Kmeans++

Boston University CS 506 - Lance Galletti

K-means - Lloyd's Algorithm

Q1: 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

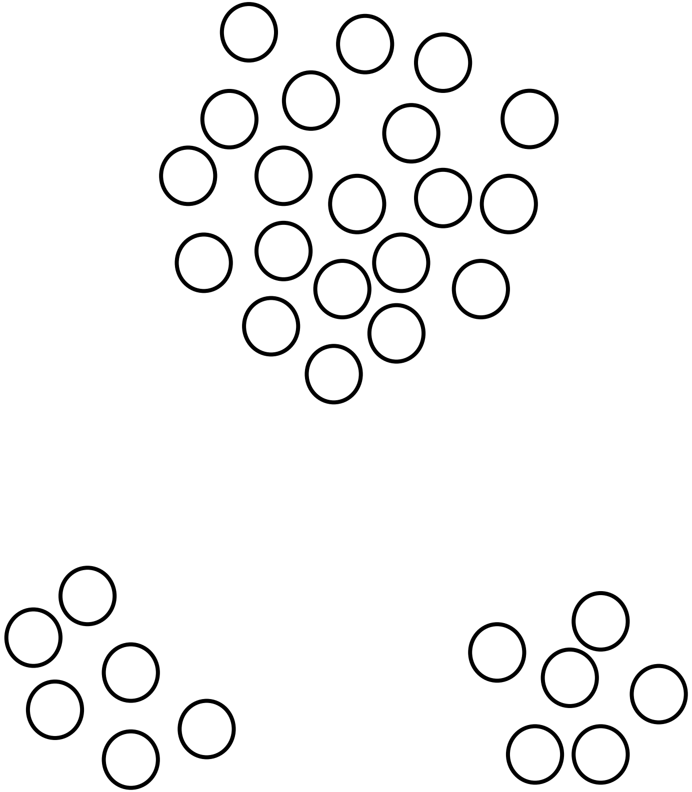
Conclusion: Lloyd's Algorithm always converges!

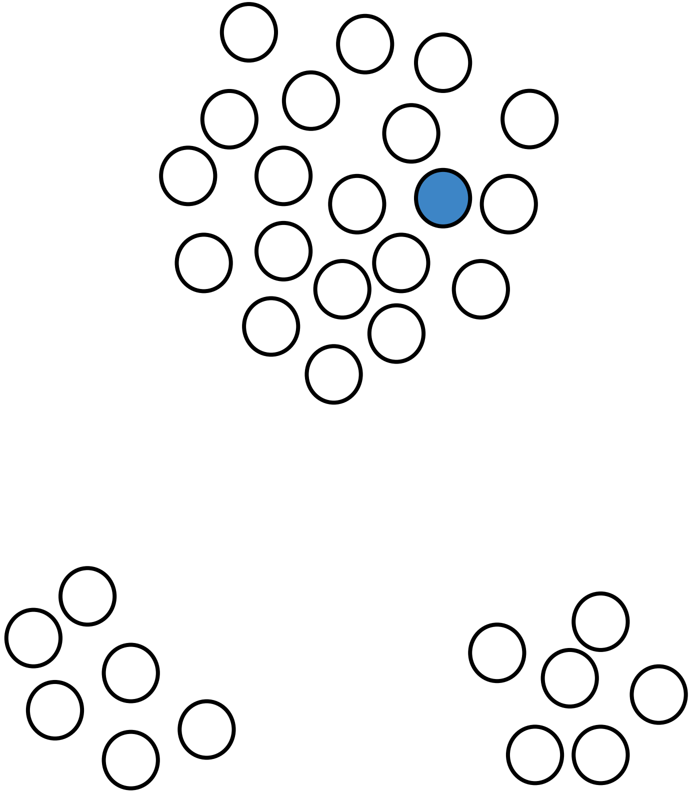
K-means - Lloyd's Algorithm

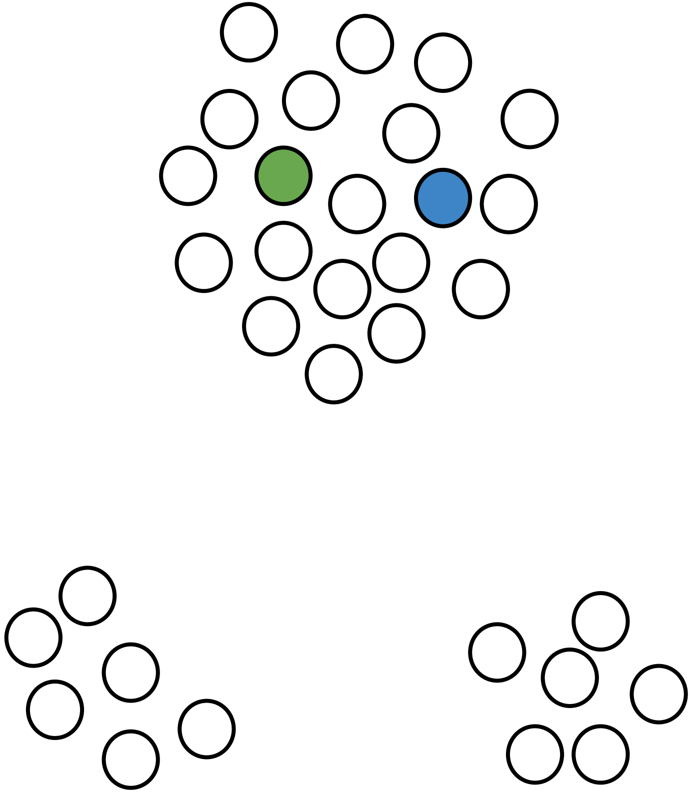
Q2: Will this always converge to the optimal solution?

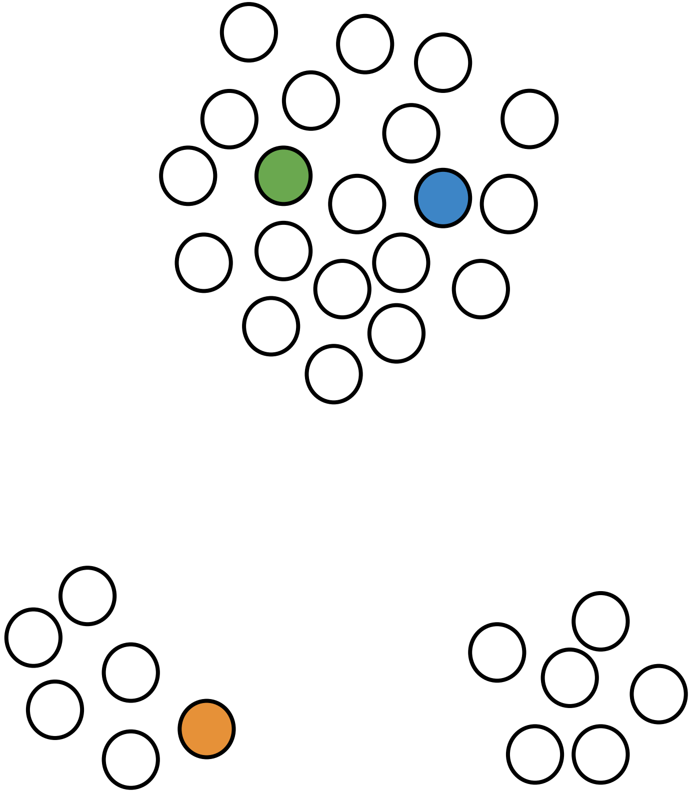
NO

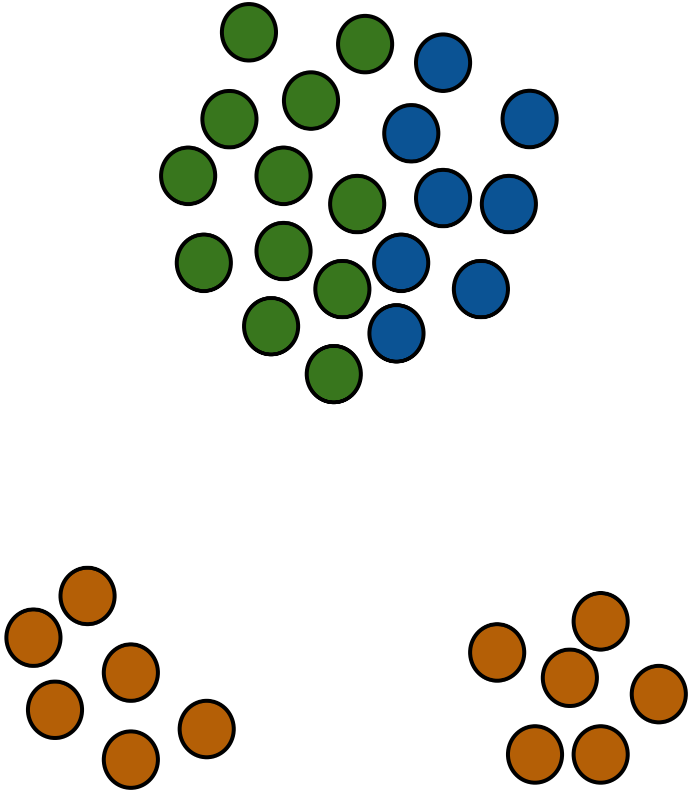
If the centers are too closed together, they would split up a naturally occuring cluster into 2 unnatural clusters



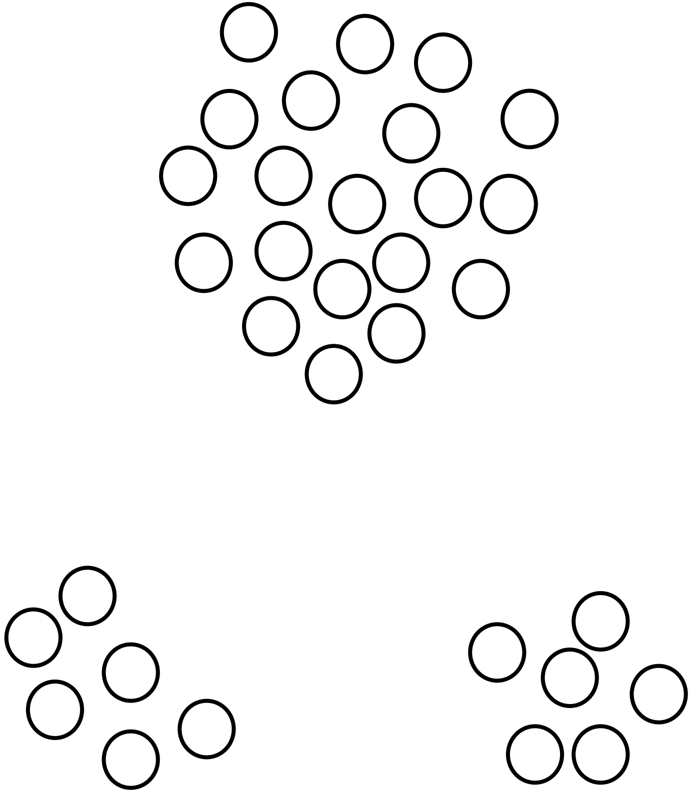


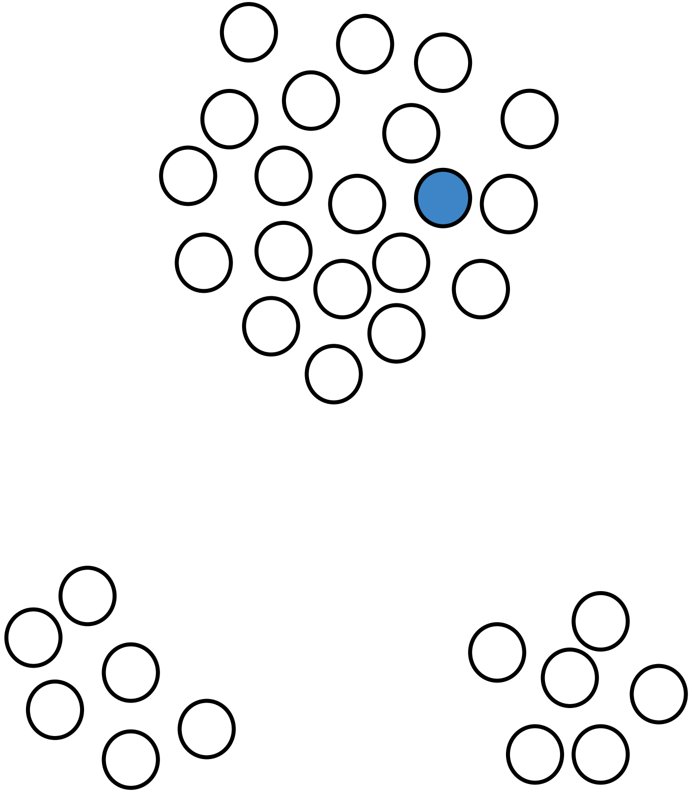


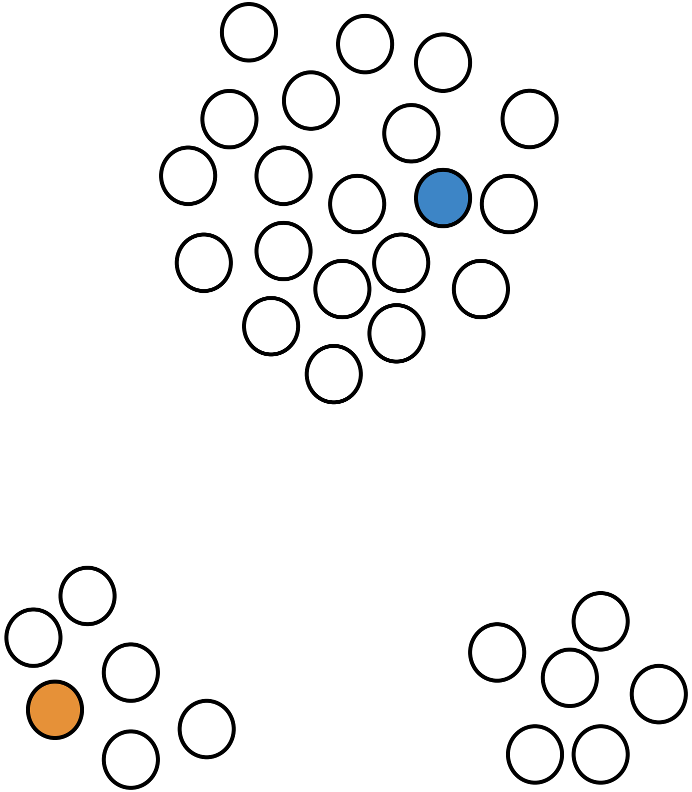


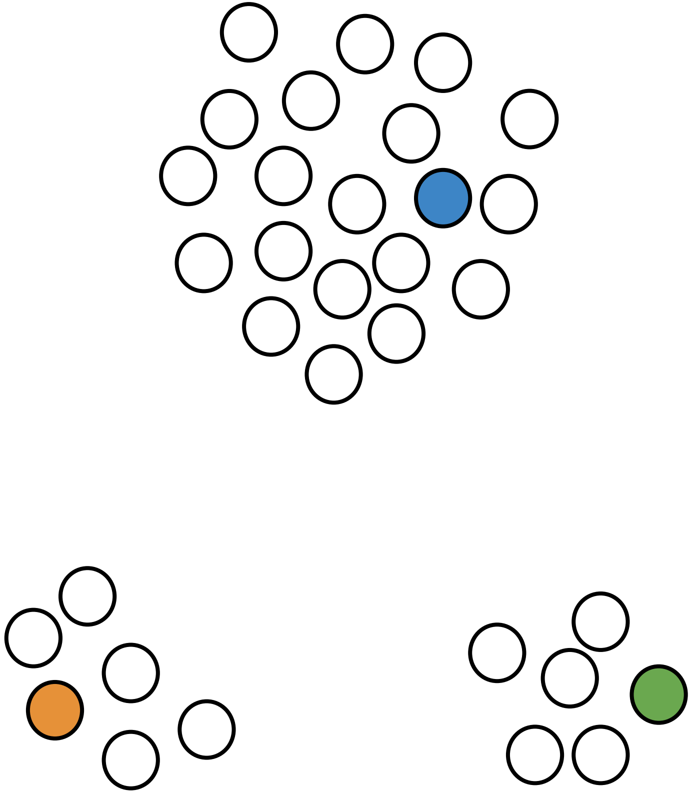


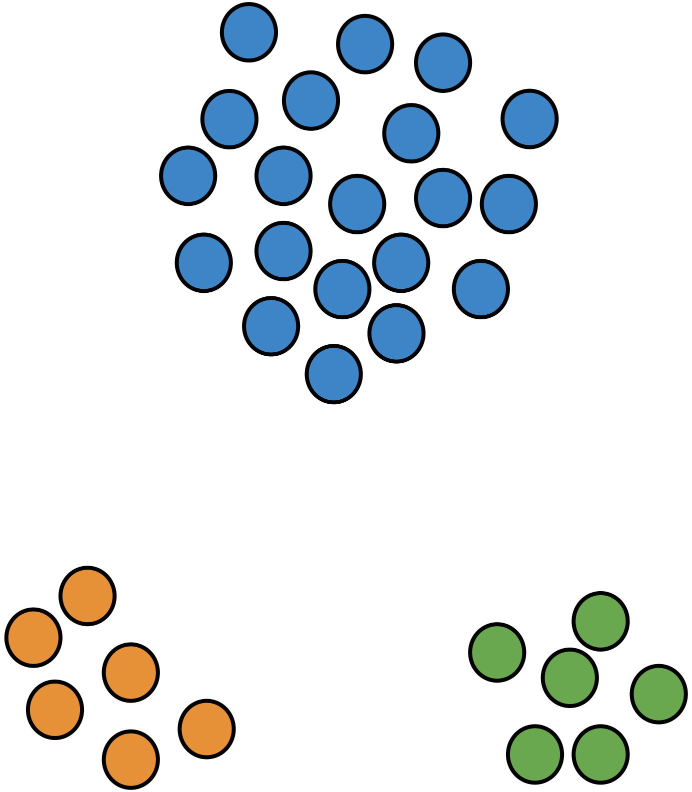
What's the problem?



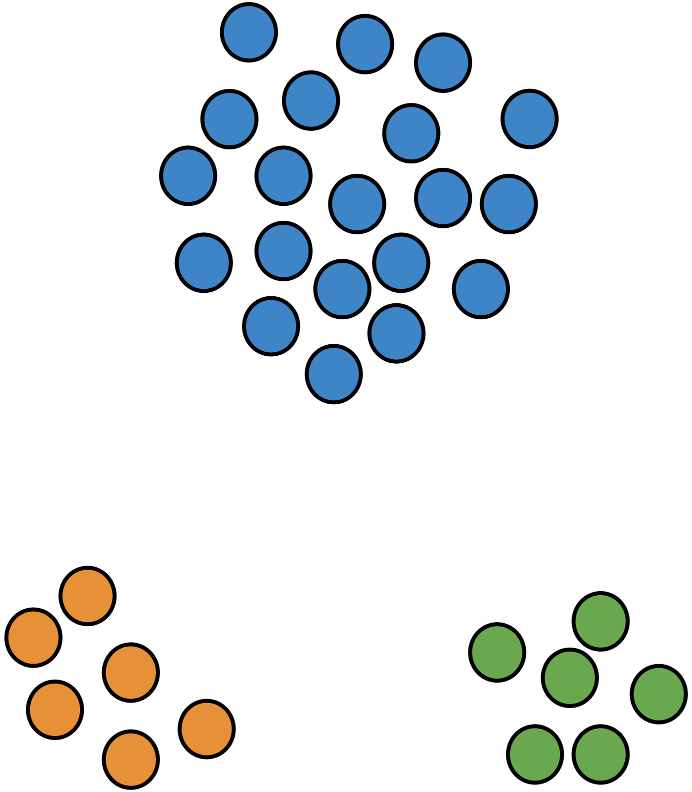






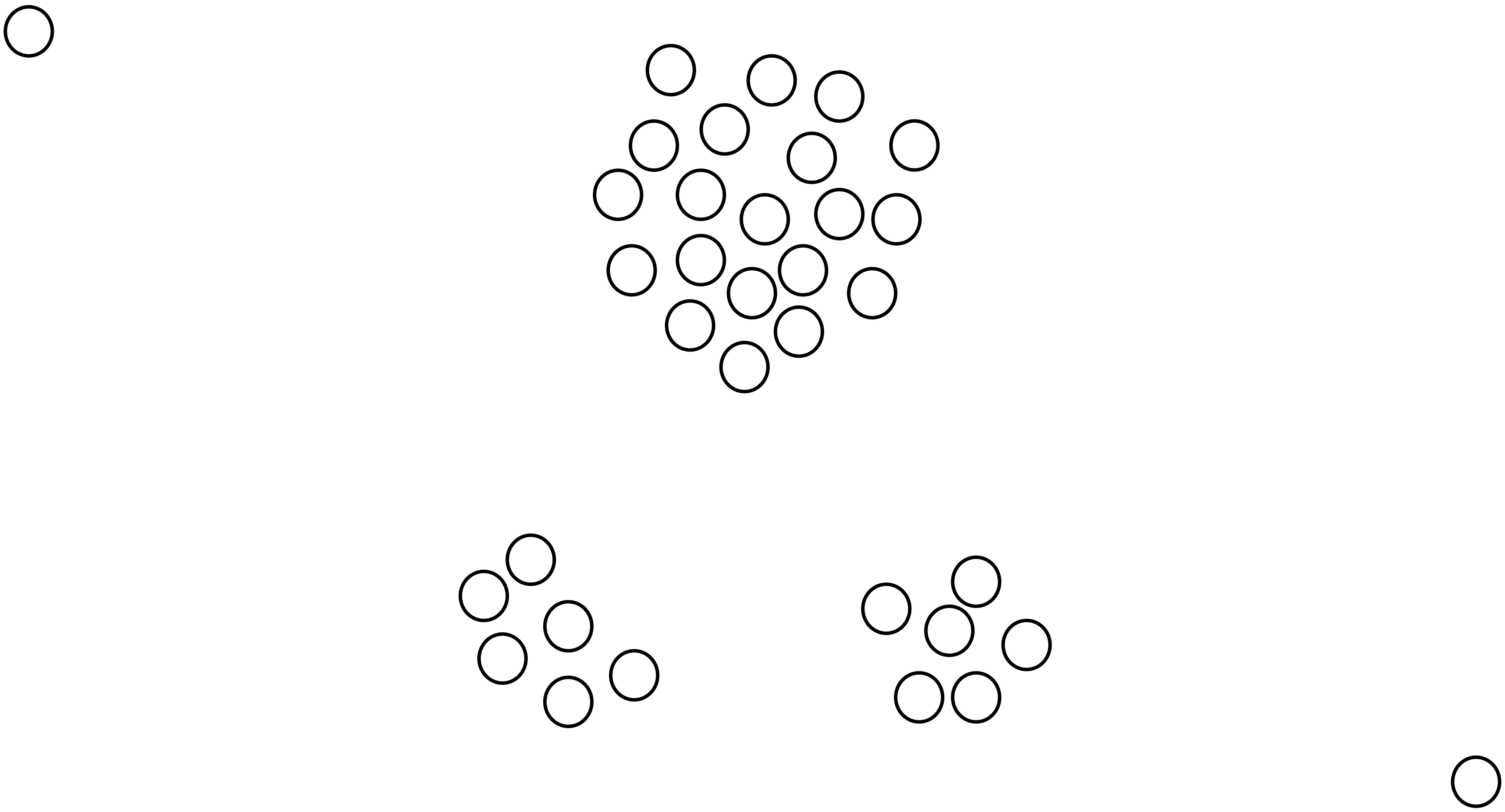


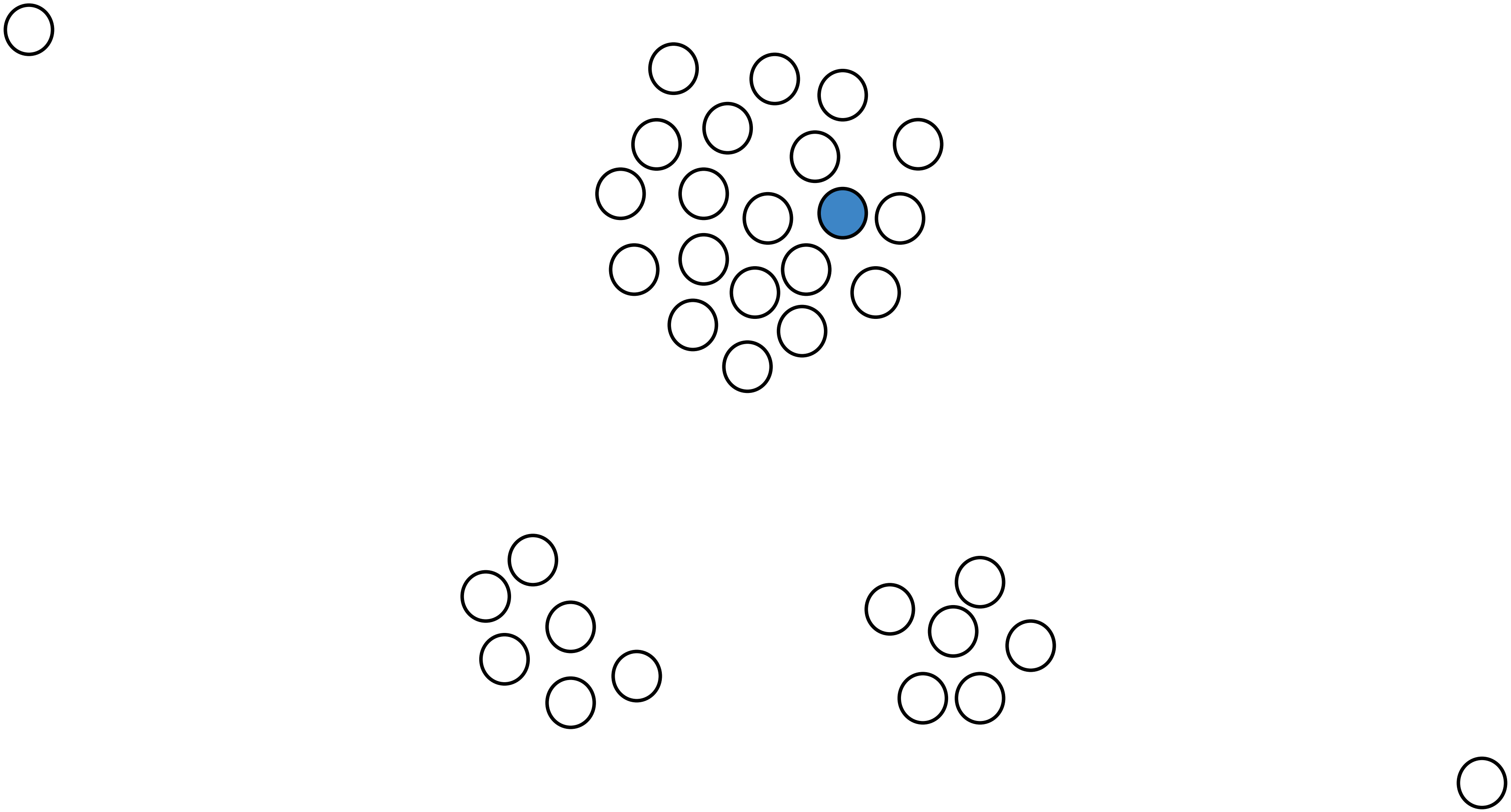
Farthest First Traversal

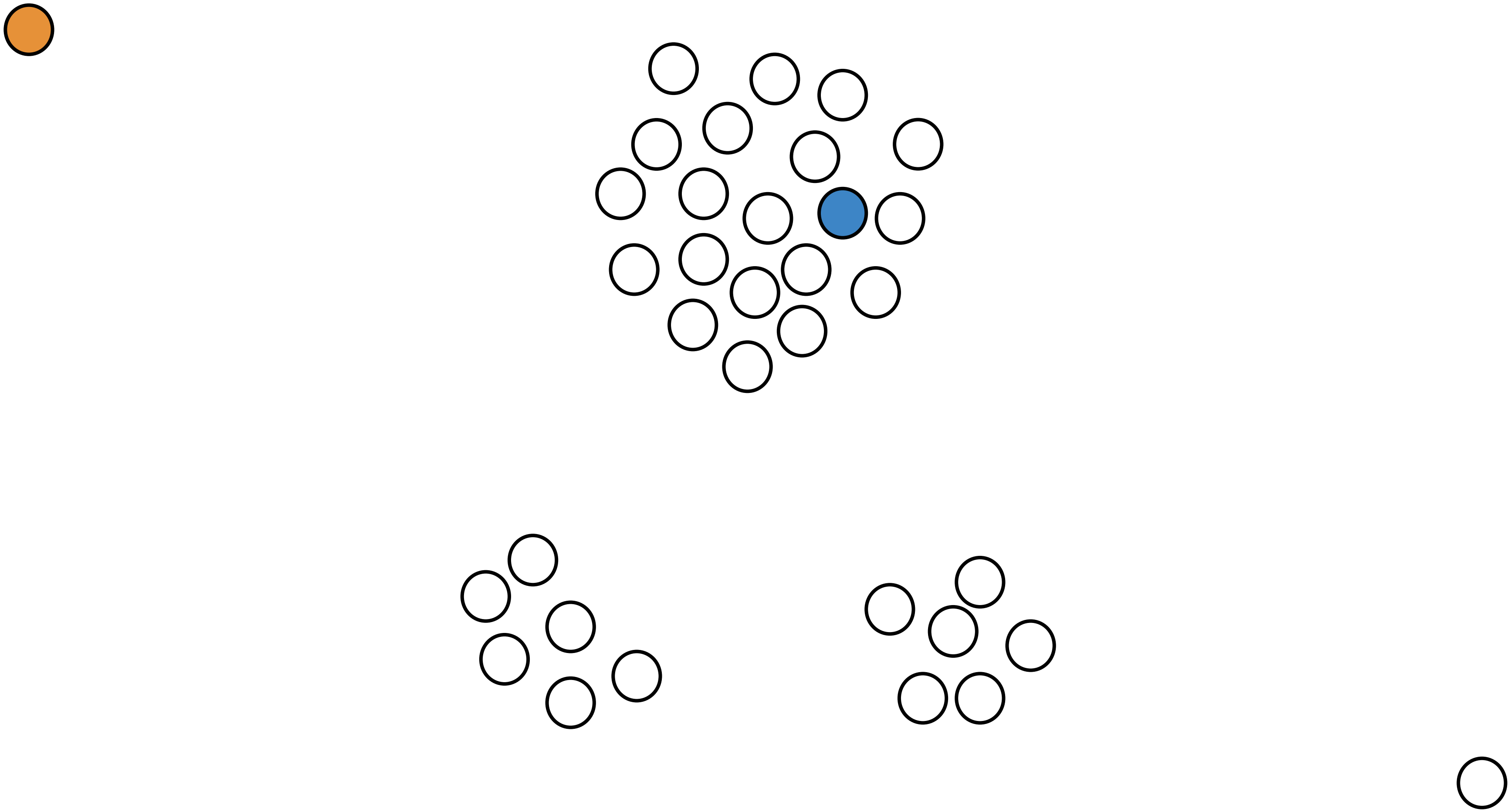


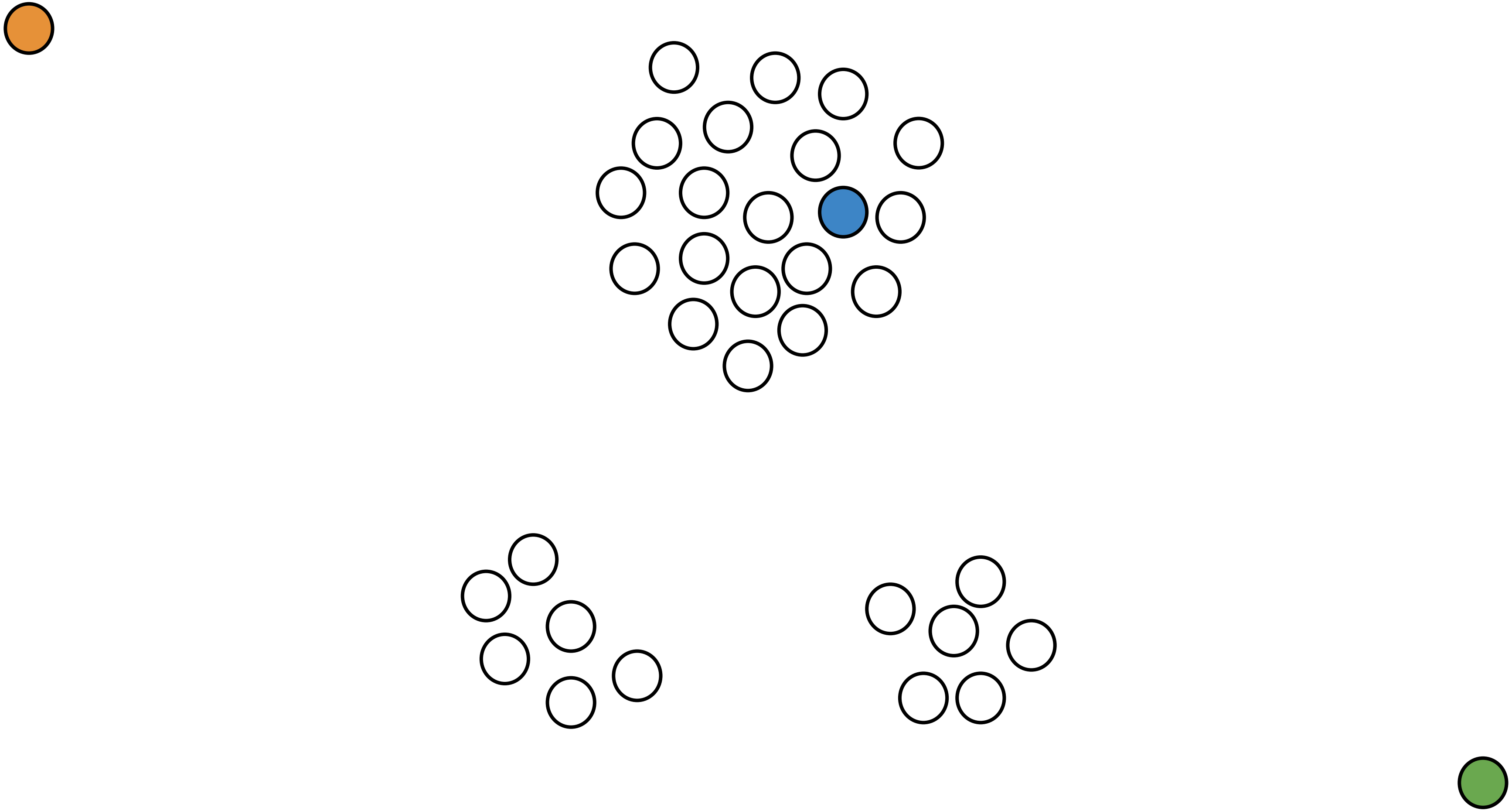
But…

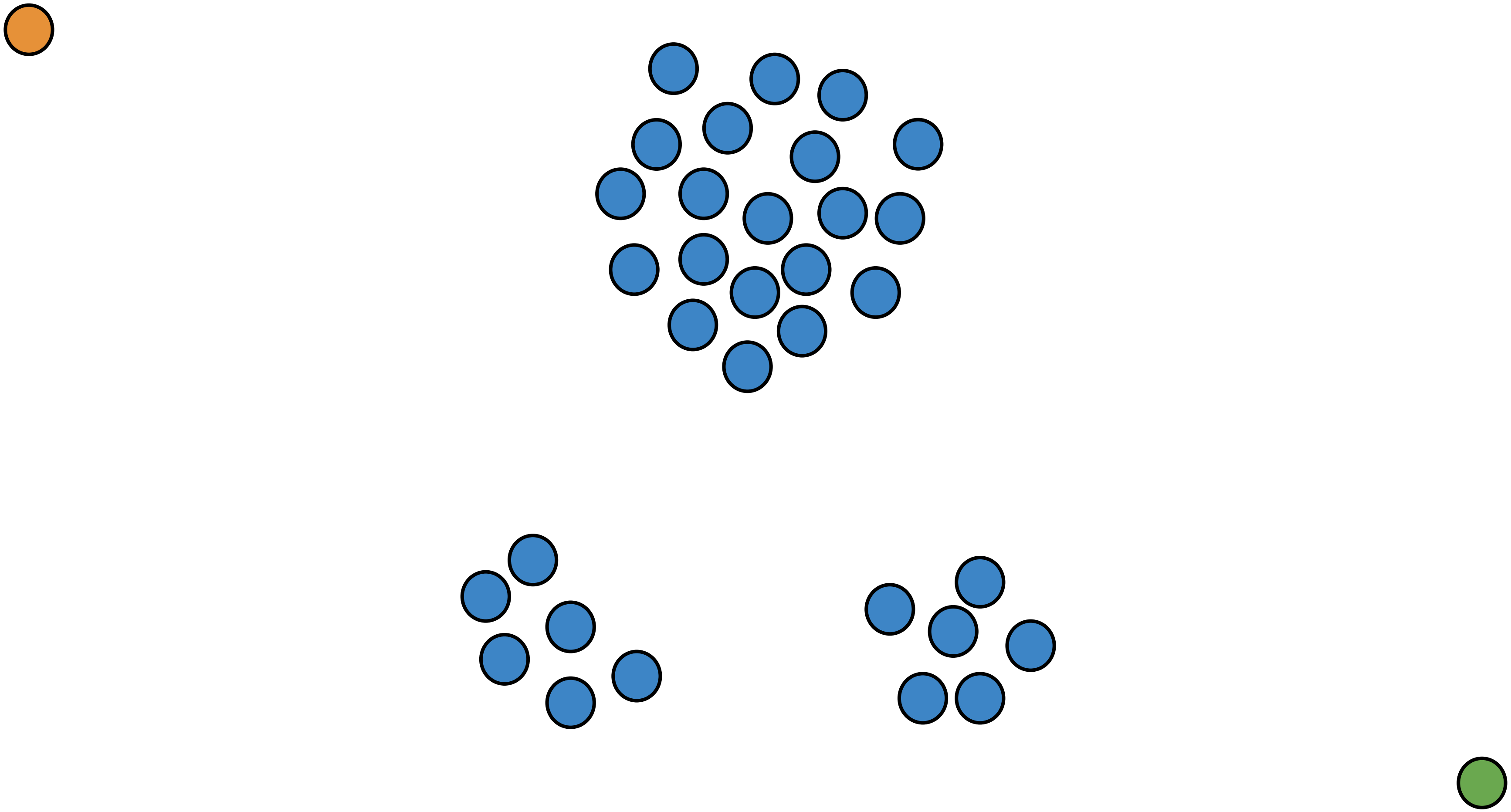
The problem is we could pick outliers as our centers



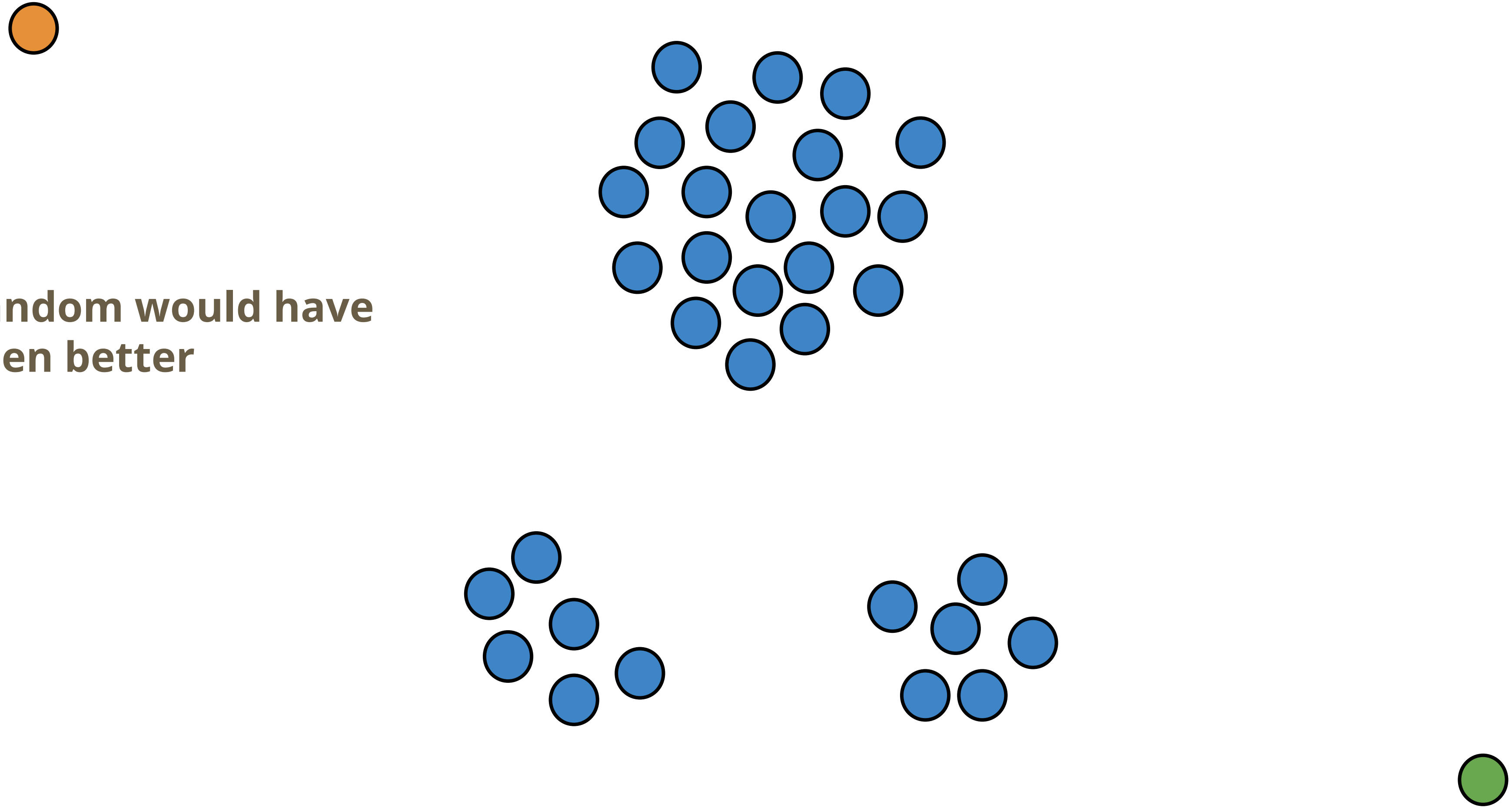








Random would have been better

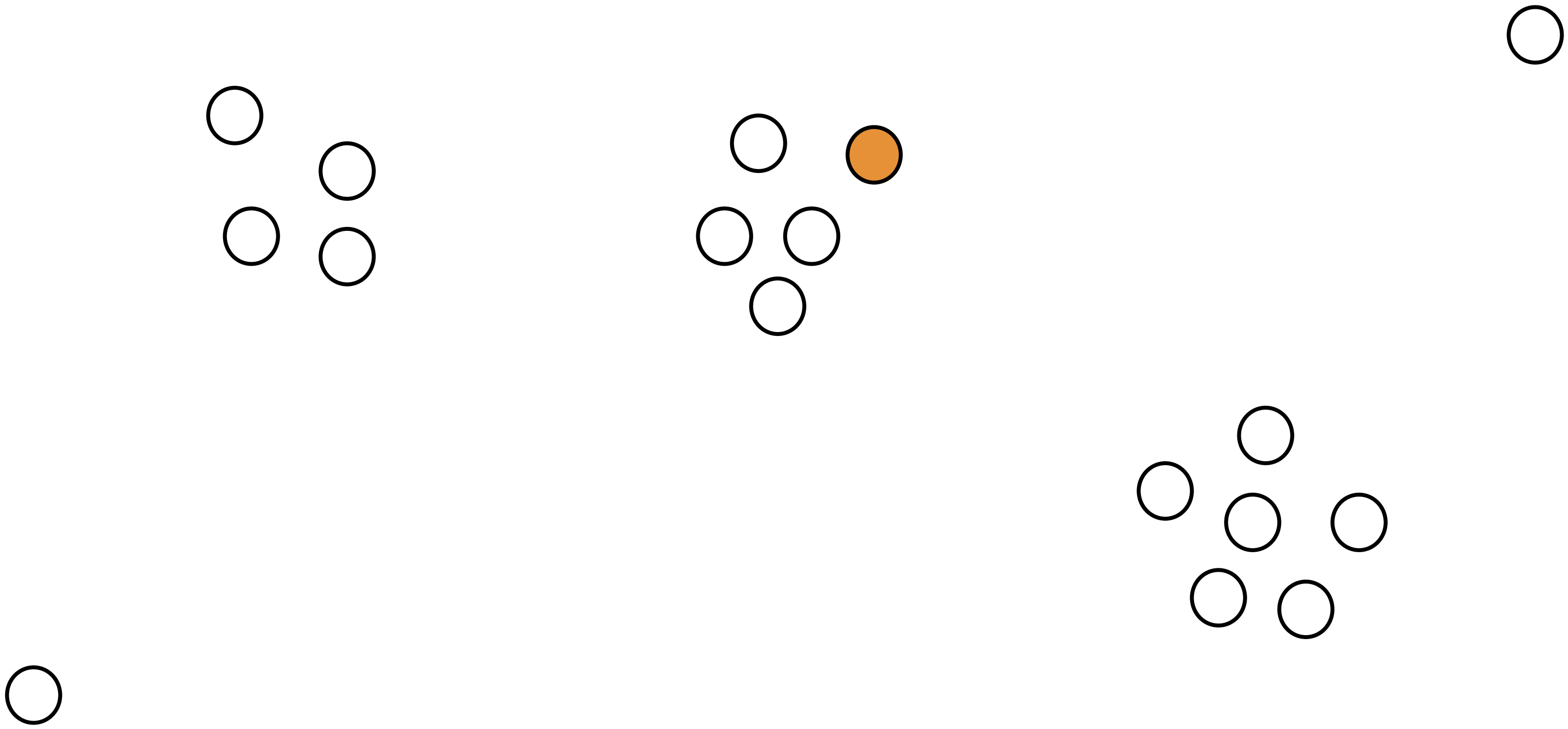


K-means++

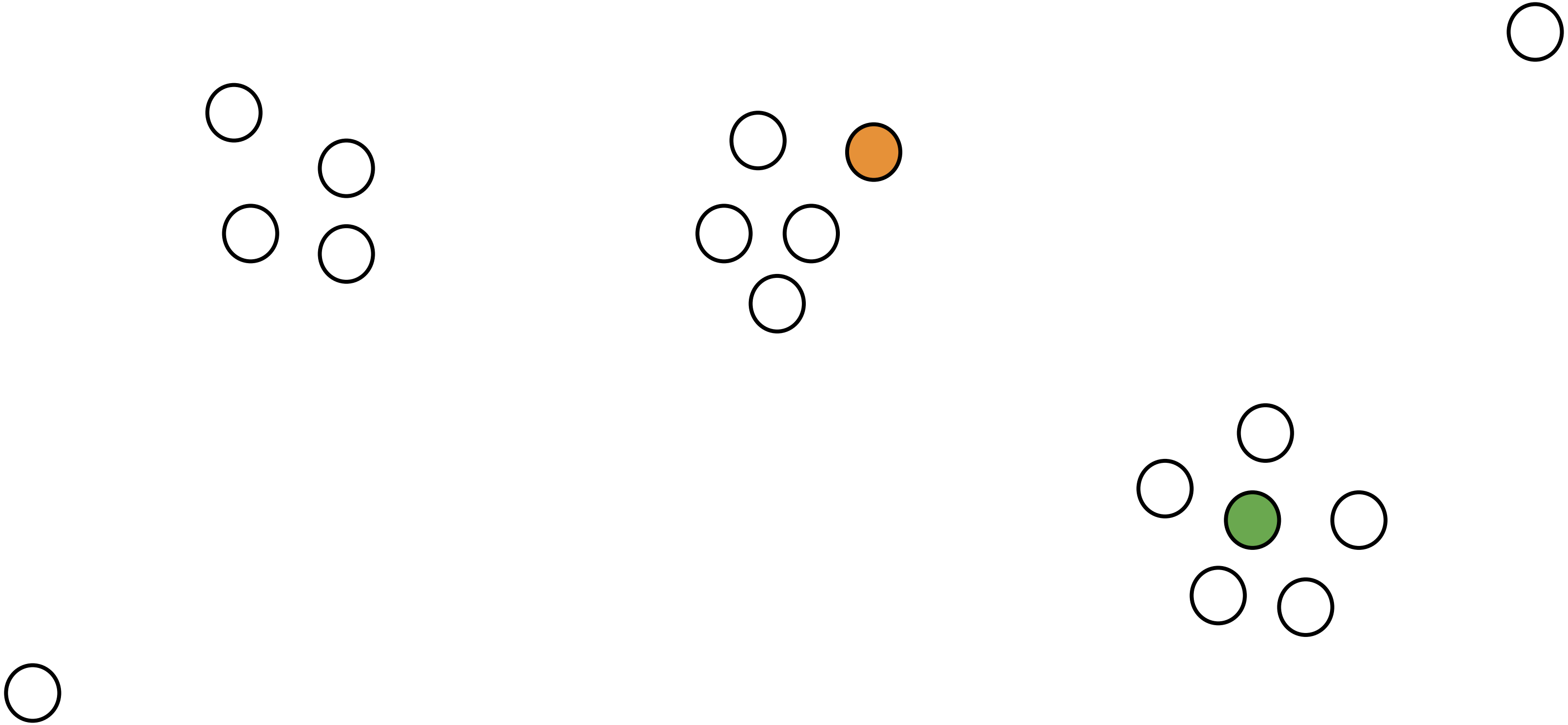
Initialize with a combination of the two methods:

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

K-means++



K-means++



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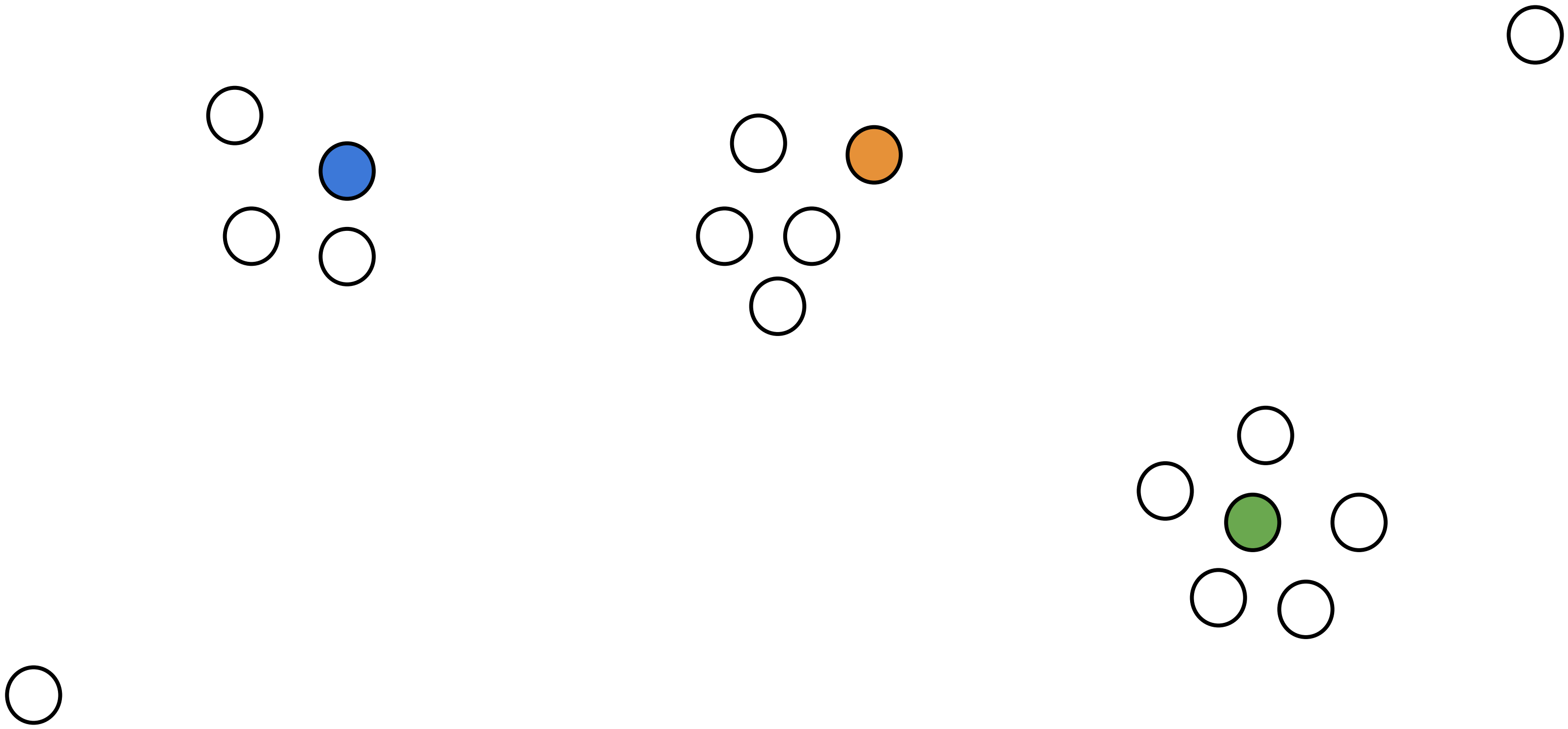

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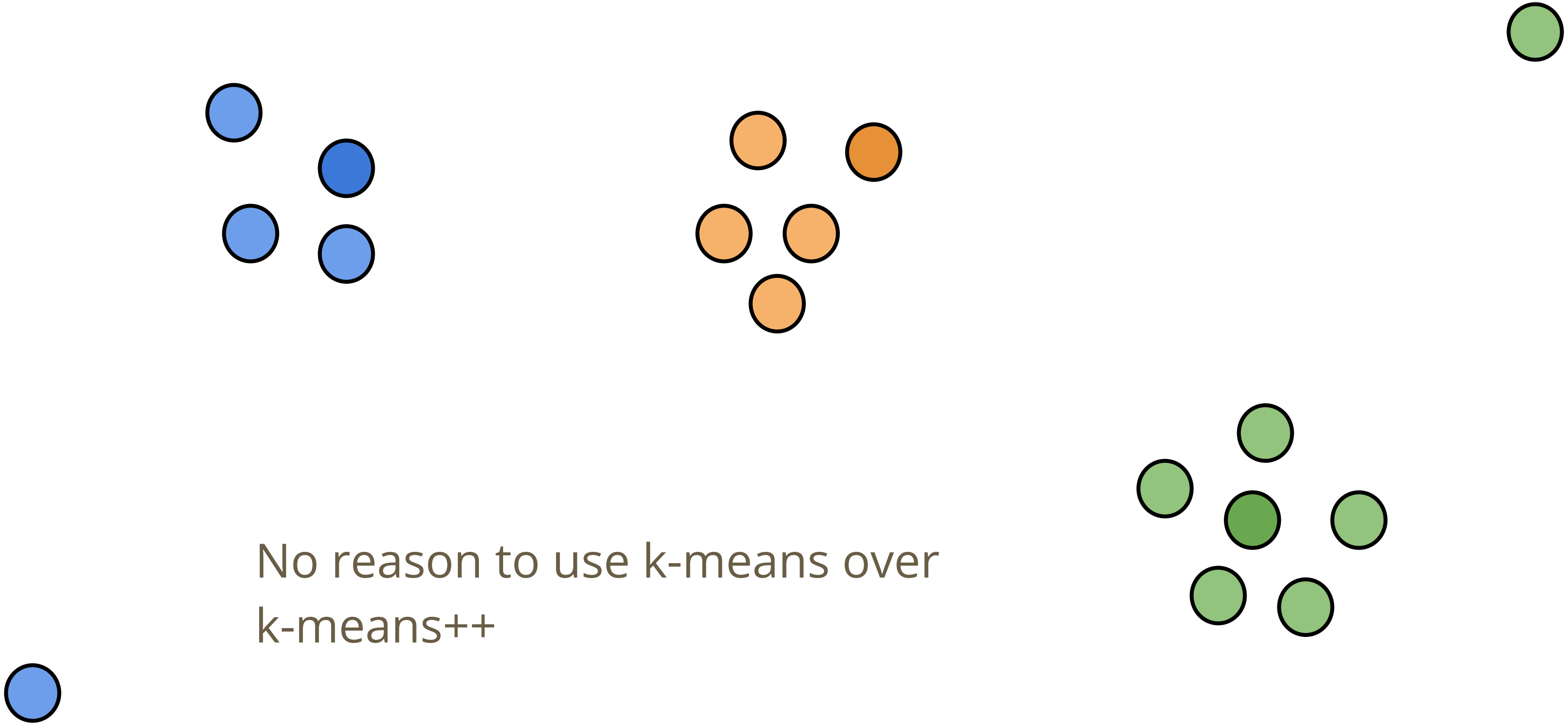

No reason to use k-means over k-means++

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 $\mathbf{D(x)^2}$?

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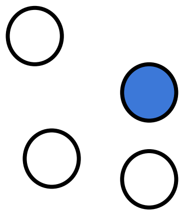

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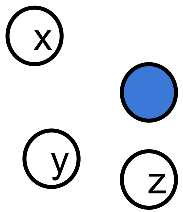
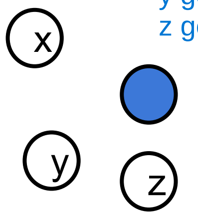


$\mathbf{D(x)^2 = 3^2 = 9}$
$\mathbf{D(y)^2 = 2^2 = 4}$
$\mathbf{D(z)^2 = 1^2 = 1}$

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 **$D(x)^2$**?

9+4+1 = 14
so x gets 9 out of 14 spots
y gets 4 out of 14
z gets 1 out of 14



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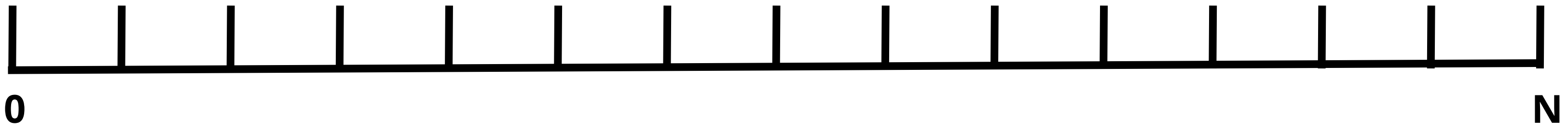

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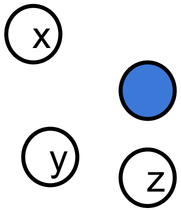

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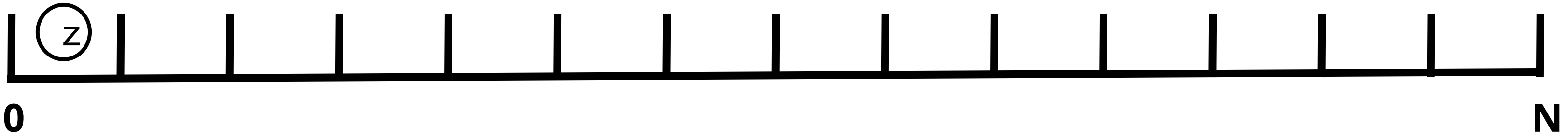

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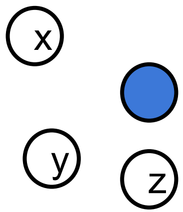

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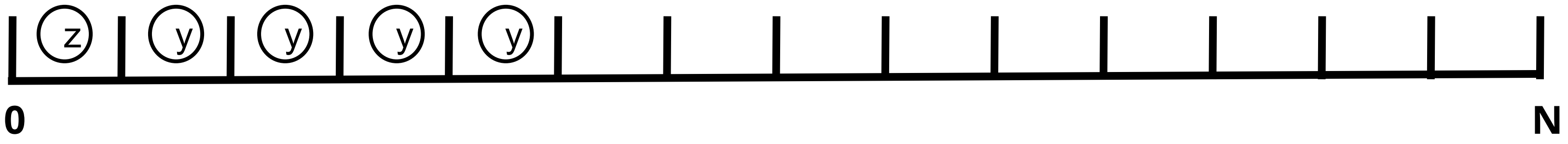

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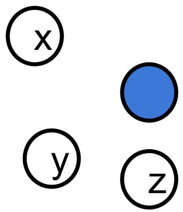

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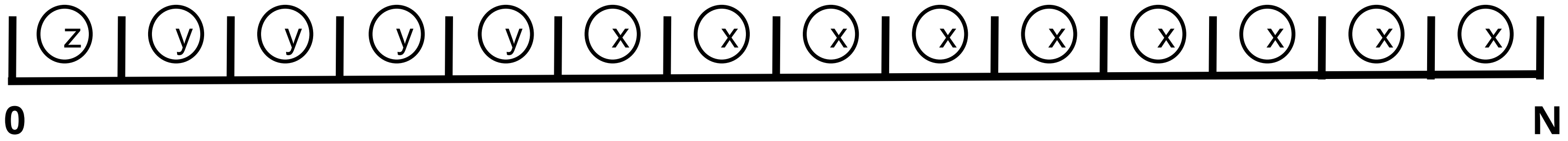

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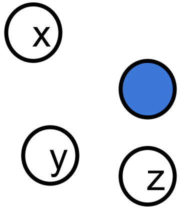

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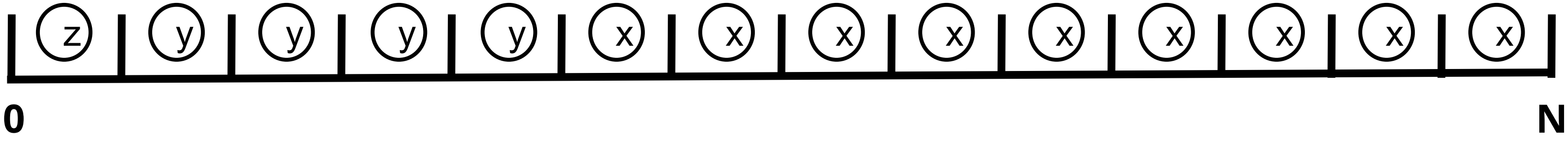

$= D(x)^2 + D(y)^2 + D(z)^2 = 14$

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 $\mathbf{D(x)^2}$?

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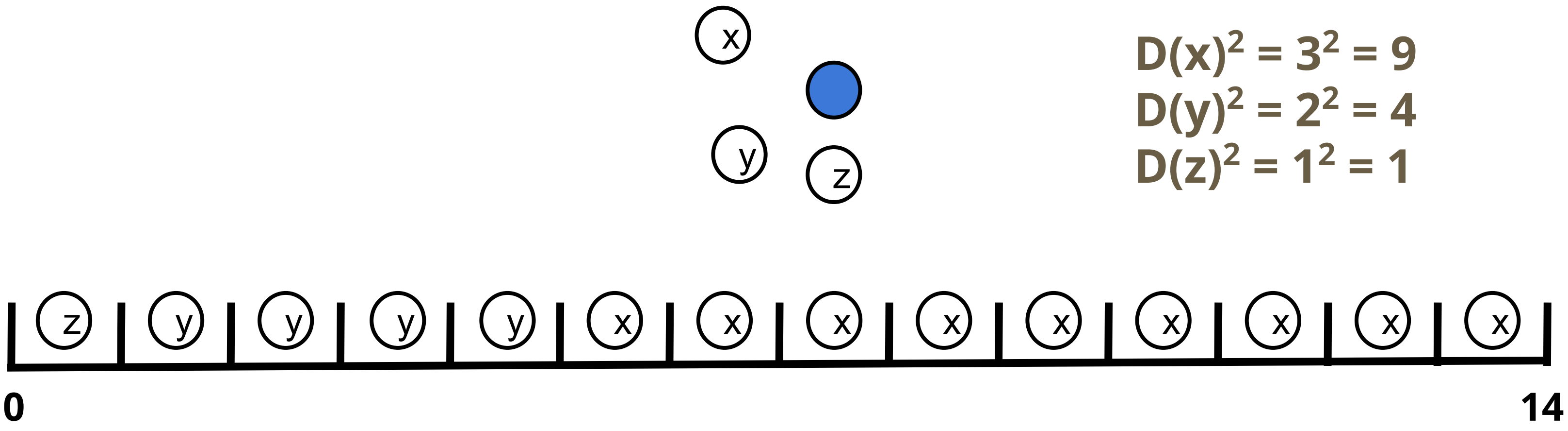
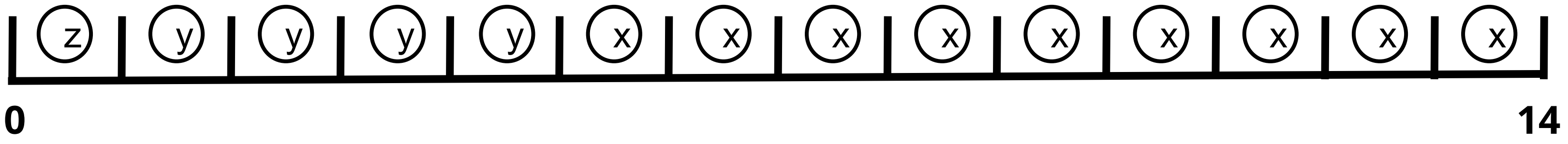


K-means++

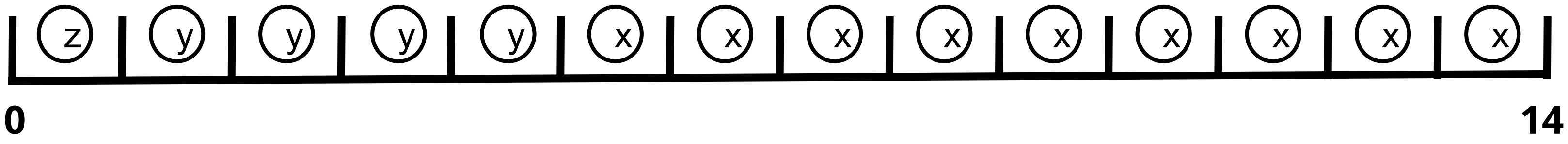
Q3: the black box returns “12” as the random number generated. Which point do we choose for the next center (x, y, or z) ?

x



K-means++

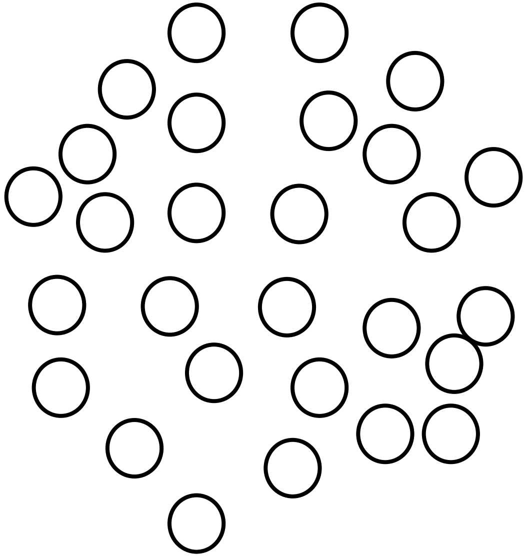
Q4: the black box returns “4” as the random number generated. Which point do we choose for the next center (x, y, or z) ? y

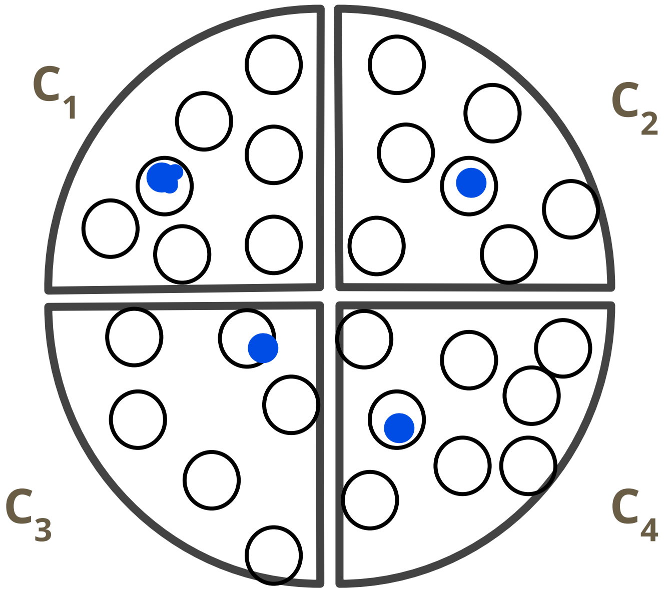


K-means++

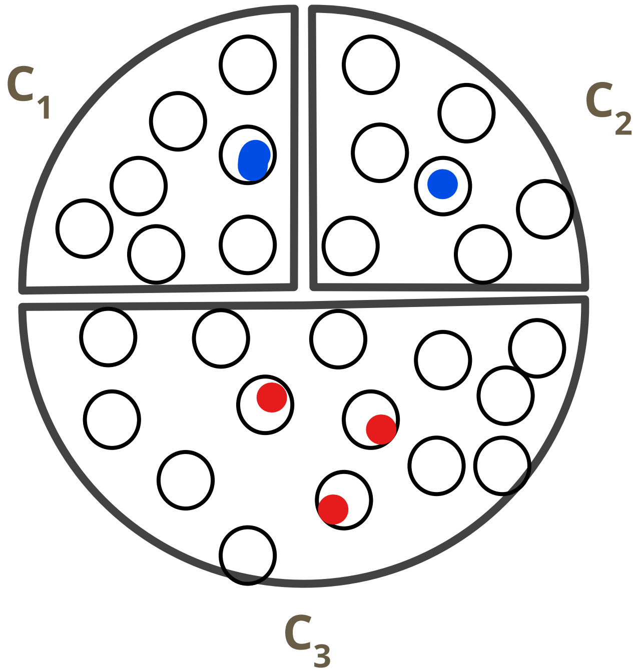
What happens if the black box can only generate numbers between 0 and 1?

Kmeans Quizz (take 2)

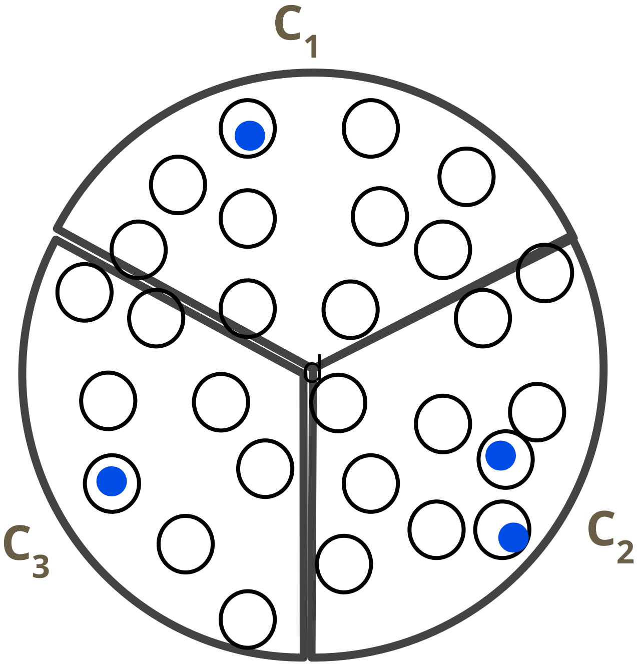


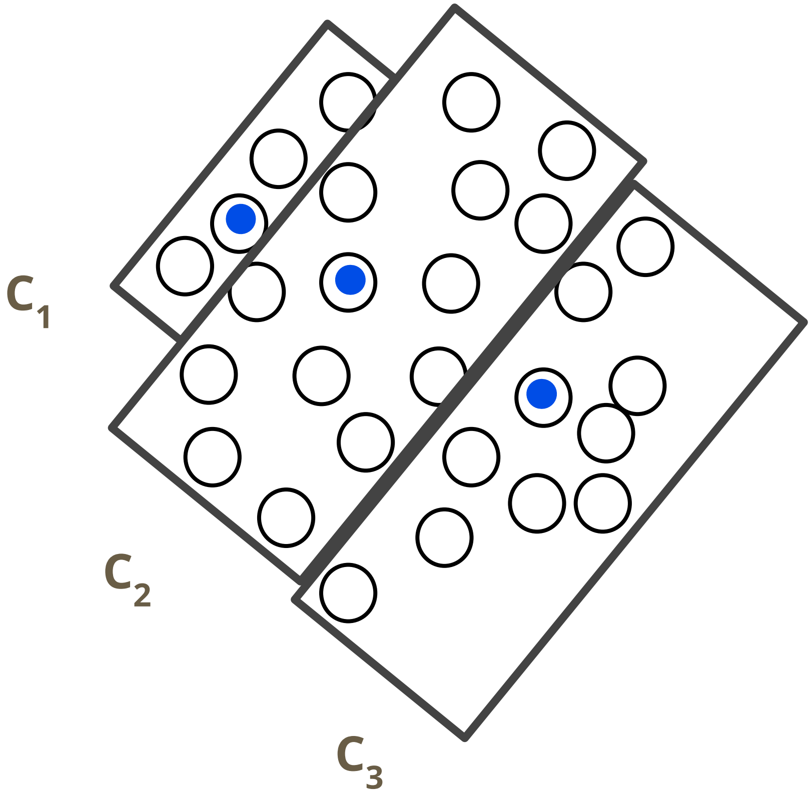


C_1
C_2
C_3
C_4

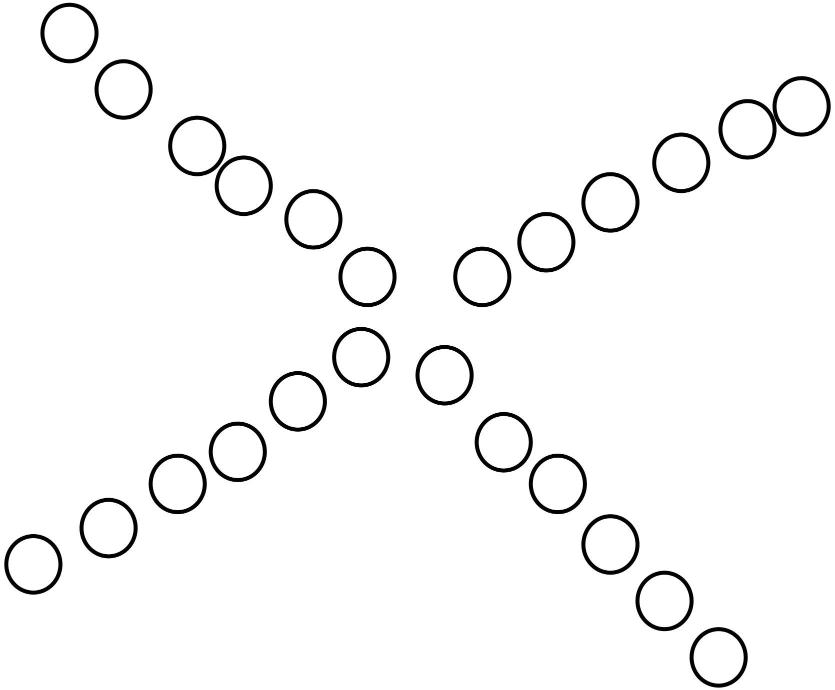


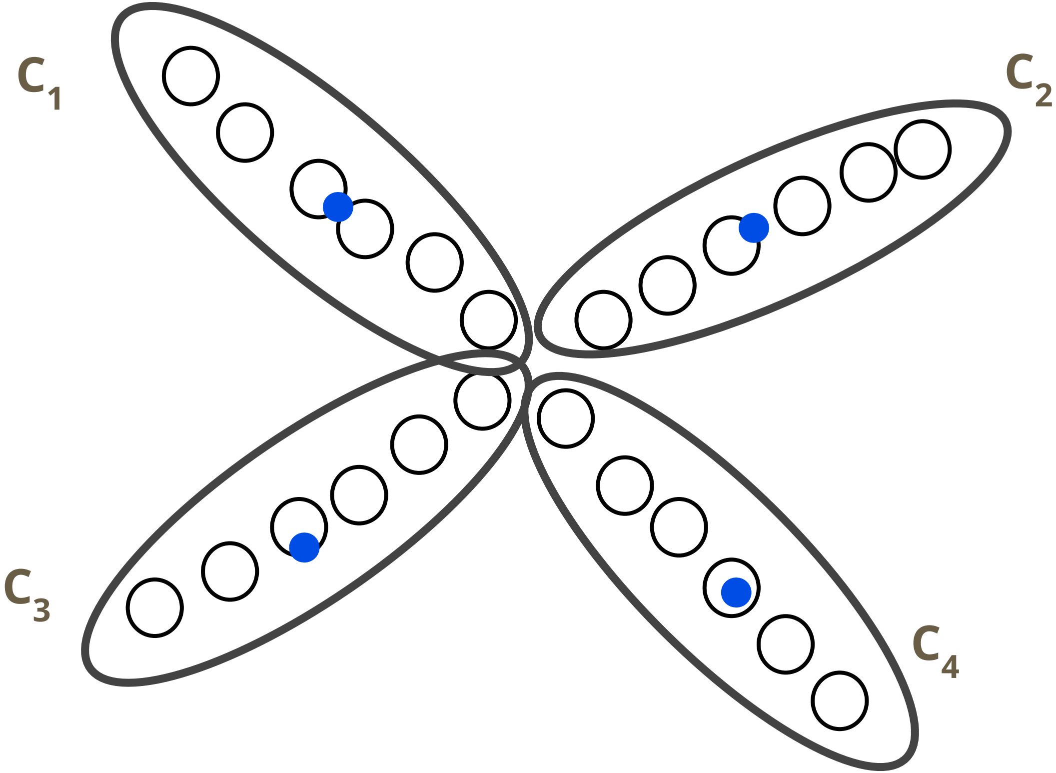
C_1
C_2
C_3


C1
C2
C3

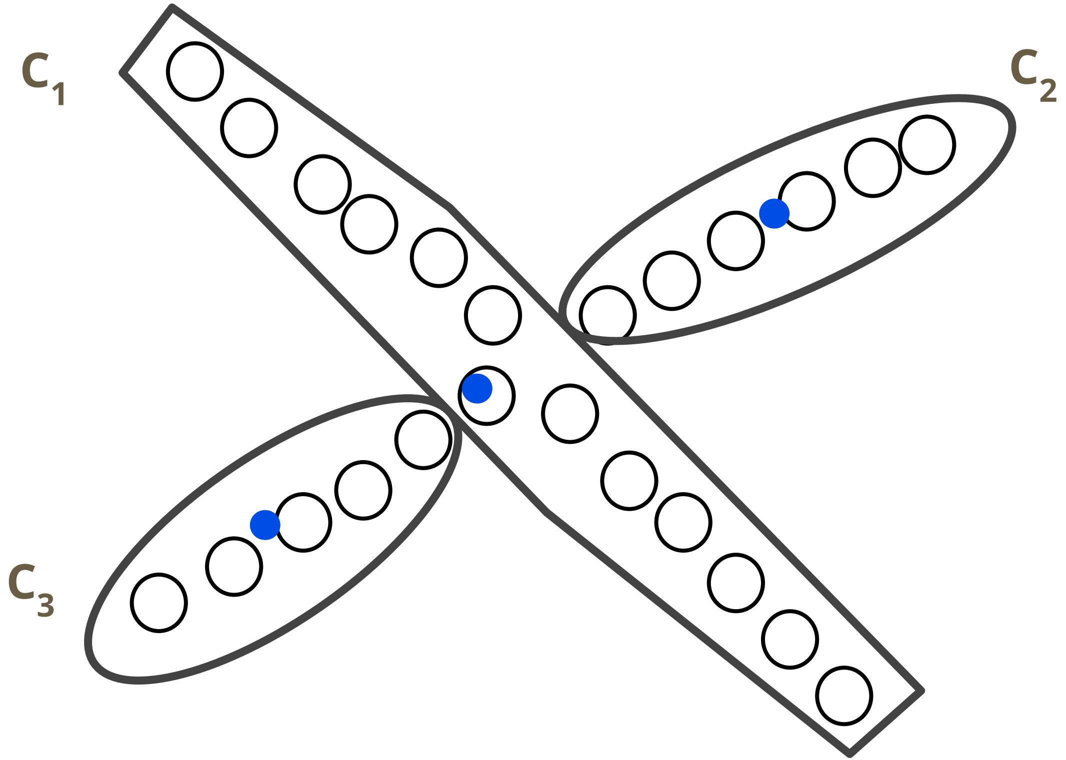


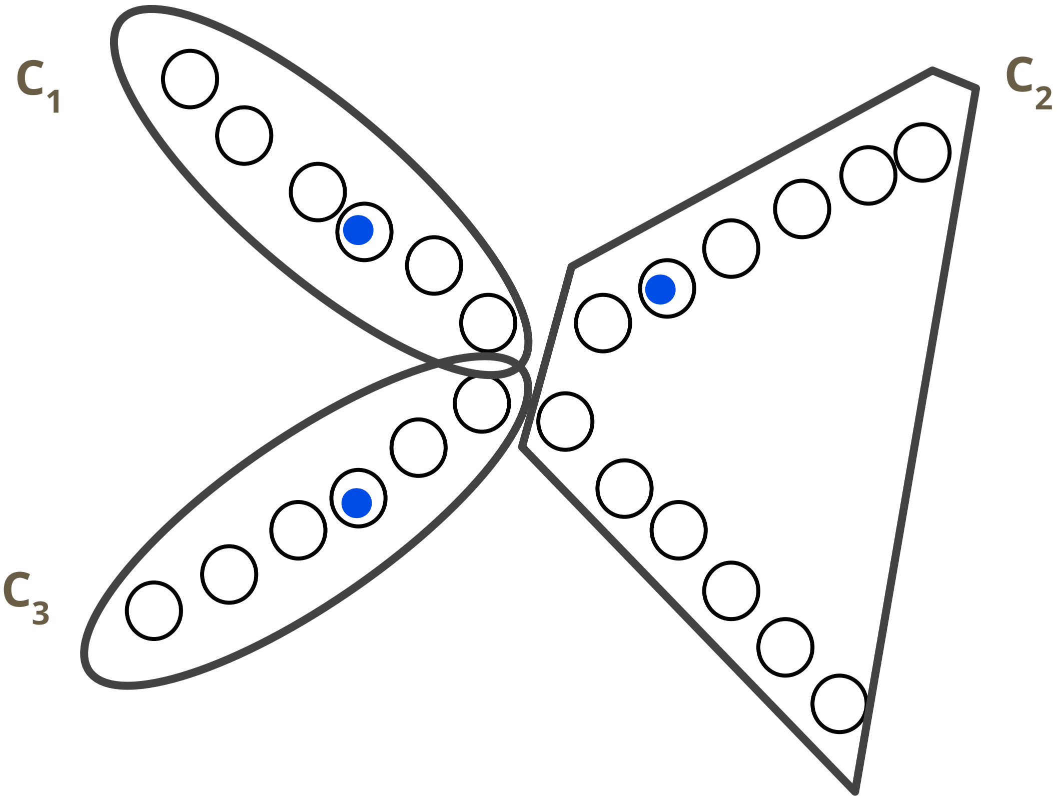
C_1
C_2
C_3

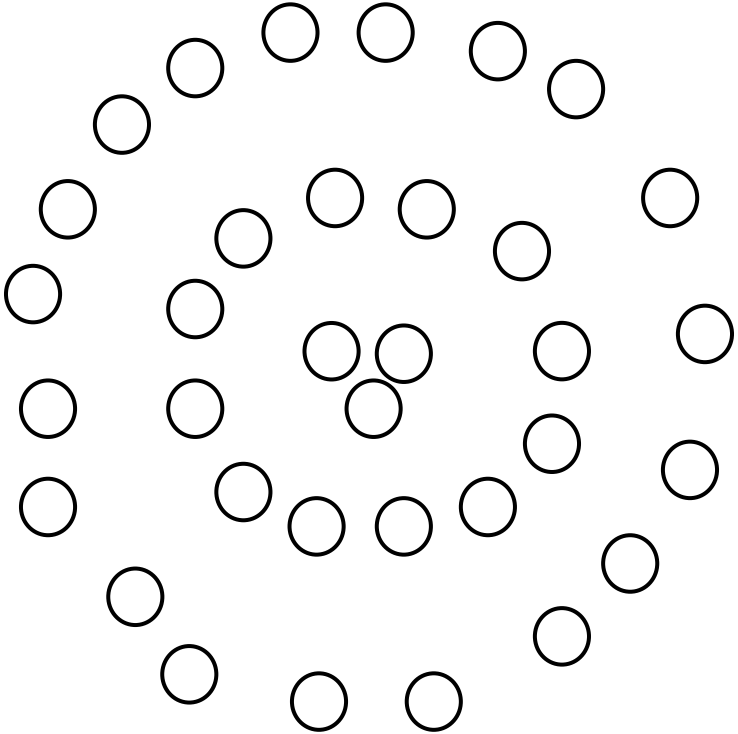


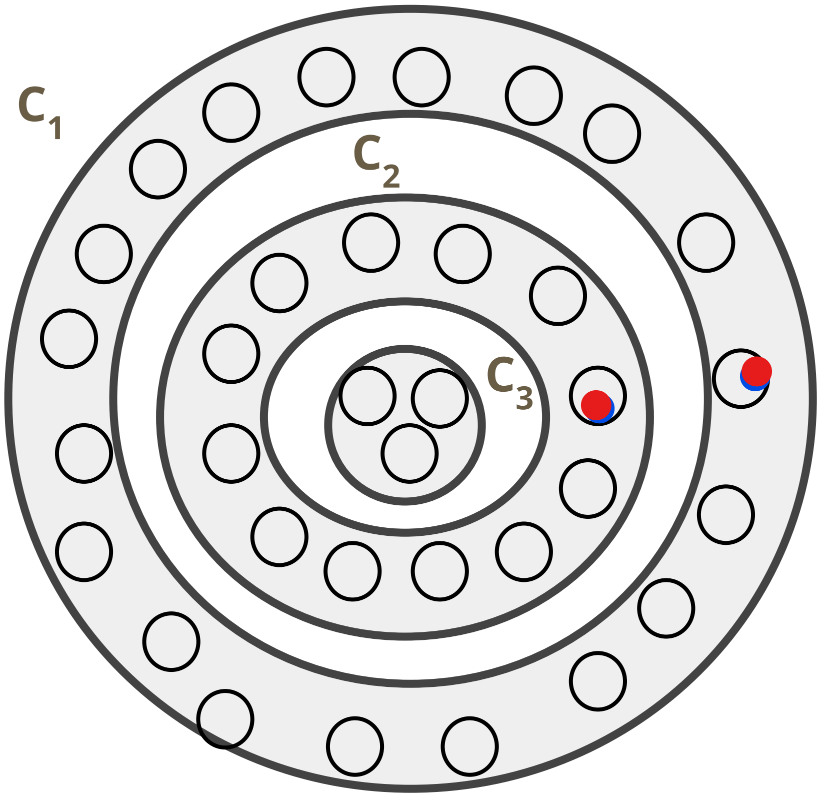


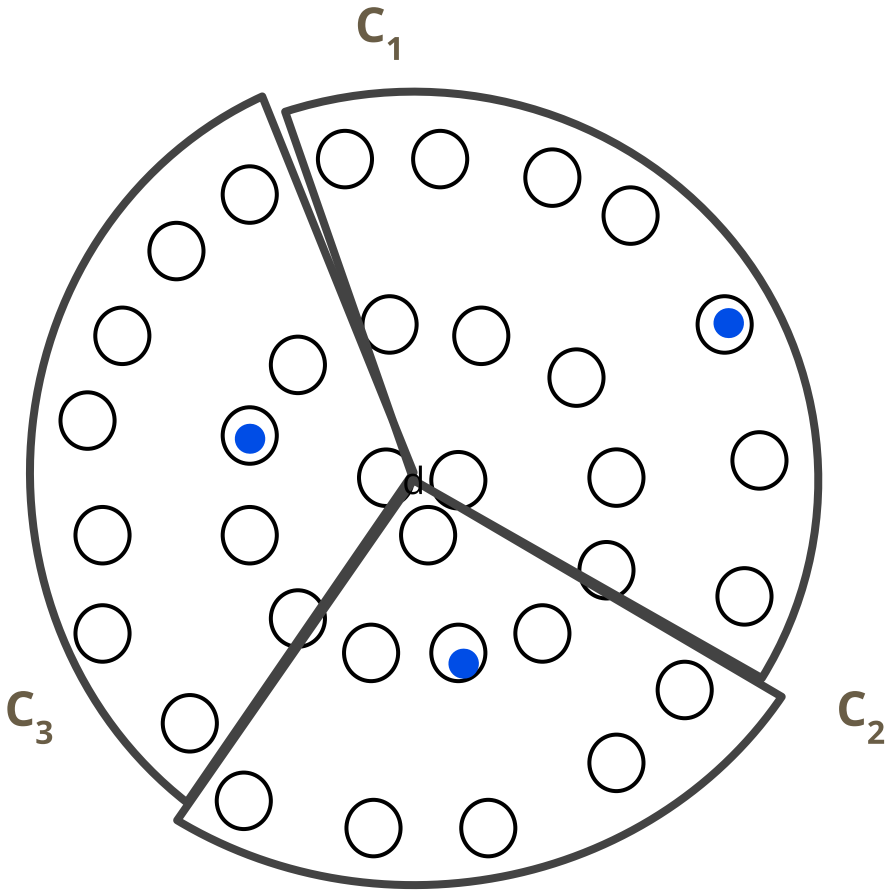
C_1
C_2
C_3
C_4


C_1
C_2
C_3

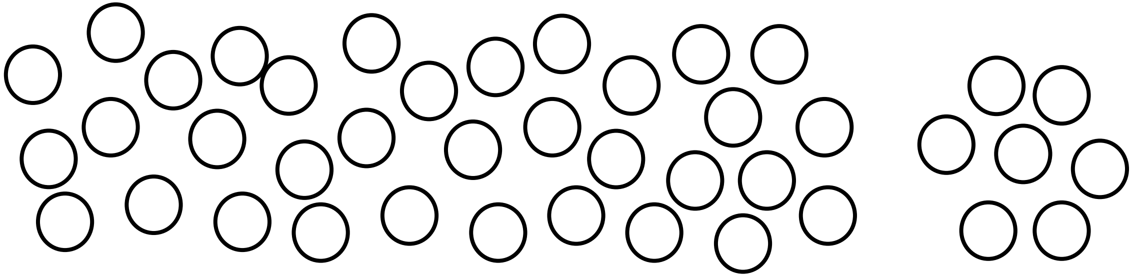

C_1
C_2
C_3

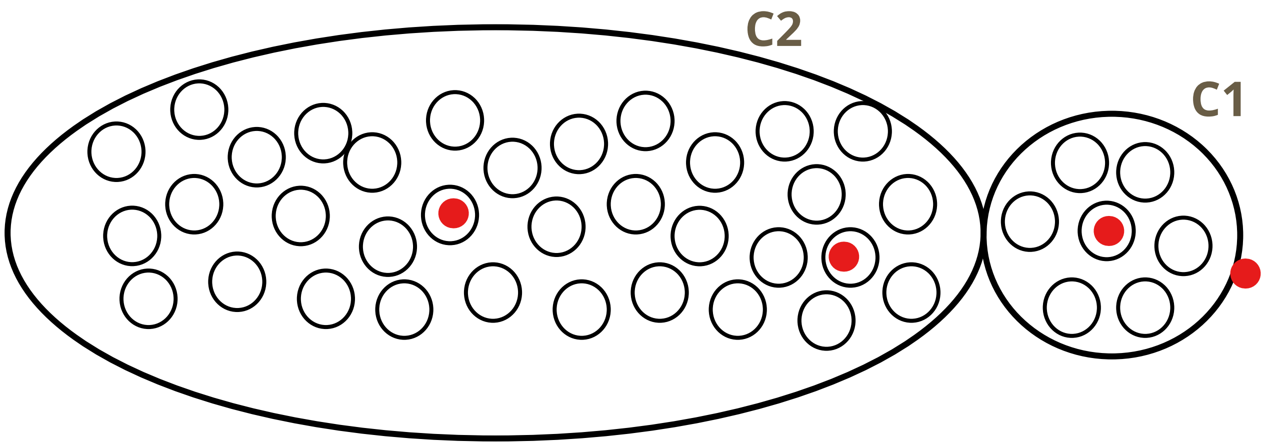



C_1
C_2
C_3



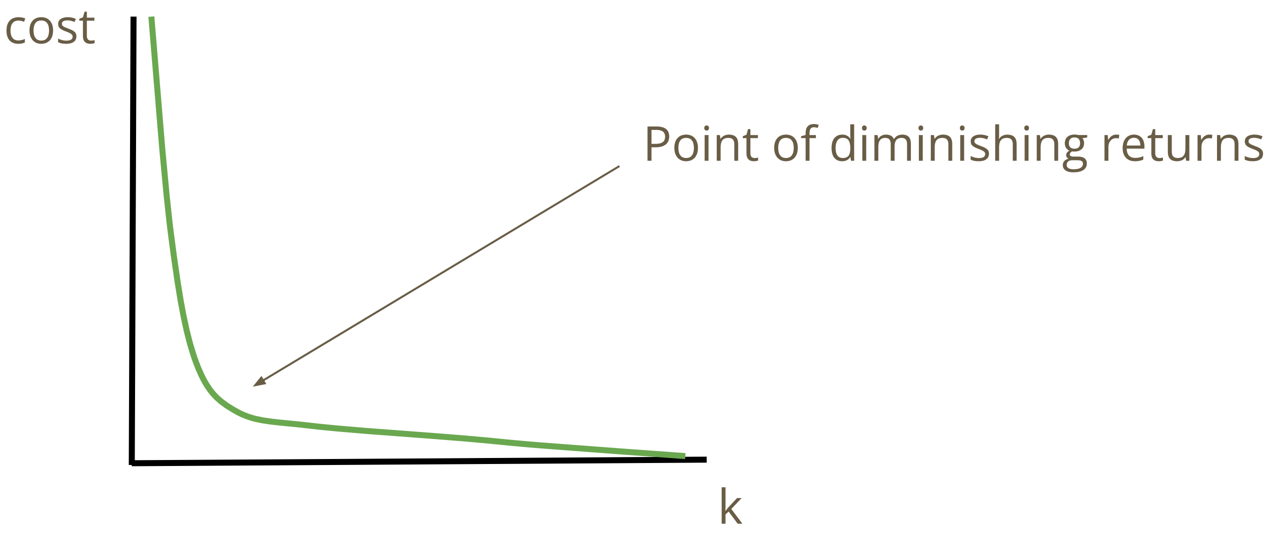
C_1
d
C_3
C_2




C2
C1

How to choose the right k?

1. Iterate through different values of k (elbow method)



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**

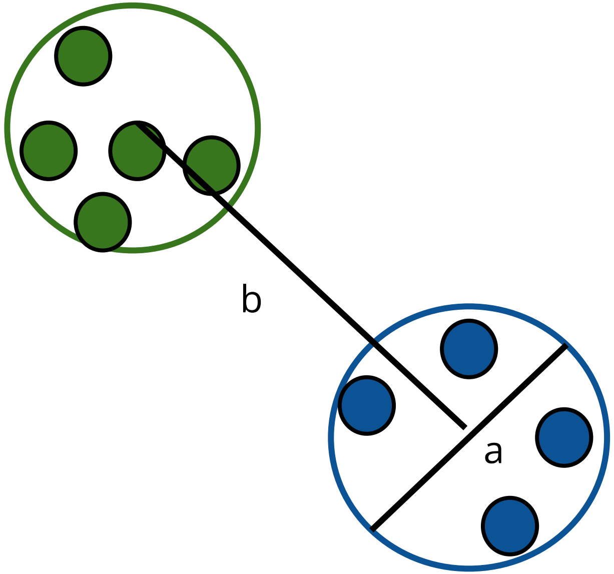
Evaluation

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?

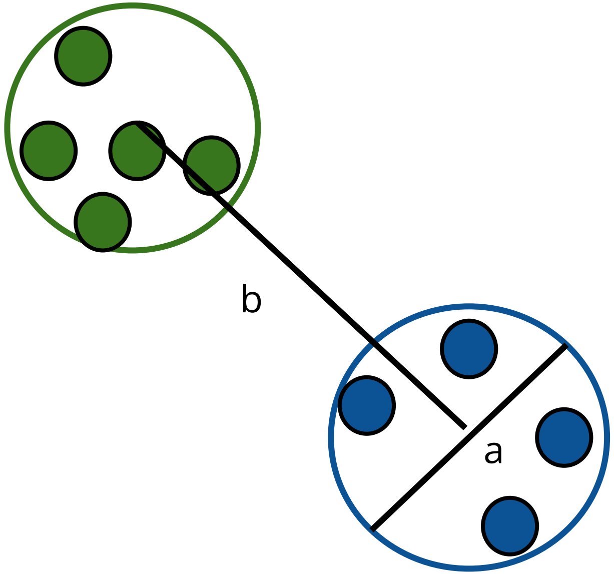
Discuss - 5min

Define a metric that evaluates how spread out the clusters are from one another.



a: average within-cluster distance

b: average intra-cluster distance



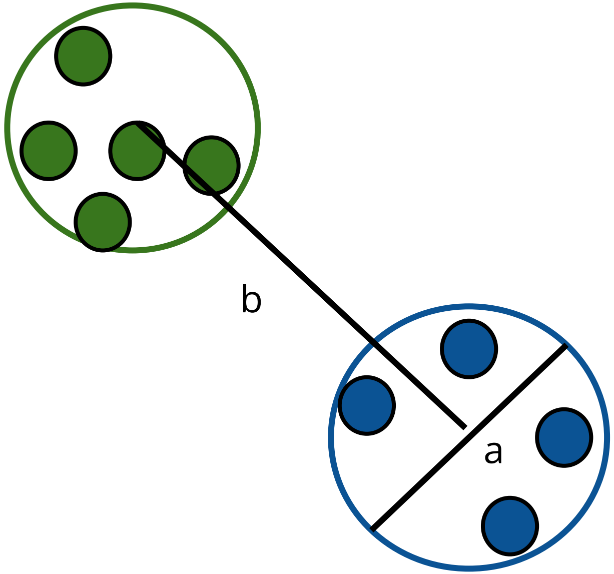
The distance within the cluster is the same as the distance between the clusters

a: average within-cluster distance

b: average intra-cluster distance

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

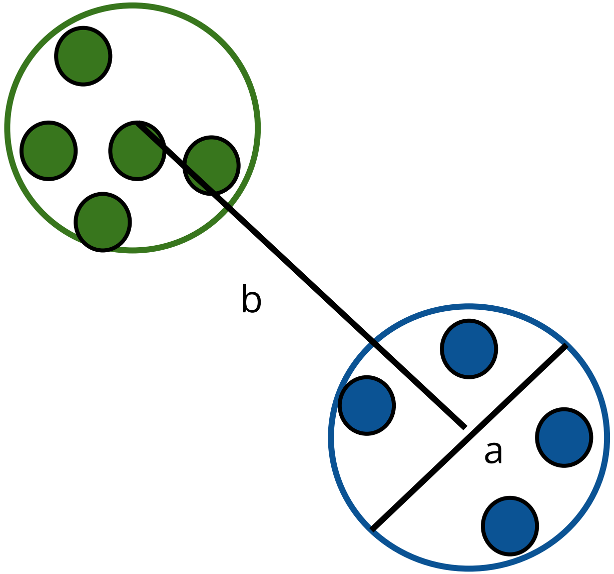
means clusters are right next to each other



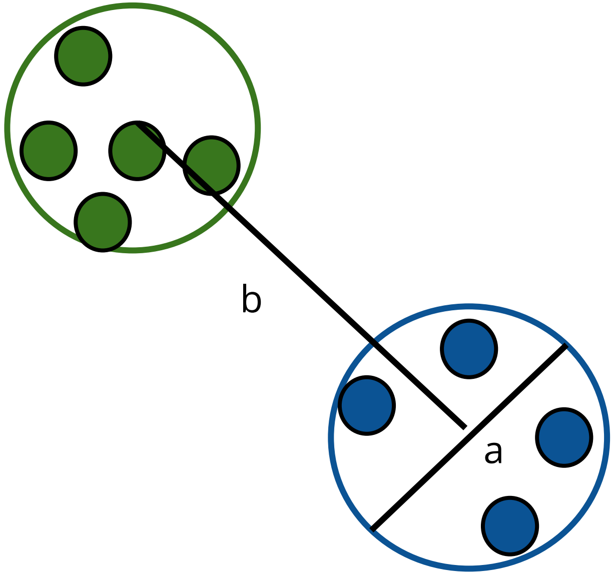
a: average within-cluster distance

b: average intra-cluster distance

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

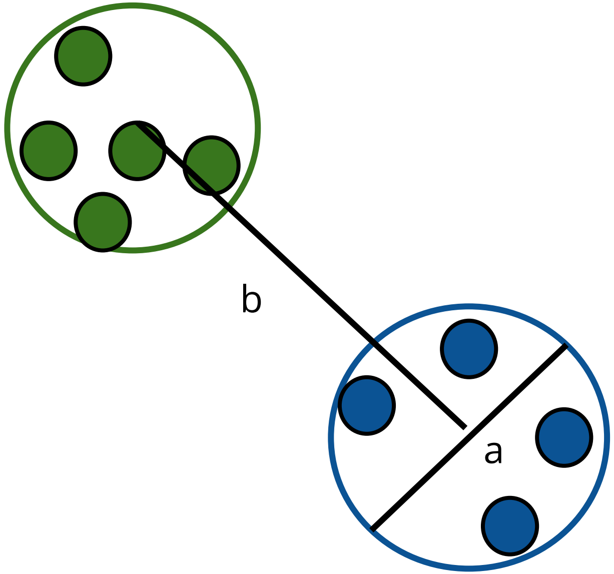


The value of (b-a) doesn't mean much by itself. Can we compare it to something so that the ratio becomes a value between 0 and 1?



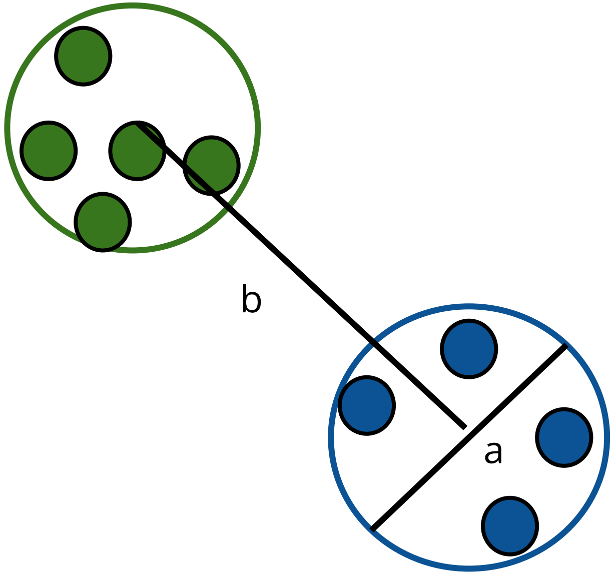
(b - a) / max(a, b)

value will be between 0 and 1



What does it mean for (b - a) / max(a, b) to be close to 1?

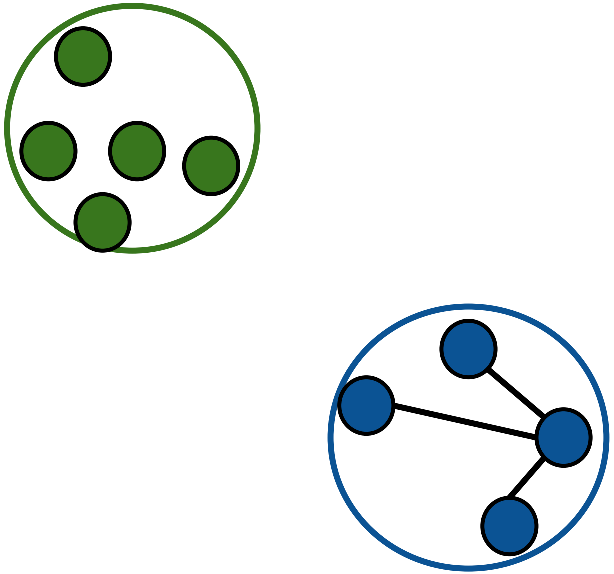
A value close to 1 indicates that the data points are well-separated from each other and from other clusters, while a value close to -1 indicates that the data points are not well-separated



What does it mean for (b - a) / max(a, b) to be close to 0?

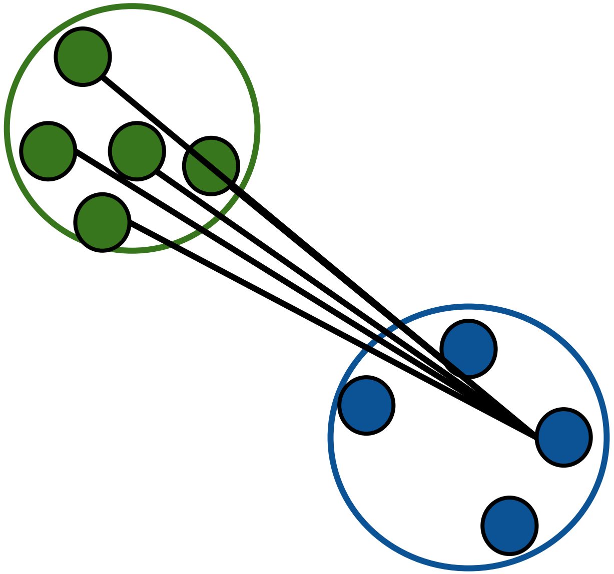
A value close to 1 indicates that the data points are well-separated from each other and from other clusters, while a value close to -1 indicates that the data points are not well-separated

Silhouette Scores



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

Silhouette Scores

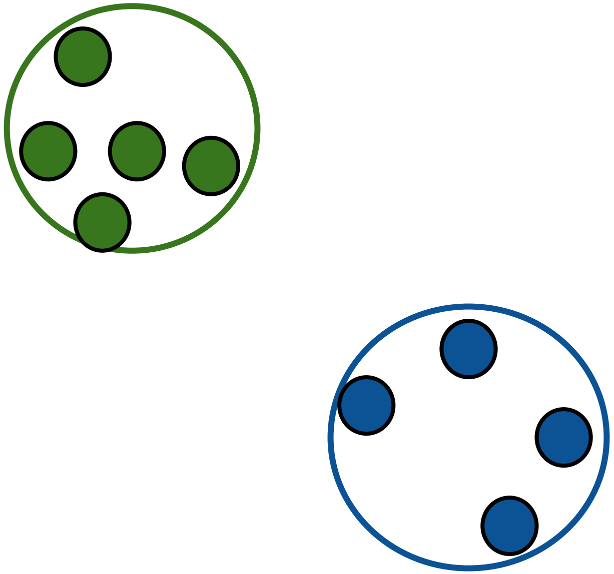


For each data point i:

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



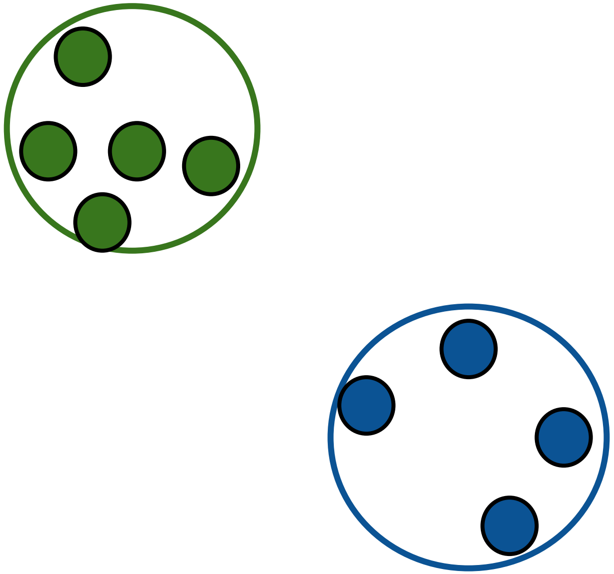
For each data point i:
a_i : mean distance from point i to every other point in its cluster
b_i : smallest mean distance from point i to every point in another cluster

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

si should be small in theory

Silhouette Scores

The silhouette score ranges from -1 to 1, where a score close to 1 indicates that the samples are well-clustered, a score close to 0 indicates overlapping clusters, and a negative score indicates that the samples might have been assigned to the wrong cluster

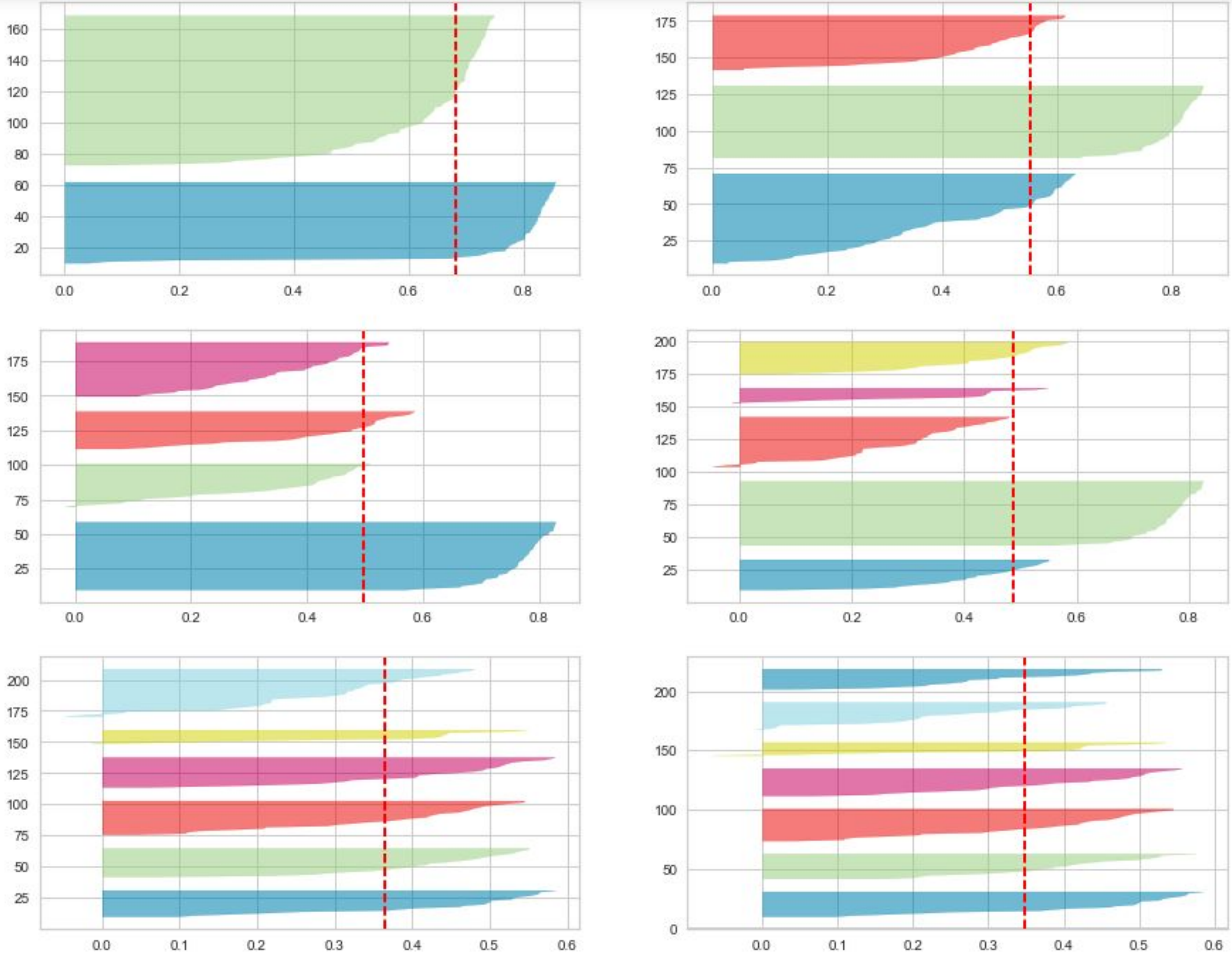


$s_i = (b_i - a_i) / \max(a_i, b_i)$

Silhouette score plot

OR

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



160
140
120
100
80
60
40
20
0.0 0.2 0.4 0.6 0.8
175
150
125
100
75
50
25
0.0 0.2 0.4 0.6 0.8
175
150
125
100
75
50
25
0.0 0.2 0.4 0.6 0.8
200
175
150
125
100
75
50
25
0.0 0.2 0.4 0.6 0.8
200
175
150
125
100
75
50
25
0.0 0.1 0.2 0.3 0.4 0.5 0.6
200
150
100
50
0
0.0 0.1 0.2 0.3 0.4 0.5 0.6

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)