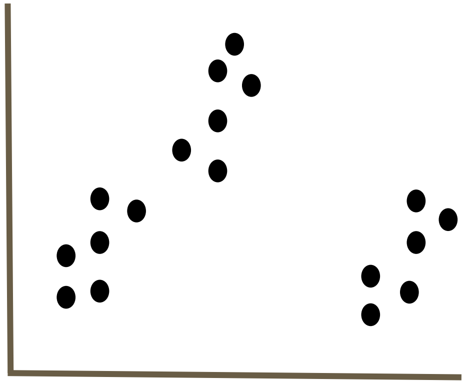
Clustering - Kmeans

Boston University CS 506 - Lance Galletti

What is a Clustering



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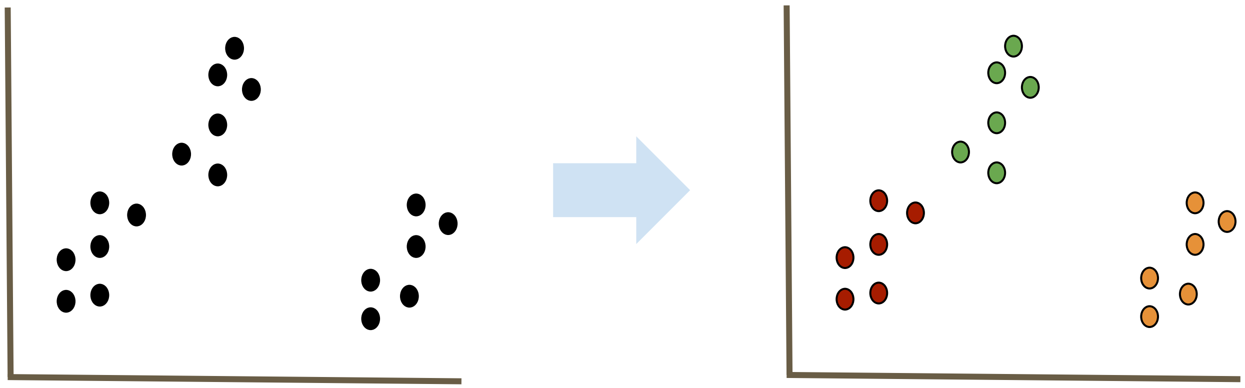
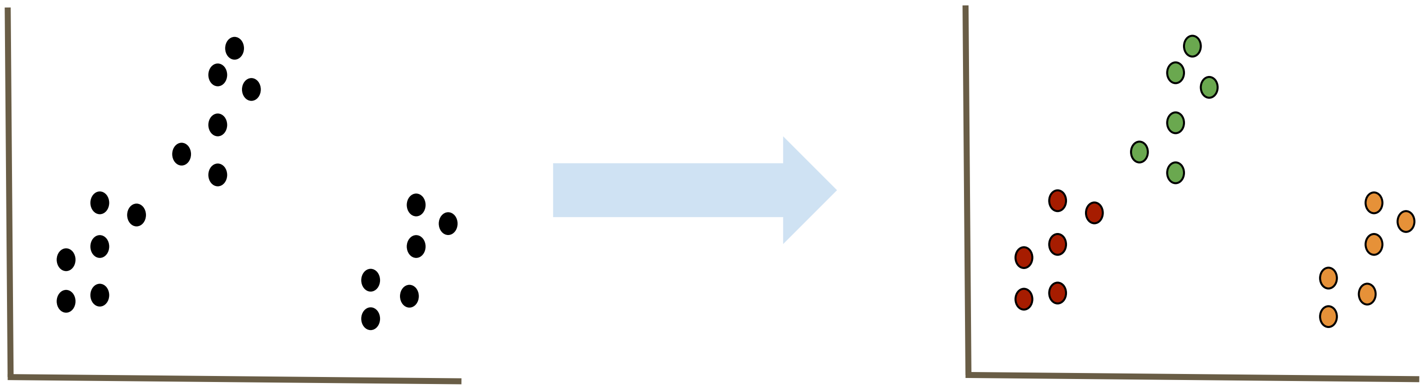


What is a Clustering

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

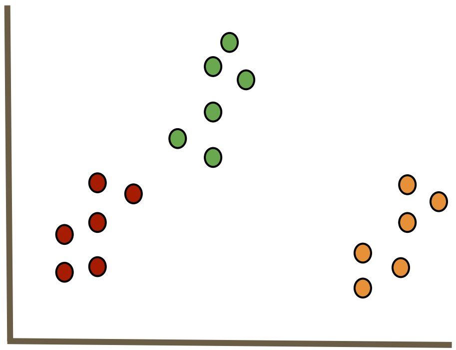
- similar to one another
- dissimilar to objects in other groups

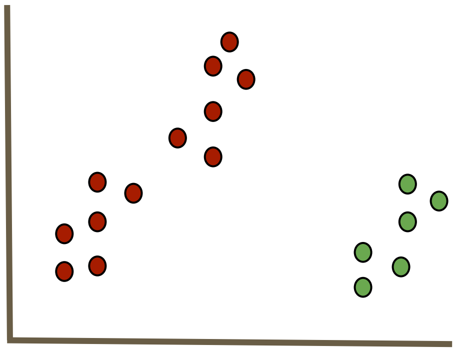


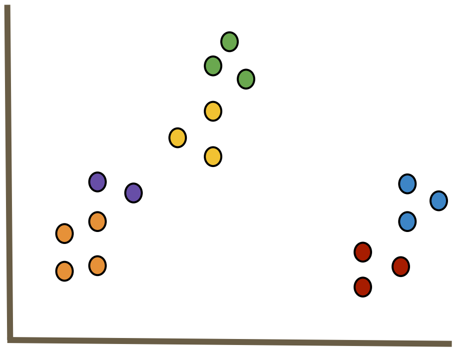
Applications

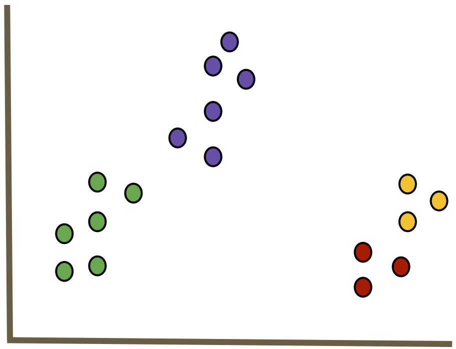
- Outlier detection / anomaly detection
  - Data Cleaning / Processing
  - Credit card fraud, spam filter etc.
- Feature Extraction
- Filling Gaps in your data
  - Using the same marketing strategy for similar people
  - Infer probable values for gaps in the data (similar users could have similar hobbies,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

Clusters can be Ambiguous









Types of Clusterings

Partitional

Each object belongs to exactly one cluster (k partitions)

Hierarchical (high level hierarchy of data points)

A set of nested clusters organized in a tree

Density-Based (create data clusters)

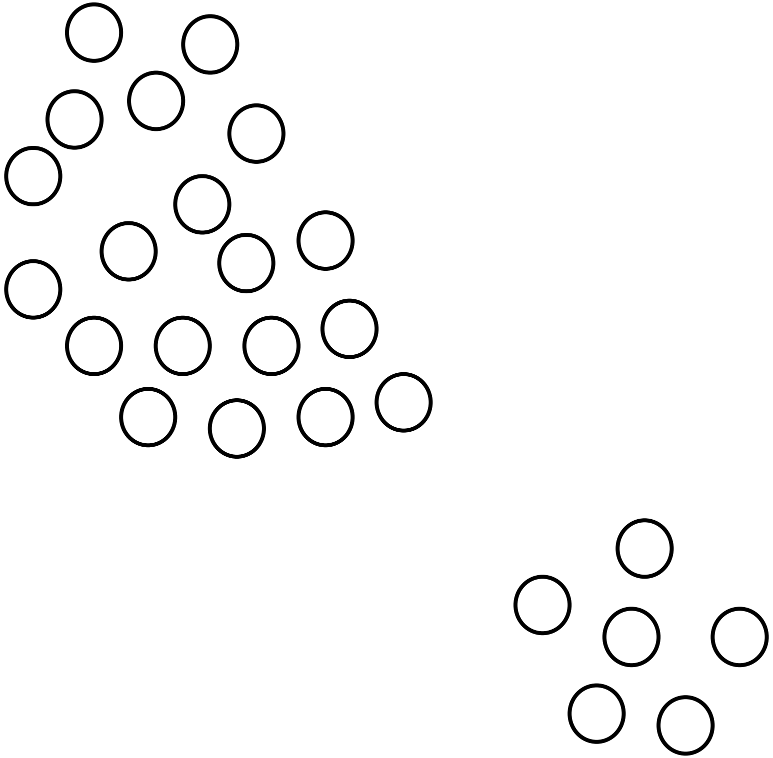
Defined based on the local density of points

Soft Clustering (“probabilistic” clustering)

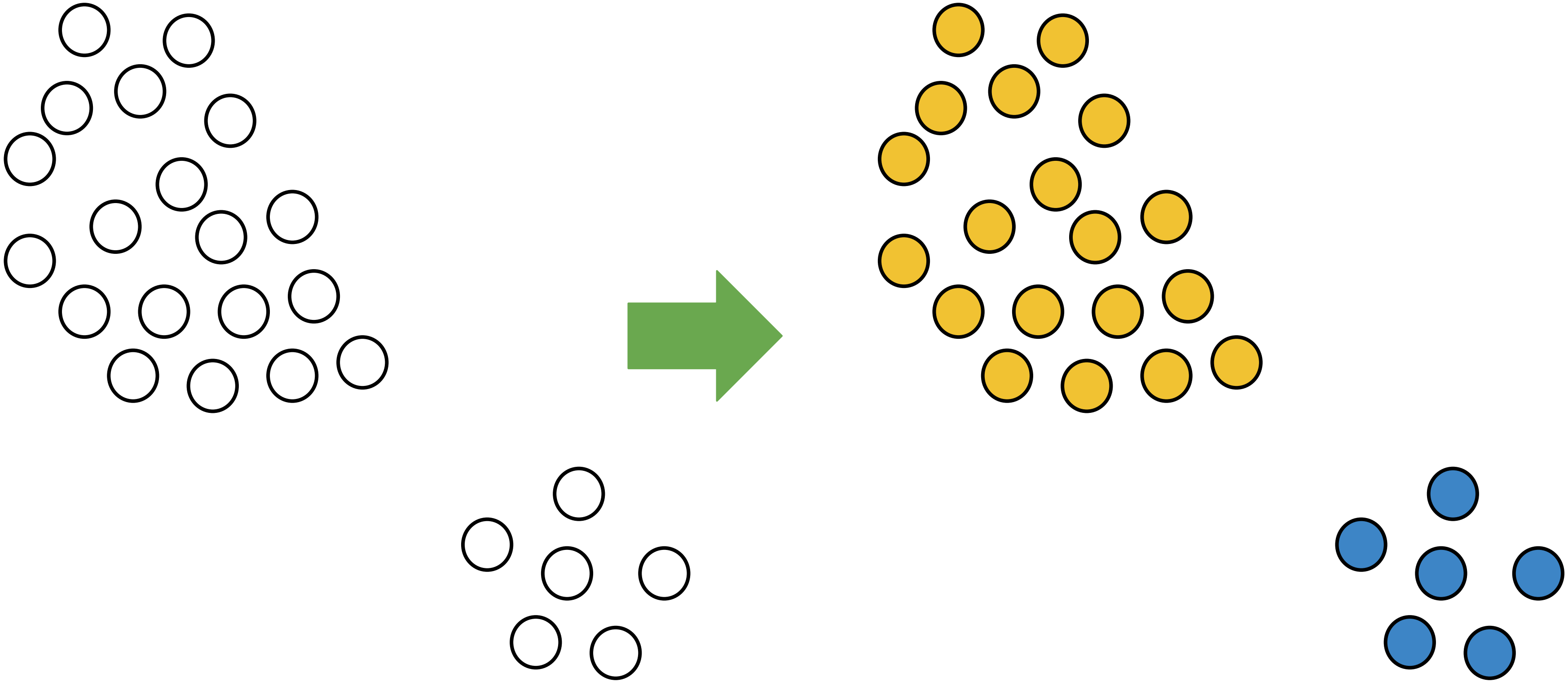
Each point is assigned to every cluster with a certain probability

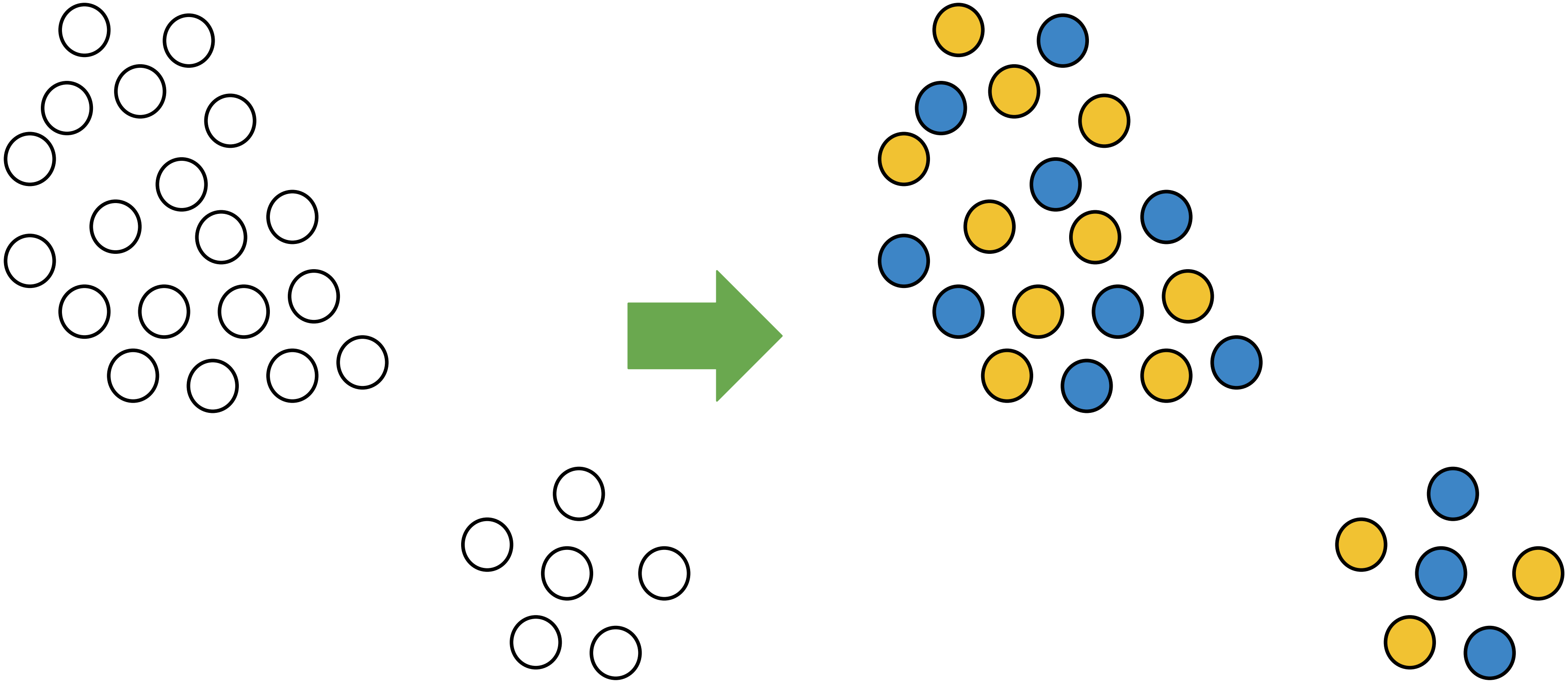
Partitional Clustering

Partitional Clustering

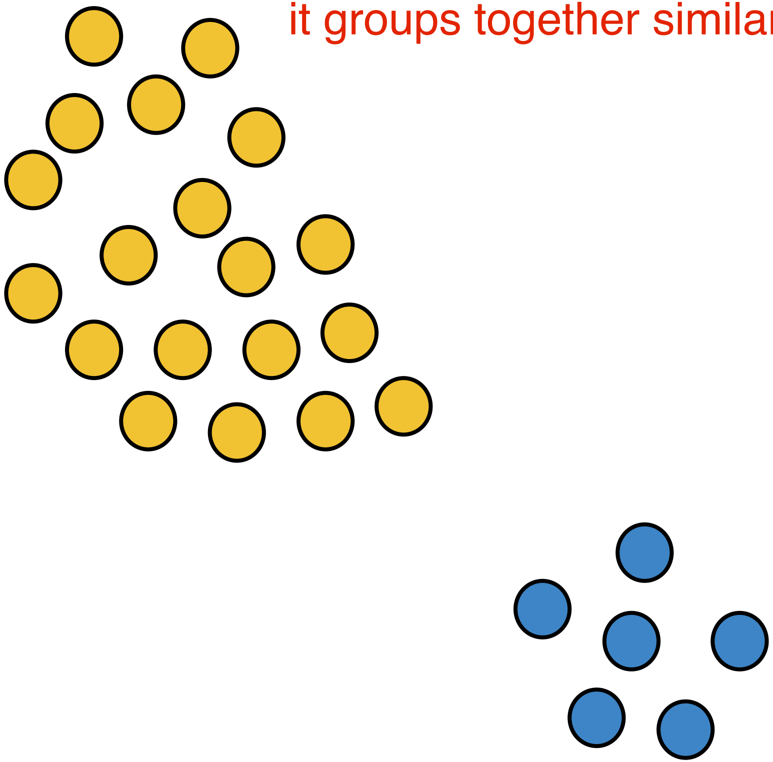


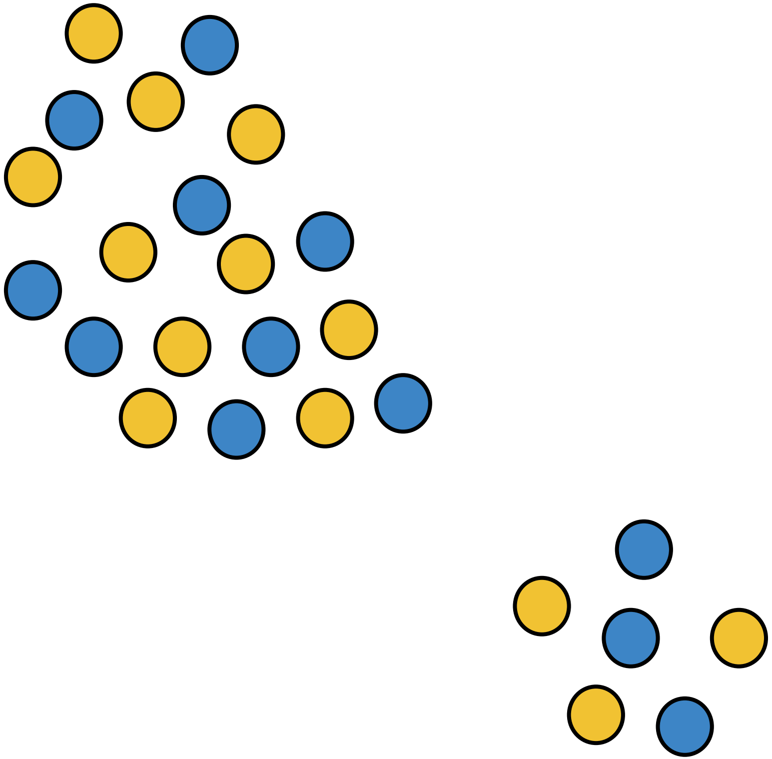
Goal: partition dataset into k partitions

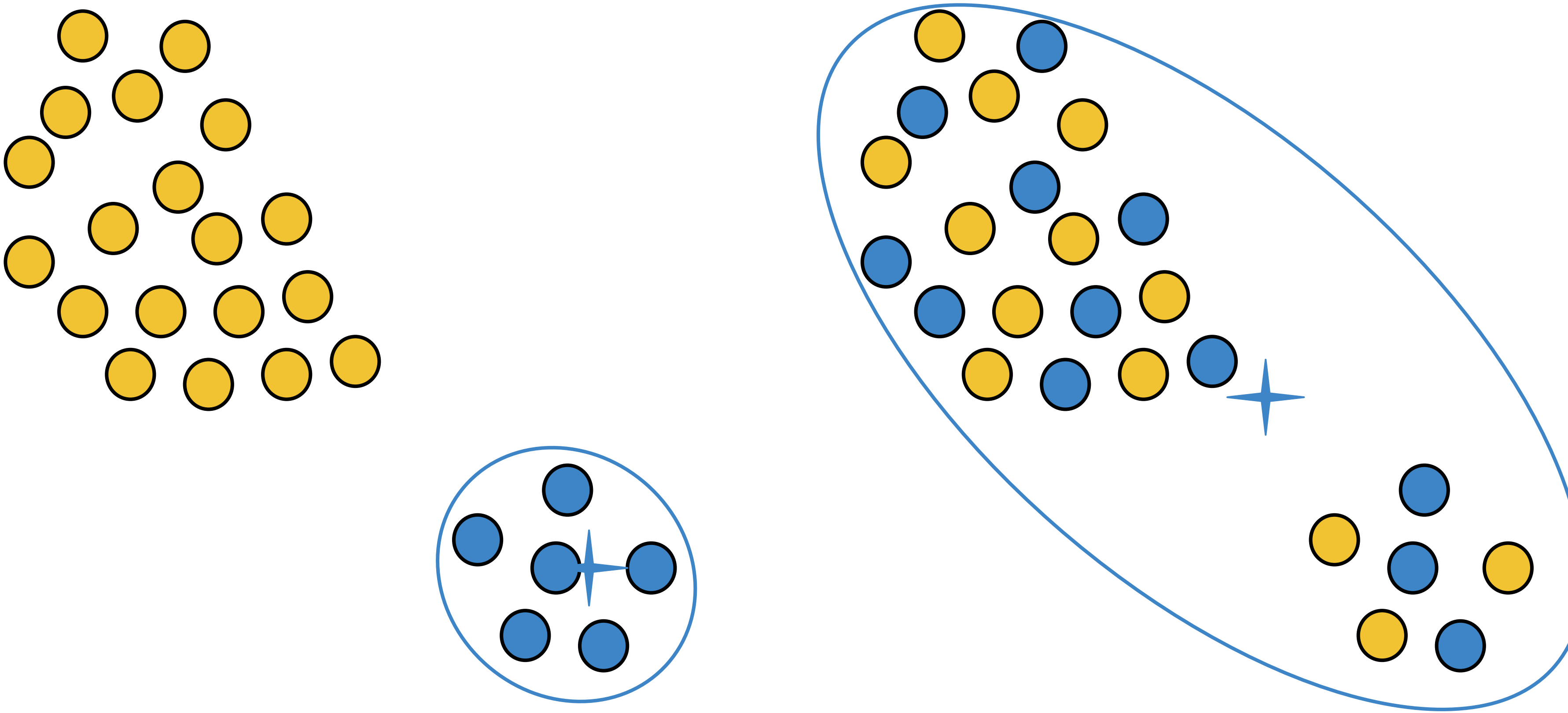




both of these are partitions,
however the first one is better because
it groups together similar data

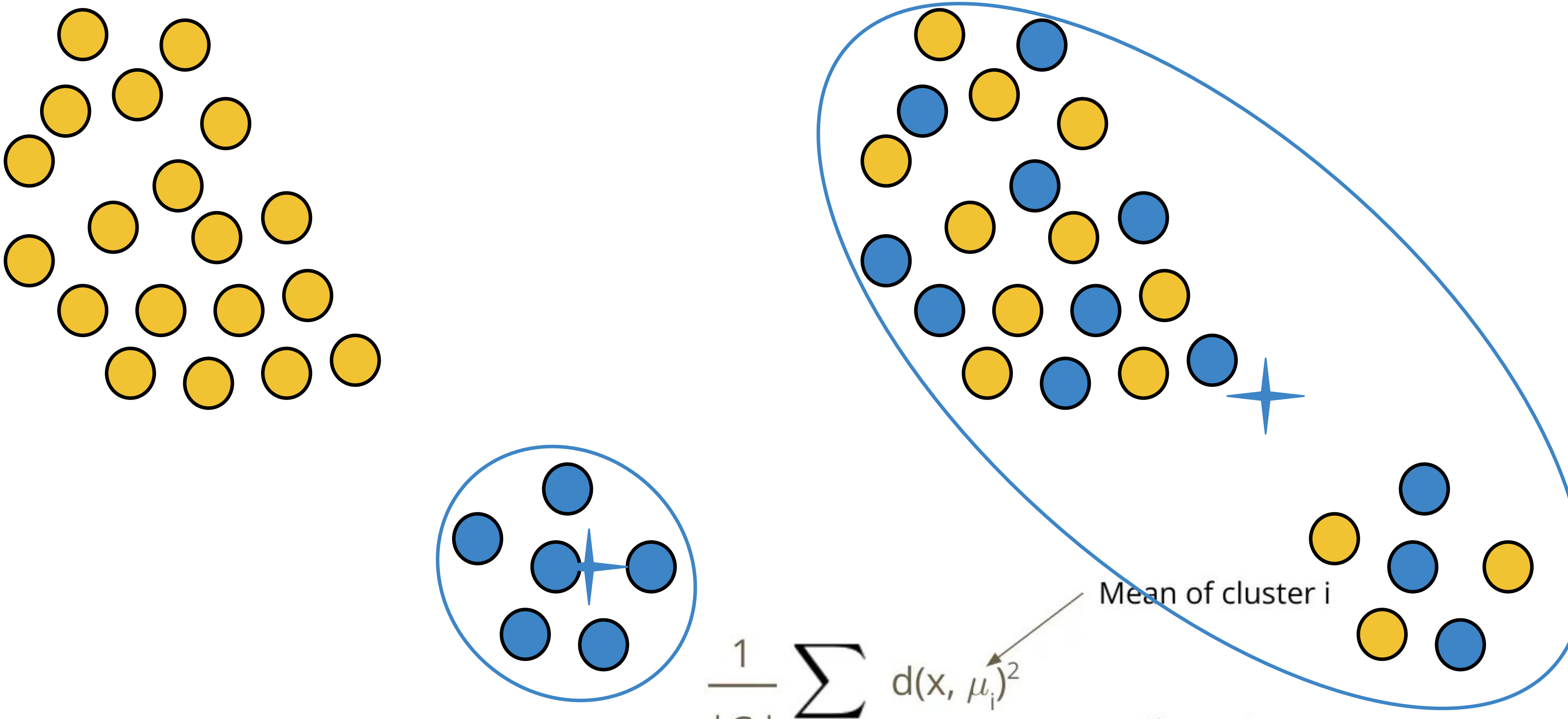






smaller value from cost function

larger value from cost function



$$\frac{1}{|C_i|}\sum_{x\in C_i} d(x, \mu_i)^2$$

Cost Function

for every cluster, take the total sum of the squared distance of each point and mean of cluster i

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

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

K-means

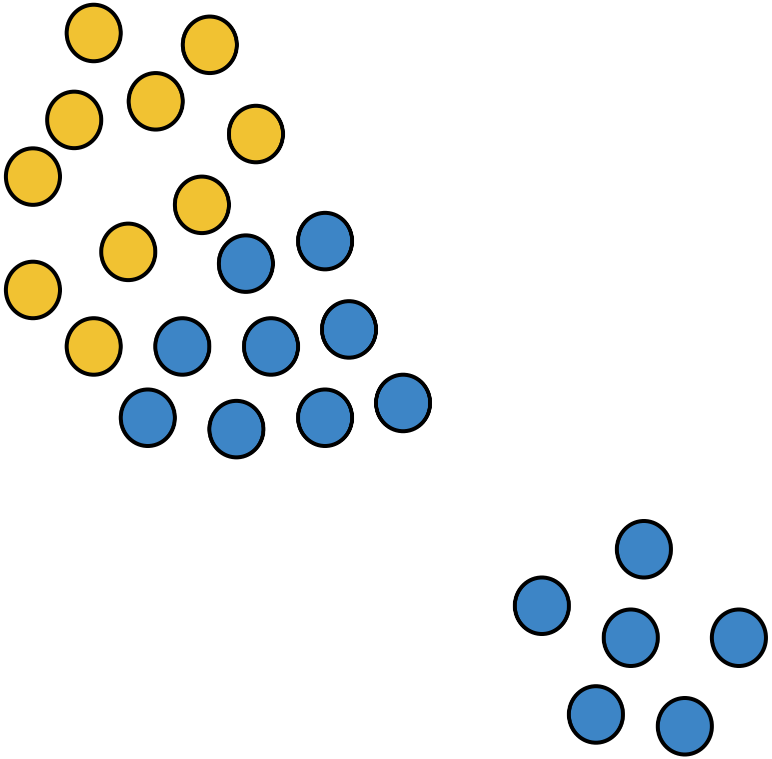
Given $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ our dataset, **d** the euclidean distance, and **k**

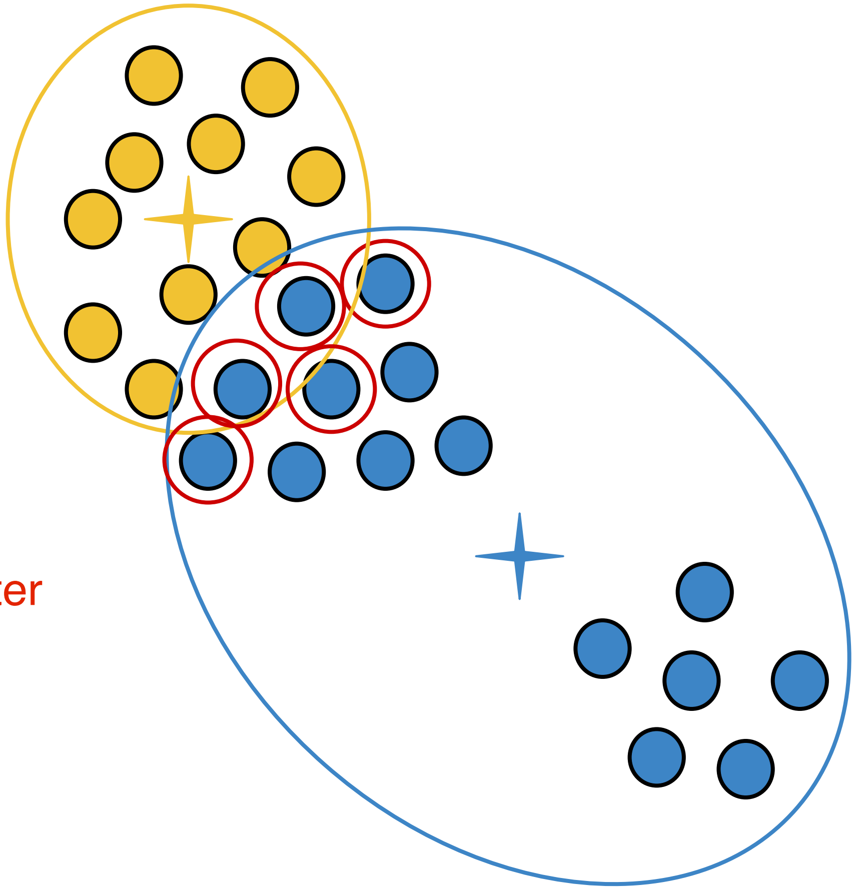
Find **k** centers $\{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k\}$ that minimize the **cost function**:

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

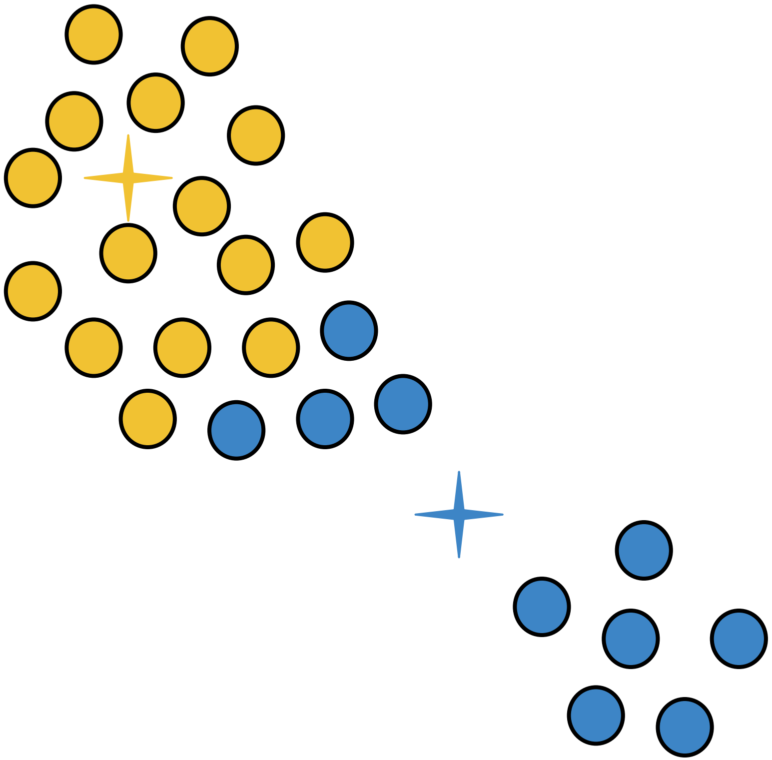
When **k=1** and **k=n** this is easy. Why? The optimal cost func. is 0. Occurs when k=n

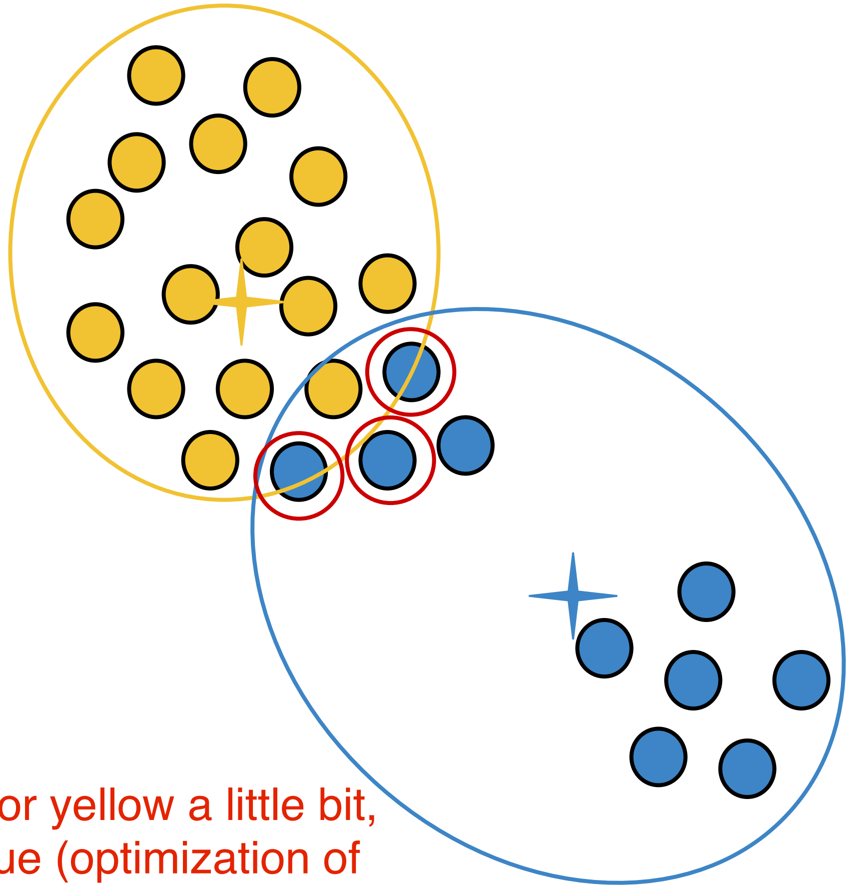
When $\mathbf{x}_i$ lives in more than 2 dimensions, this is a very difficult (**NP-hard**) problem



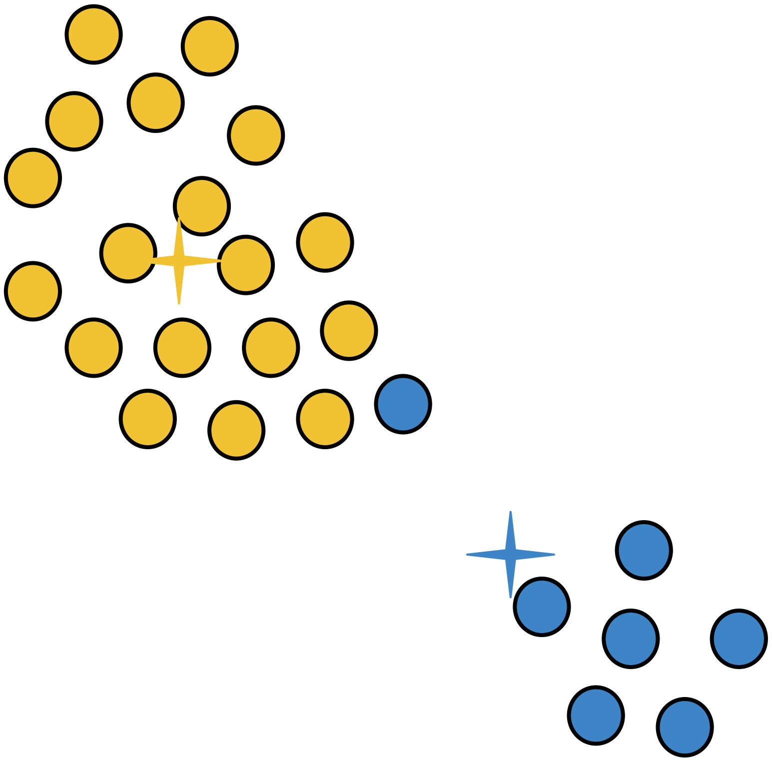


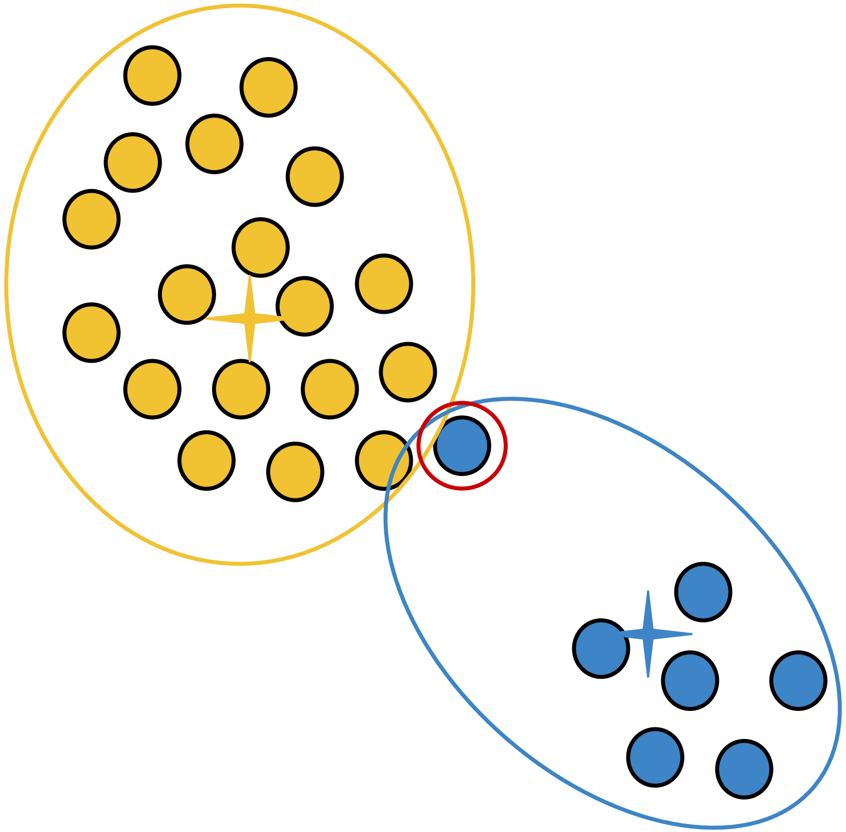
points in red are closer to
yellow mean (the center)
compared to the blue center



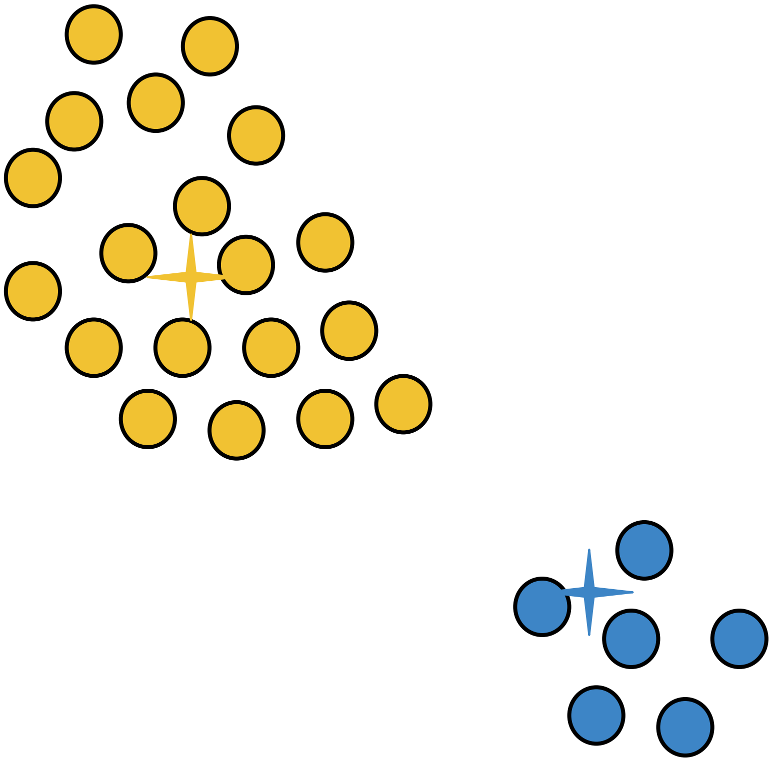


increasing the sum of squares for yellow a little bit, but drastically decreasing for blue (optimization of cost function)





optimized clusters
for cost function

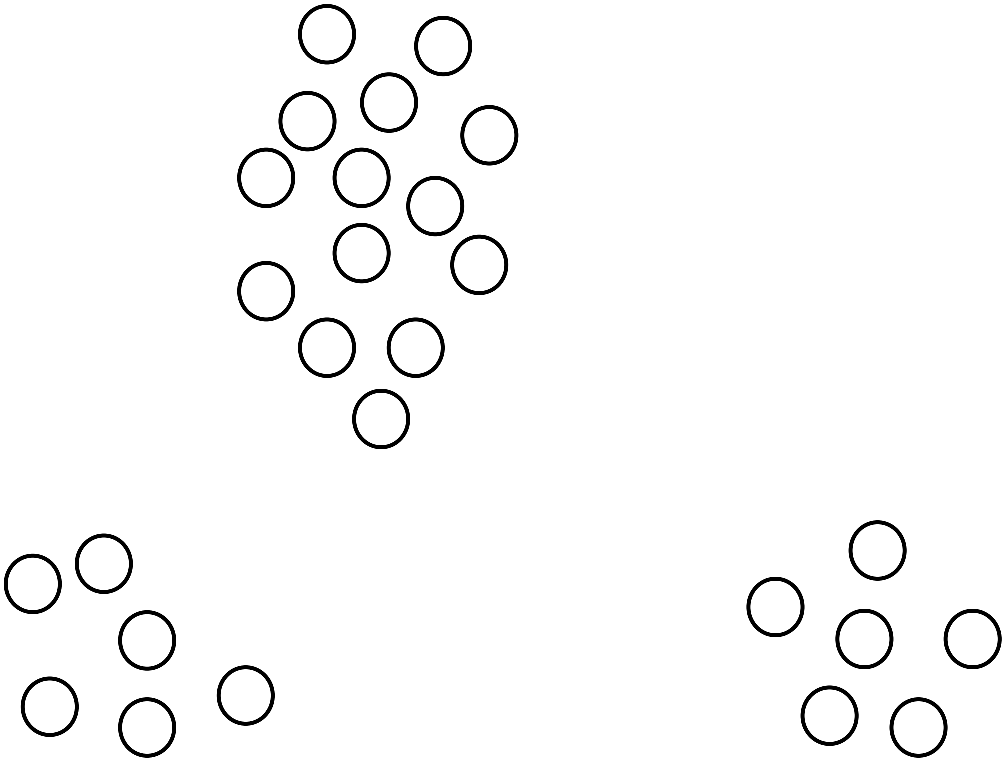


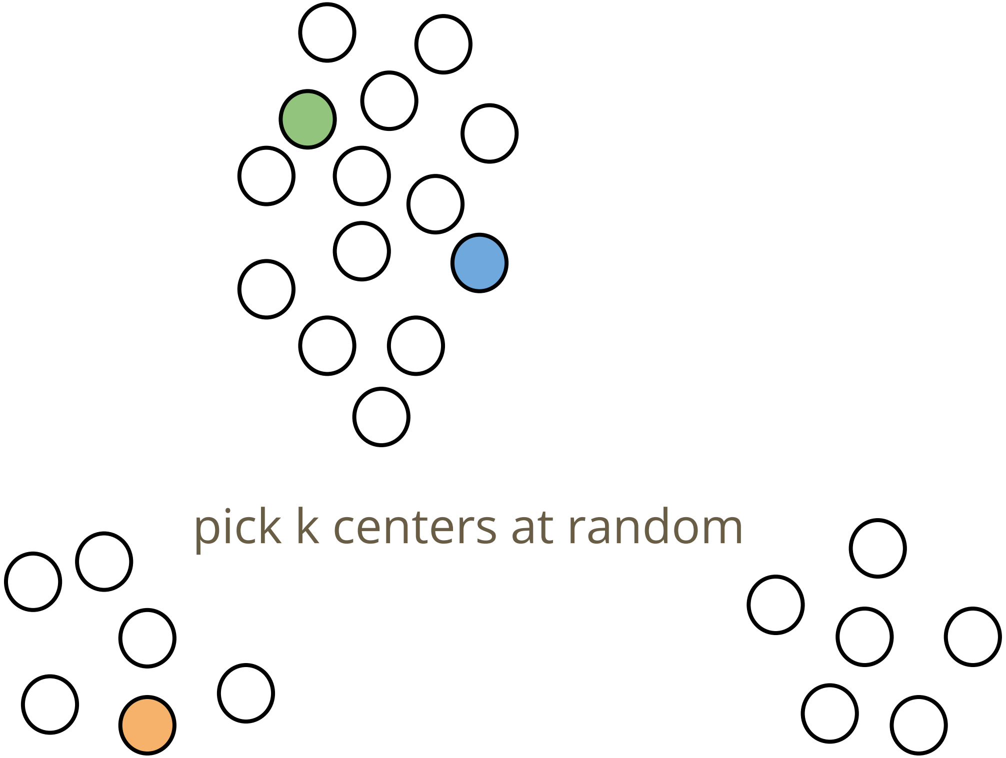
K-means - Lloyd's Algorithm

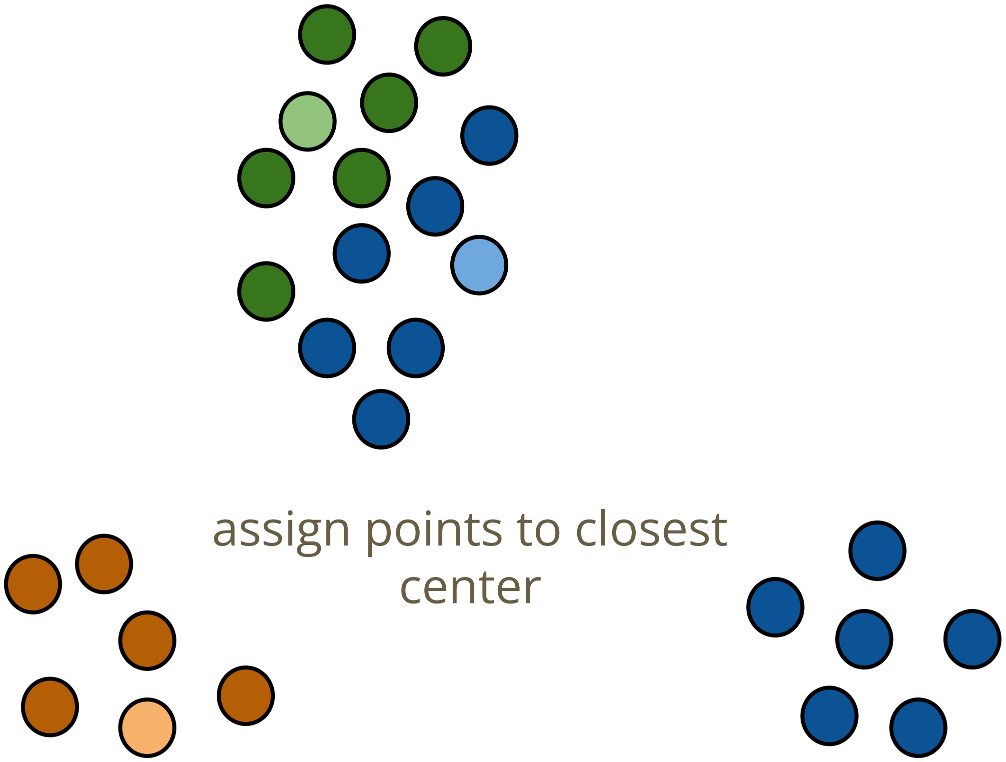
1. Randomly pick **k** centers **{$\mu_1, \ldots, \mu_k$}**
2. Assign each point in the dataset to its closest center
3. Compute the new centers as the means of each cluster
4. Repeat 2 & 3 until convergence

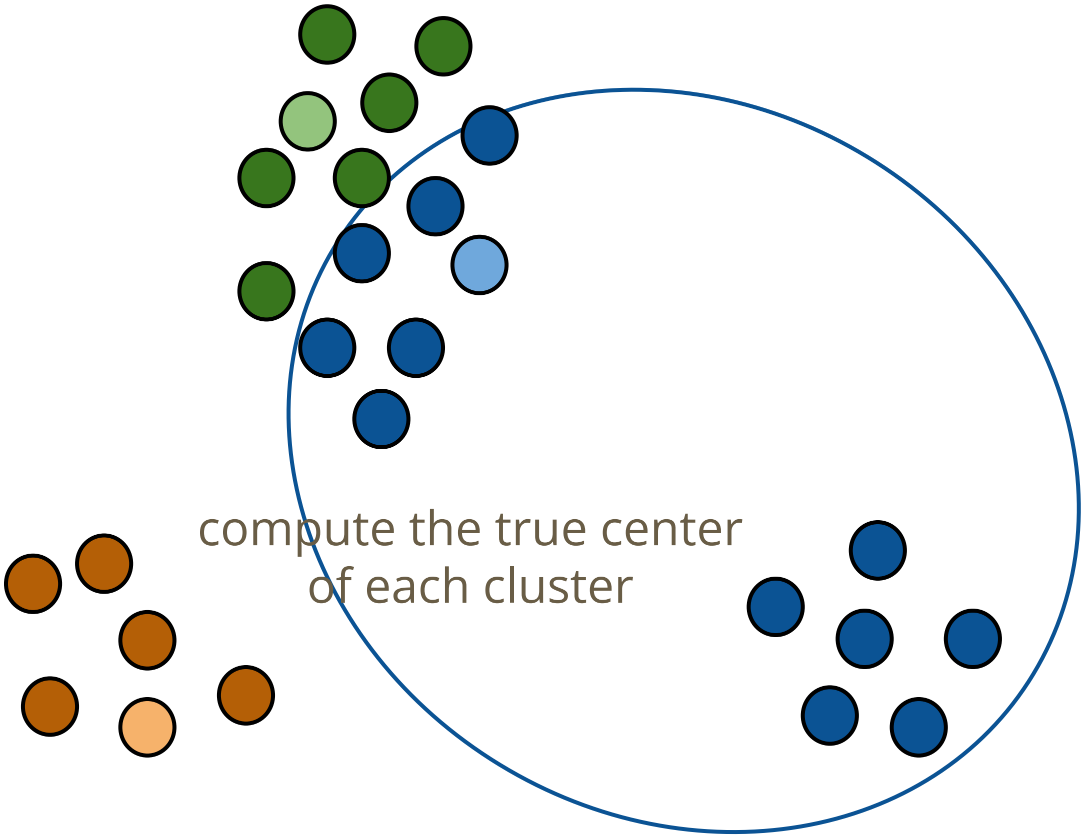
pick points closest to
center to create cluster

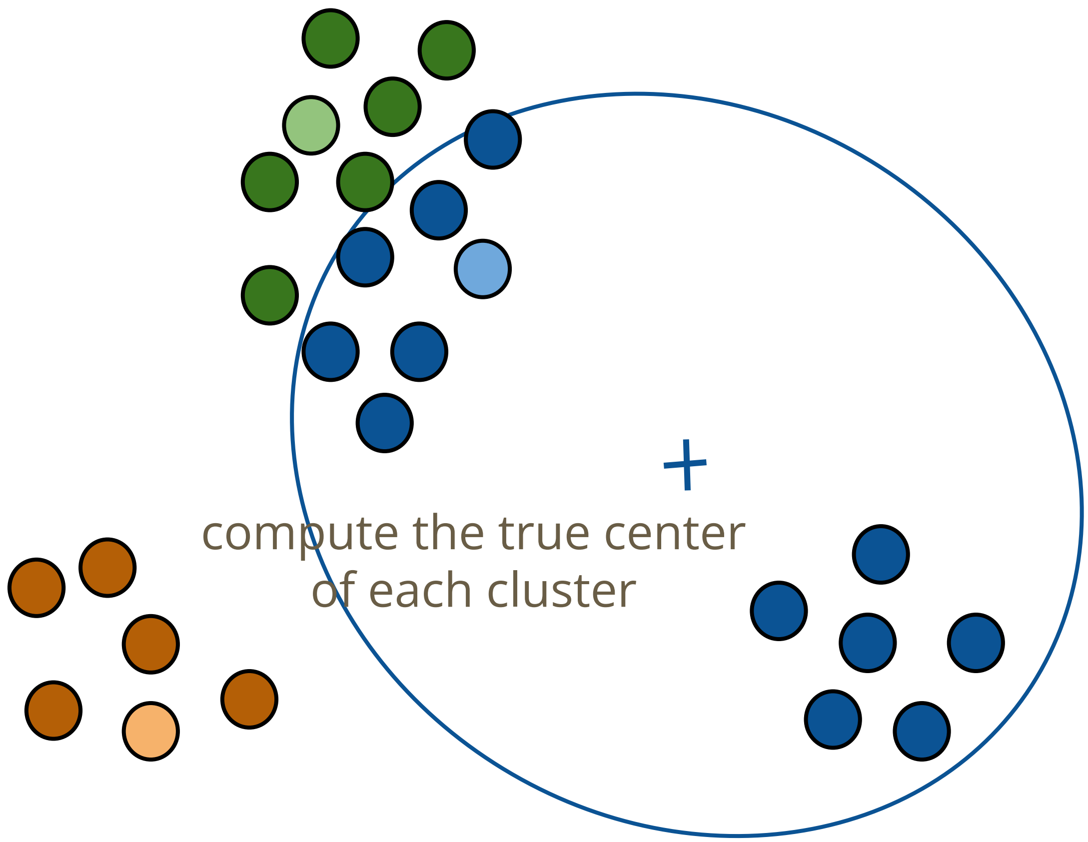
adjust centers by calculating mean
and recalculating for new centers




pick k centers at random


assign points to closest center


compute the true center
of each cluster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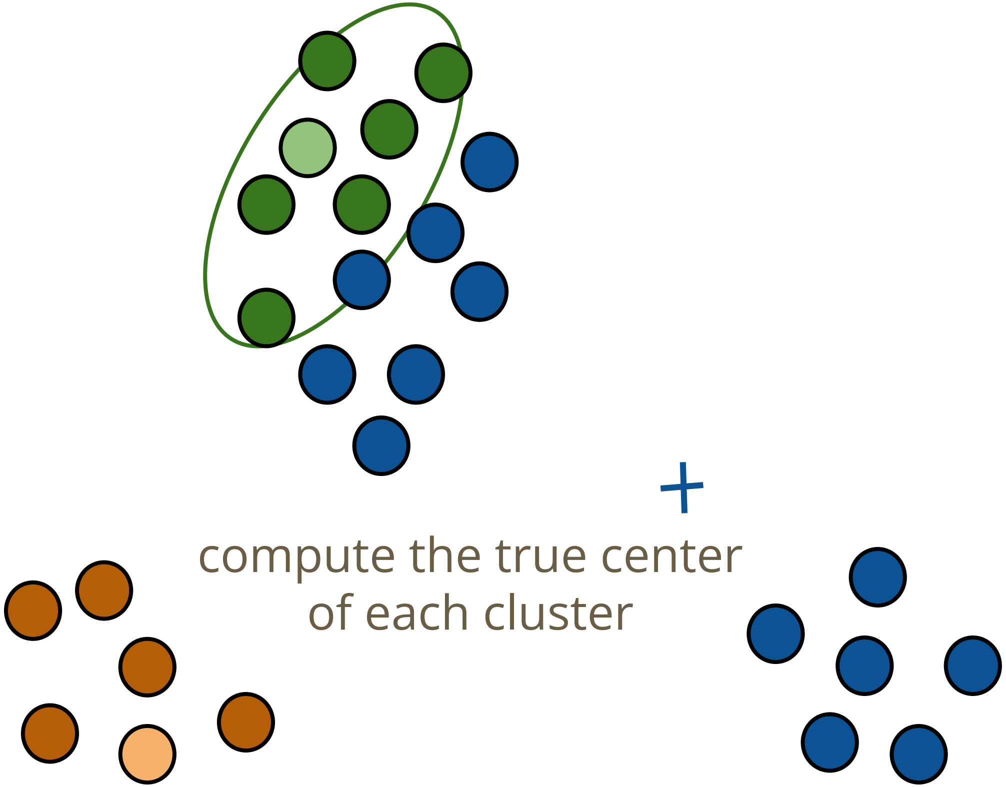
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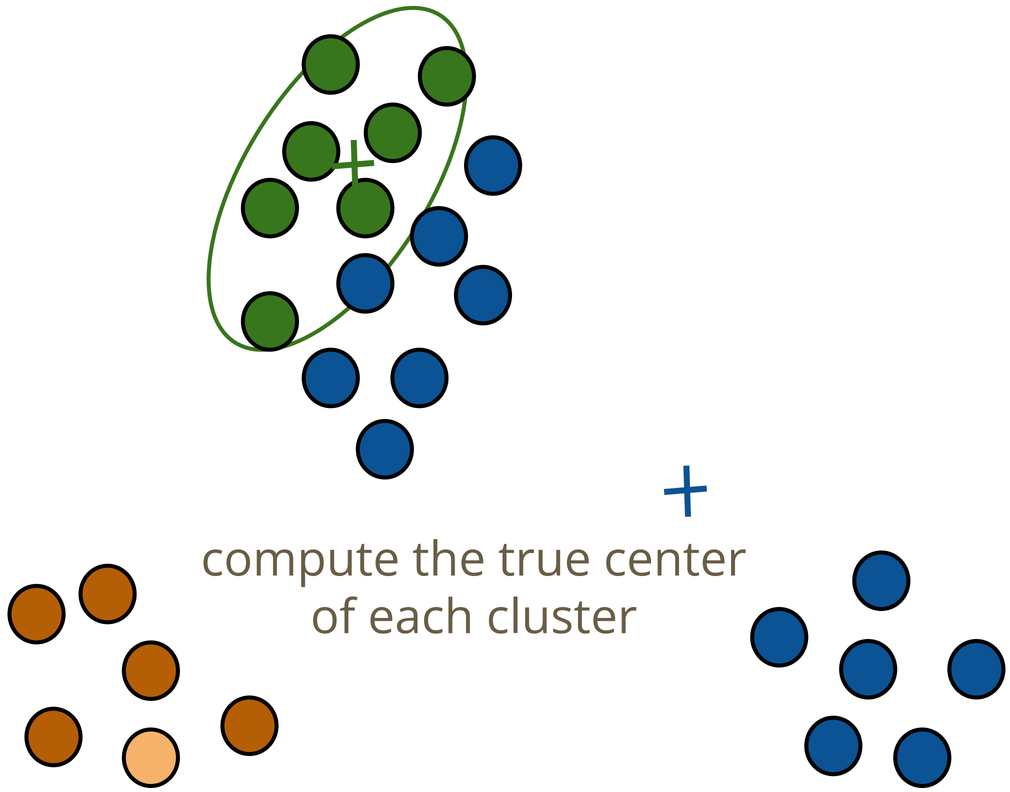
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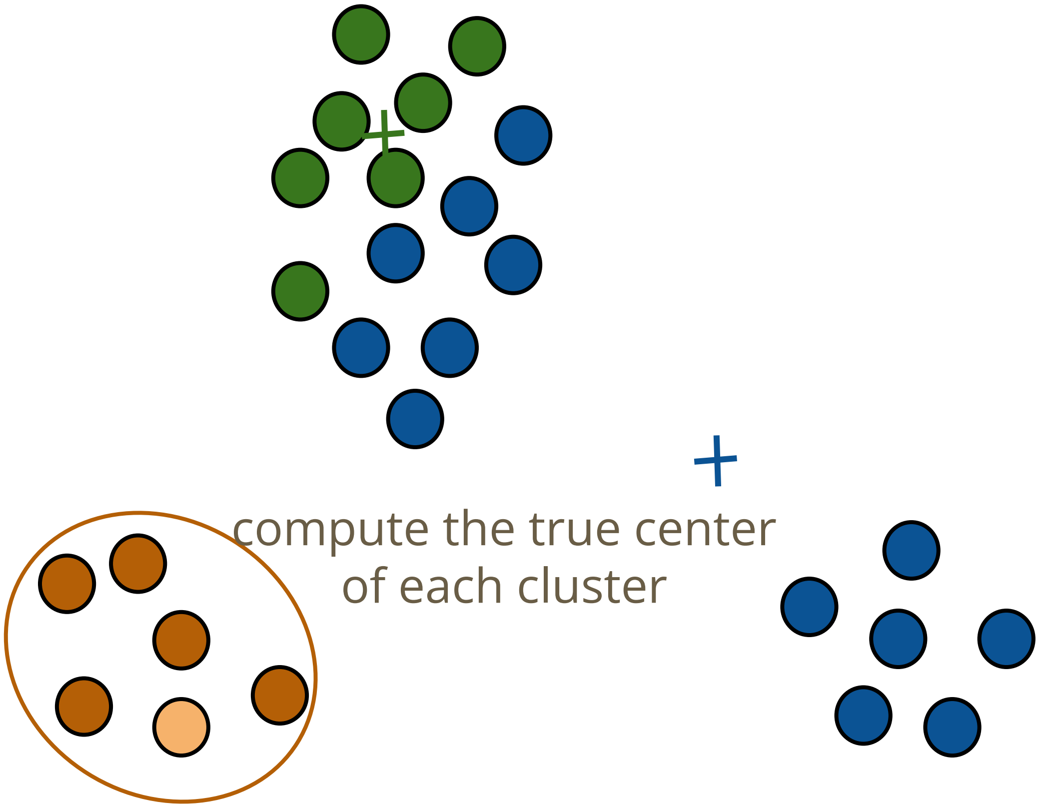
compute the true center
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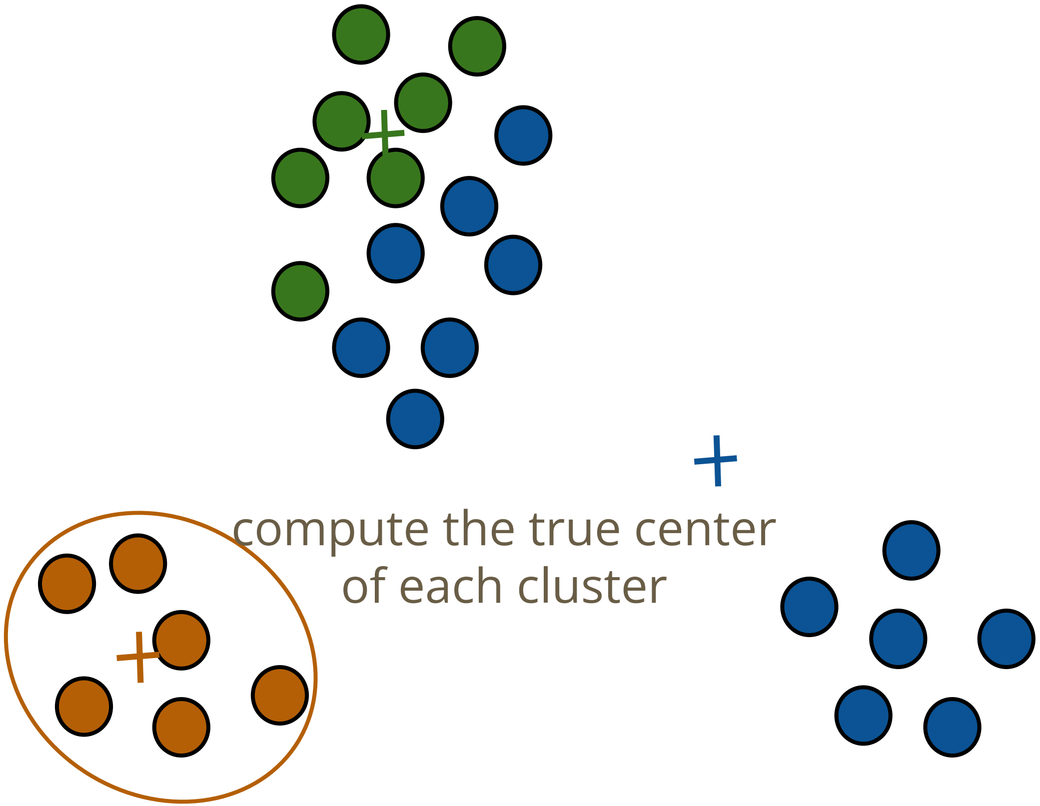
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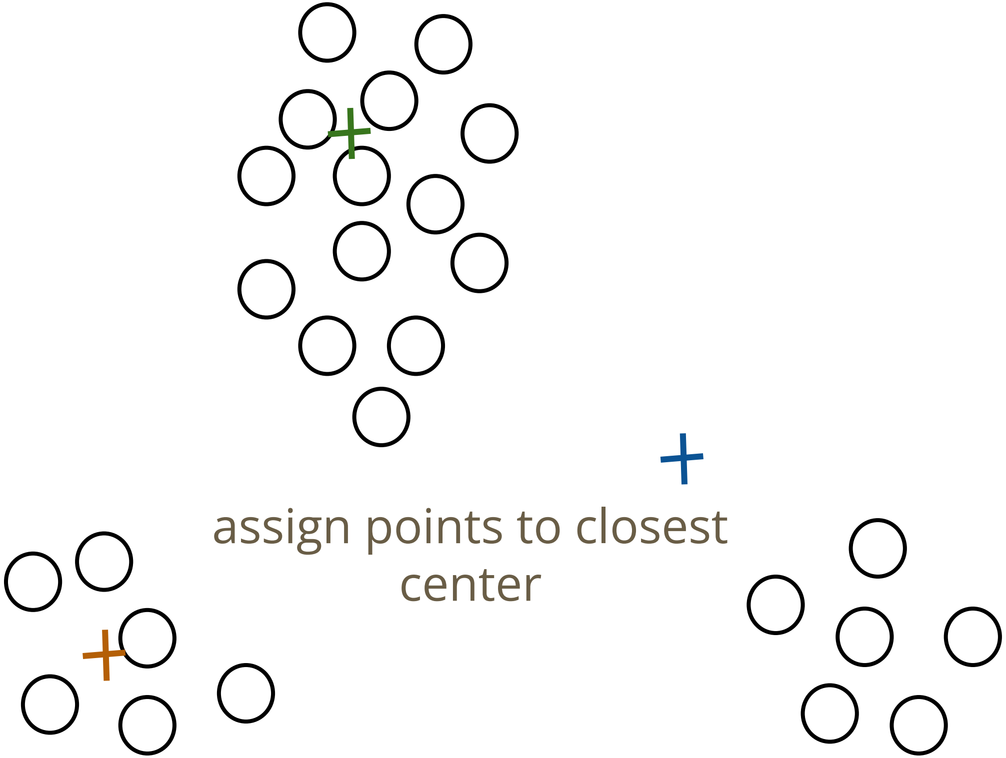
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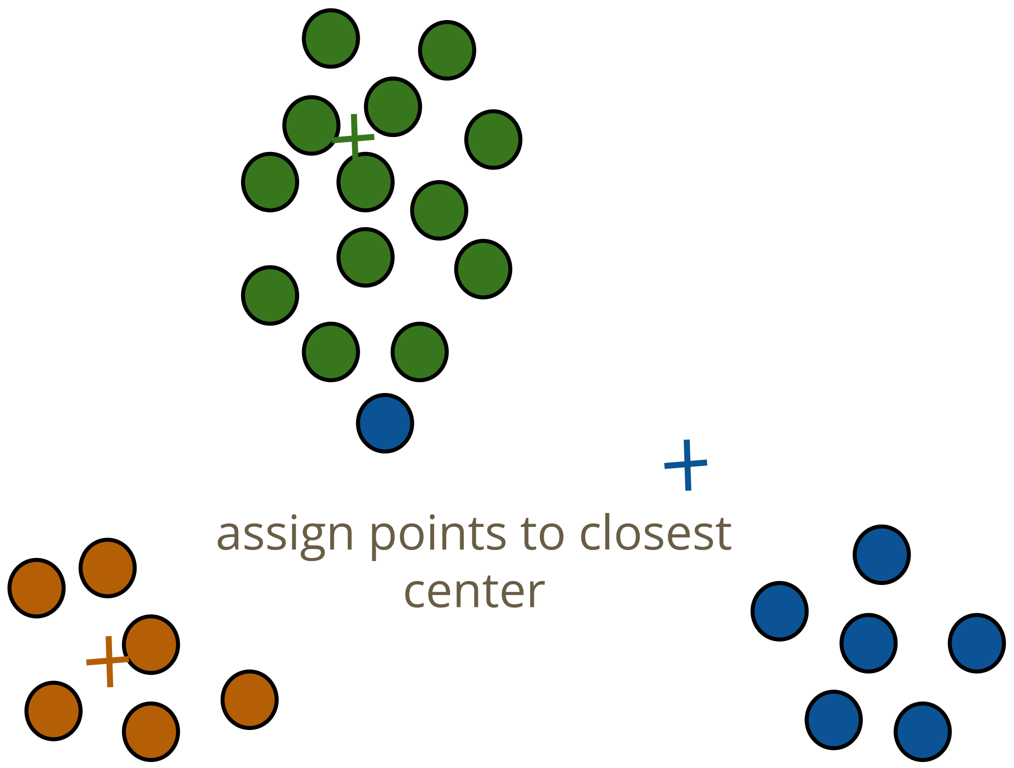
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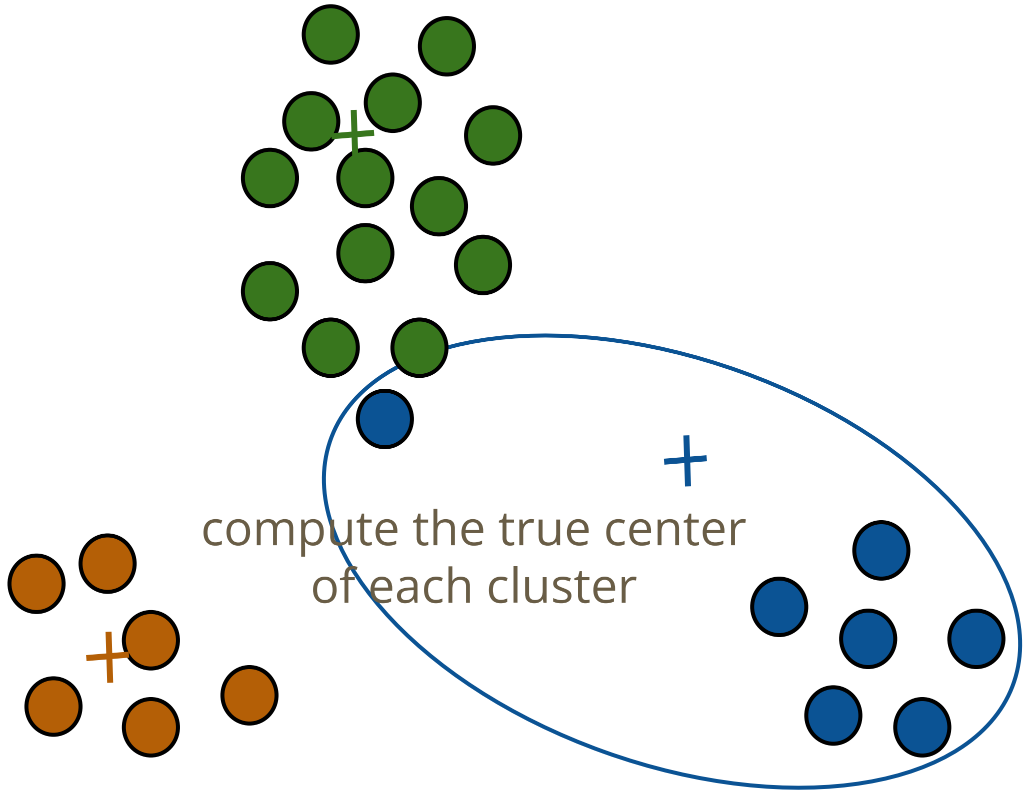
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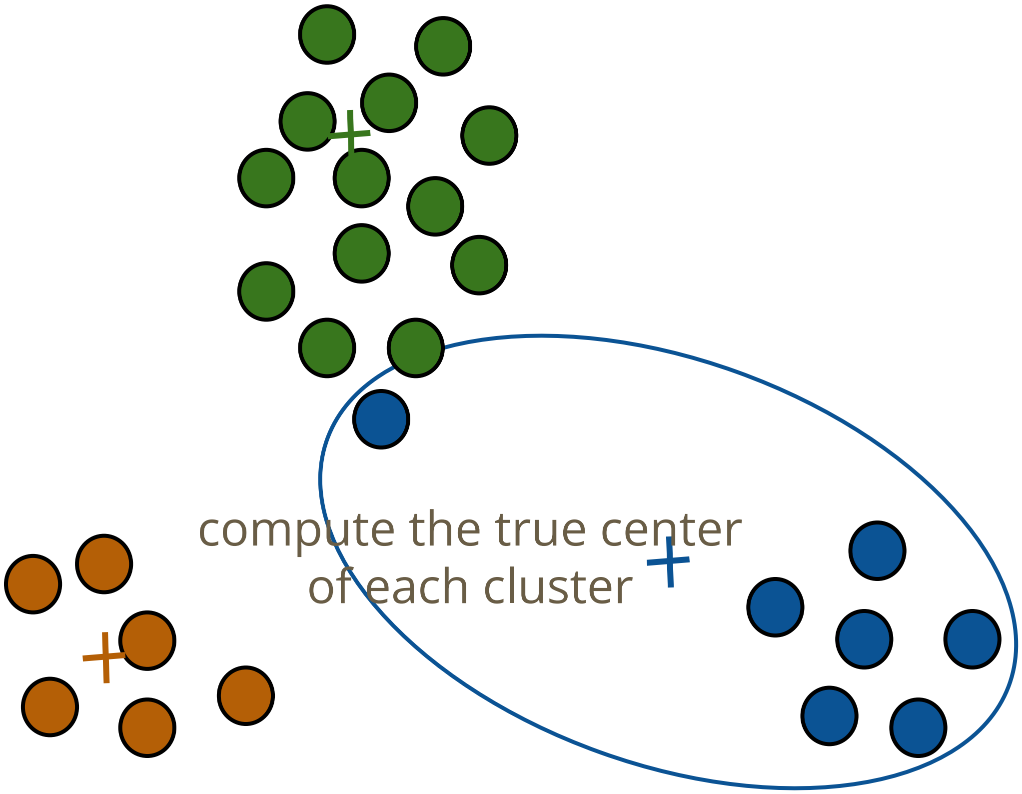
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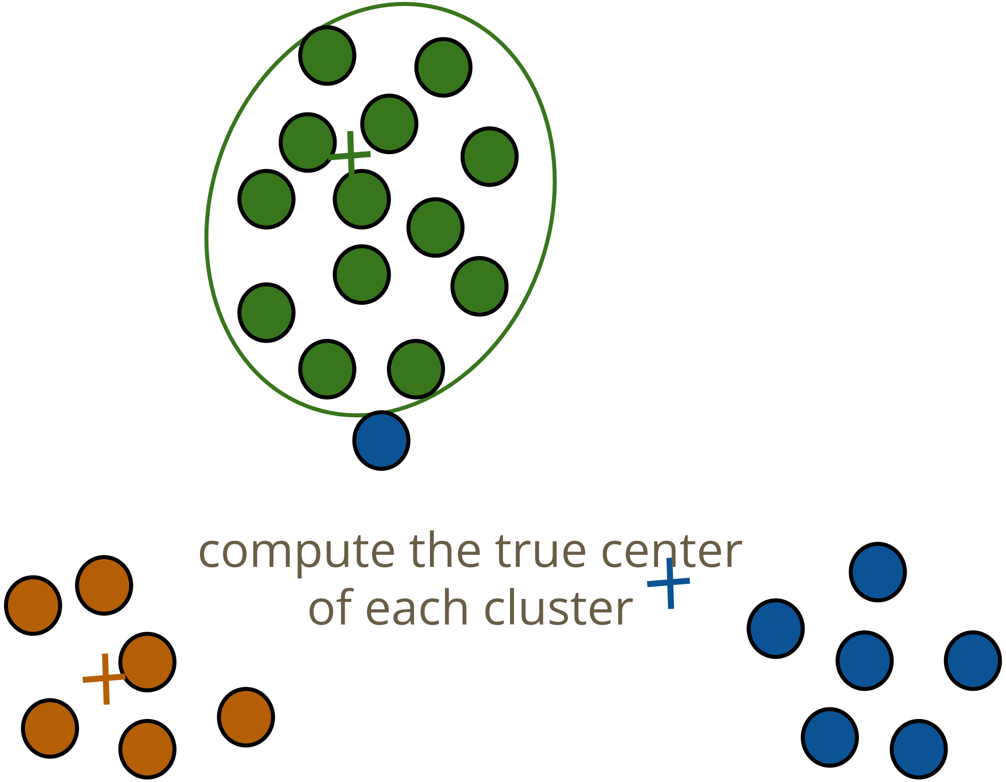
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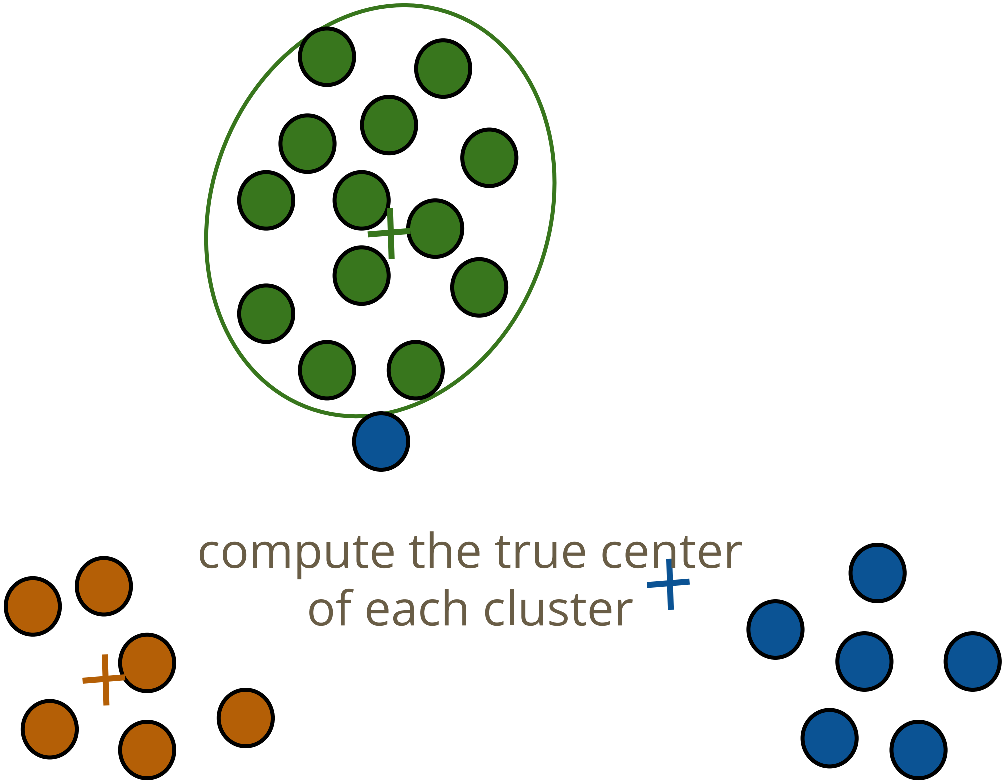
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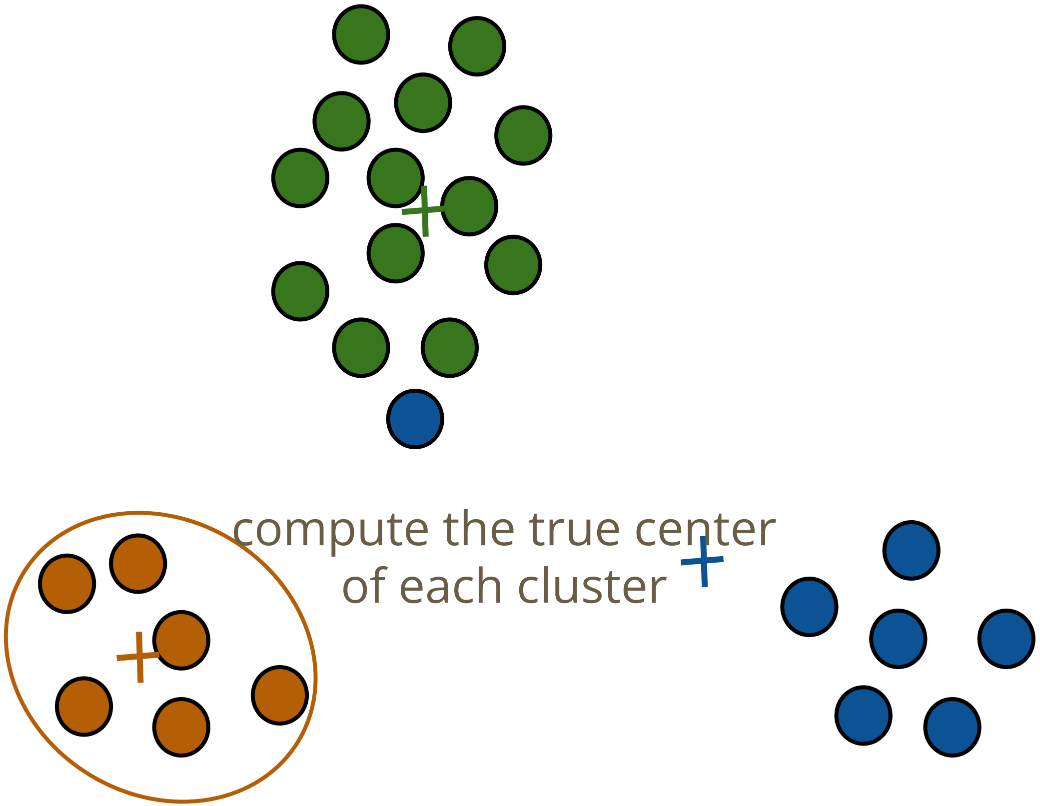
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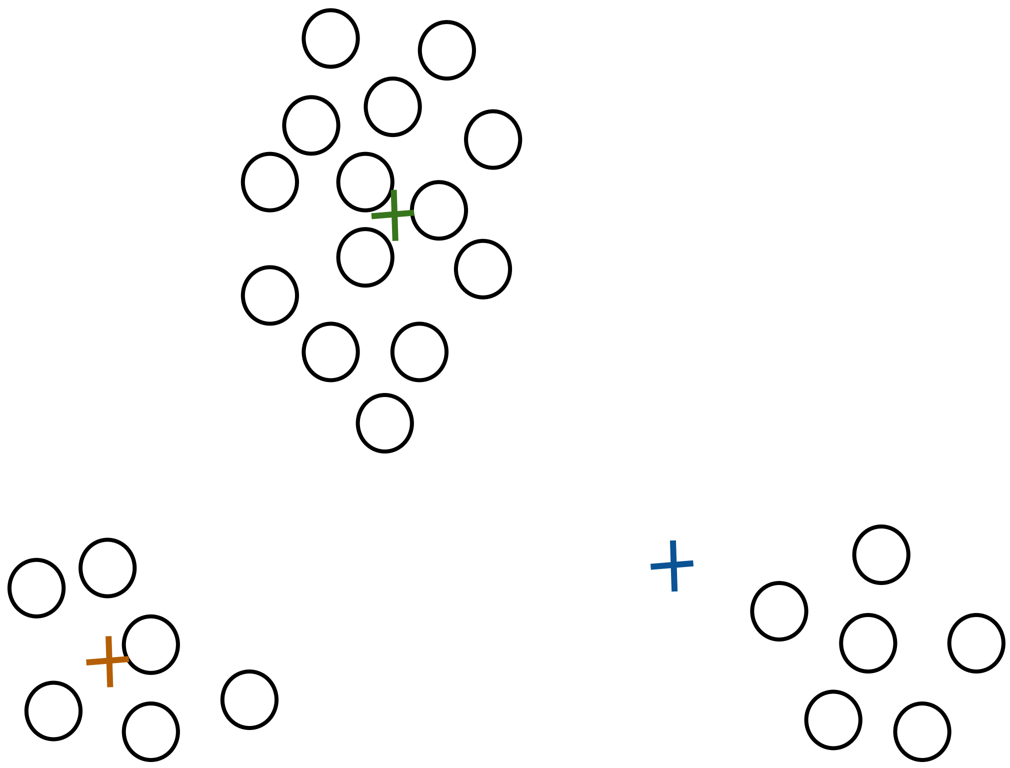
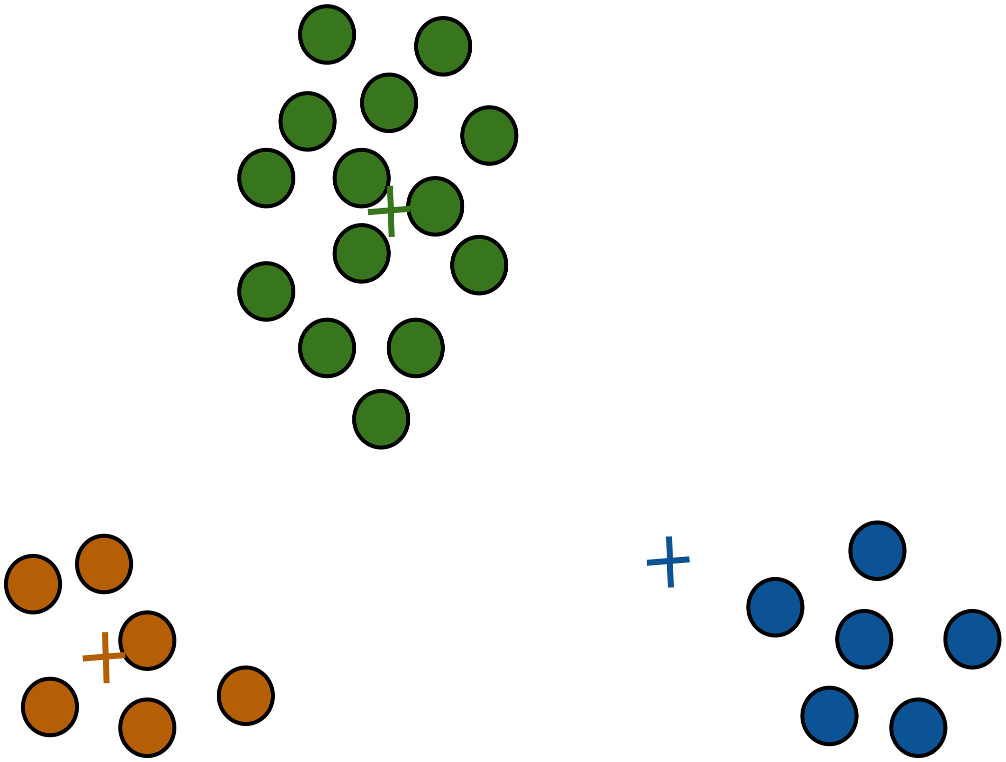
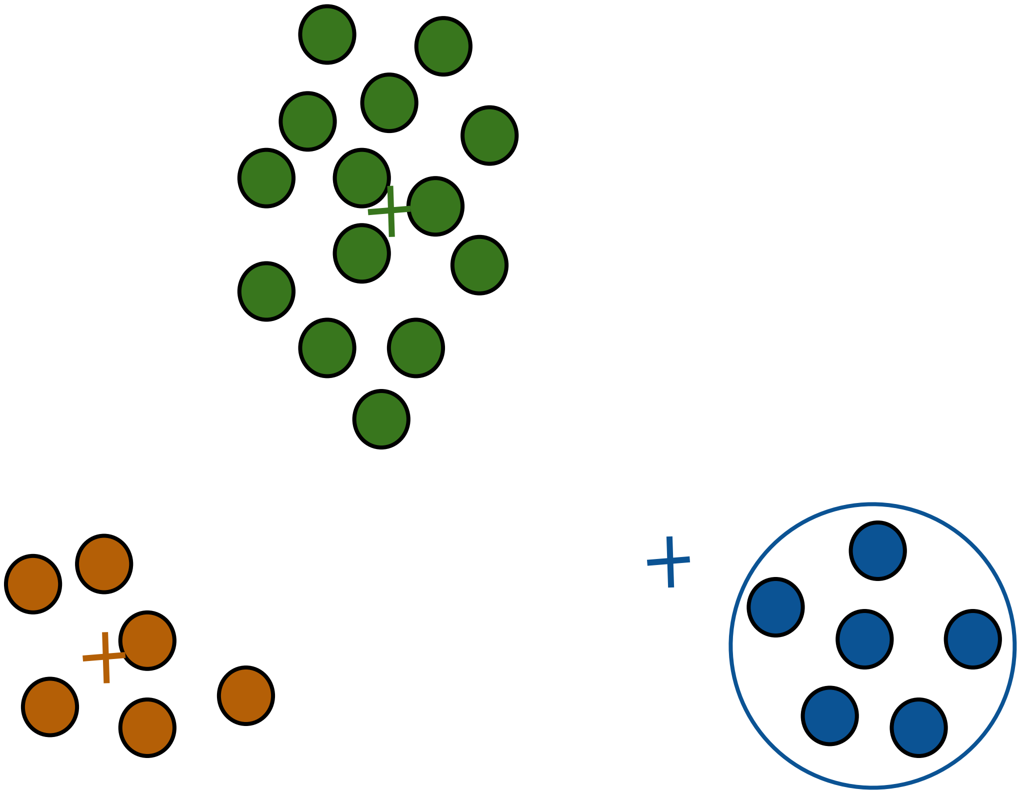
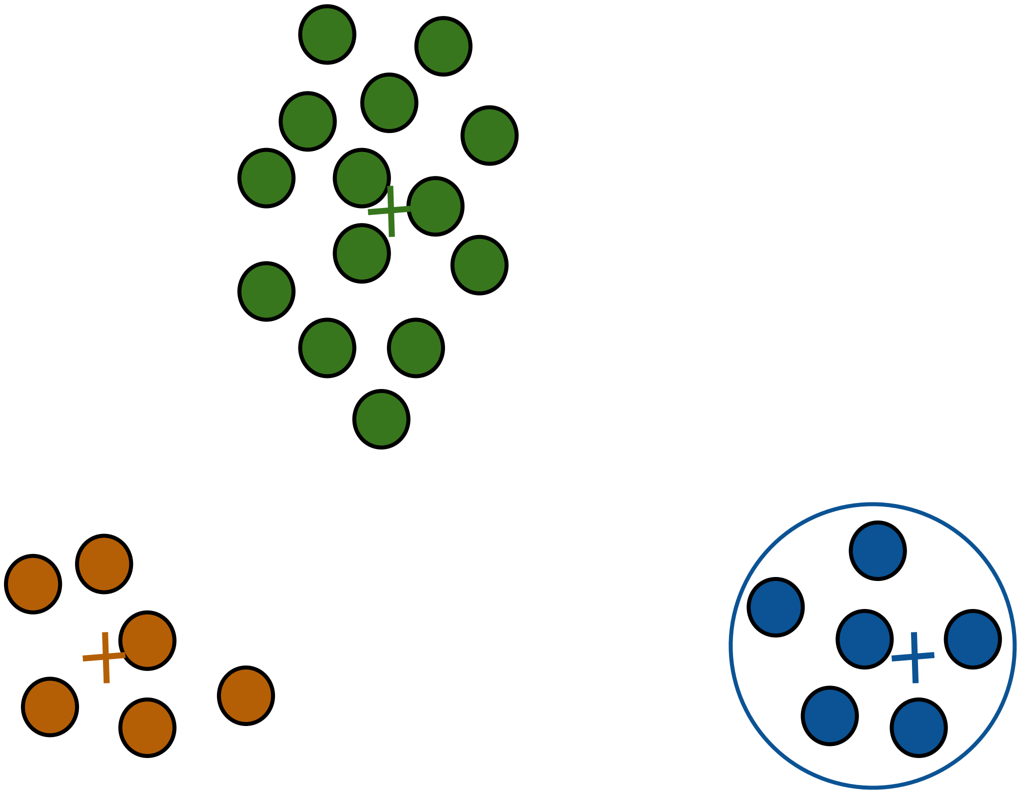
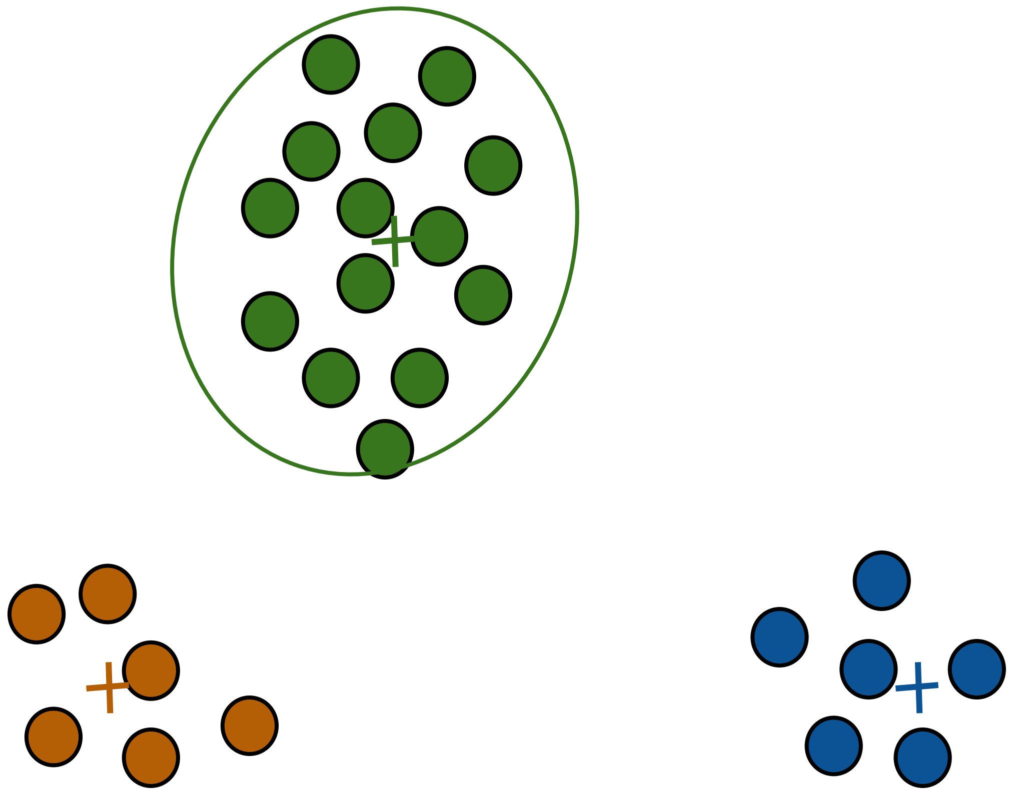
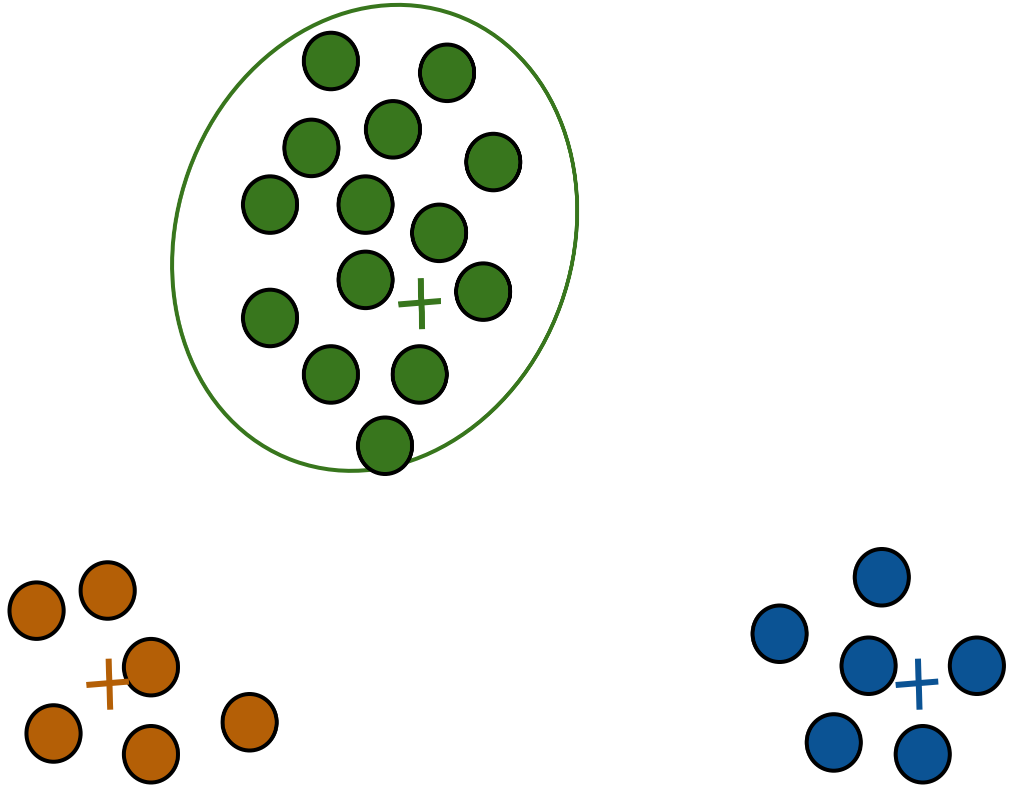


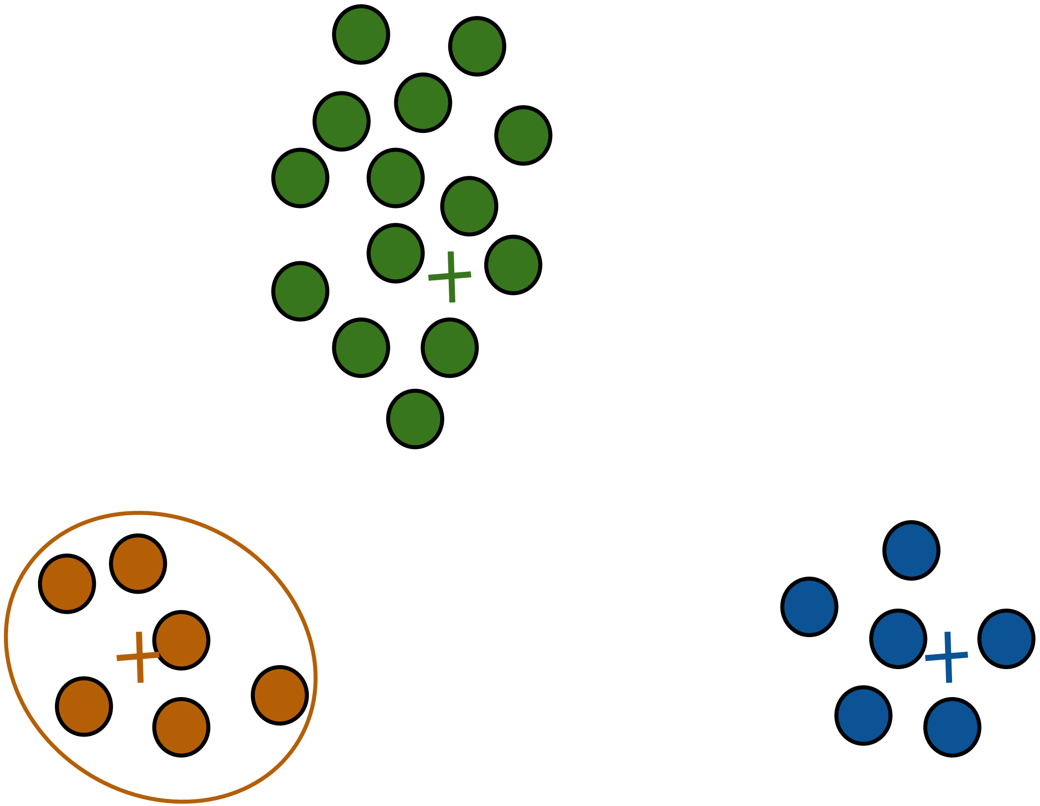


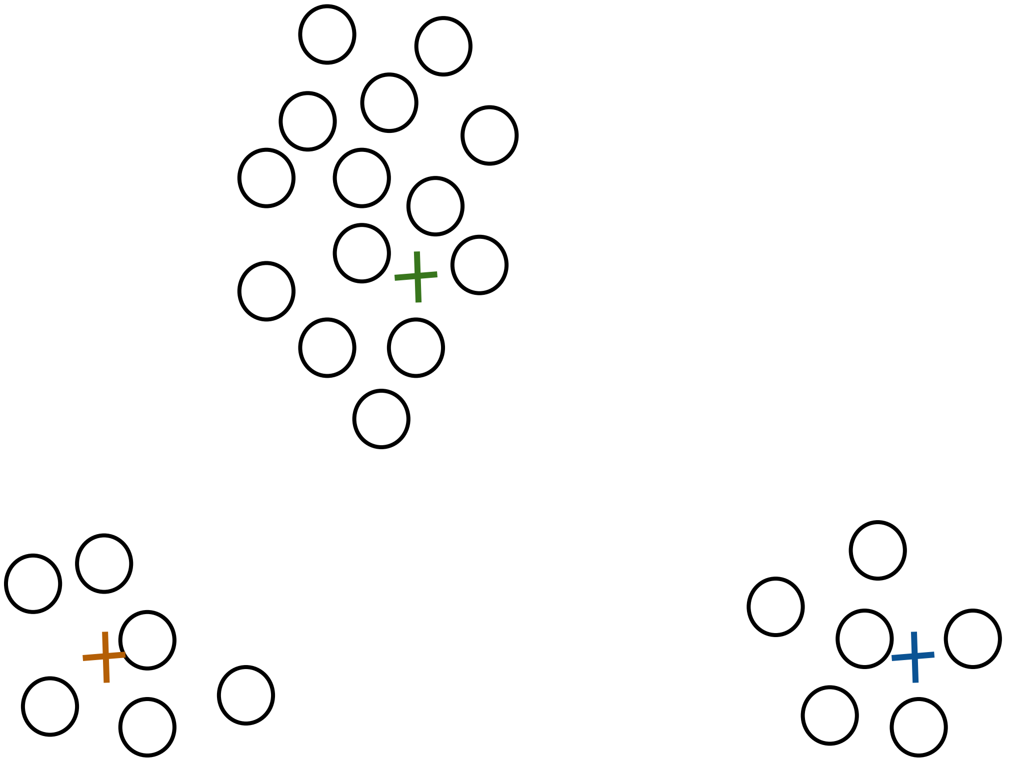


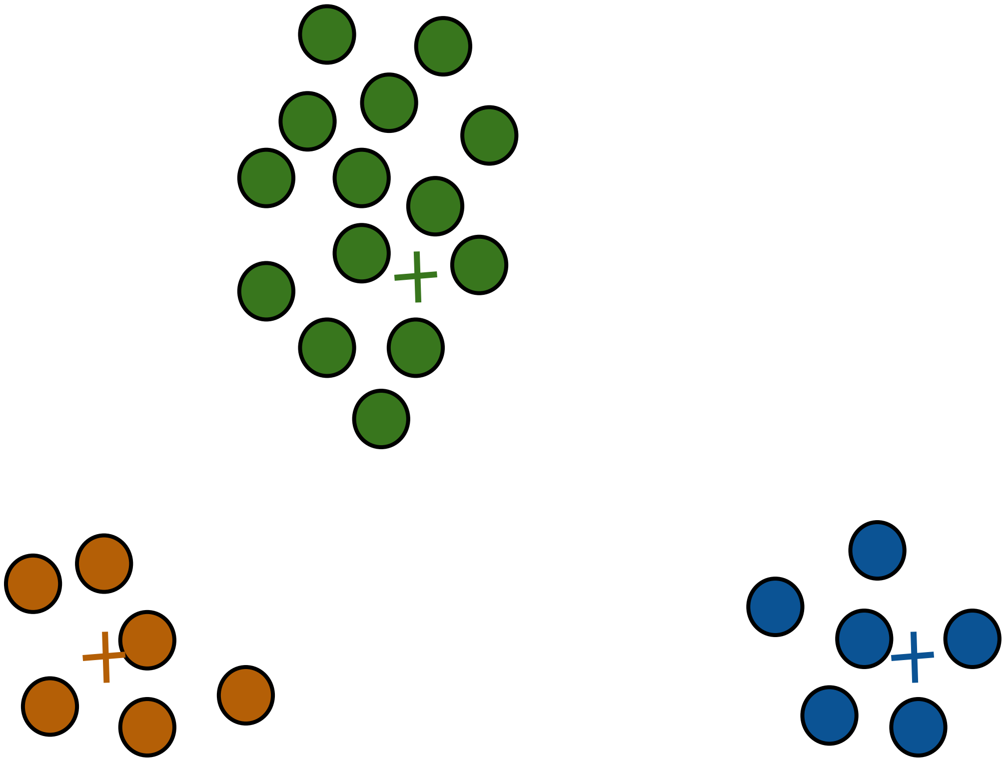


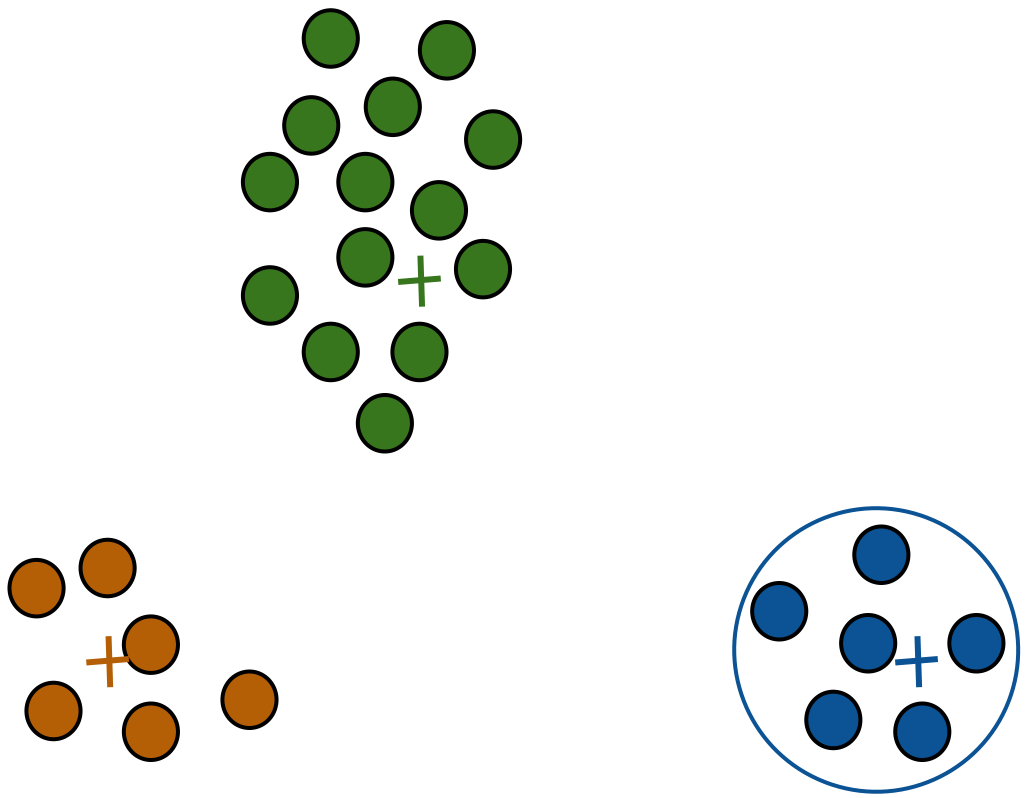


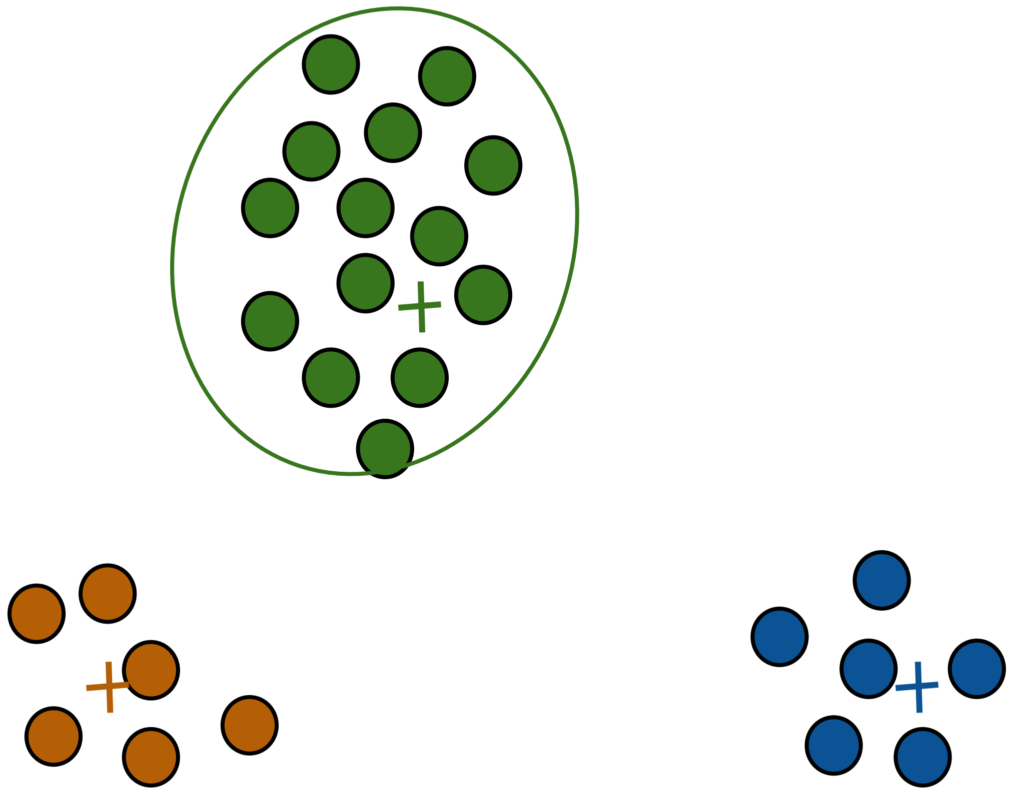


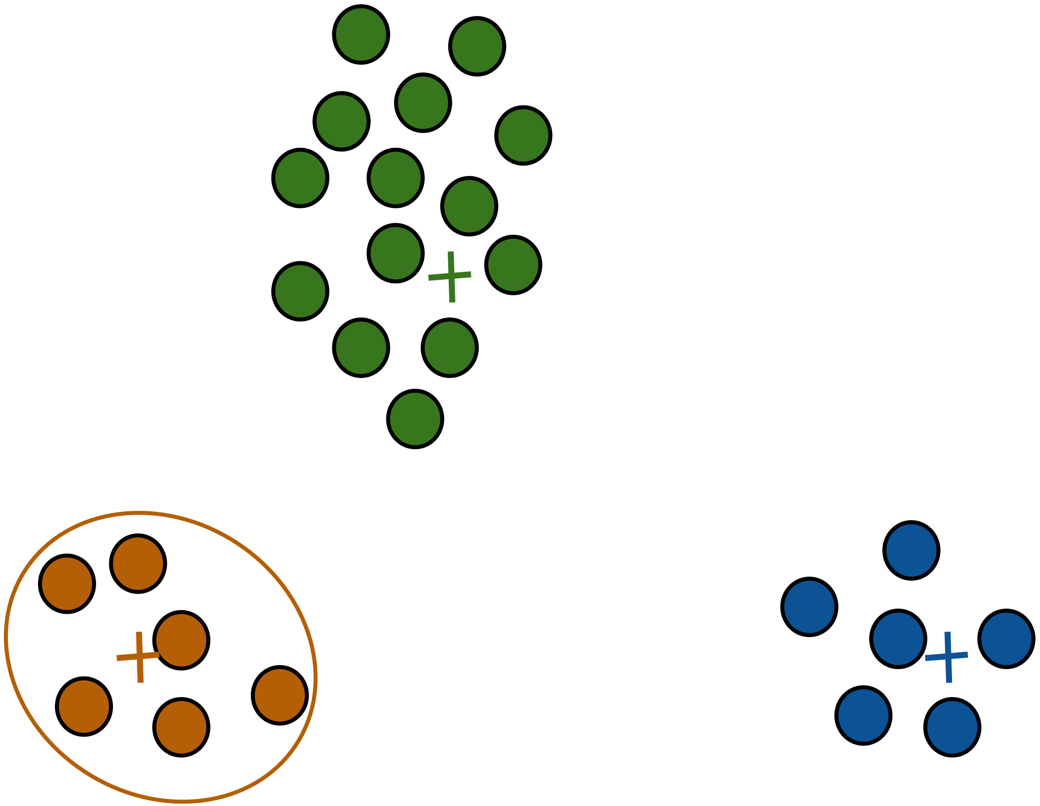


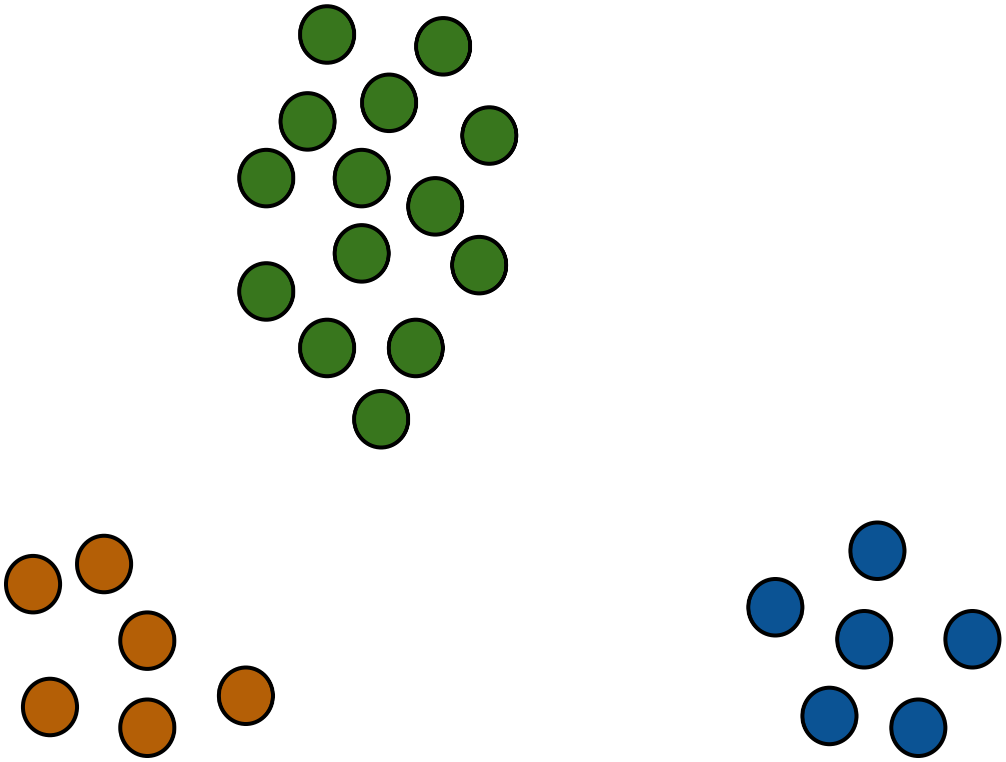




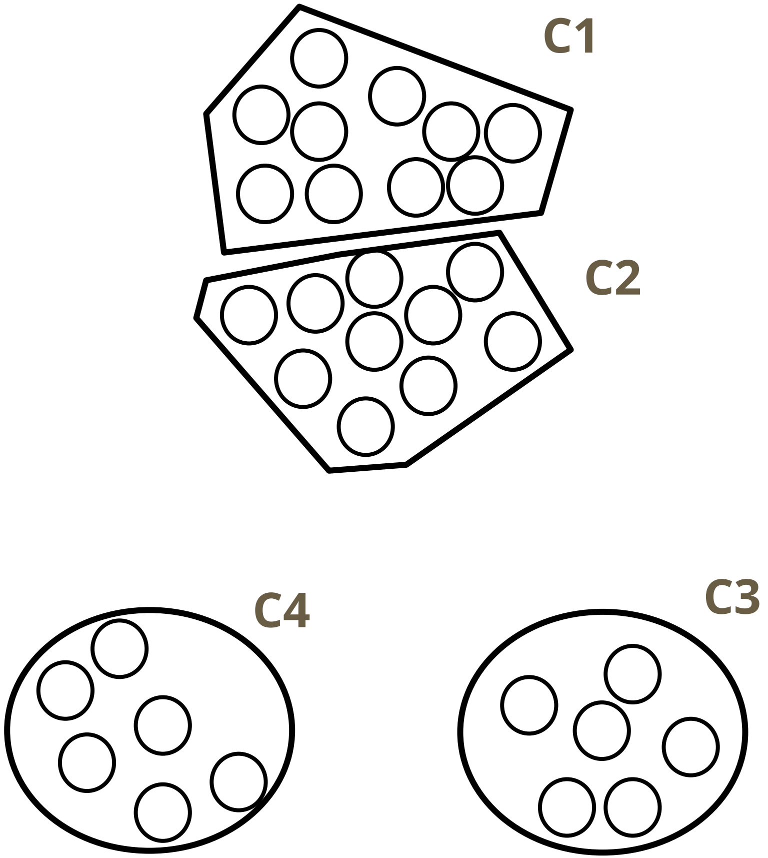


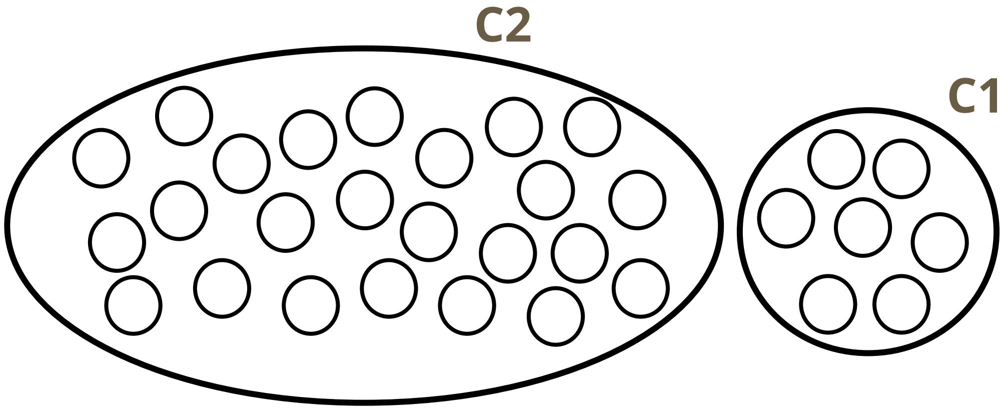


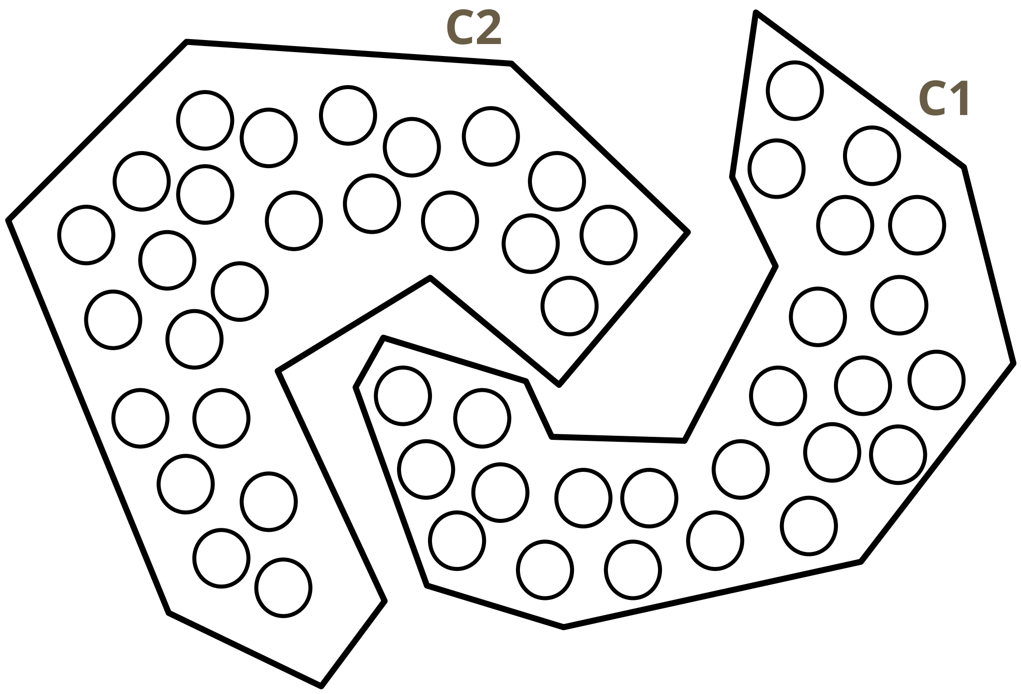




Questions


C1
C2
C4
C3


C2
C1


C2
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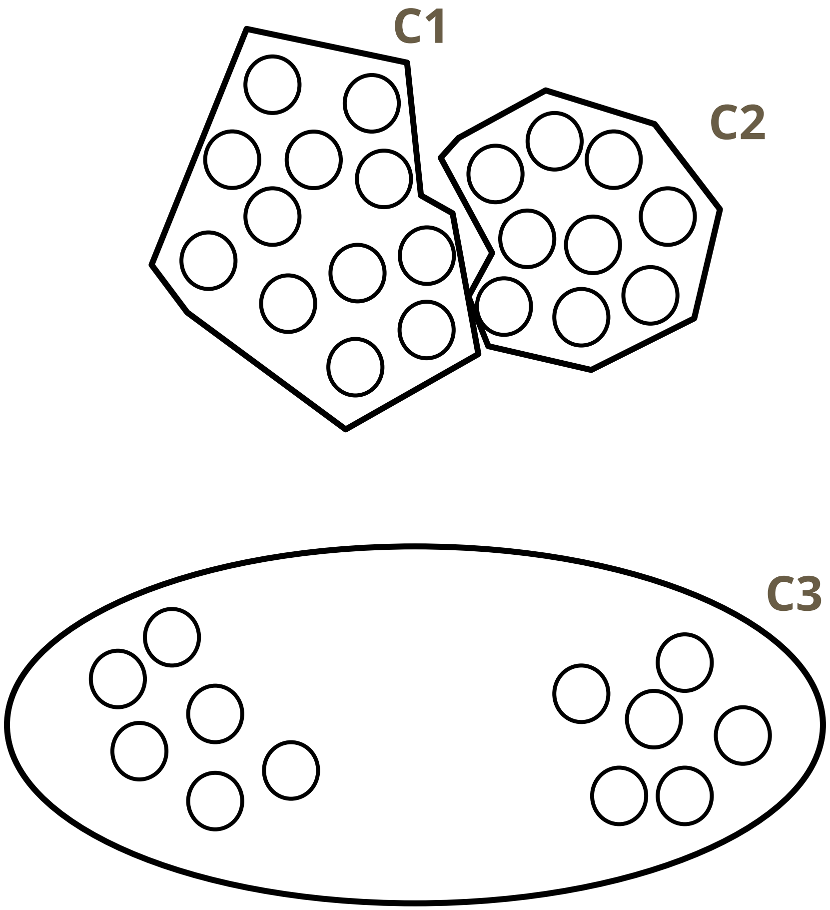
C1
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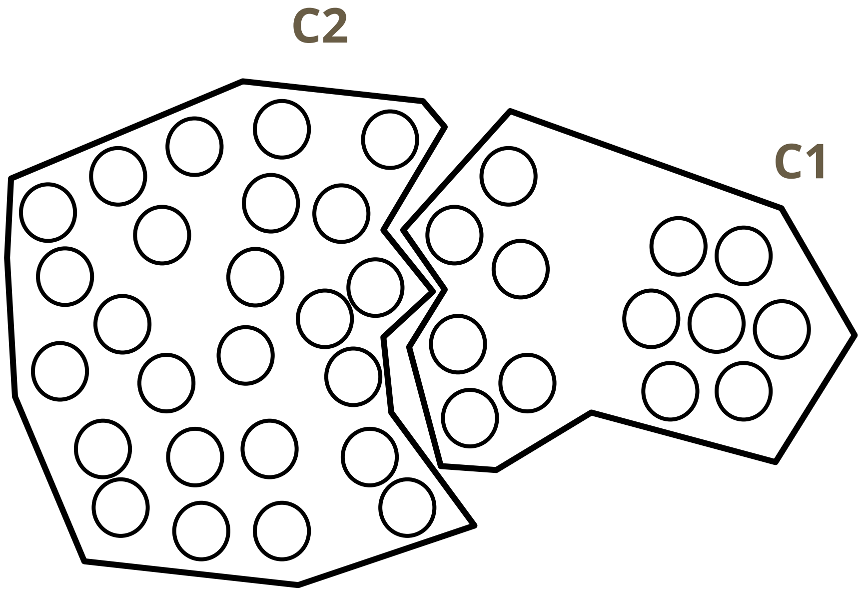
C3


C2
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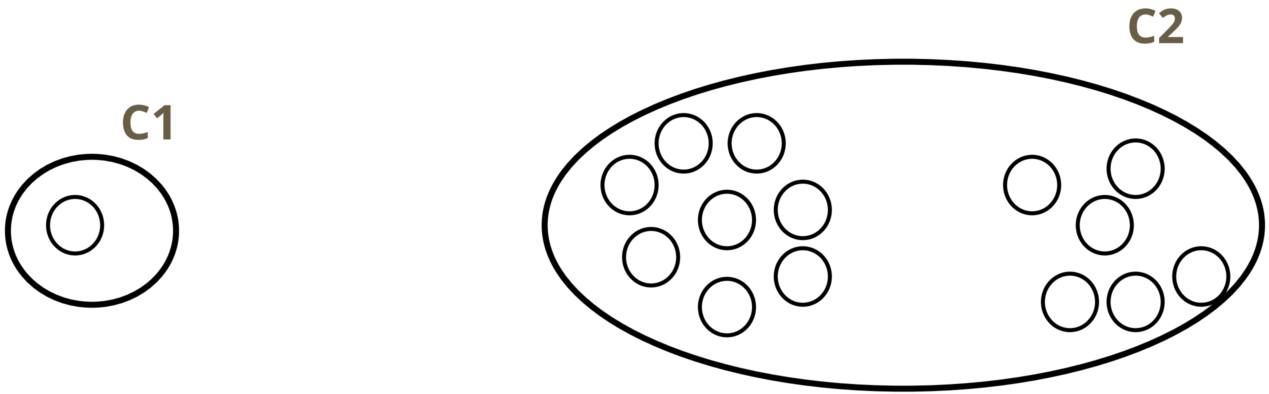
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