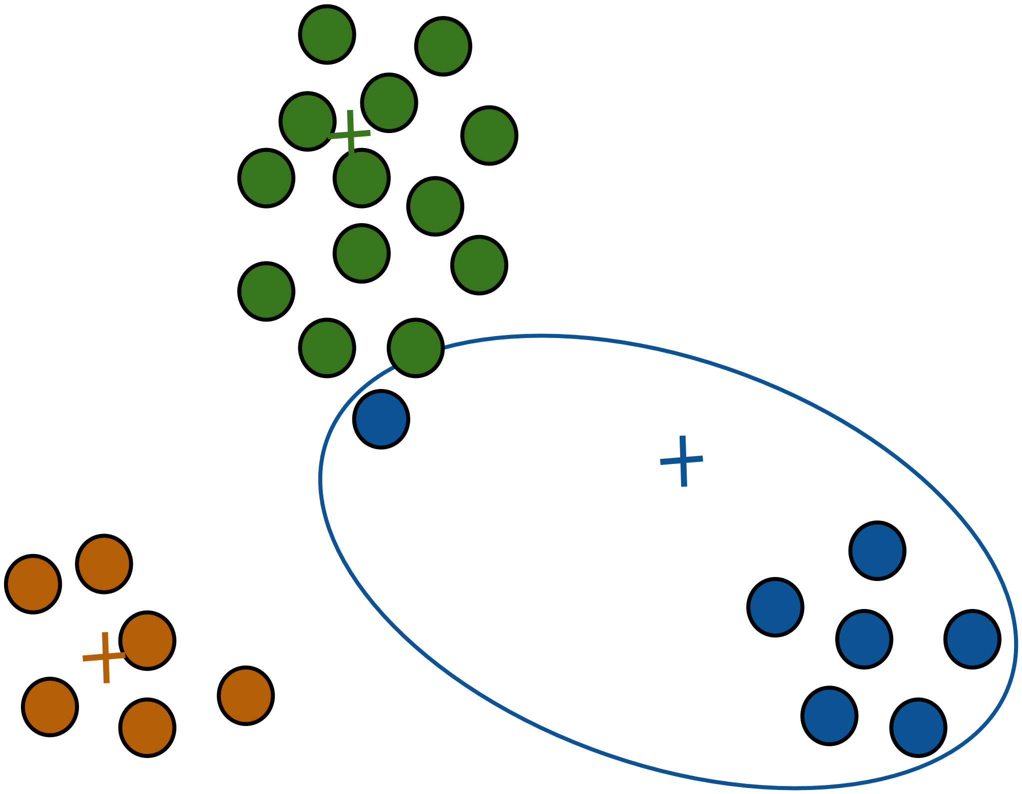


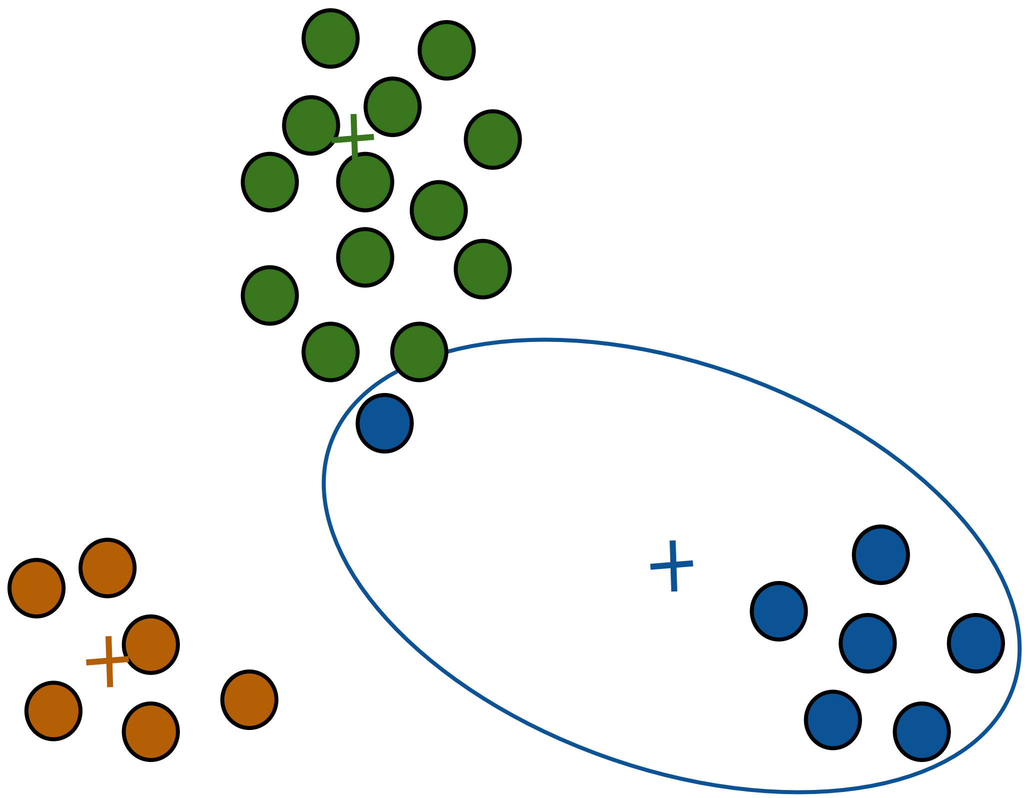


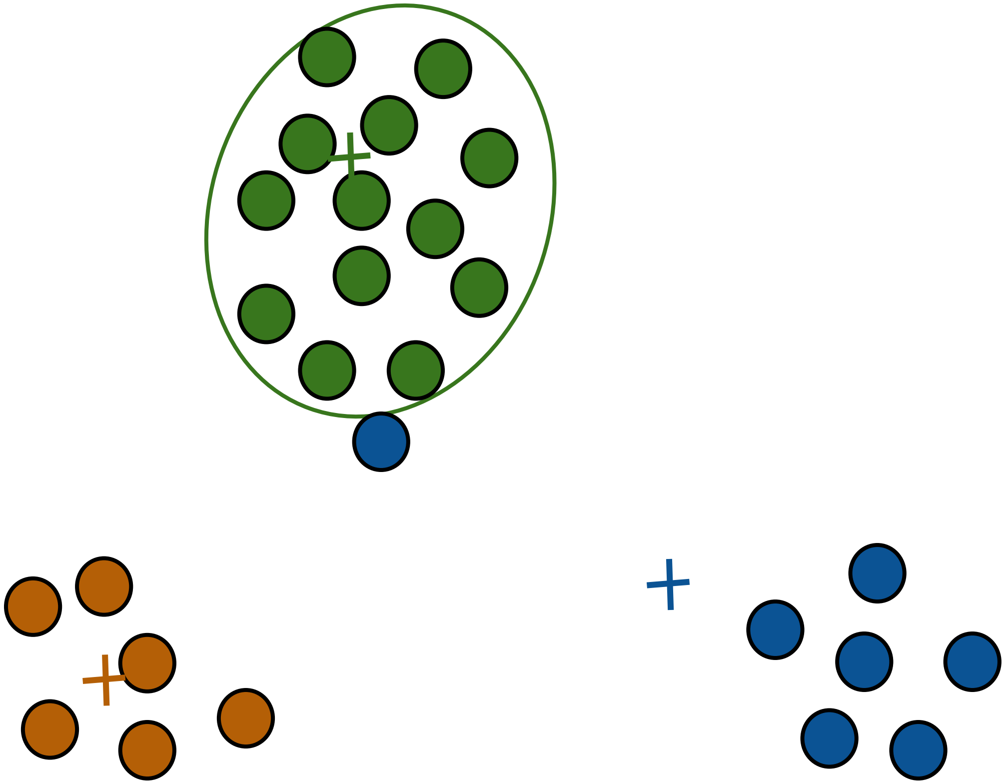


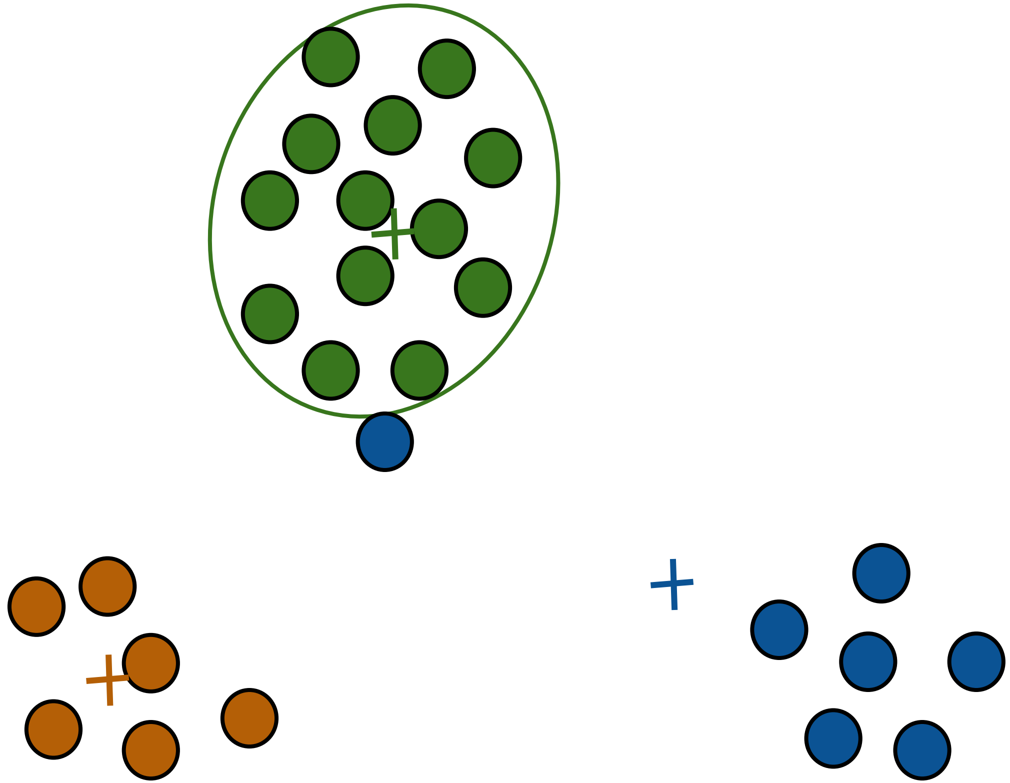


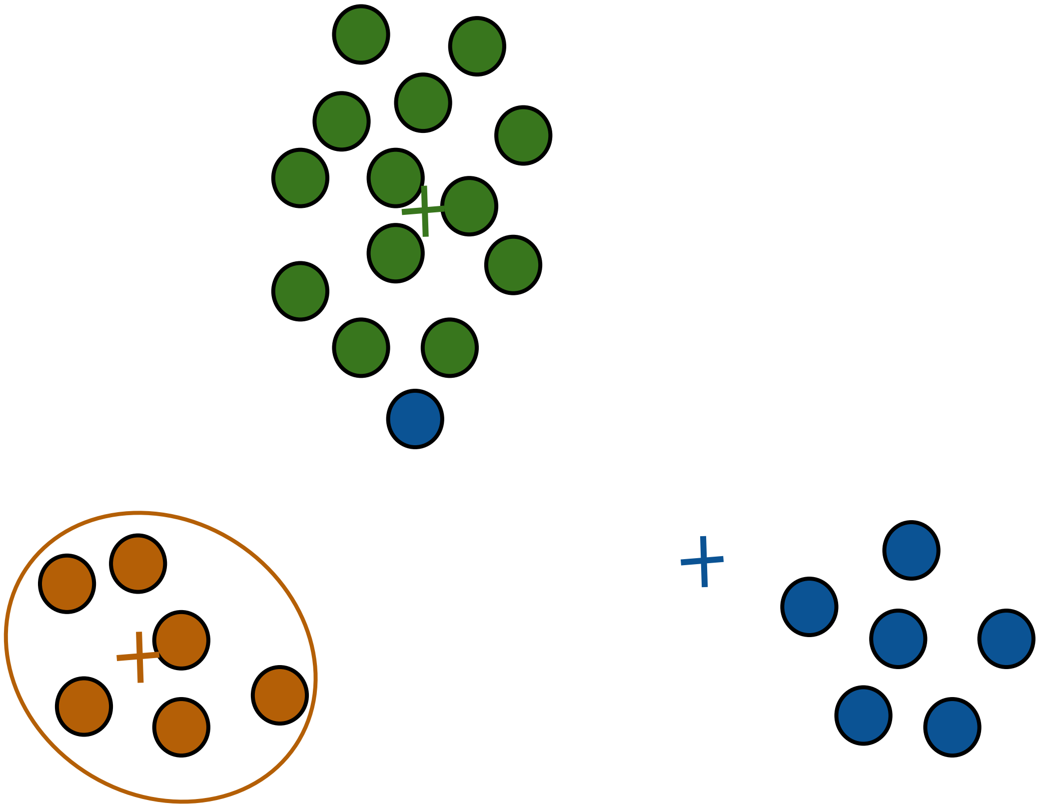


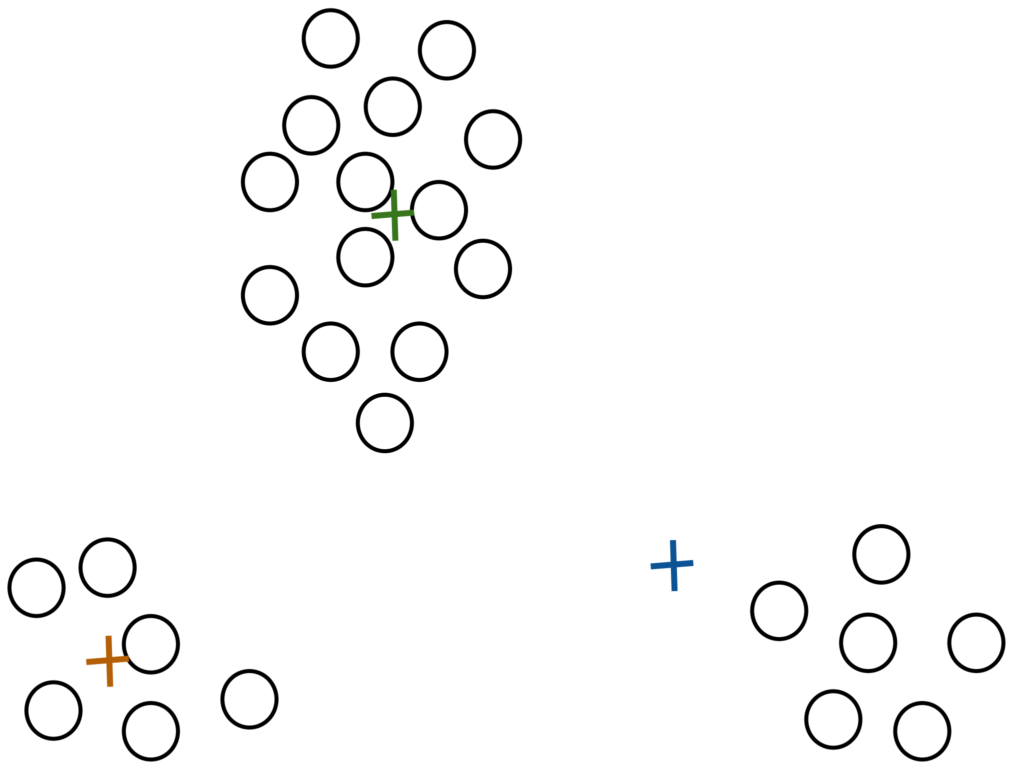


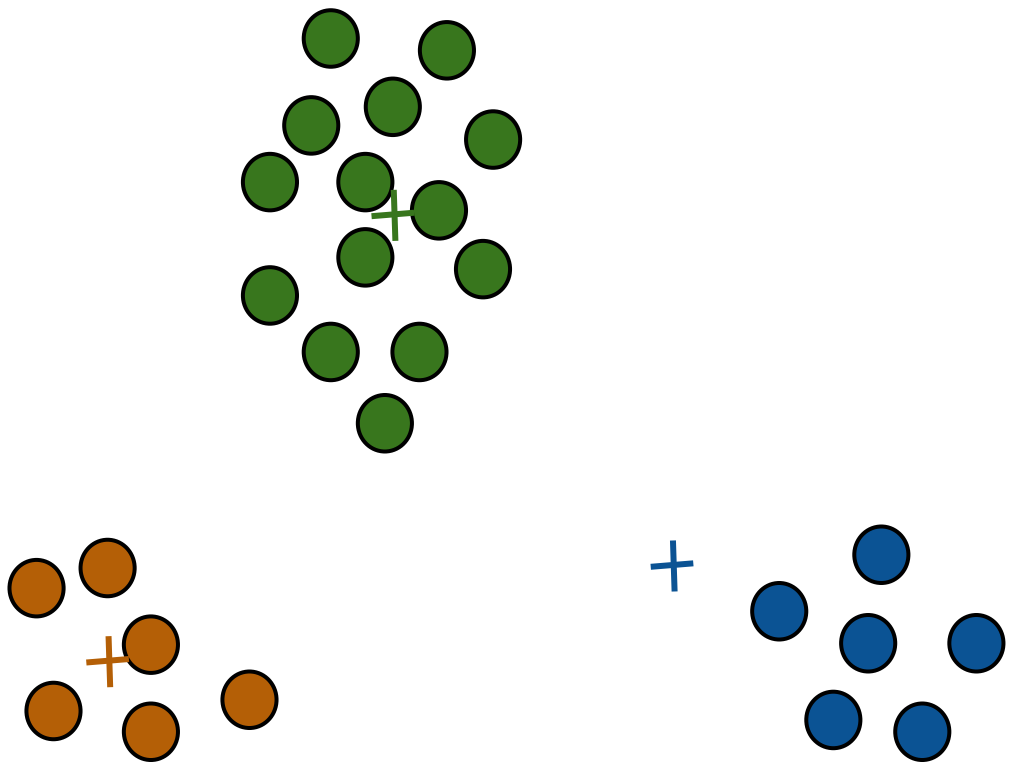


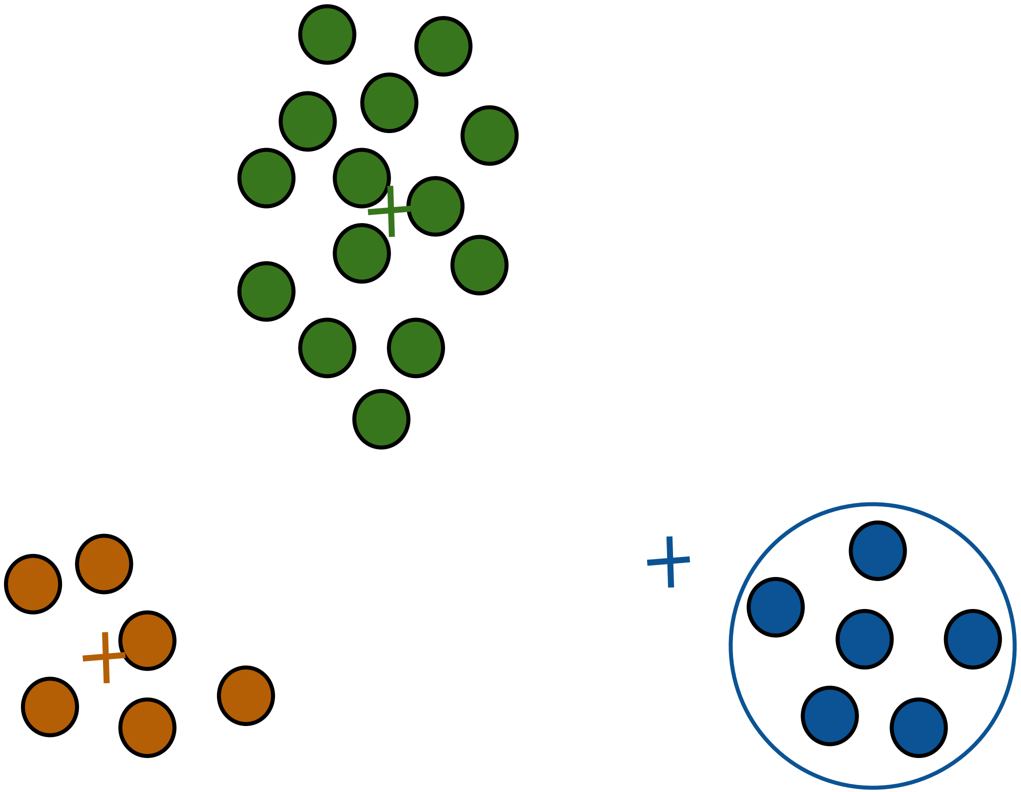


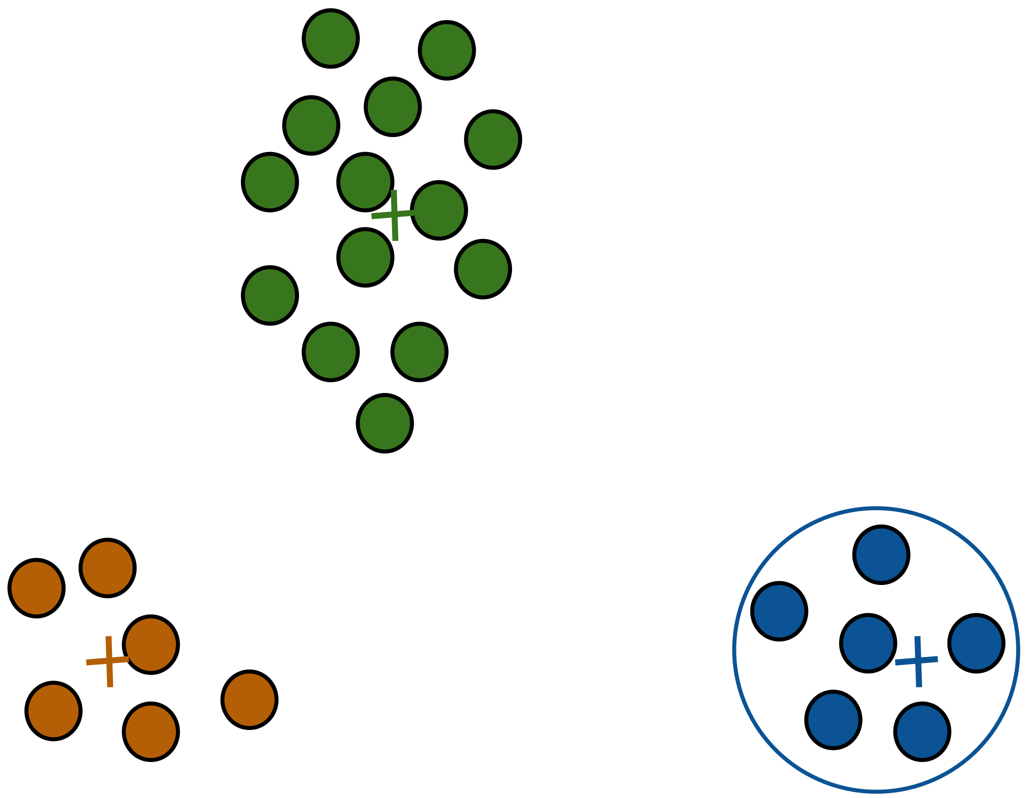


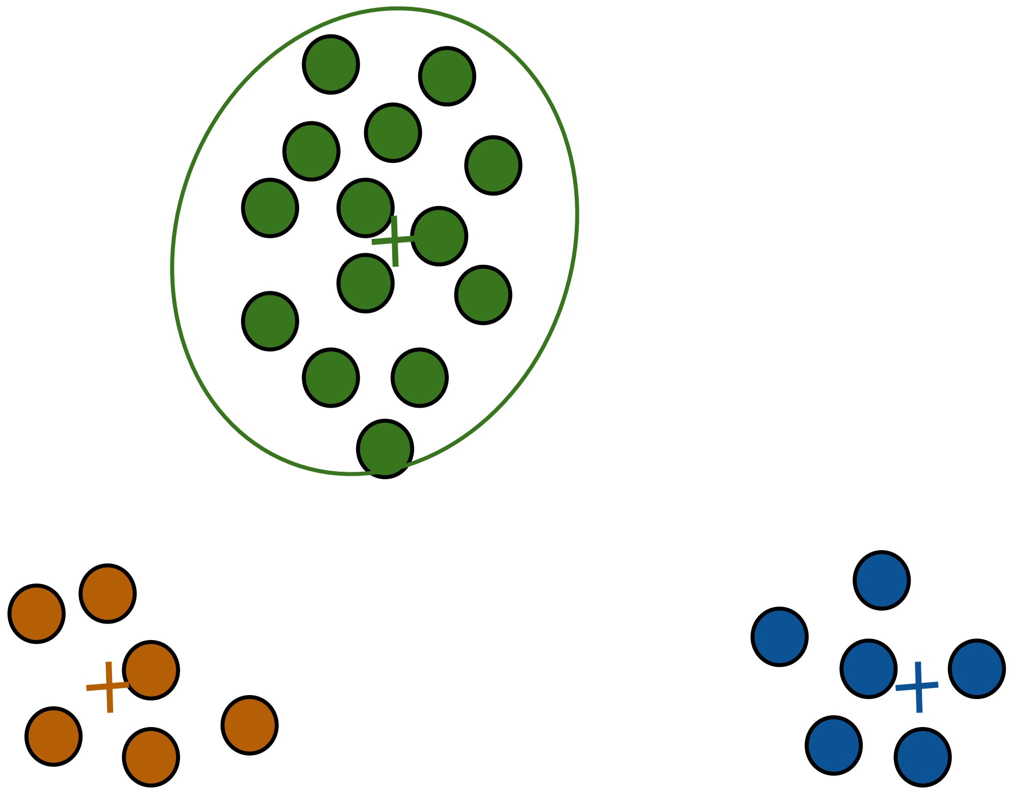


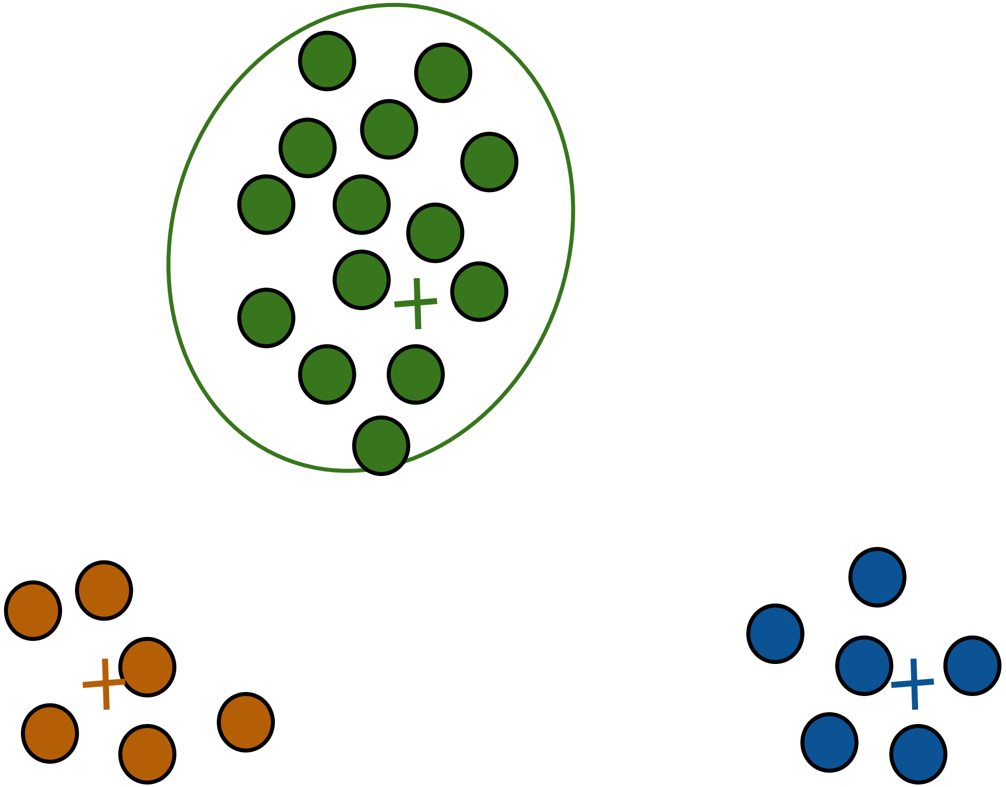


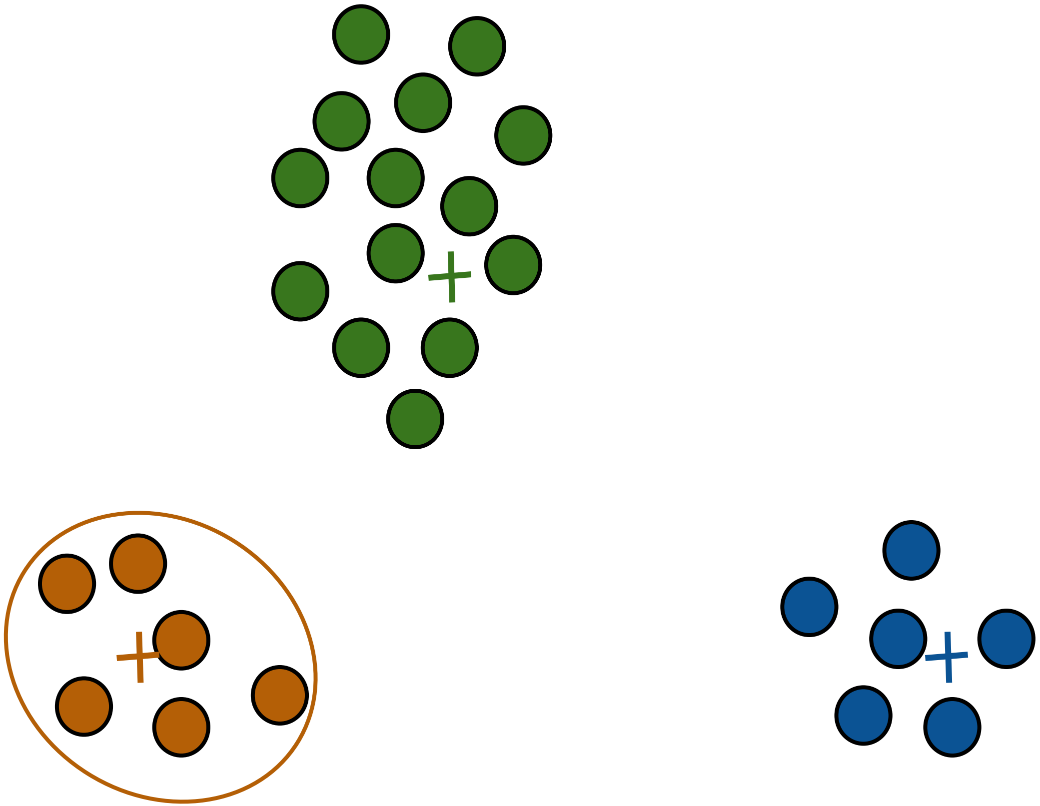


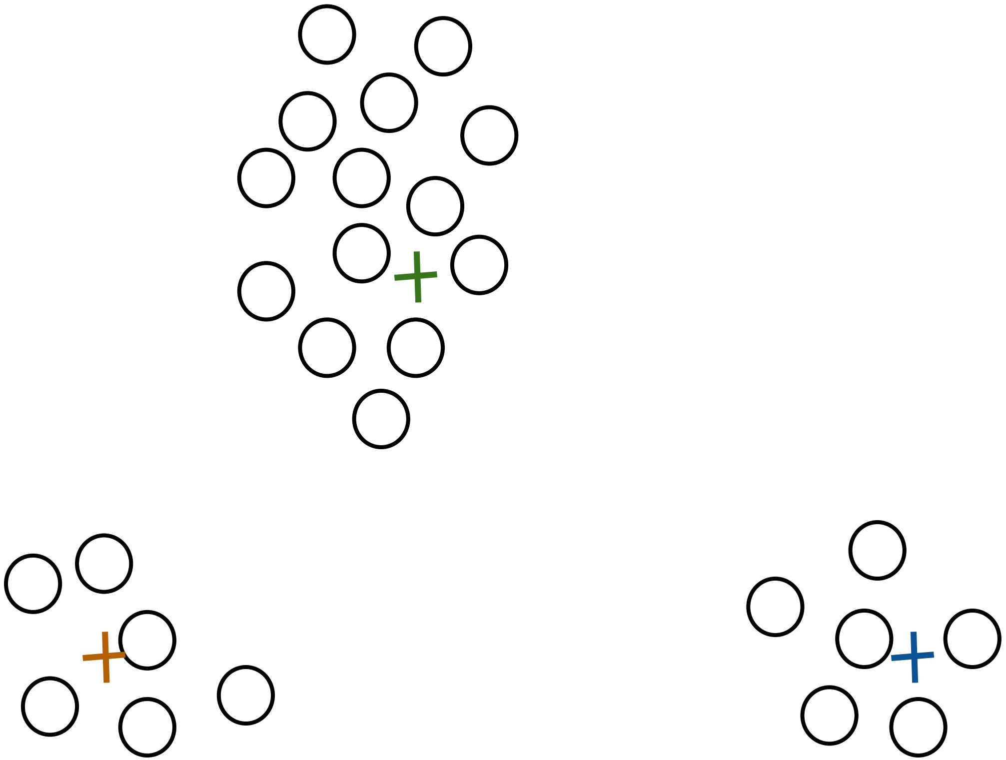


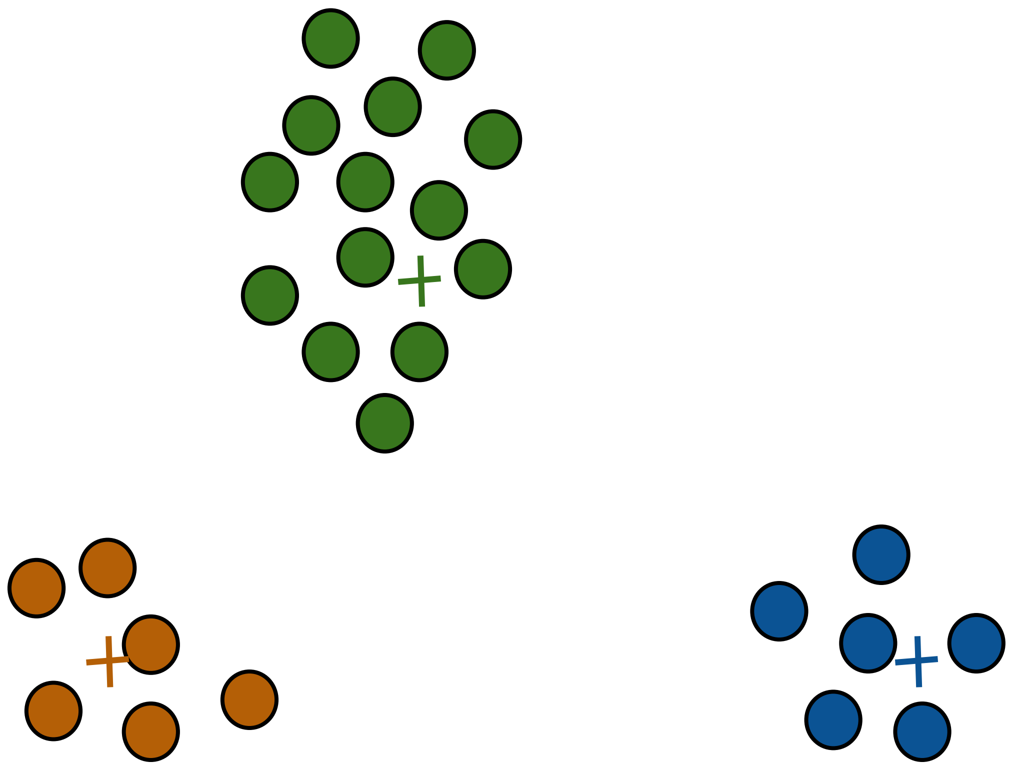


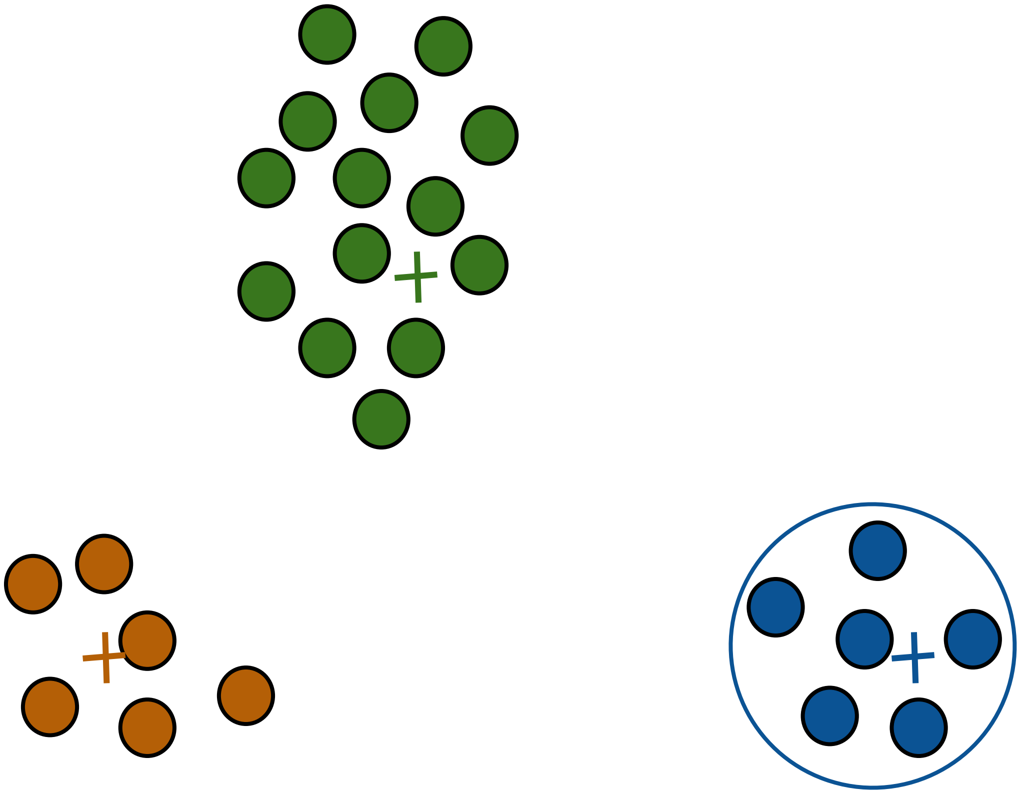


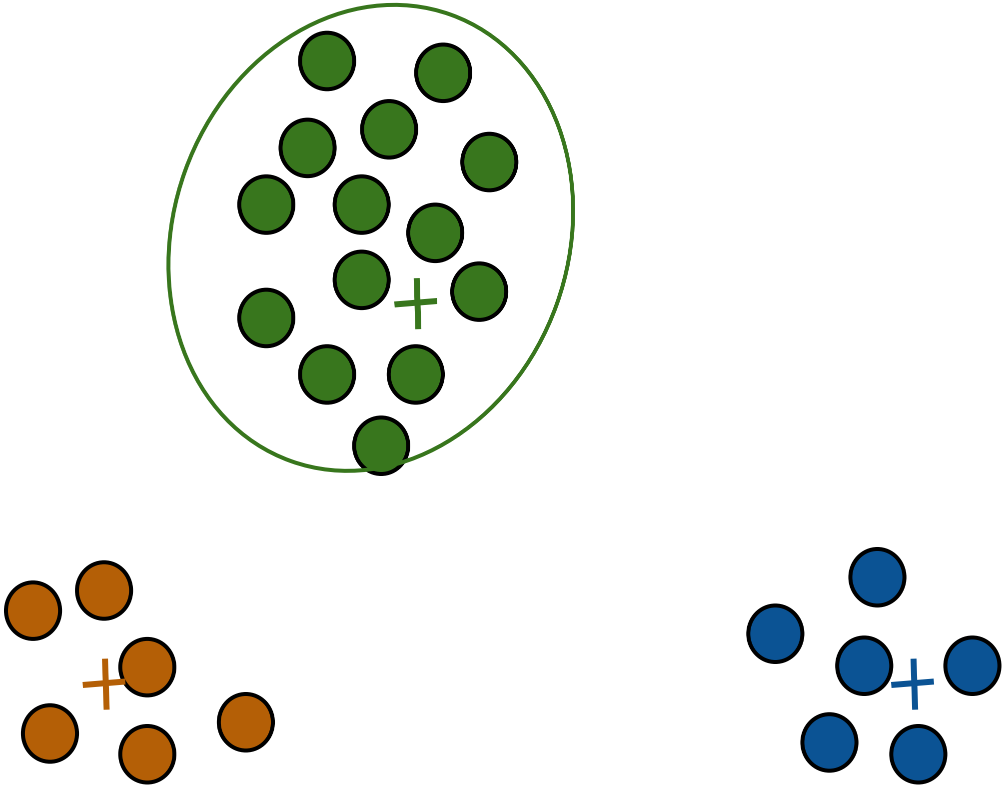


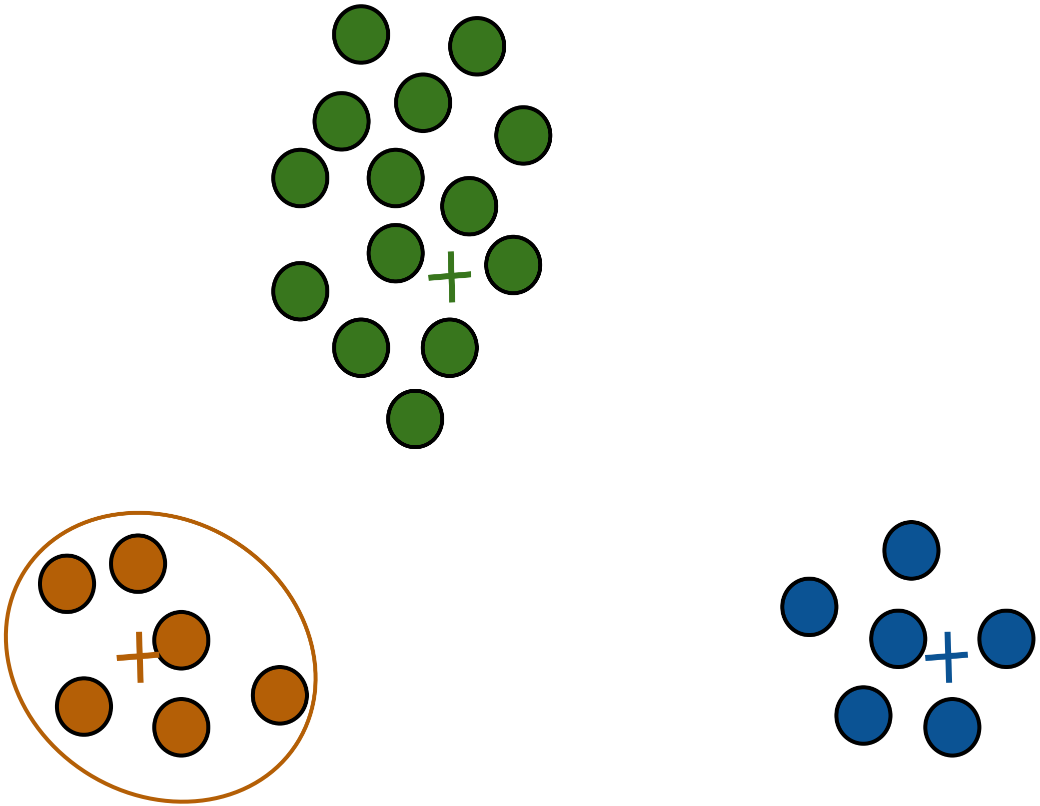


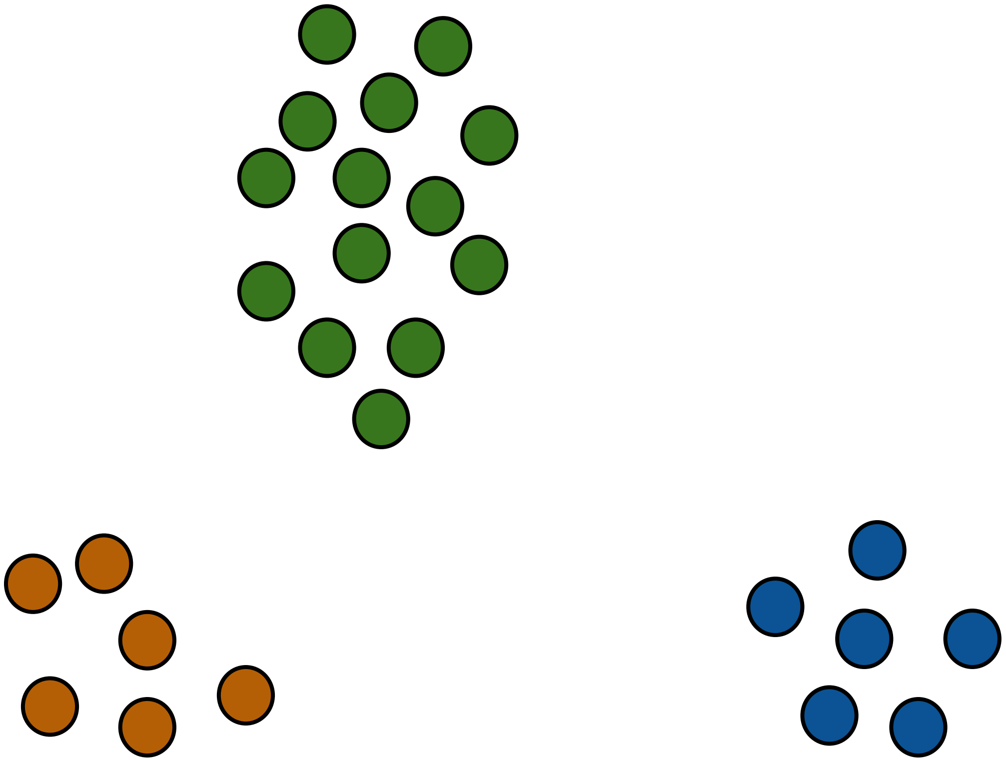




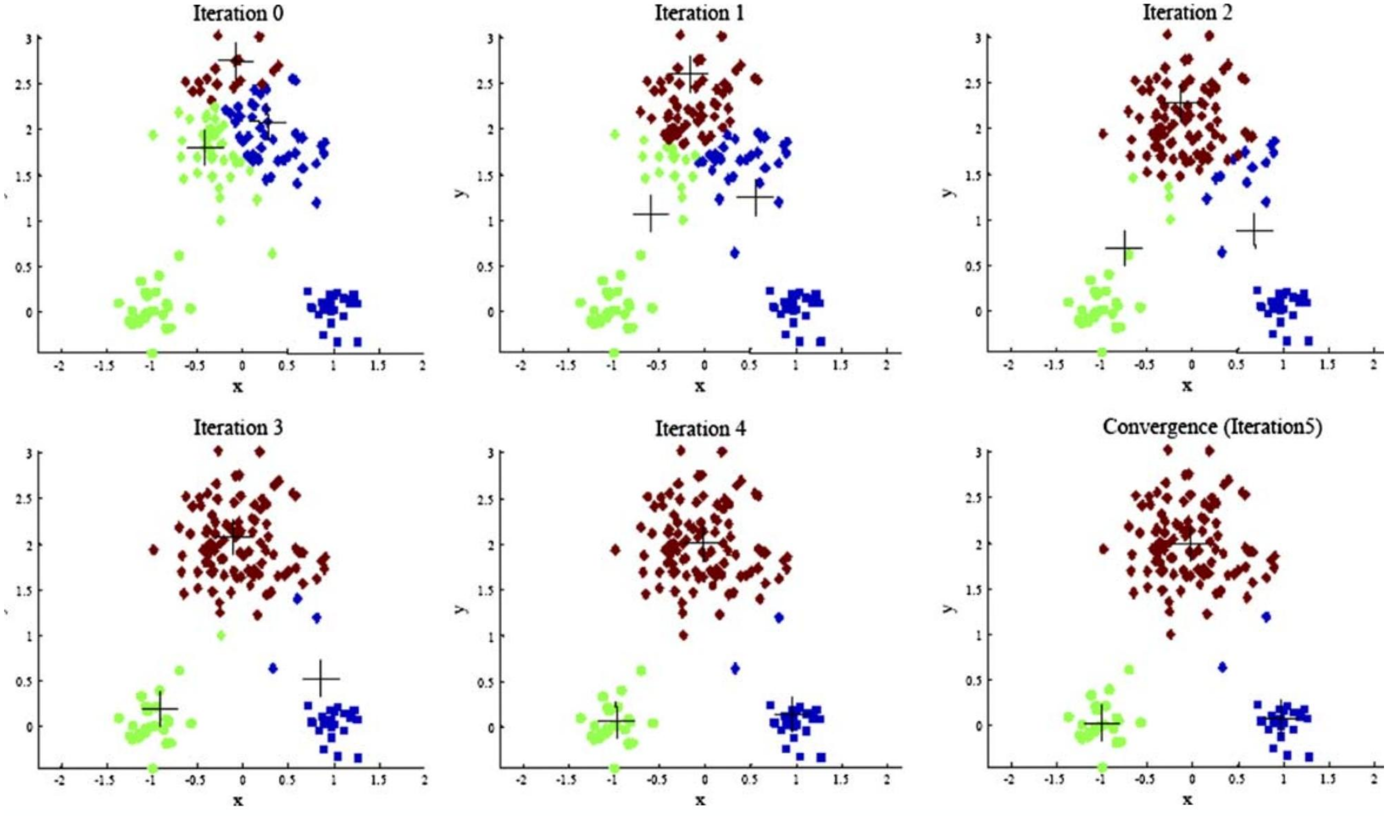








K-means - Lloyd's Algorithm



Worksheet -5min

Please do a) -> d) of the worksheet with the person sitting next to you.

Worksheet - 5min

Share your answers with the group next to you. Discuss / debate if you have different answers.

K-means - Lloyd's Algorithm

Will this algorithm always converge?

Proof (by contradiction): Suppose it does not converge. Then, either:

1. The minimum of the cost function is only reached in the limit (i.e. after an infinite number of iterations).
   Impossible because we are iterating over a finite set of partitions

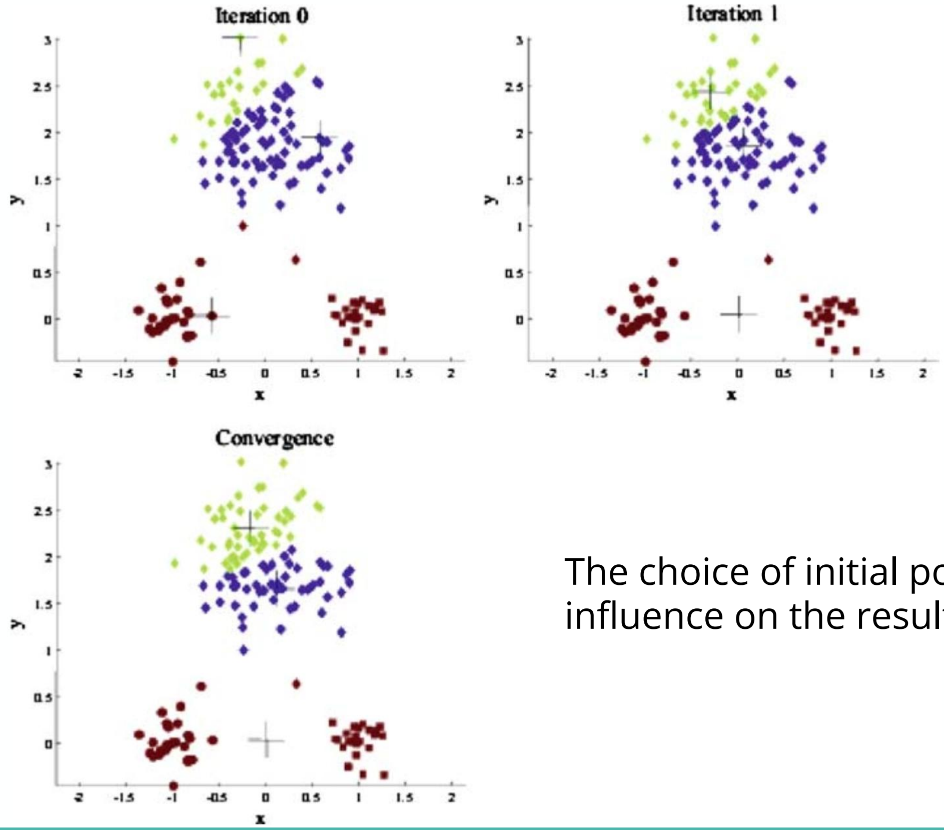
1. The algorithm gets stuck in a cycle / loop
   Impossible since this would require having a clustering that has a lower cost than itself and we know:
   - If old ≠ new clustering then the cost has improved
   - If old = new clustering then the cost is unchanged

Conclusion: Lloyd's Algorithm always converges!

K-means - Lloyd's Algorithm

Will this always converge to the optimal solution?

K-means - Lloyd's Algorithm



The choice of initial points has a large influence on the resulting clustering

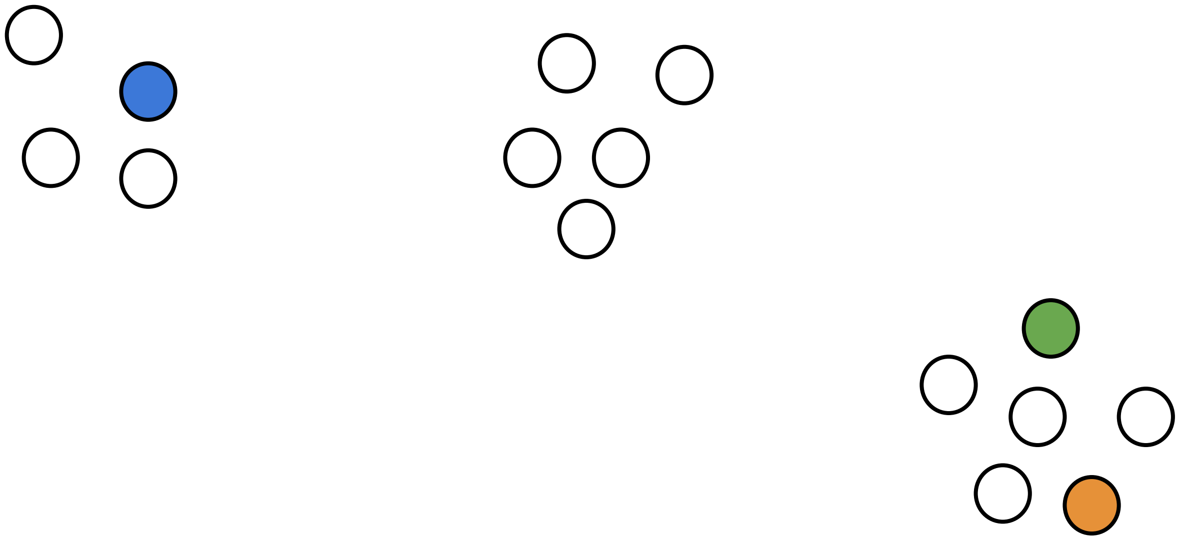
K-means - Initialization

One solution: Run Lloyd’s algorithm multiple times and choose the result with the lowest cost.

This can still lead to bad results because of randomness.

Another solution: Try different initialization methods

K-means - Random



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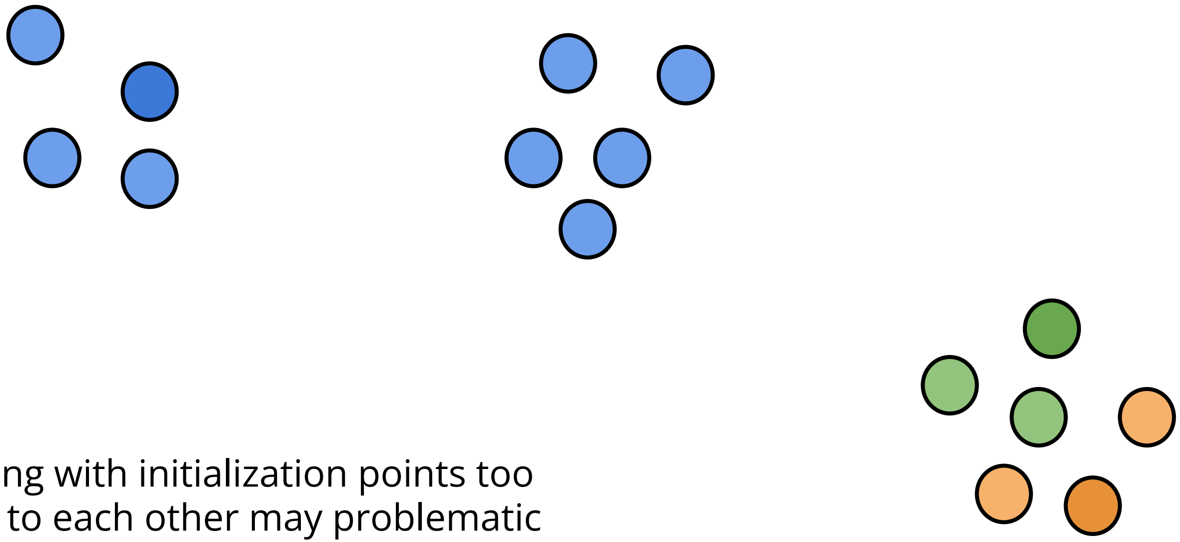
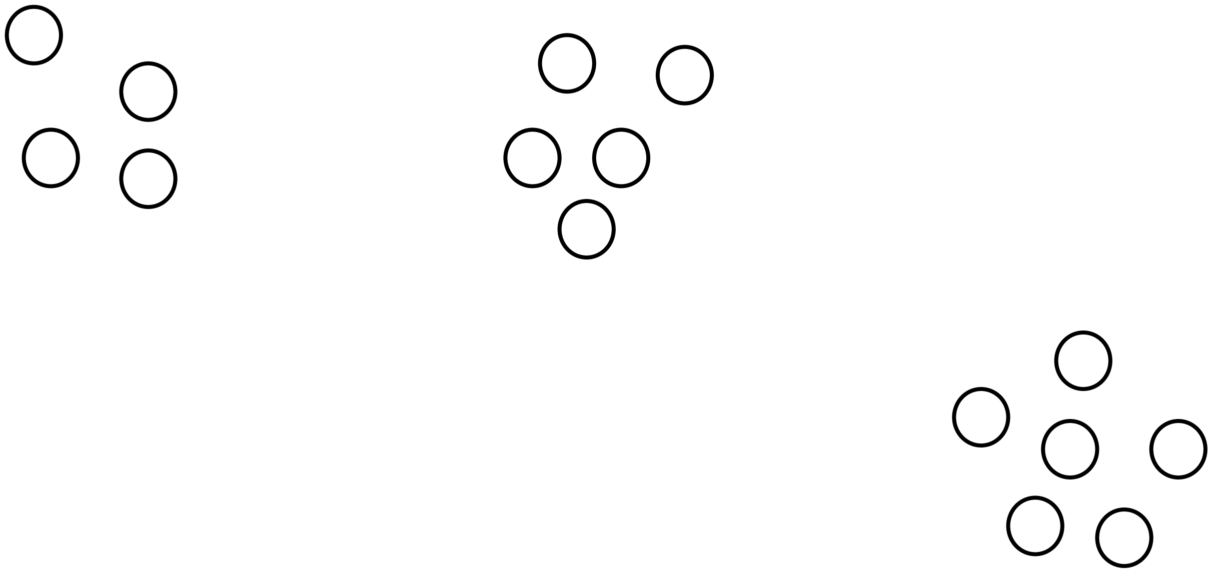
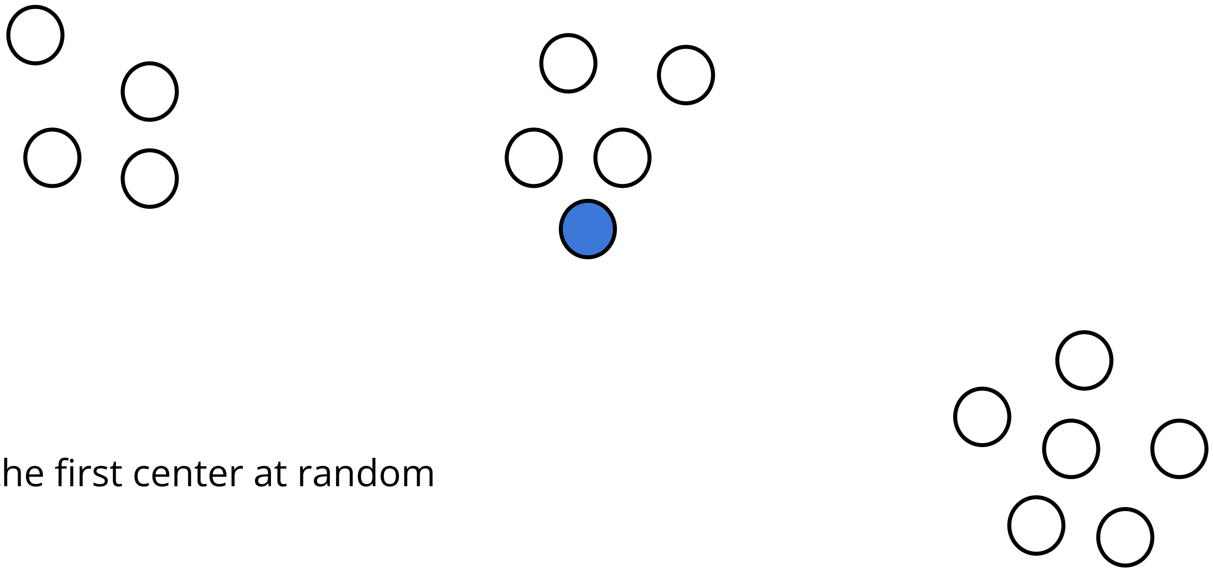


Starting with initialization points too
close to each other may problematic

K-means - Farthest First Traversal

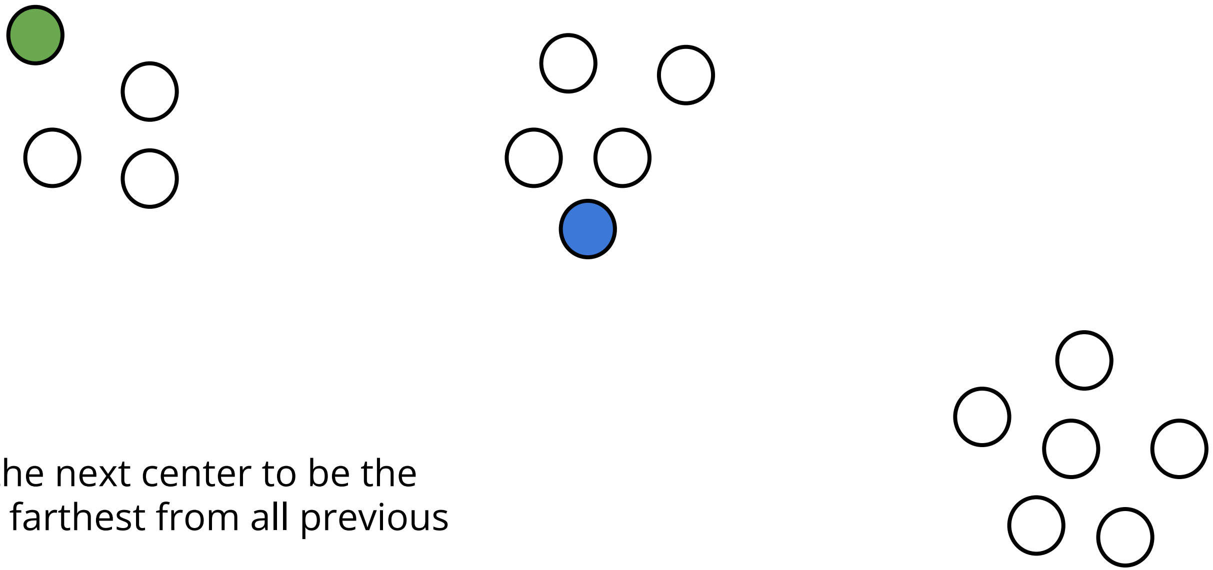


K-means - Farthest First Traversal



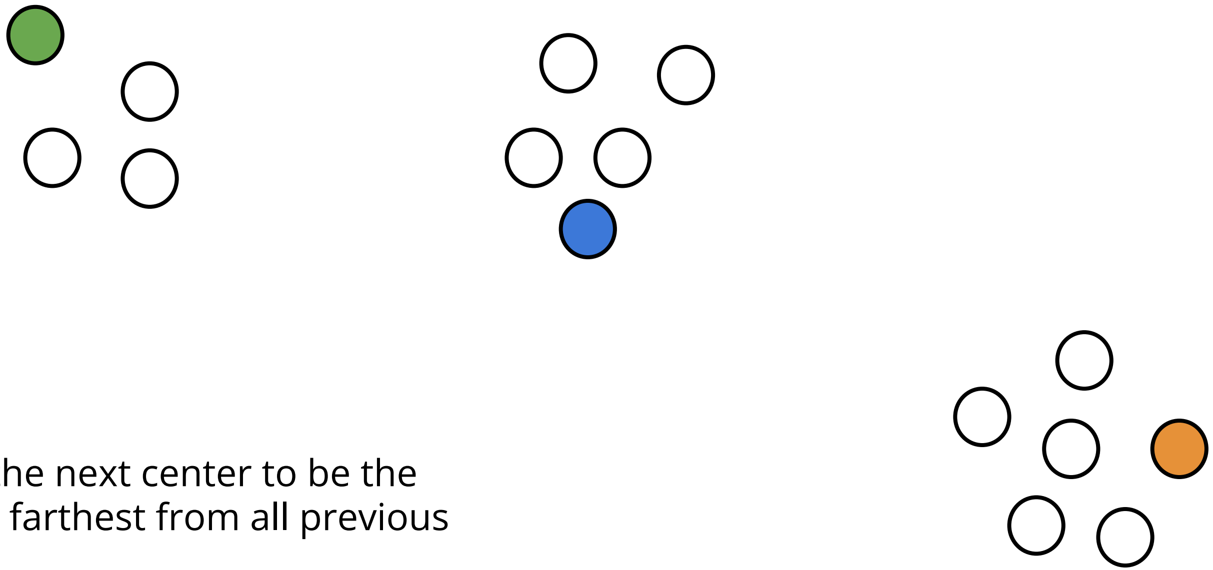
Pick the first center at random

K-means - Farthest First Traversal



Pick the next center to be the point farthest from all previous

K-means - Farthest First Traversal



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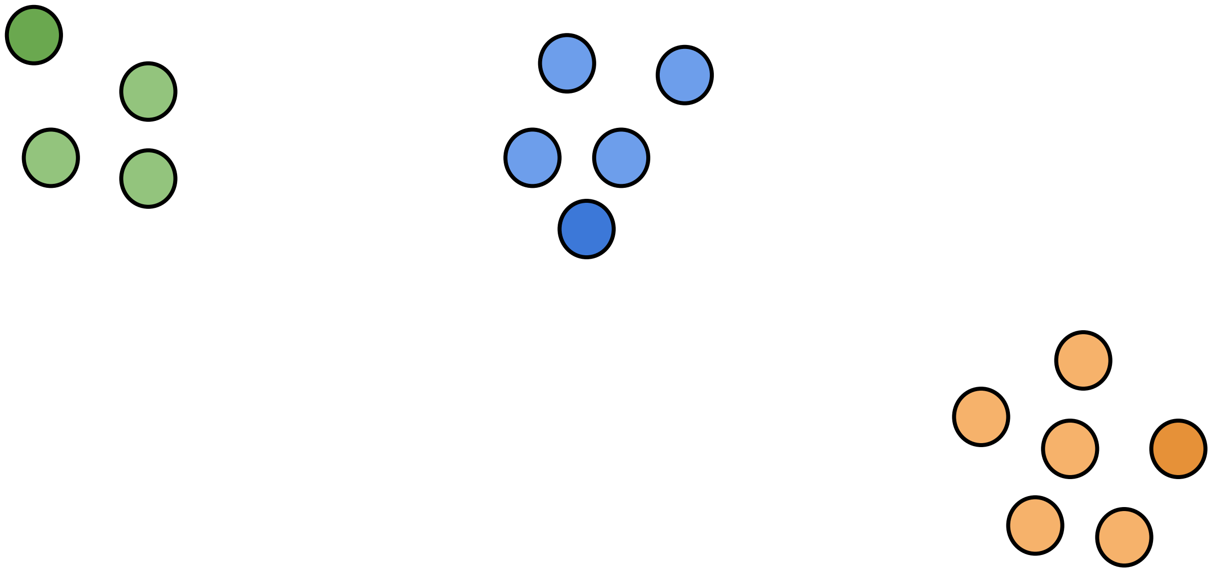
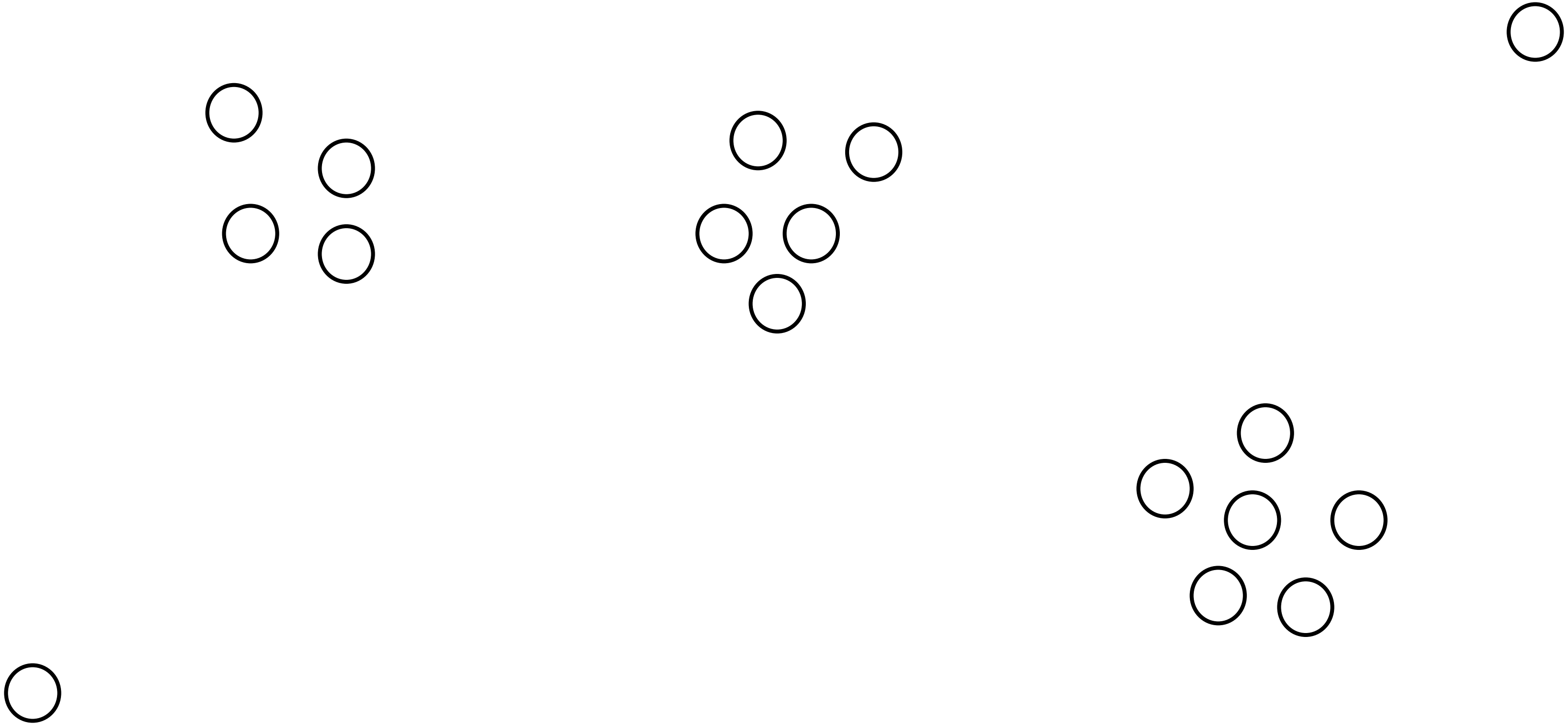
K-means - Farthest First Traversal



K-means - FFT and outliers



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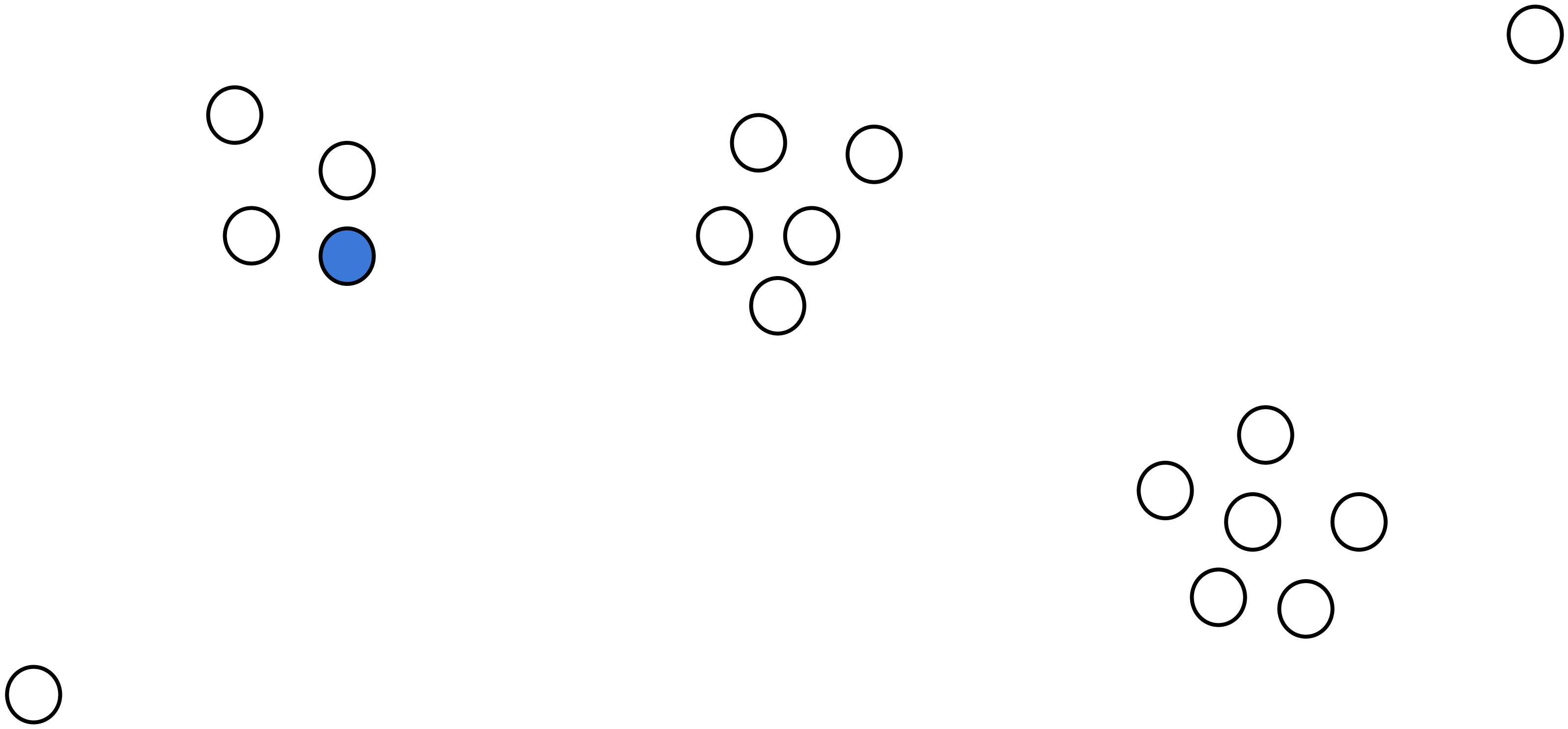

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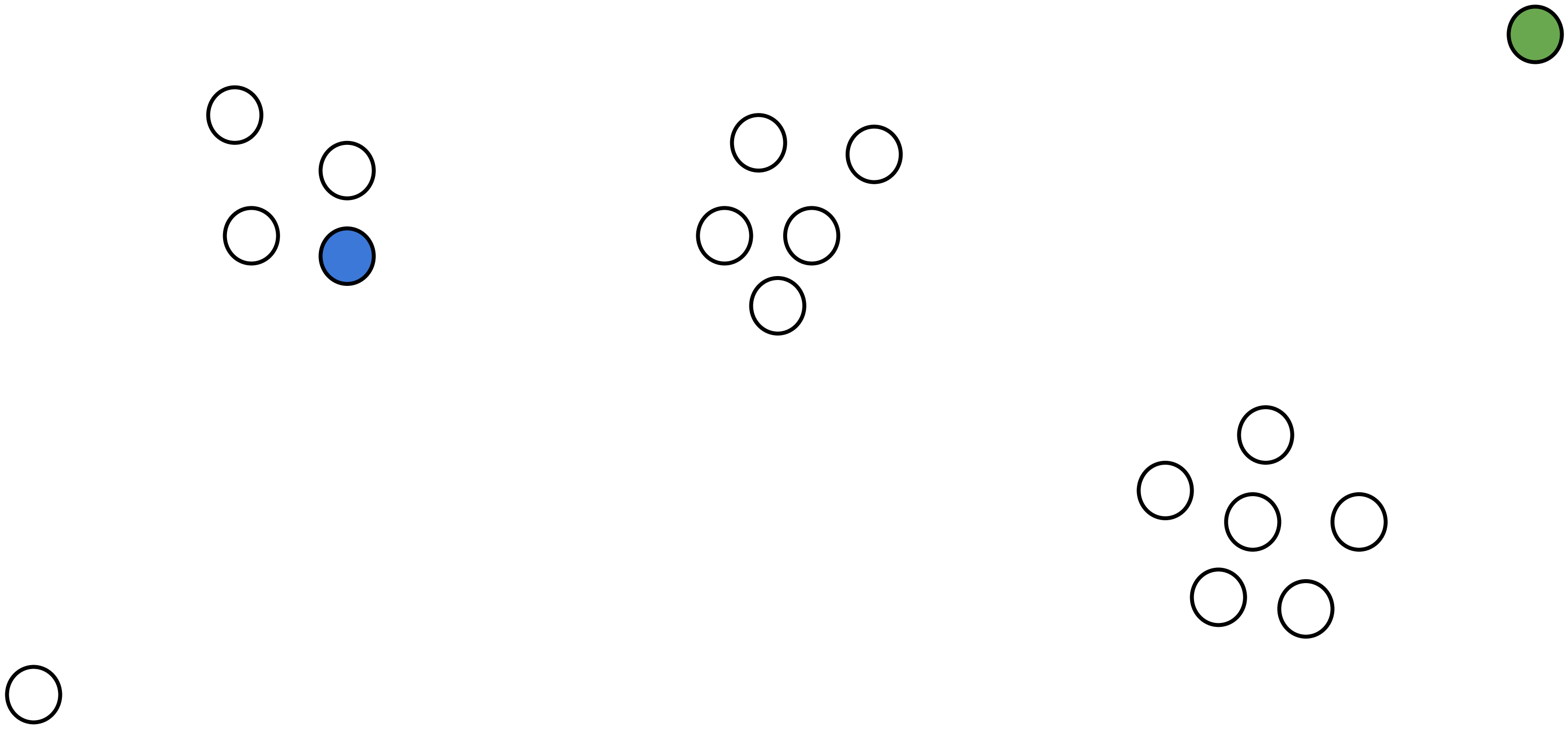

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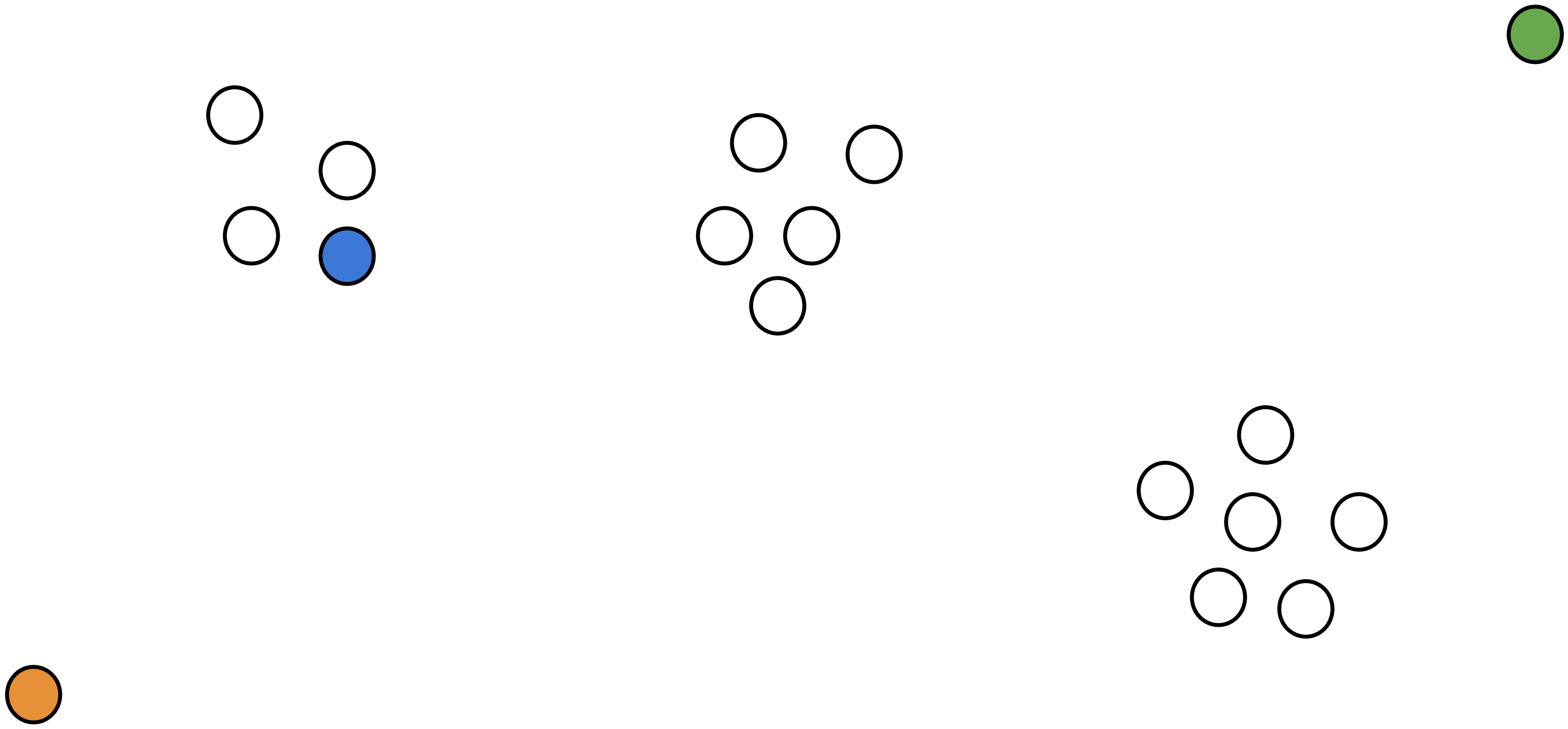

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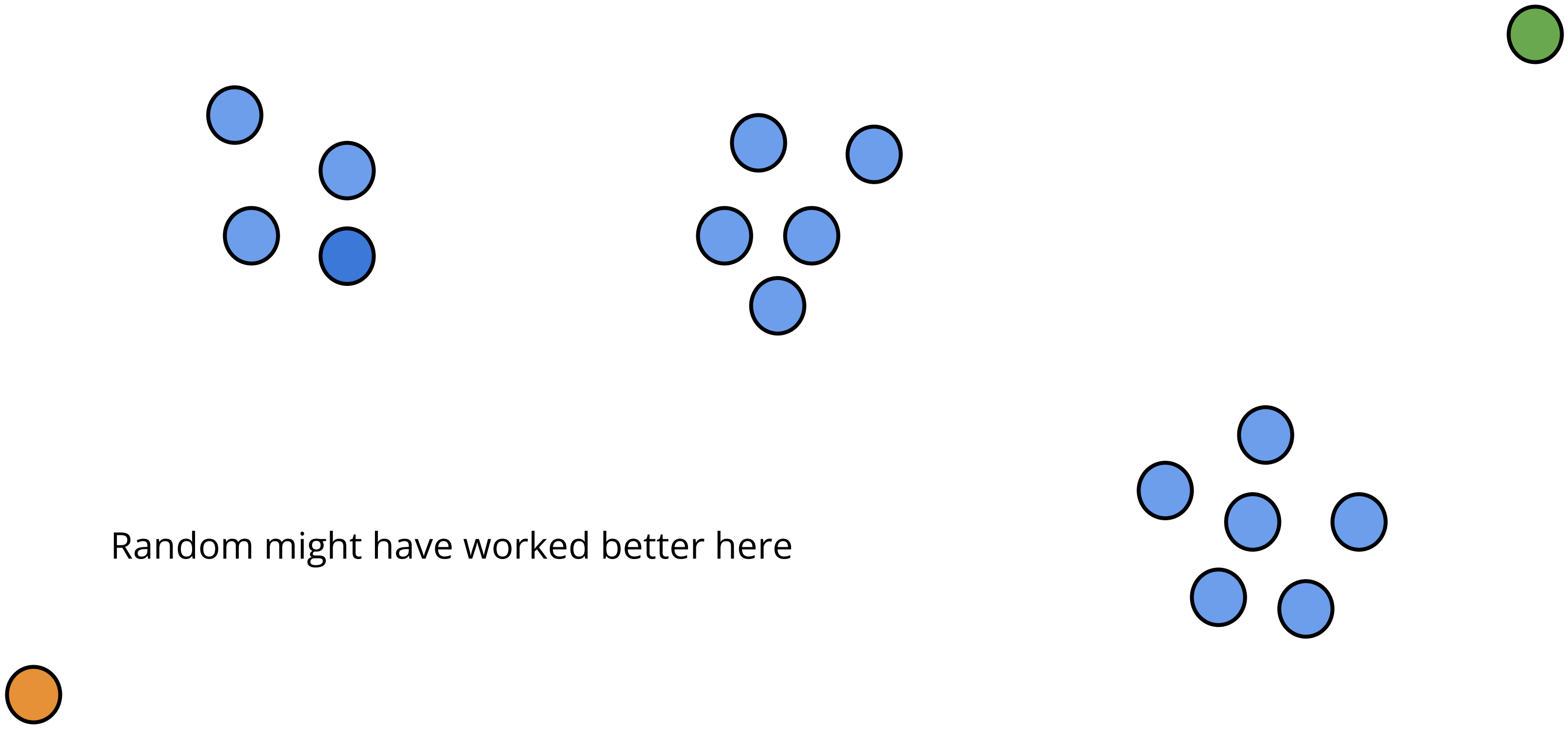


K-means++

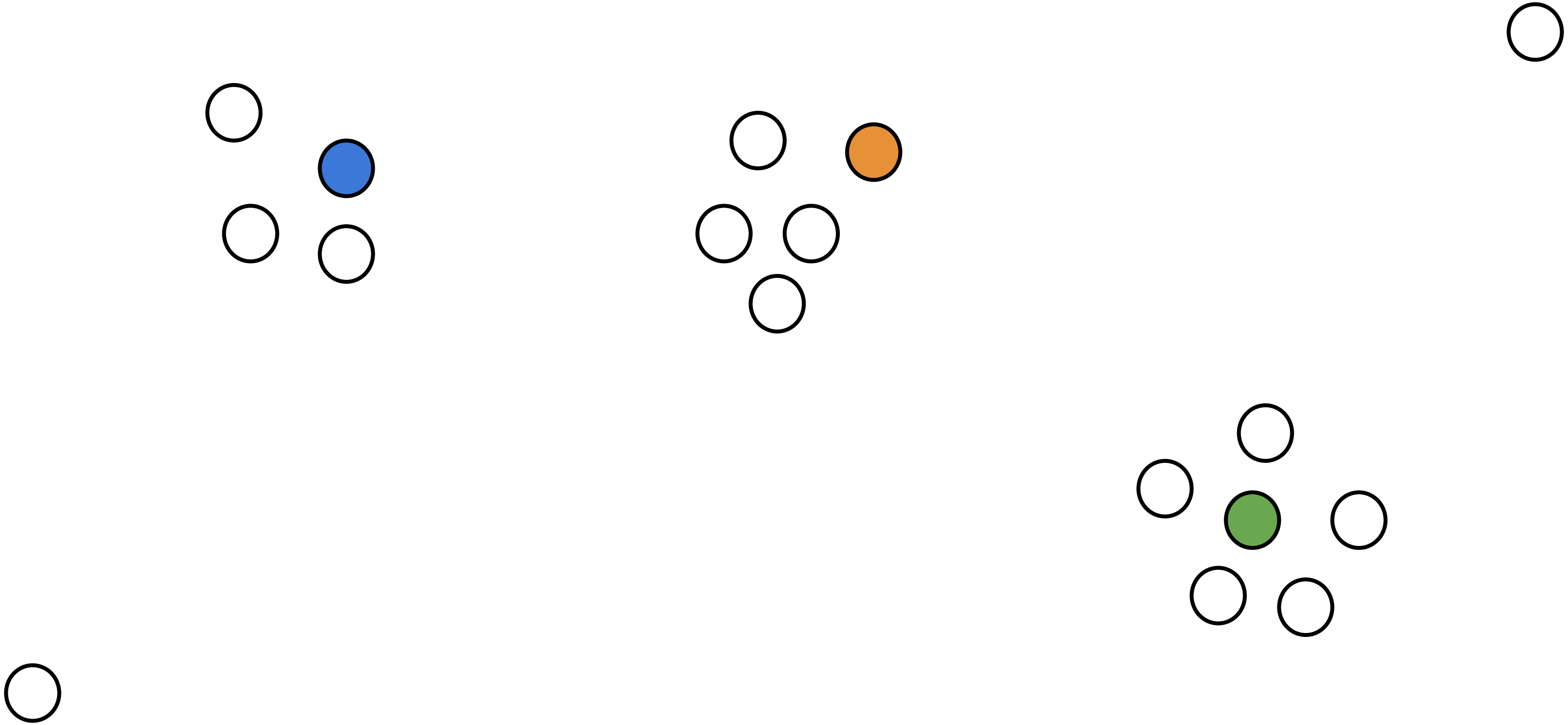
Initialize with a combination of the two methods:

1. Start with a random center
2. Let **D(x)** be the distance between **x** and the centers selected so far. Choose the next center with probability proportional to $\mathbf{D(x)^a}$

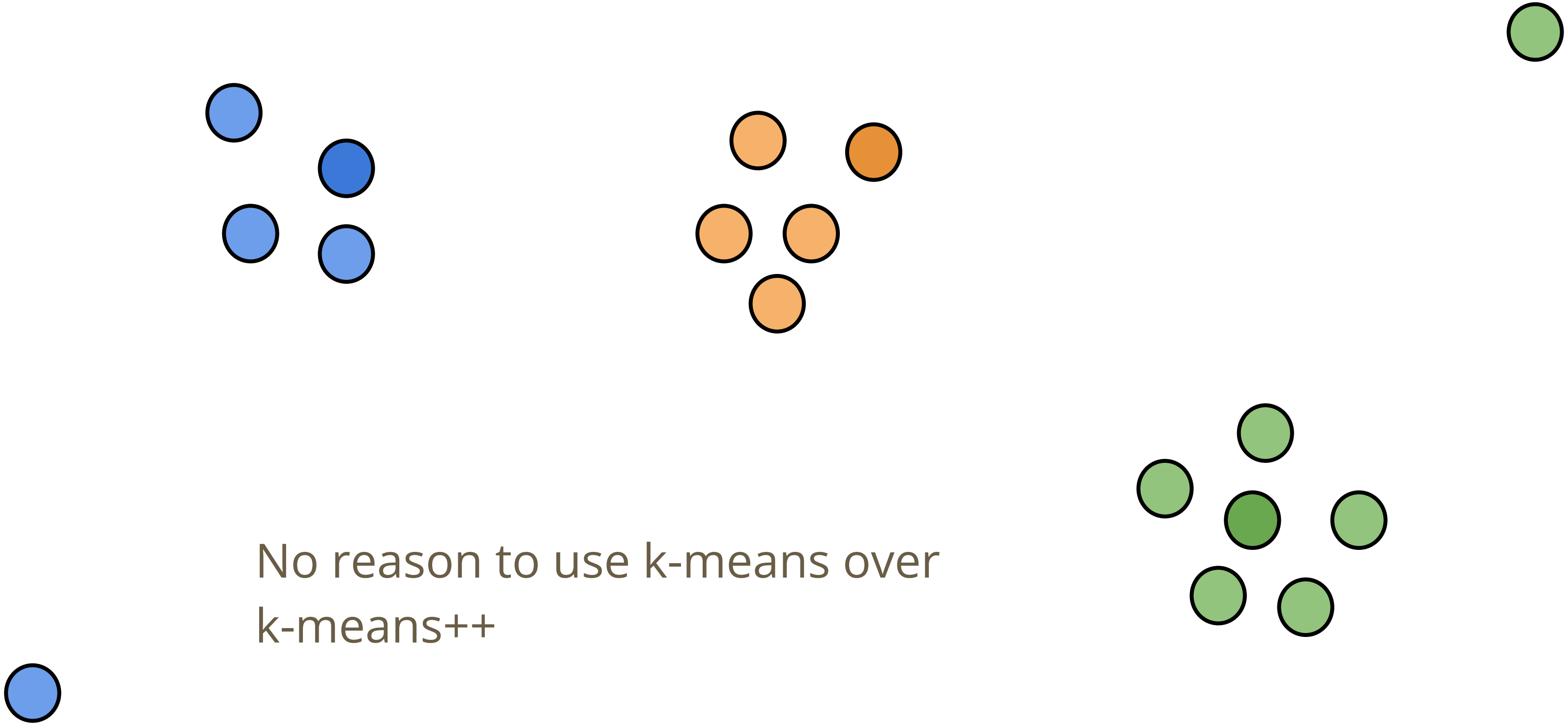
When:

- **a = 0** : random initialization (all points have equal probability)
- **a = ∞** : farthest first traversal
- **a = 2** : K-means++

K-means++



K-means++



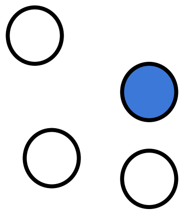
No reason to use k-means over k-means++

K-means++

Suppose we are given a black box that will generate a uniform random number between 0 and any **N**. How can we use this black box to select points with probability proportional to $\mathbf{D(x)^a}$?

K-means++

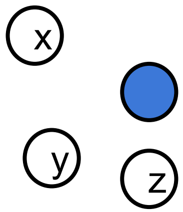
Suppose we are given a black box that will generate a uniform random number between 0 and any **N**. How can we use this black box to select points with probability proportional to $\mathbf{D(x)^a}$?



K-means++

Suppose we are given a black box that will generate a uniform random number between 0 and any **N**. How can we use this black box to select points with probability proportional to $\mathbf{D(x)^2}$?

Let's set $\mathbf{a = 2}$



$\mathbf{D(x)^2 = 3^2 = 9}$
$\mathbf{D(y)^2 = 2^2 = 4}$
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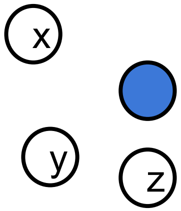

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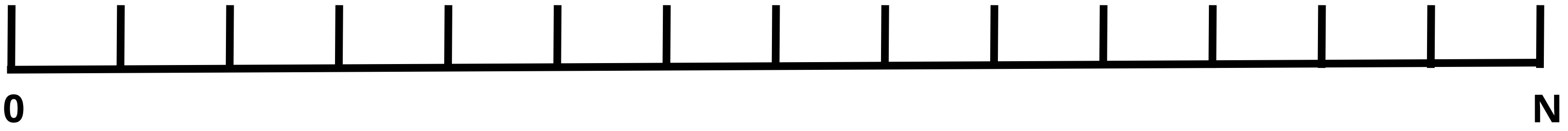

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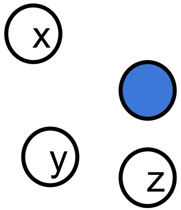

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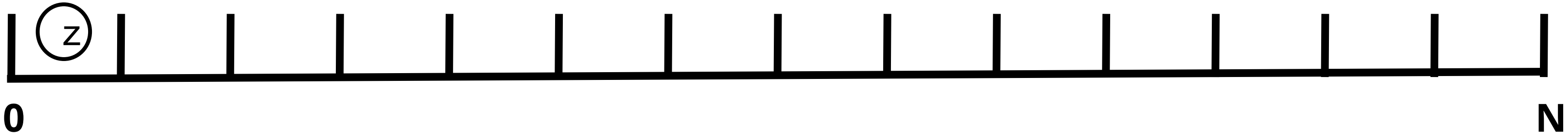

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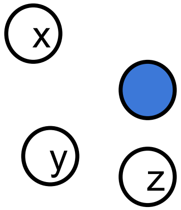

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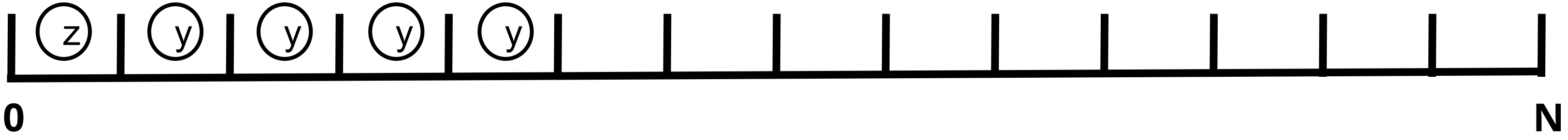

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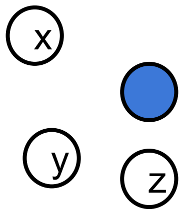

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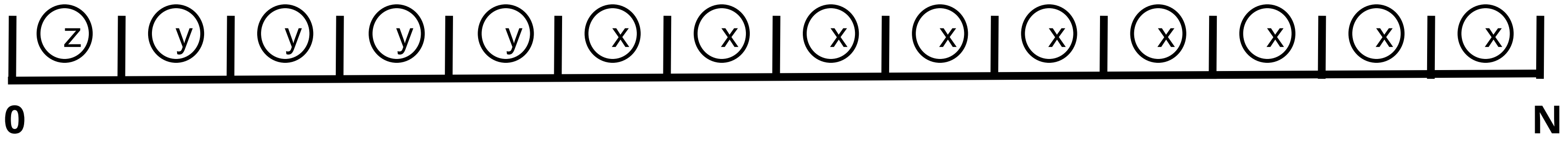

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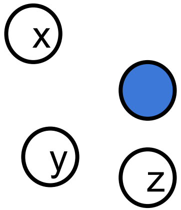

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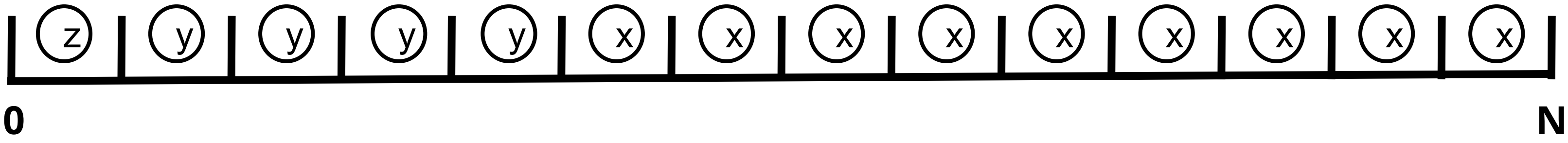

$= D(x)^2 + D(y)^2 + D(z)^2 = 14$

K-means++

Suppose we are given a black box that will generate a uniform random number between 0 and any **N**. How can we use this black box to select points with probability proportional to **$D(x)^2$**?

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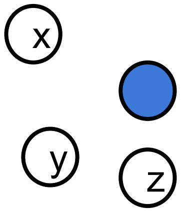

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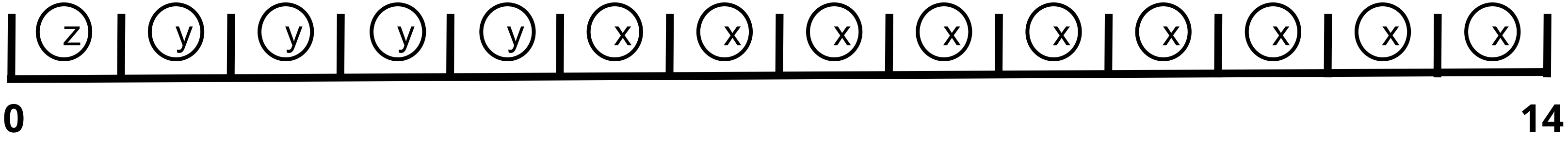
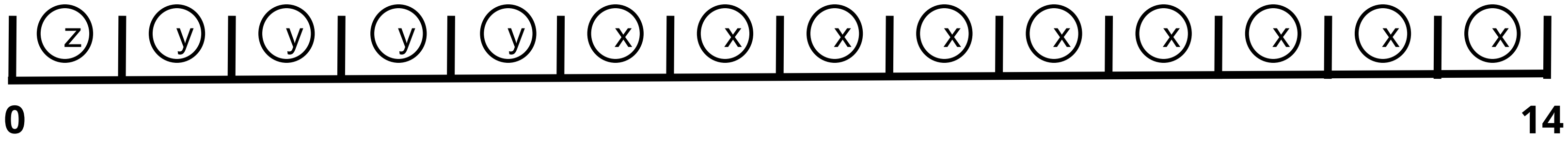


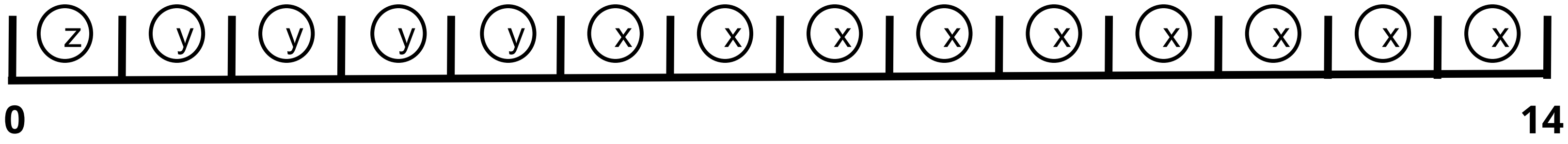
K-means++

Q: the black box returns “12” as the random number generated. Which point do we choose for the next center (x, y, or z) ?



K-means++

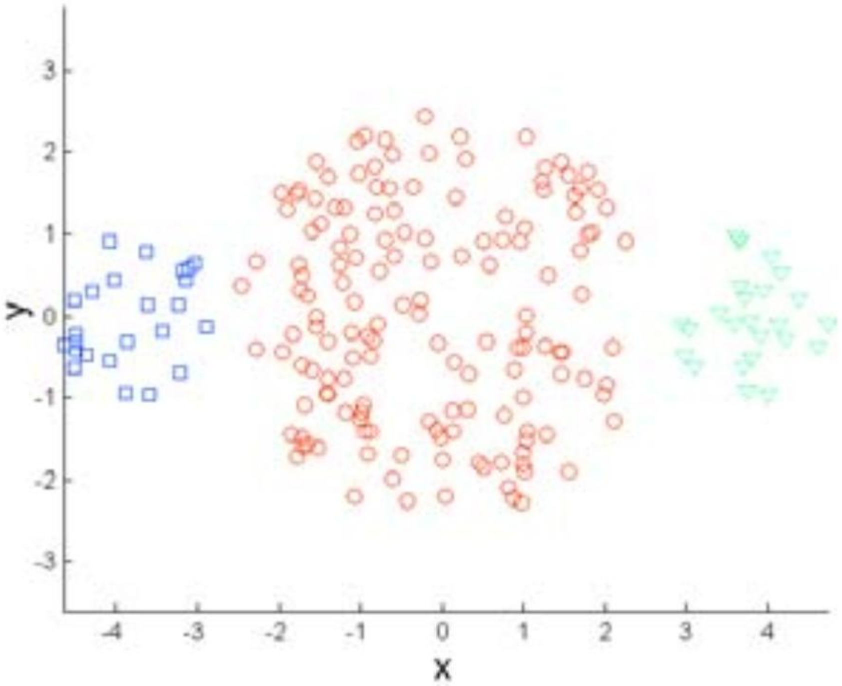
Q: the black box returns “4” as the random number generated. Which point do we choose for the next center (x, y, or z) ?

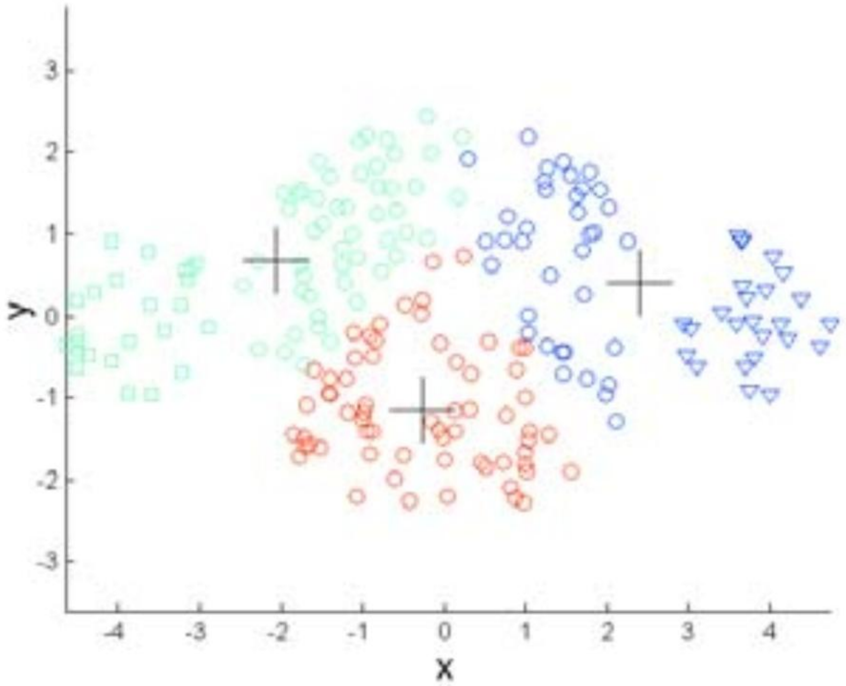


K-means++

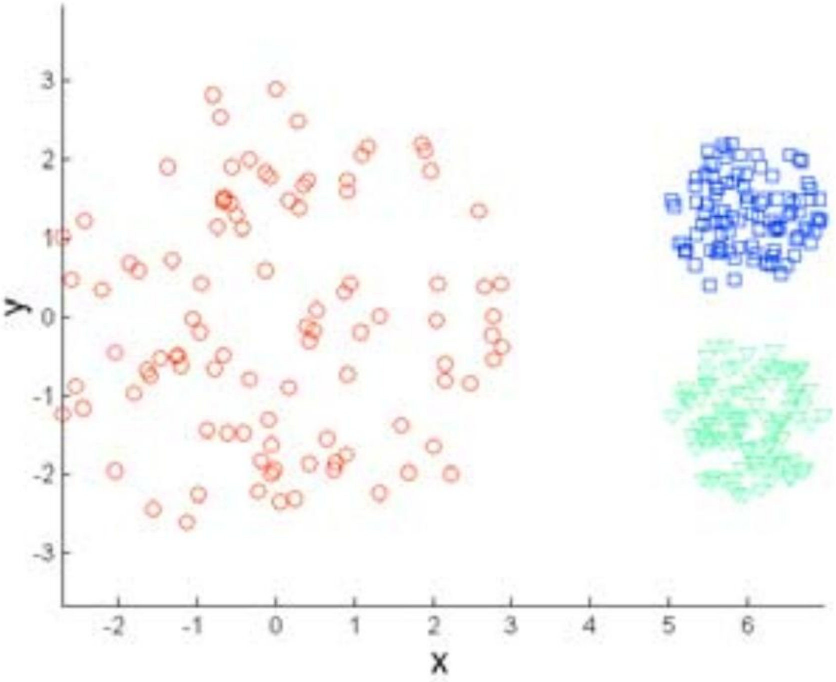
What happens if the black box can only generate numbers between 0 and 1?

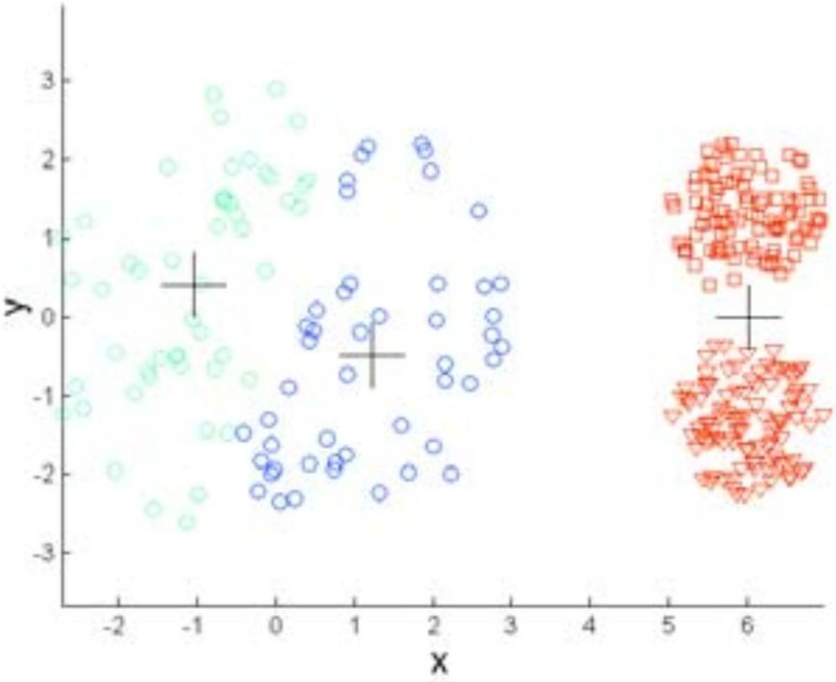
K-means / K-means++ Limitations





K-means / K-means++ Limitations





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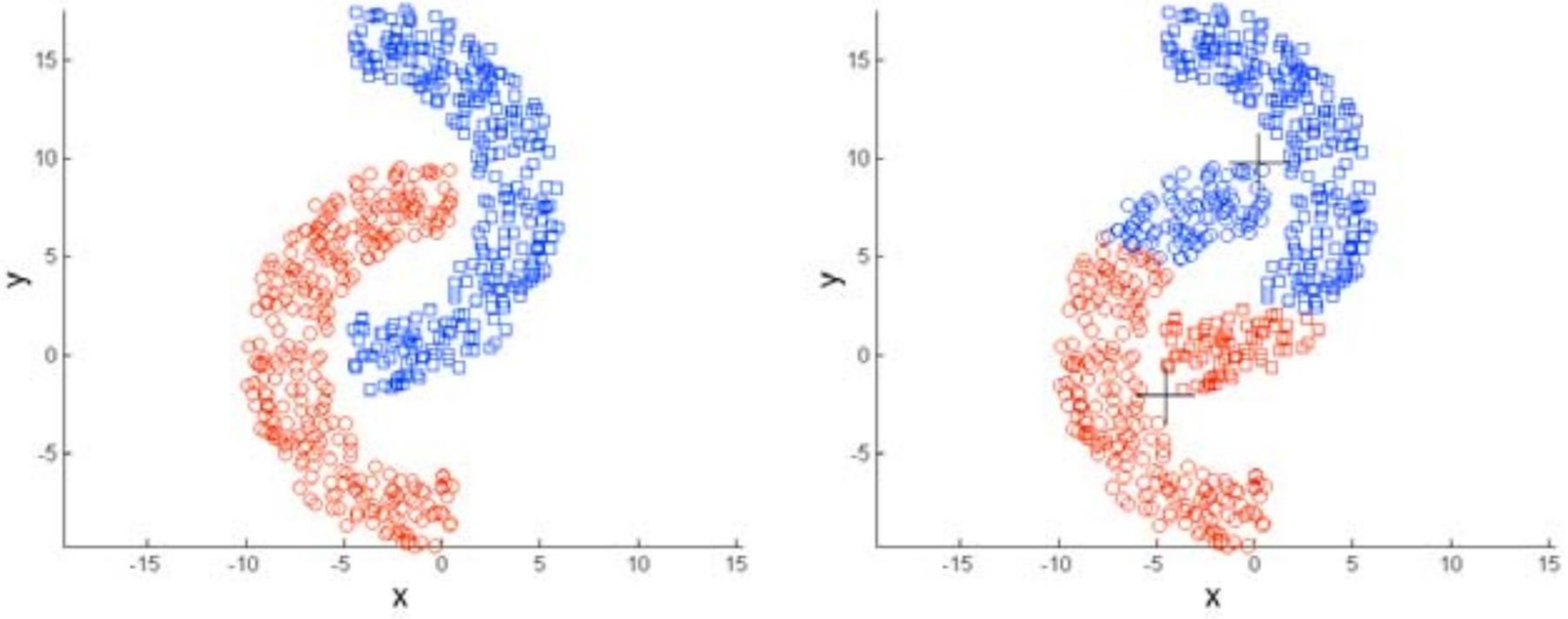


How to choose the right k?

1. Iterate through different values of k (elbow method)
2. Use empirical / domain-specific knowledge

   Example: Is there a known approximate distribution of the data? (K-means is good for spherical gaussians)
3. Metric for evaluating a clustering output

Evaluation

Recall our goal: Find a clustering such that

- **Similar** data points are in the **same cluster**
- **Dissimilar** data points are in **different clusters**

Evaluation

Recall our goal: Find a clustering such that

- **Similar** data points are in the **same cluster** ✅
- **Dissimilar** data points are in **different clusters**

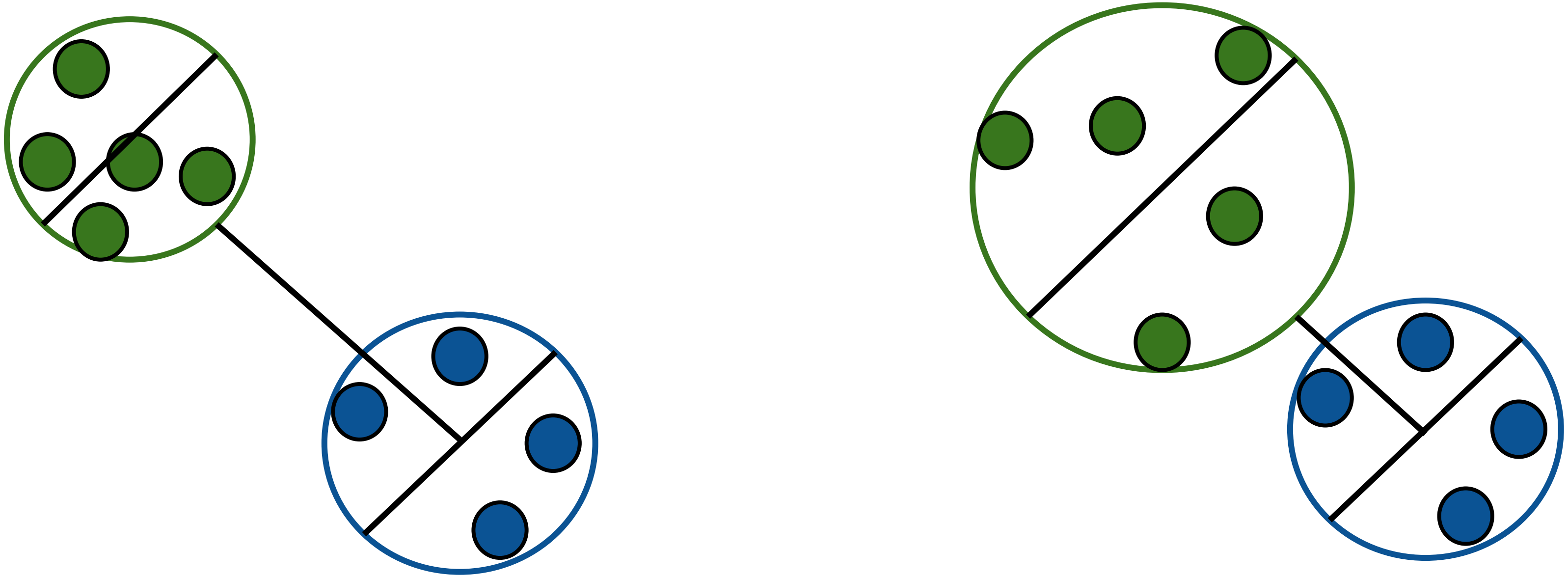
Evaluation

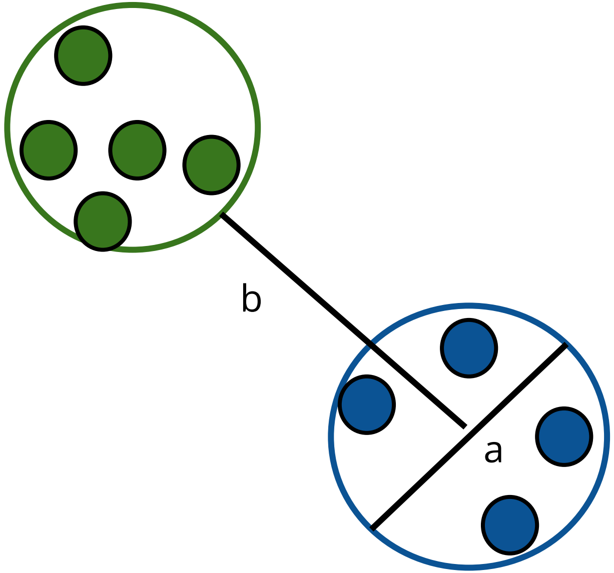
K-means cost function tells us the within-cluster distances between points will be small overall.

But what about the intra-cluster distance? Are the clusters we created far? How far? Relative to what?

Discuss - 5min

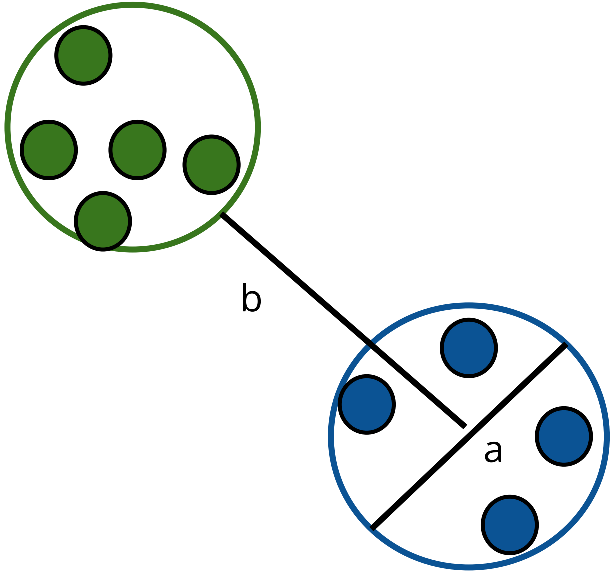
Define a few metrics that you might care about when evaluating a clustering.



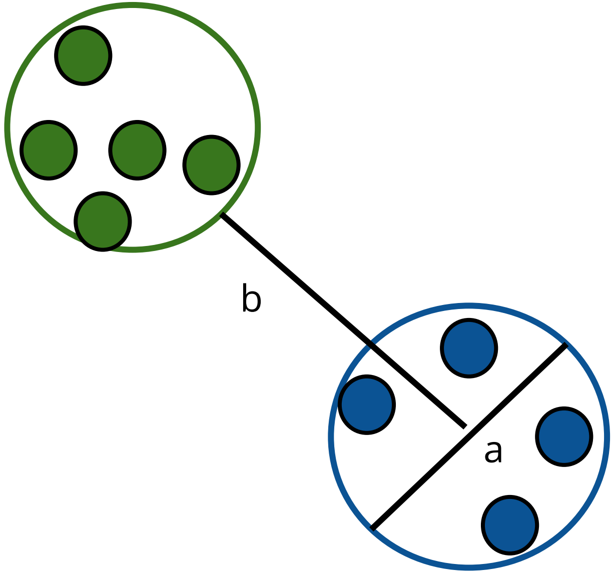


a: average within-cluster distance

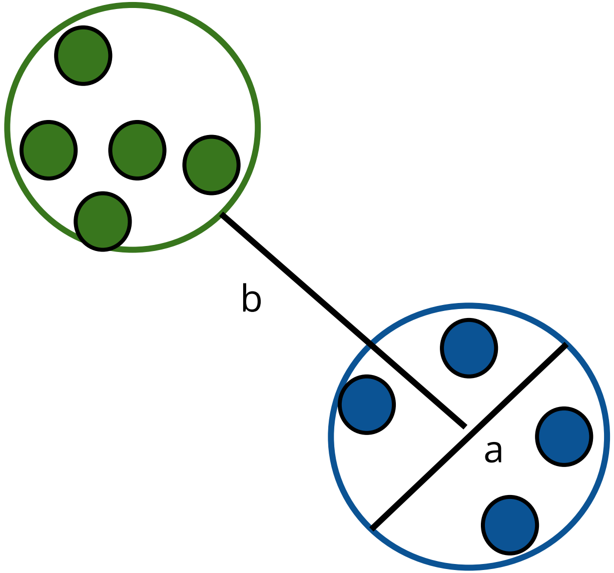
b: average intra-cluster distance



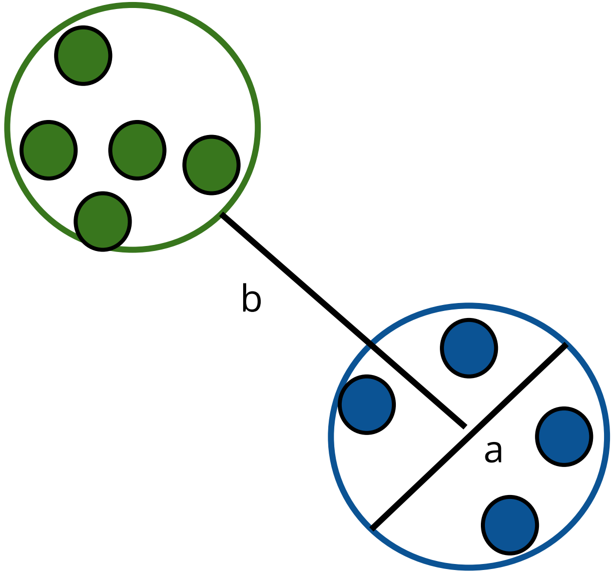
What does it mean for (b - a) to be 0?



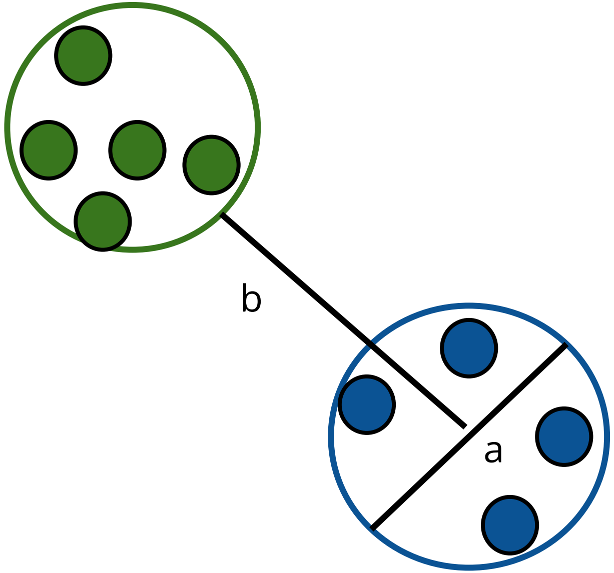
What does it mean for (b - a) to be large?



What does it mean for (b - a) to be negative?

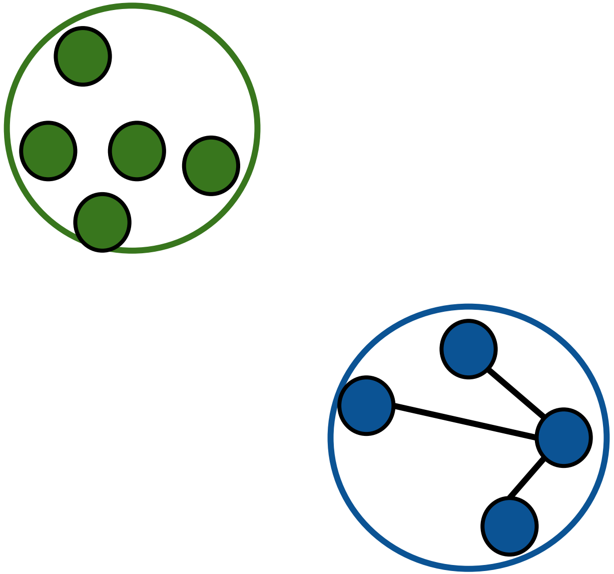


Should we compare (b - a) to some other value, in order to get a sense of how representative that average value is overall?



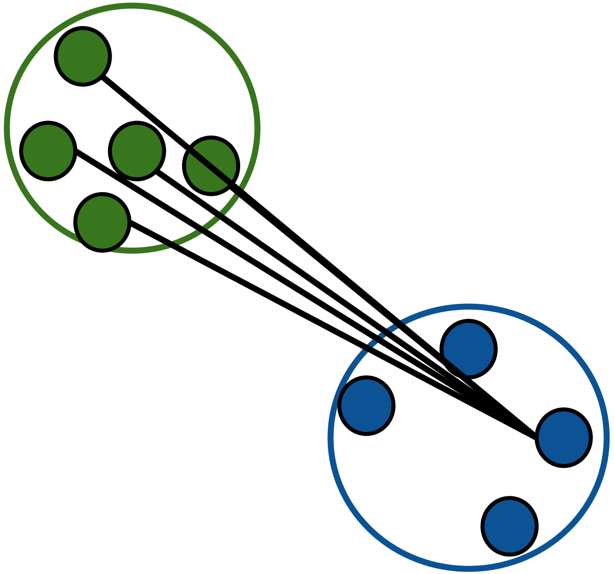
(b - a) / max(a, b)

Silhouette Scores



For each data point i:
a_i : mean distance from point i to every other point in its cluster

Silhouette Scores

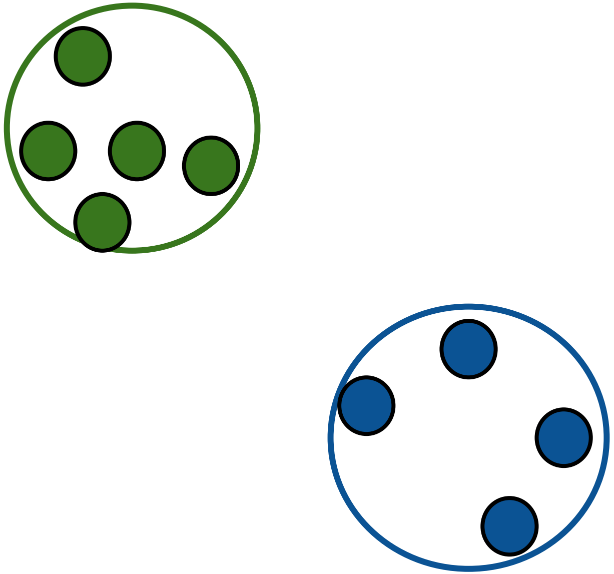


For each data point i:

a_i : mean distance from point i to every other point in its cluster

b_i : smallest mean distance from point i to every point in another cluster

Silhouette Scores



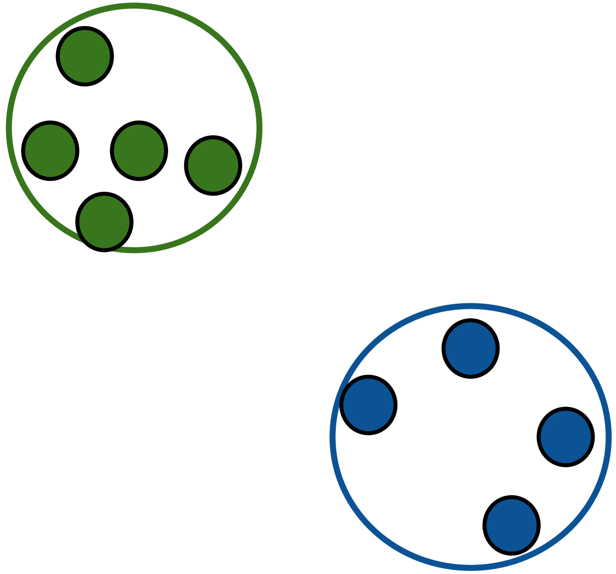
For each data point i:

a_i : mean distance from point i to every other point in its cluster

b_i : smallest mean distance from point i to every point in another cluster

$s_i = (b_i - a_i) / \max(a_i, b_i)$

Silhouette Scores



$s_i = (b_i - a_i) / \max(a_i, b_i)$

Silhouette score plot

OR

return the mean s_i over the entire dataset as a measure of goodness of fit

Discuss

Q: What is a good silhouette score value?
Q: What is a bad silhouette score value?

Worksheet - answer the last question

K-means Variations

1. K-medians (uses the L_1 norm / manhattan distance)
2. K-medoids (any distance function + the centers must be in the dataset)
3. Weighted K-means (each point has a different weight when computing the mean)