# Kmeans++

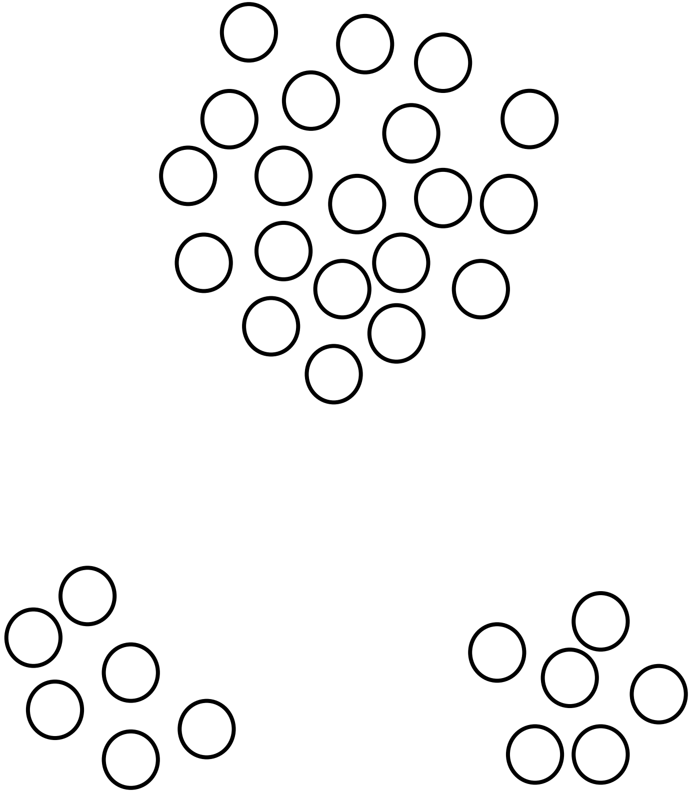
Boston University CS 506 - Lance Galletti

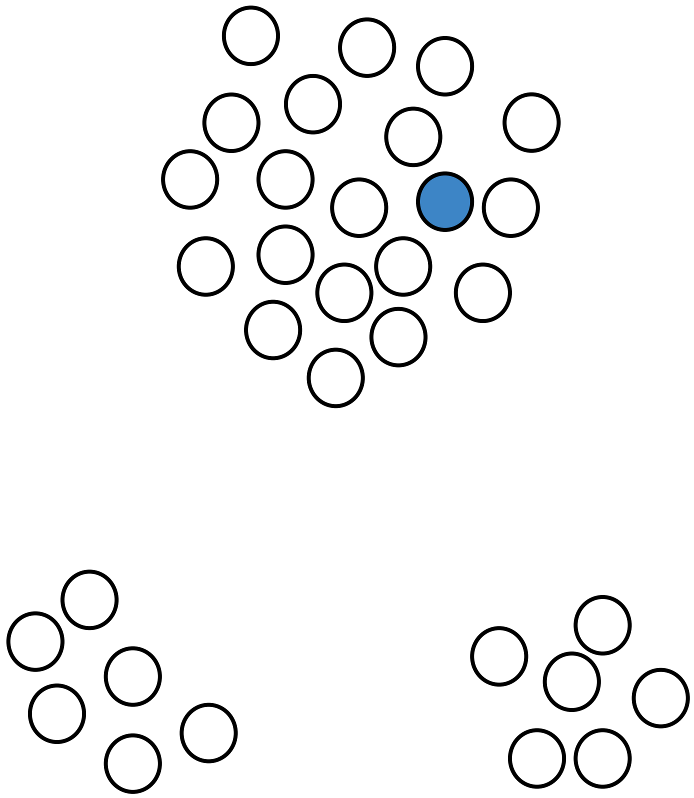
# K-means - Lloyd's Algorithm

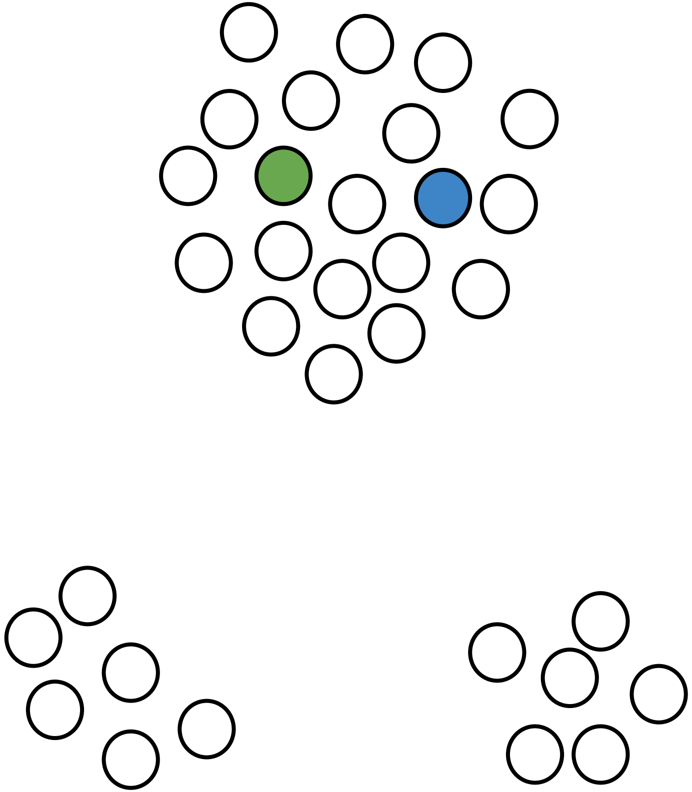
Q1: Will this algorithm always converge?

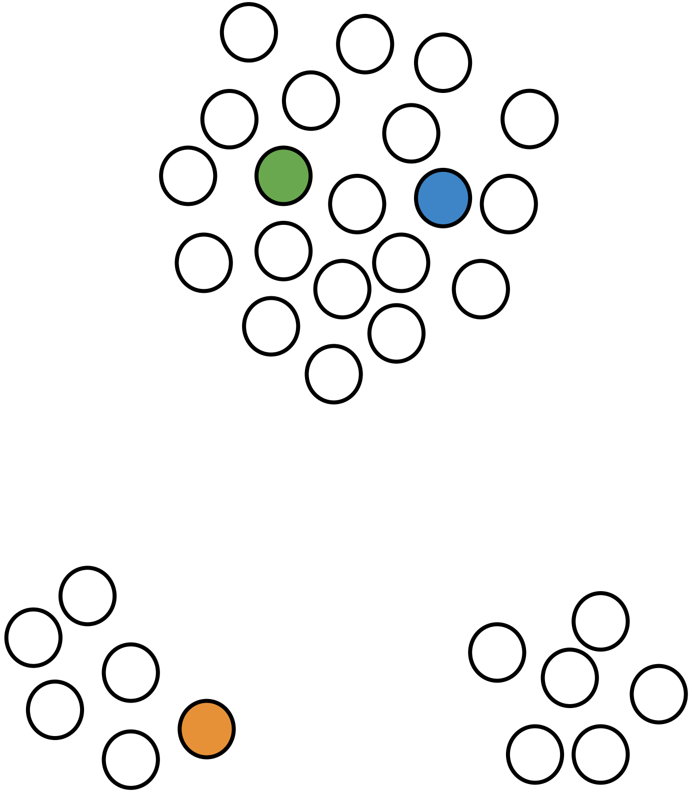
# K-means - Lloyd's Algorithm

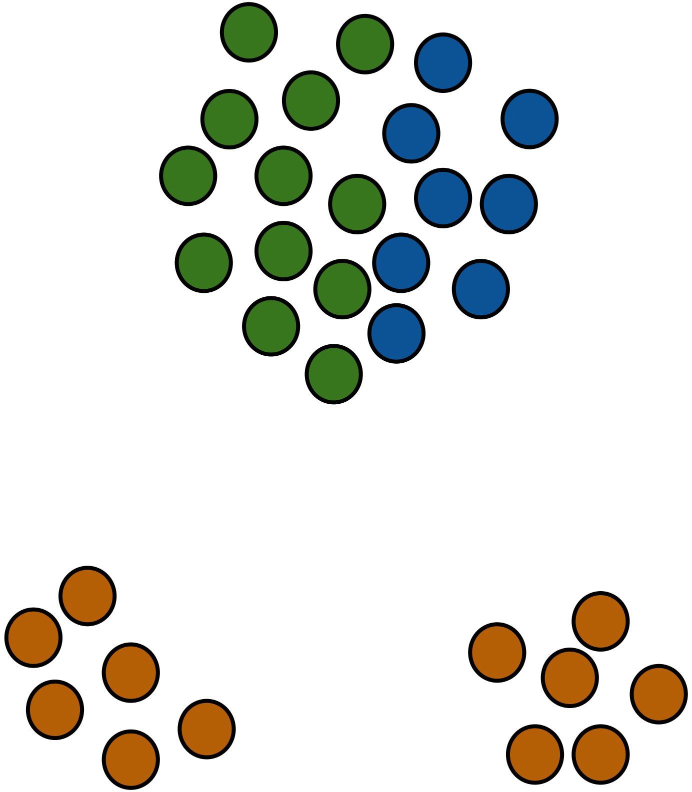
Q2: Will this always converge to the optimal solution?



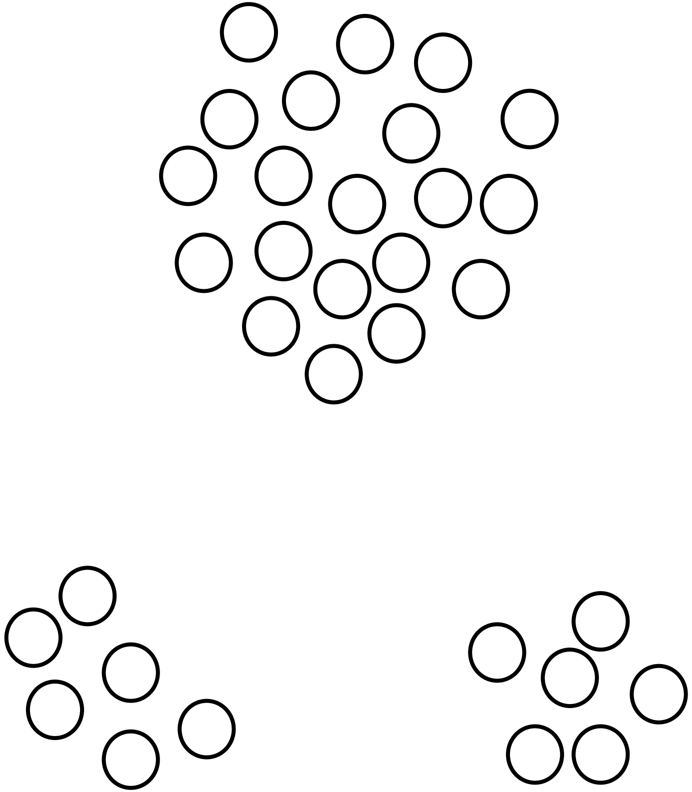


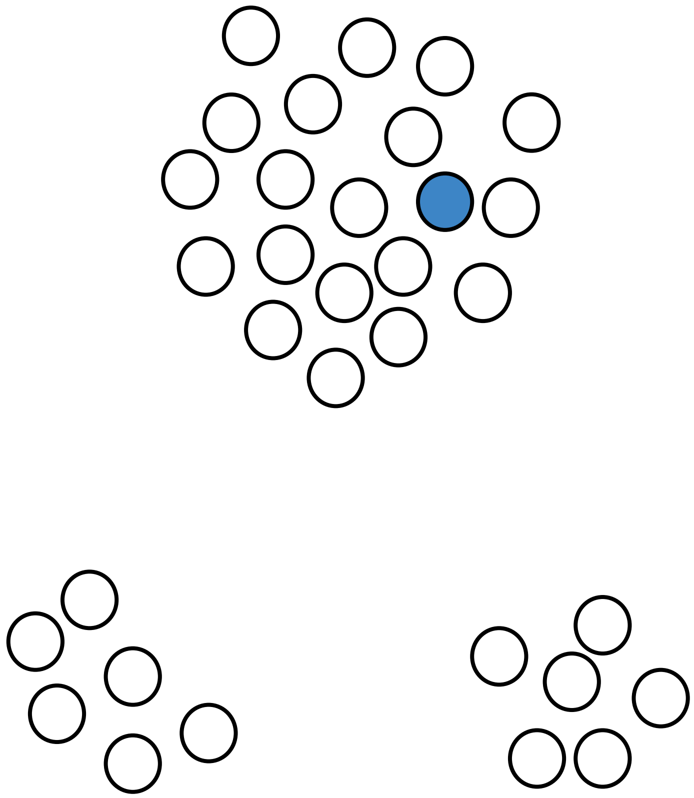


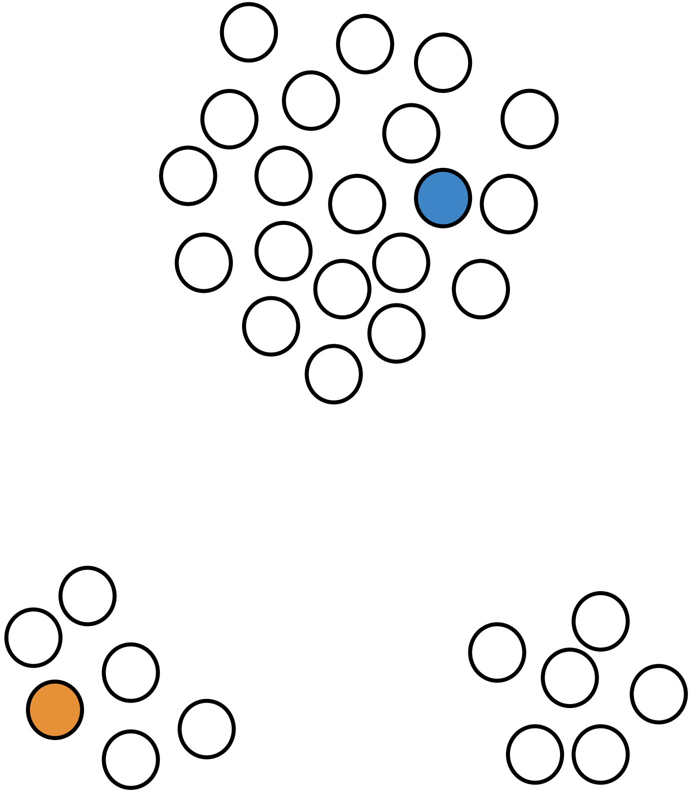


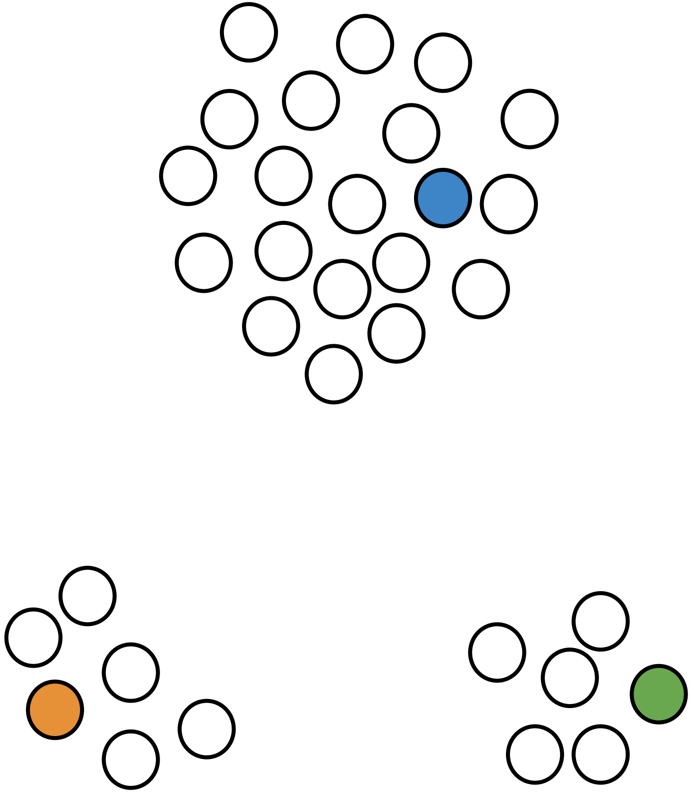


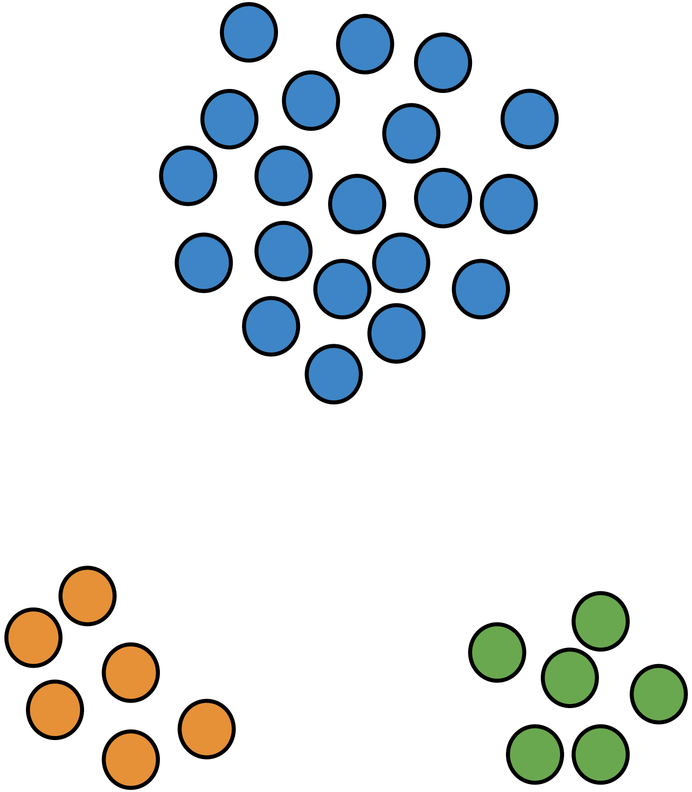
# What’s the problem?



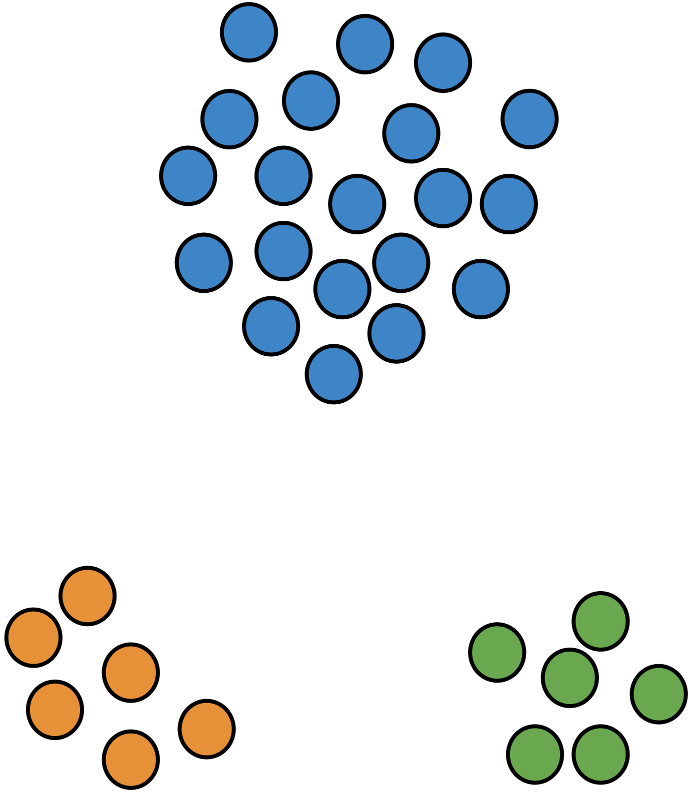




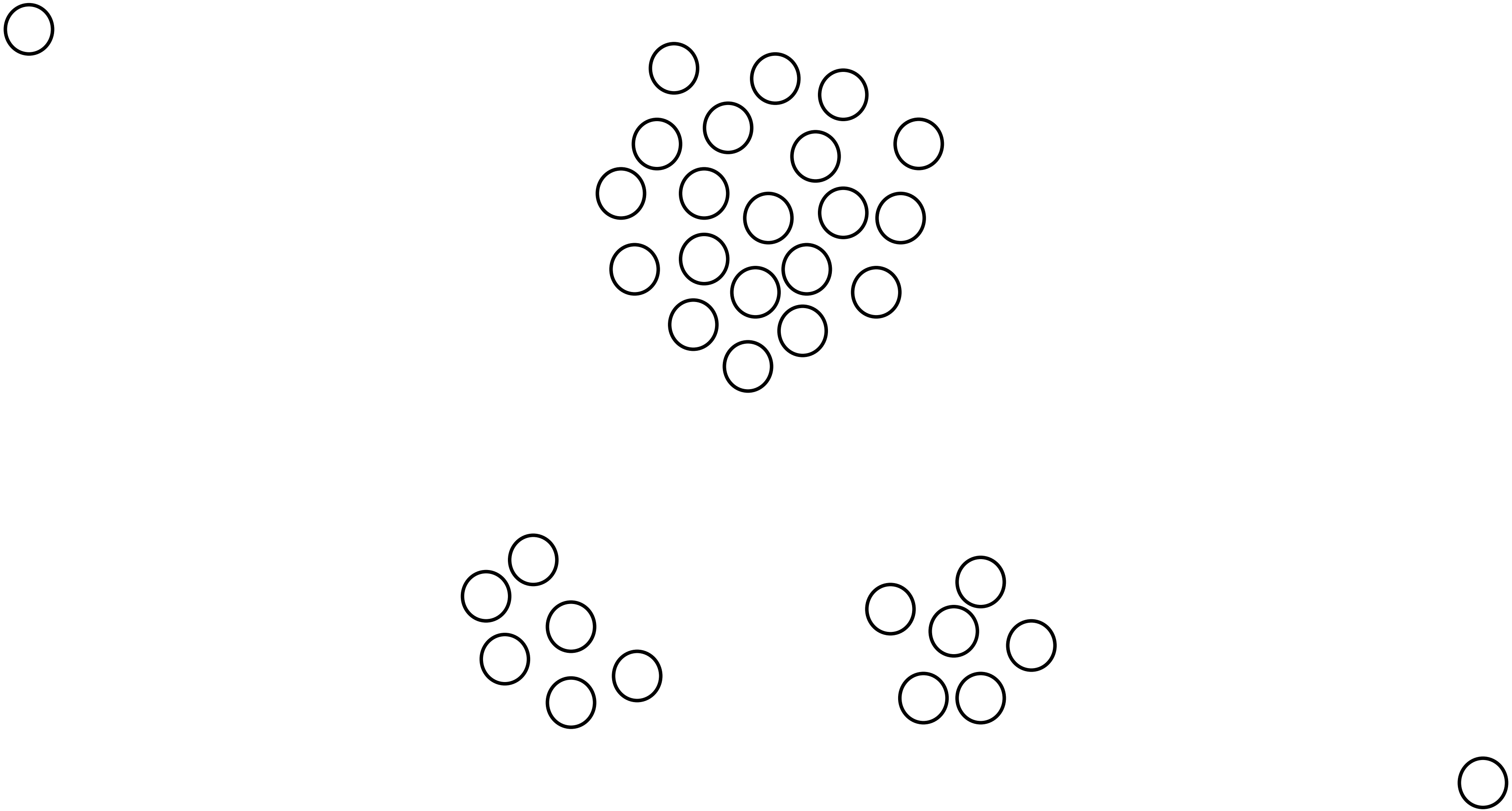


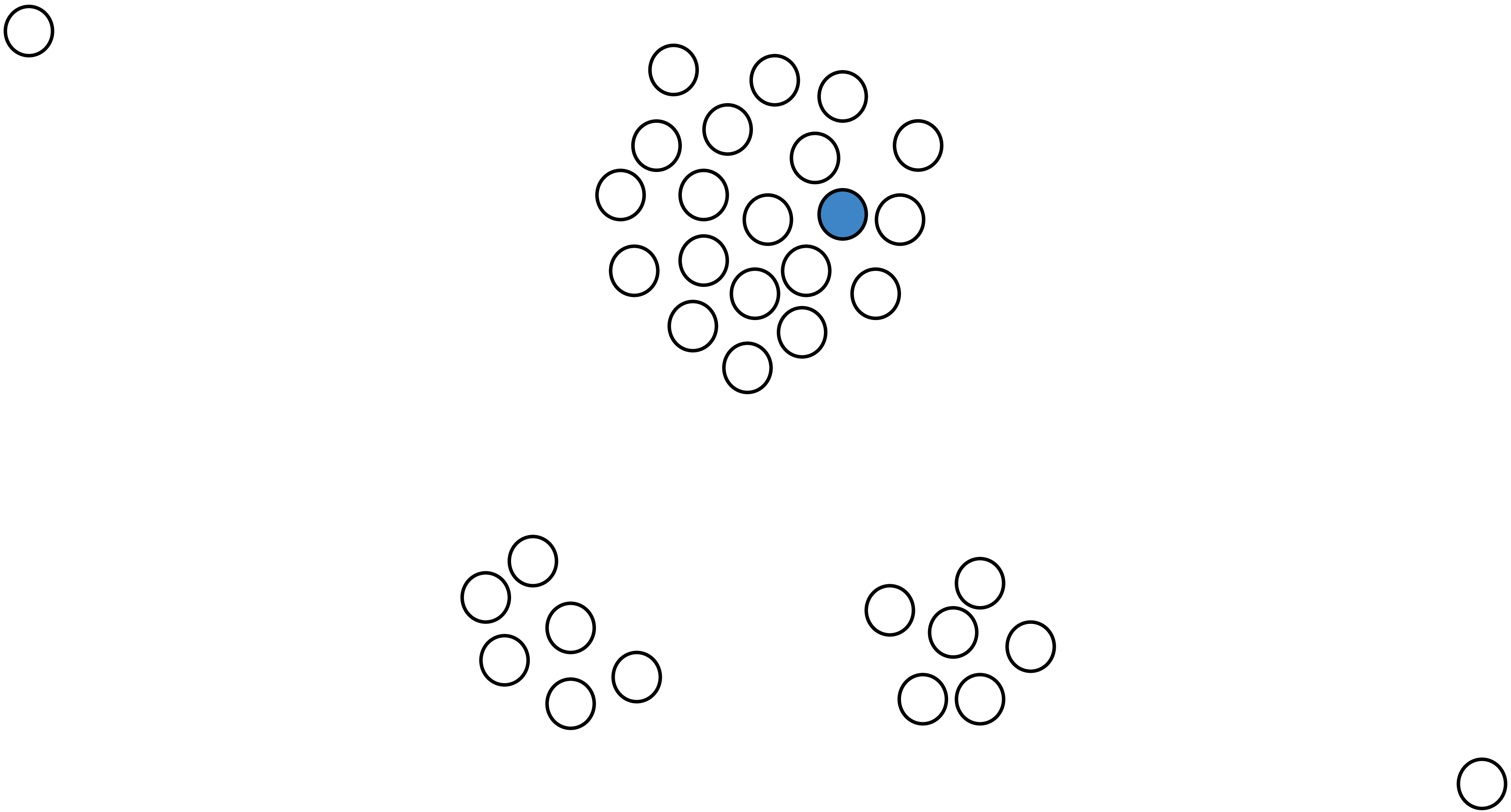


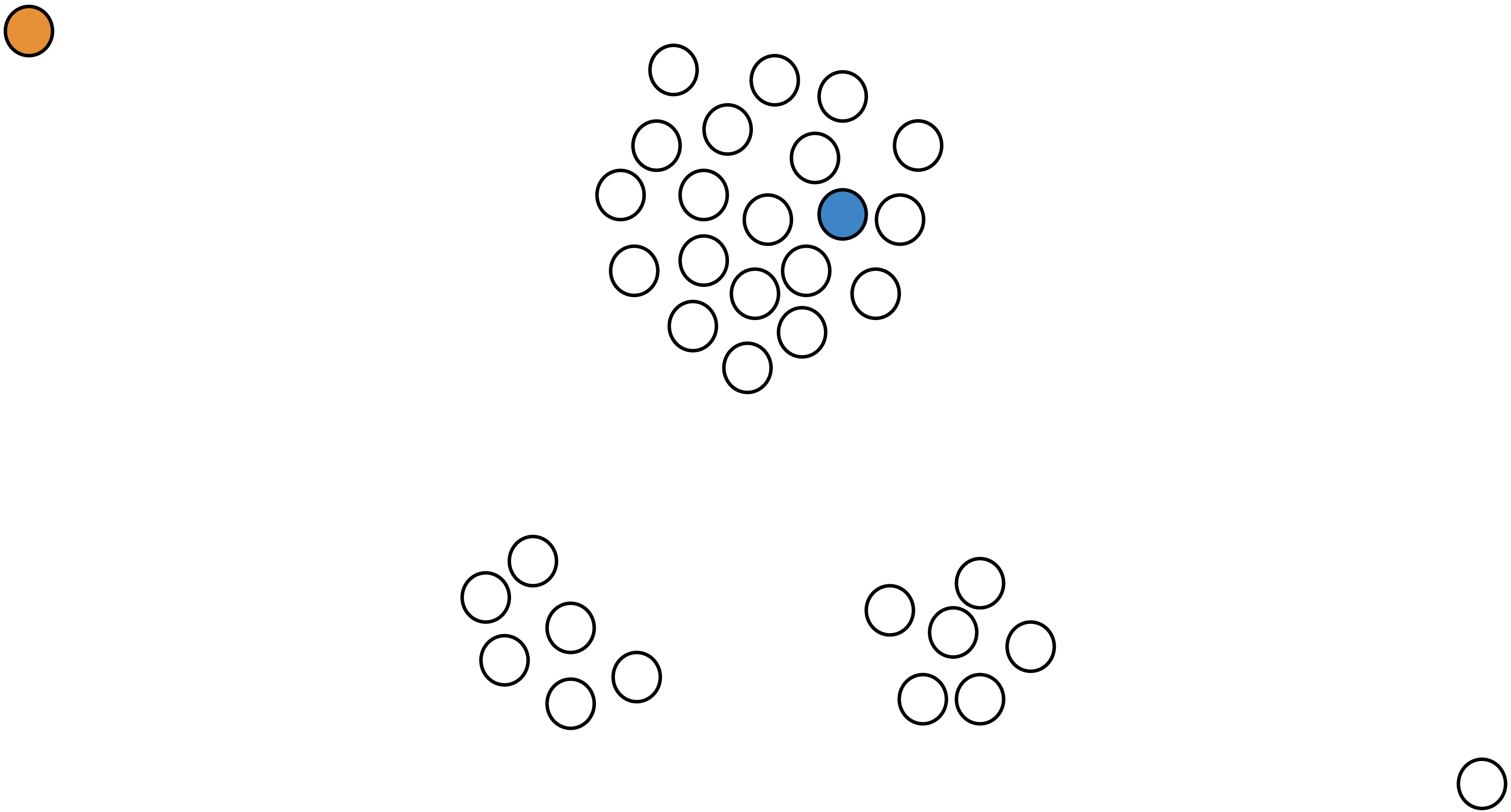
# Farthest First Traversal

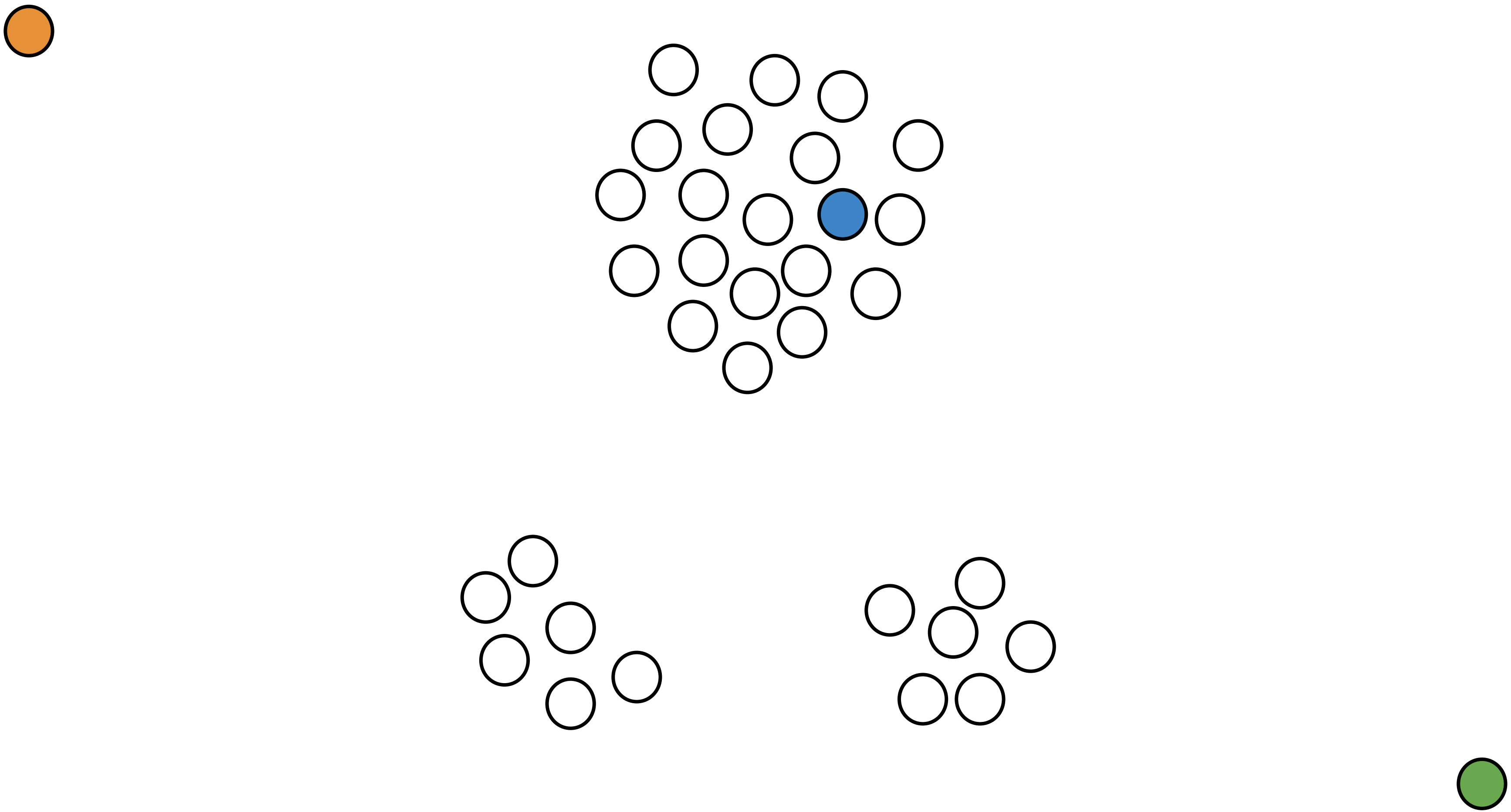


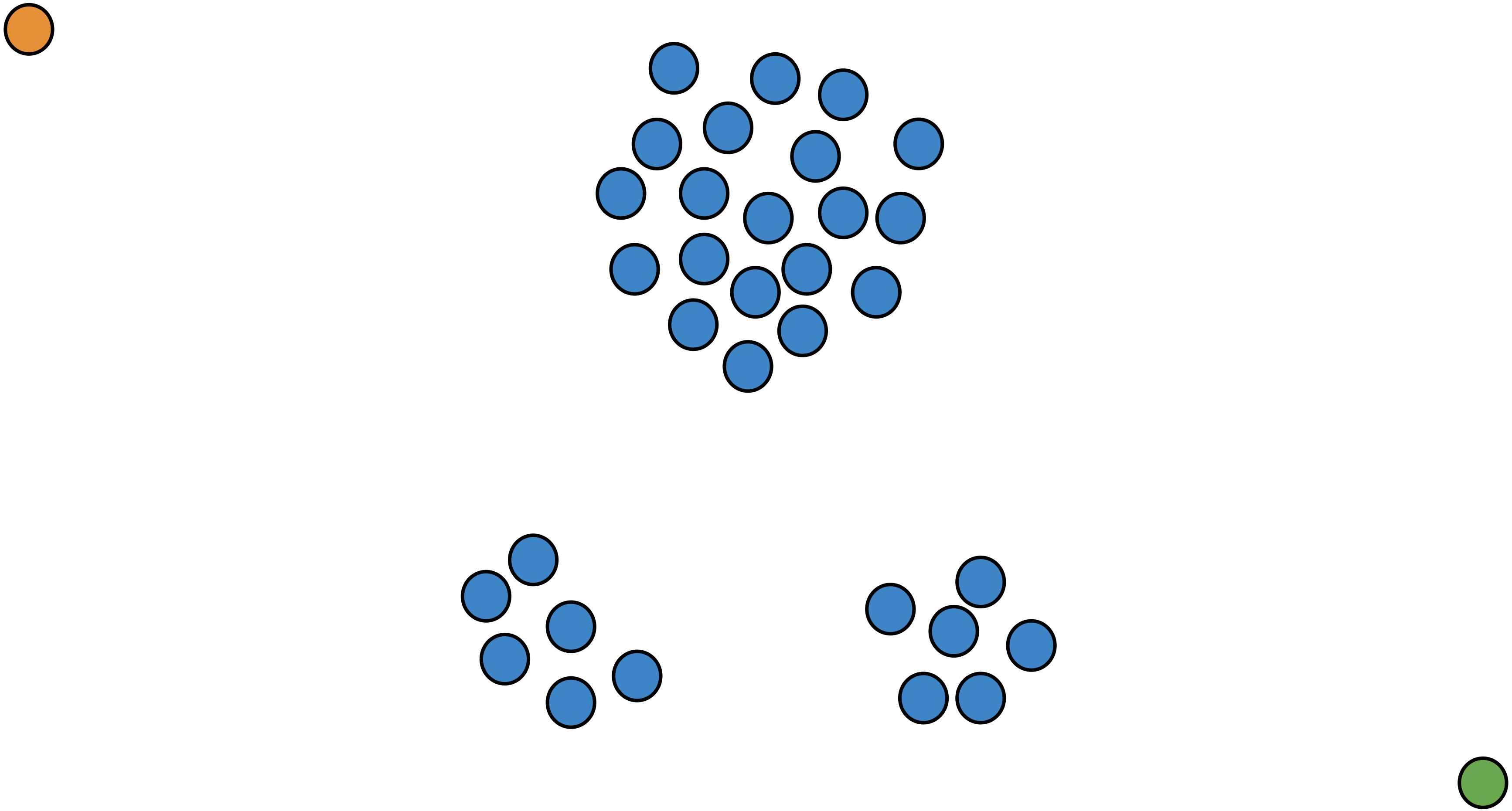
# But…



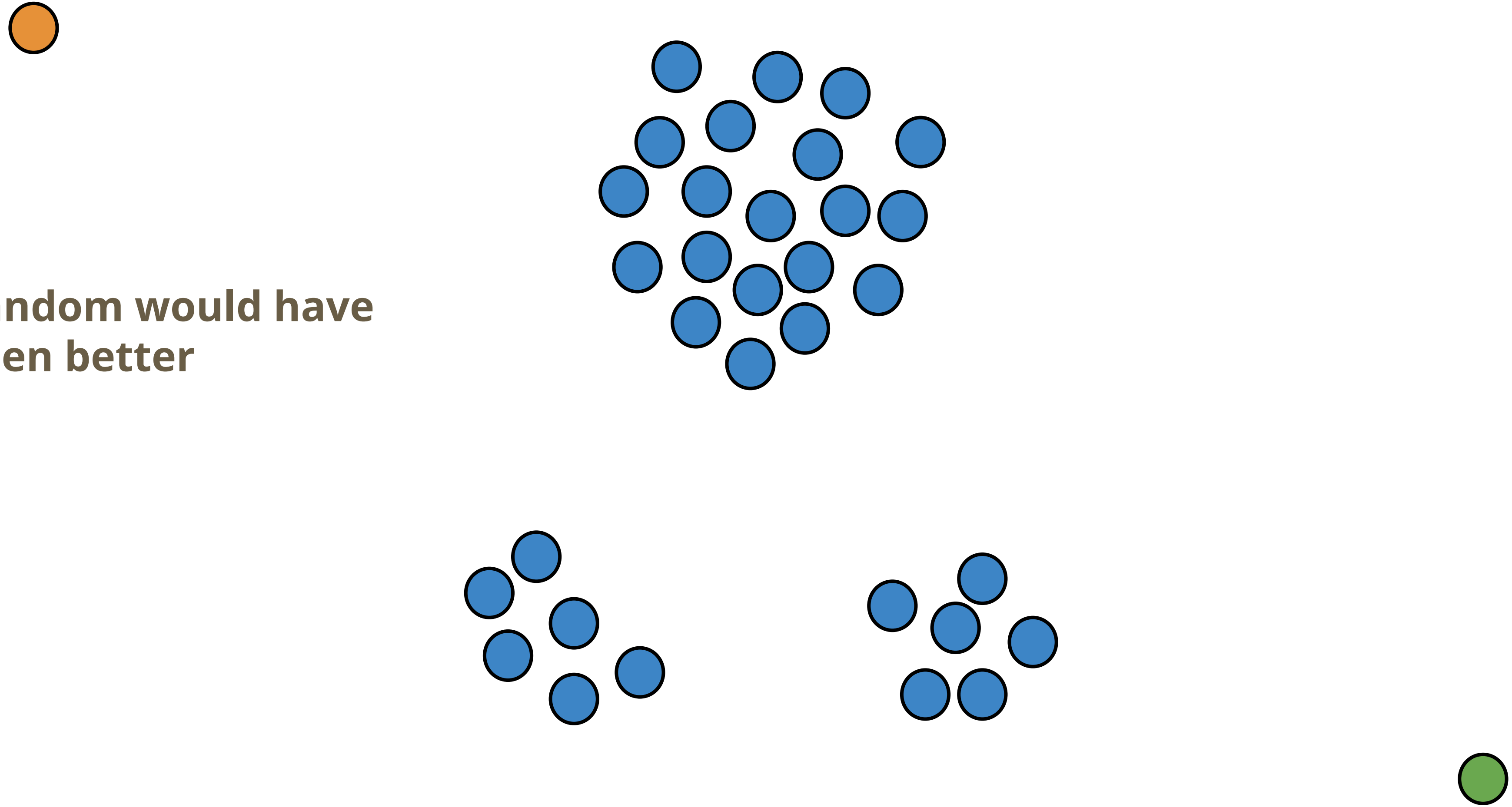








**Random would have been better**

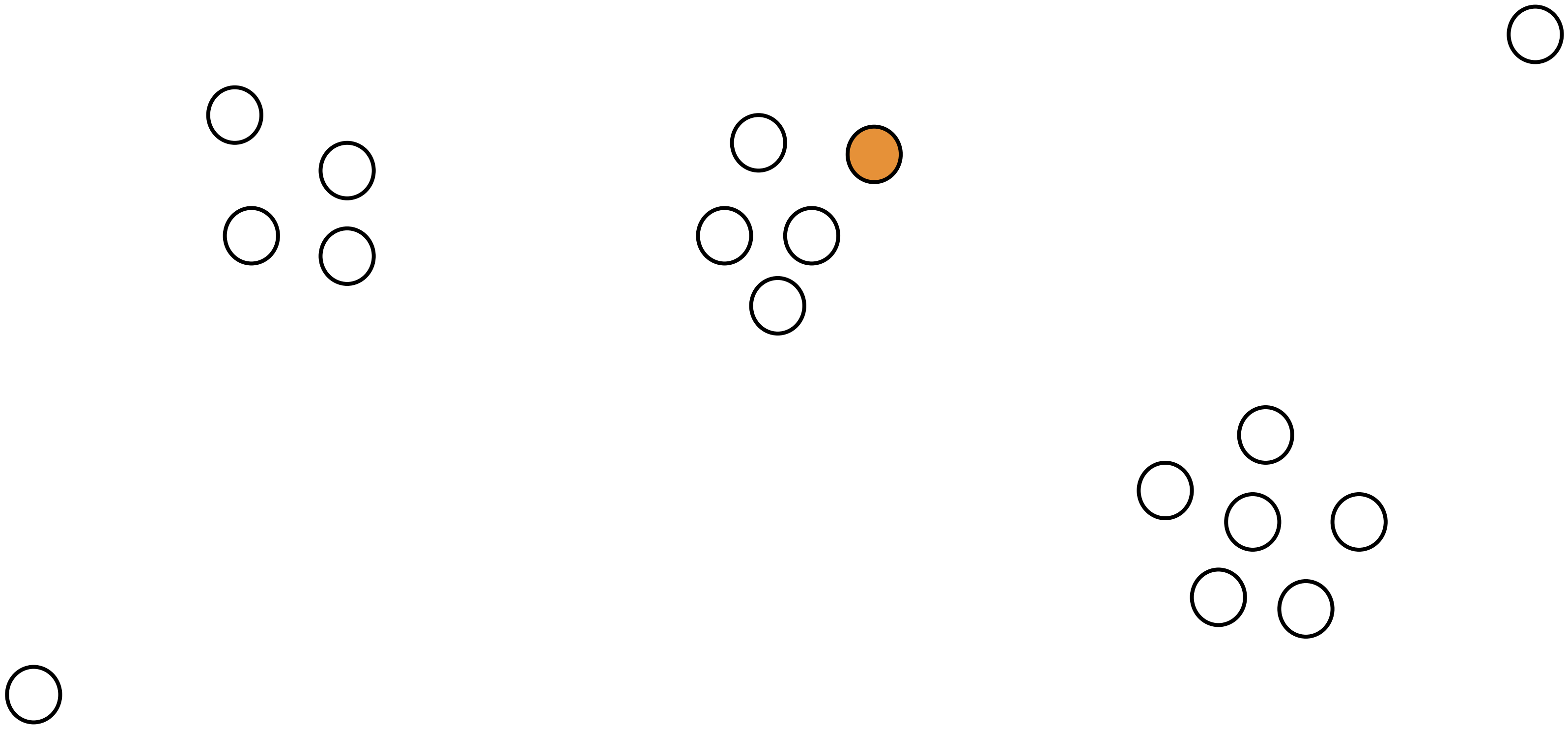


# K-means++

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++



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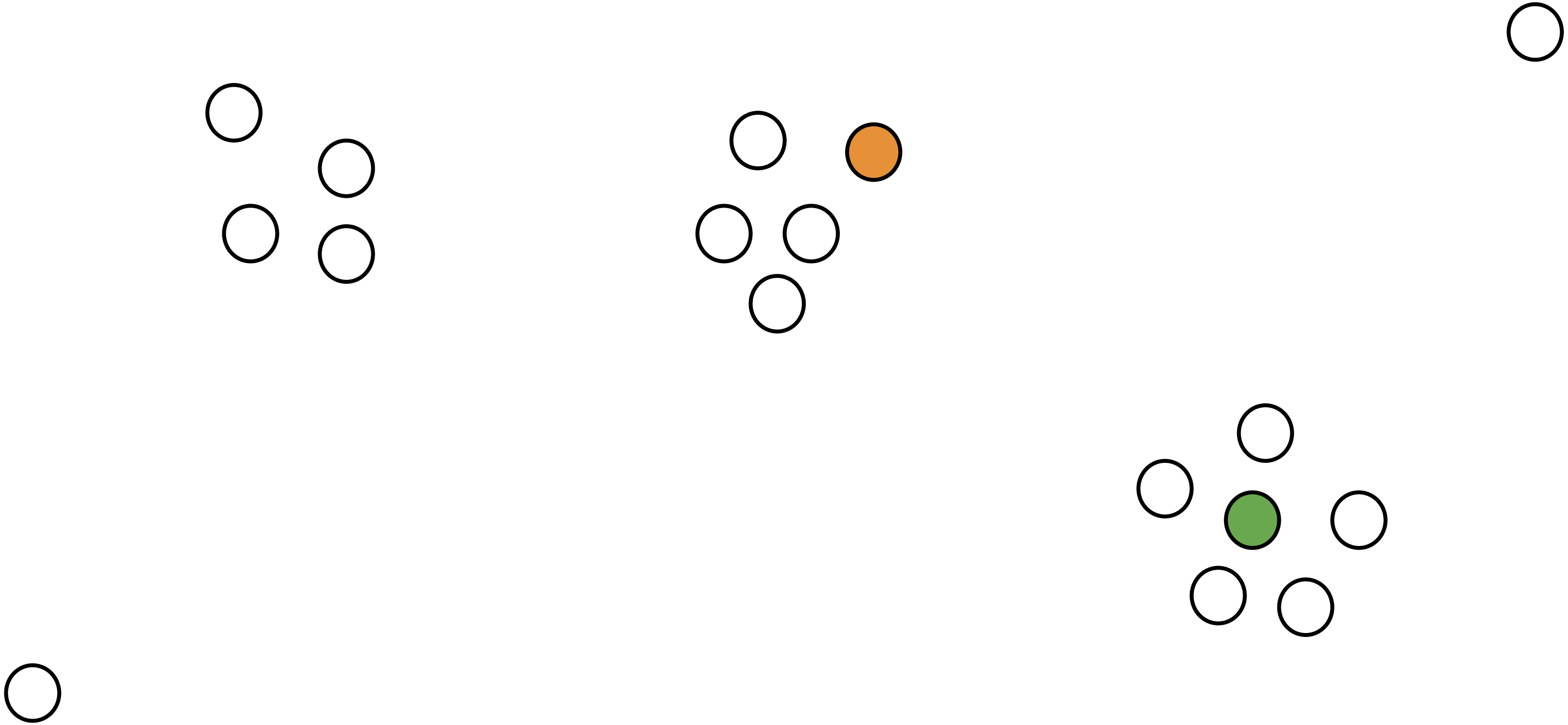

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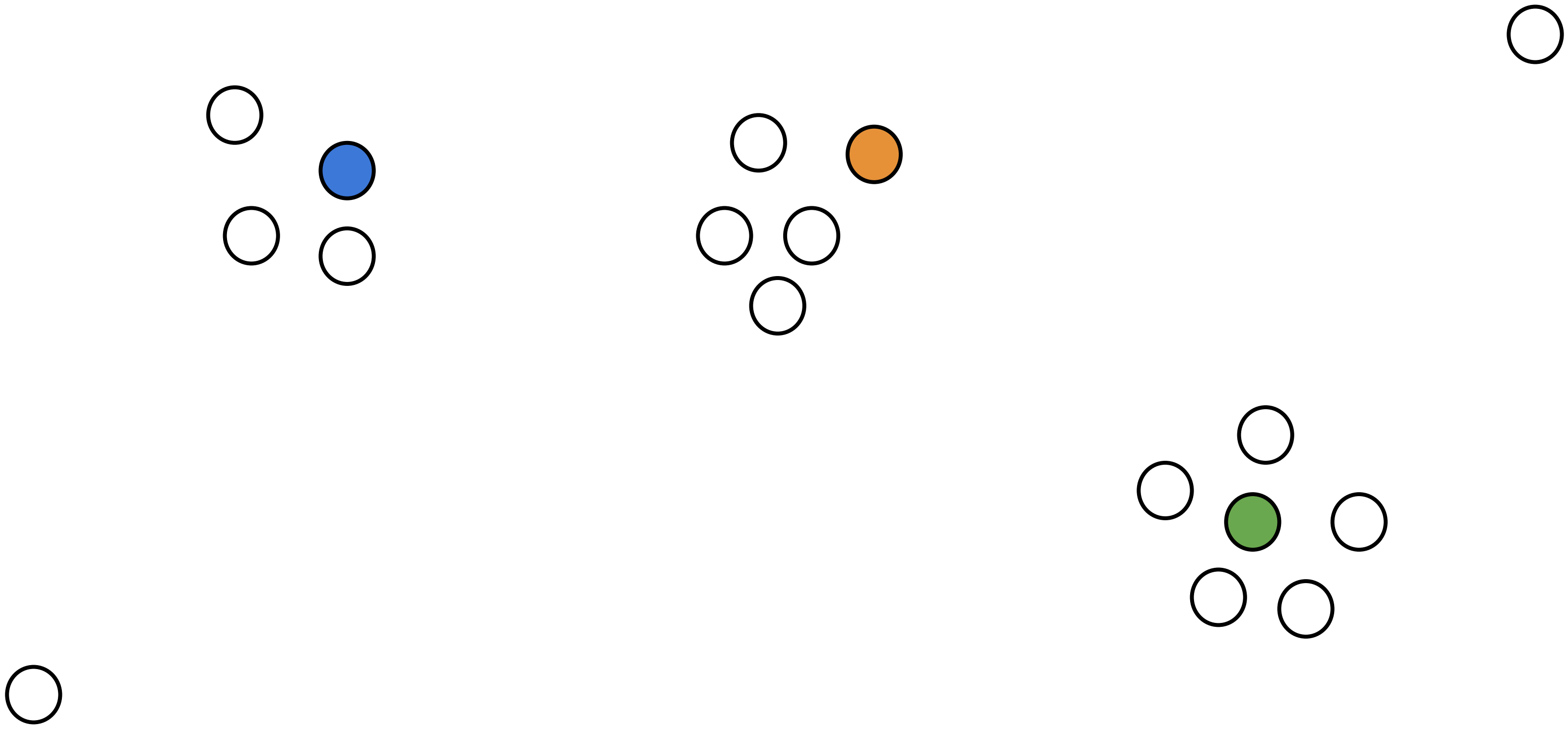

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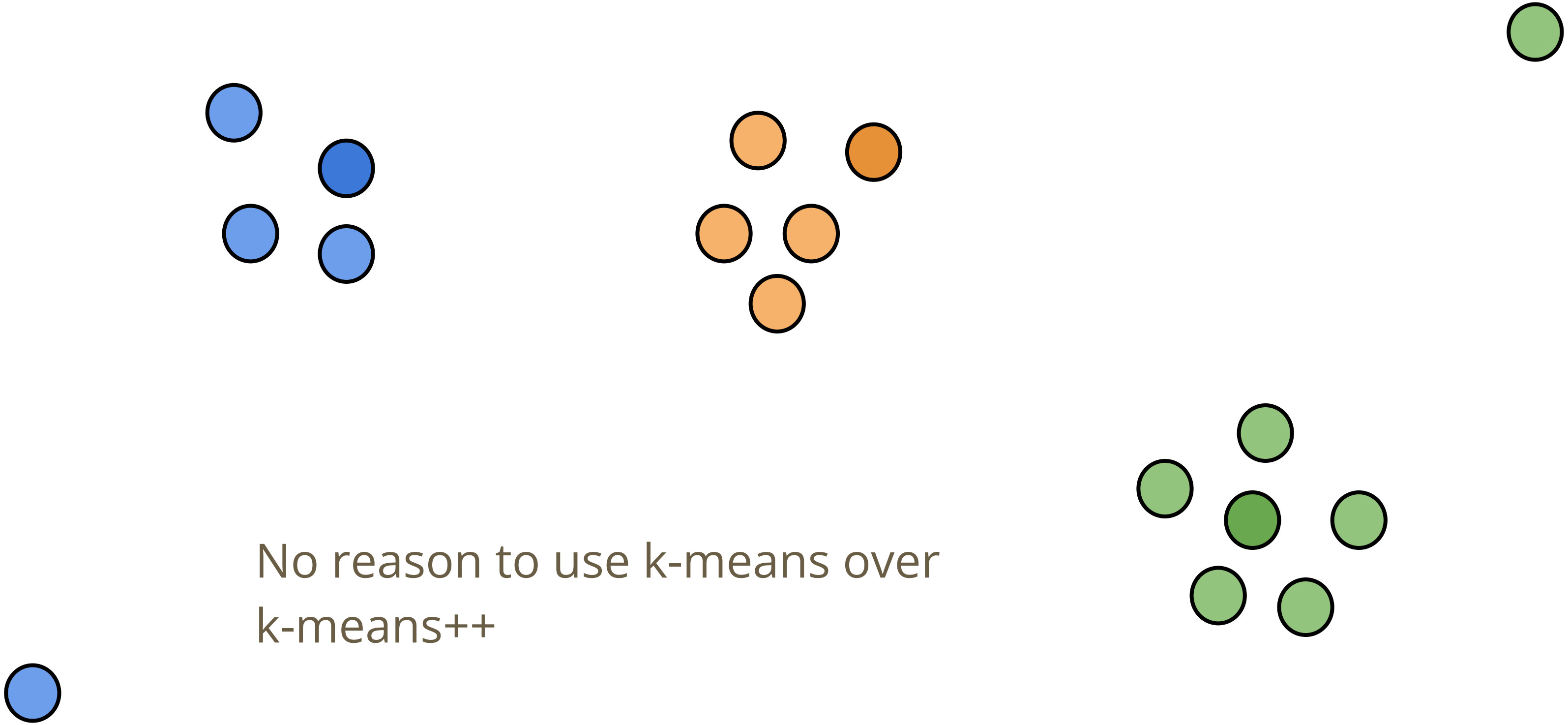

No reason to use k-means over
k-means++

# 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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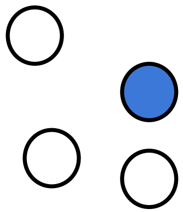

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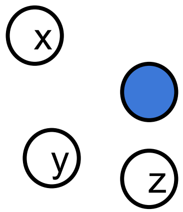
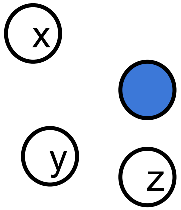



$$D(x)^2 = 3^2 = 9$$
$$D(y)^2 = 2^2 = 4$$
$$D(z)^2 = 1^2 = 1$$

# 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**?

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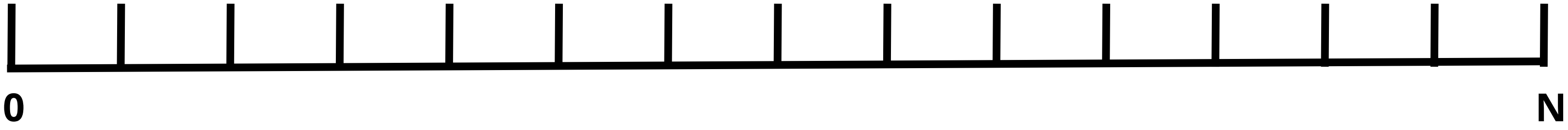

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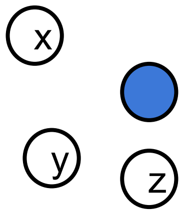


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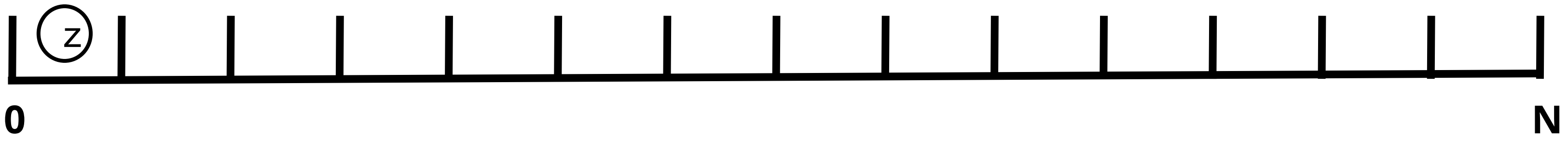

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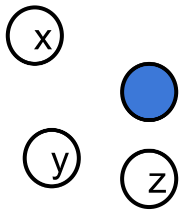


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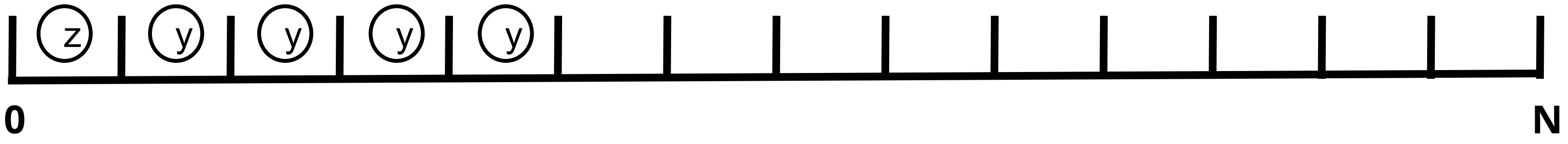

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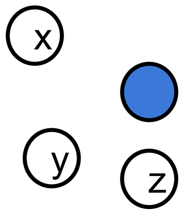


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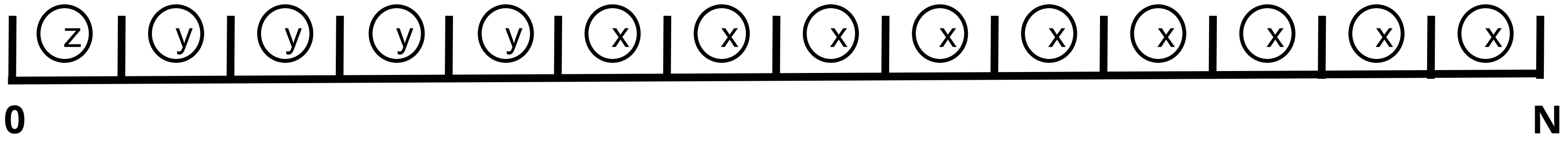

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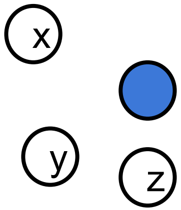


$$\mathbf{D(x)^2 = 3^2 = 9}$$
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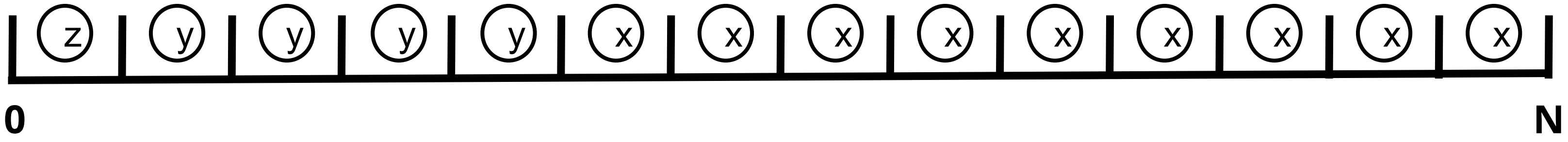
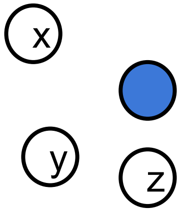



$$\mathbf{= D(x)^2 + D(y)^2 + D(z)^2 = 14}$$

# 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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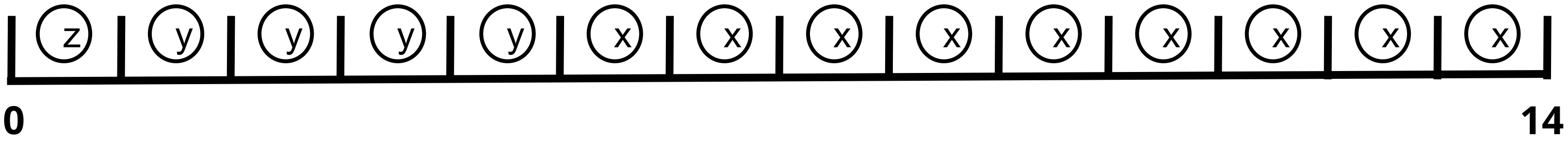
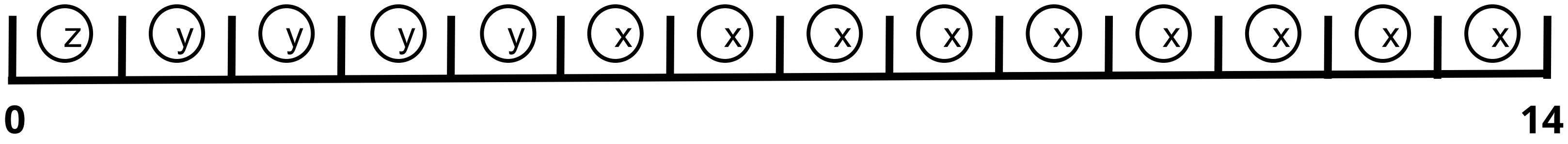


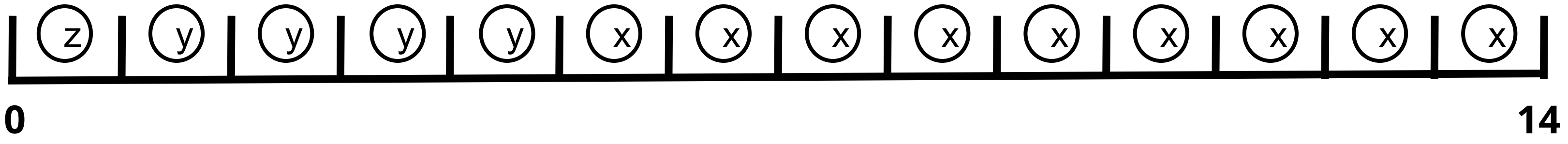
# K-means++

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



# K-means++

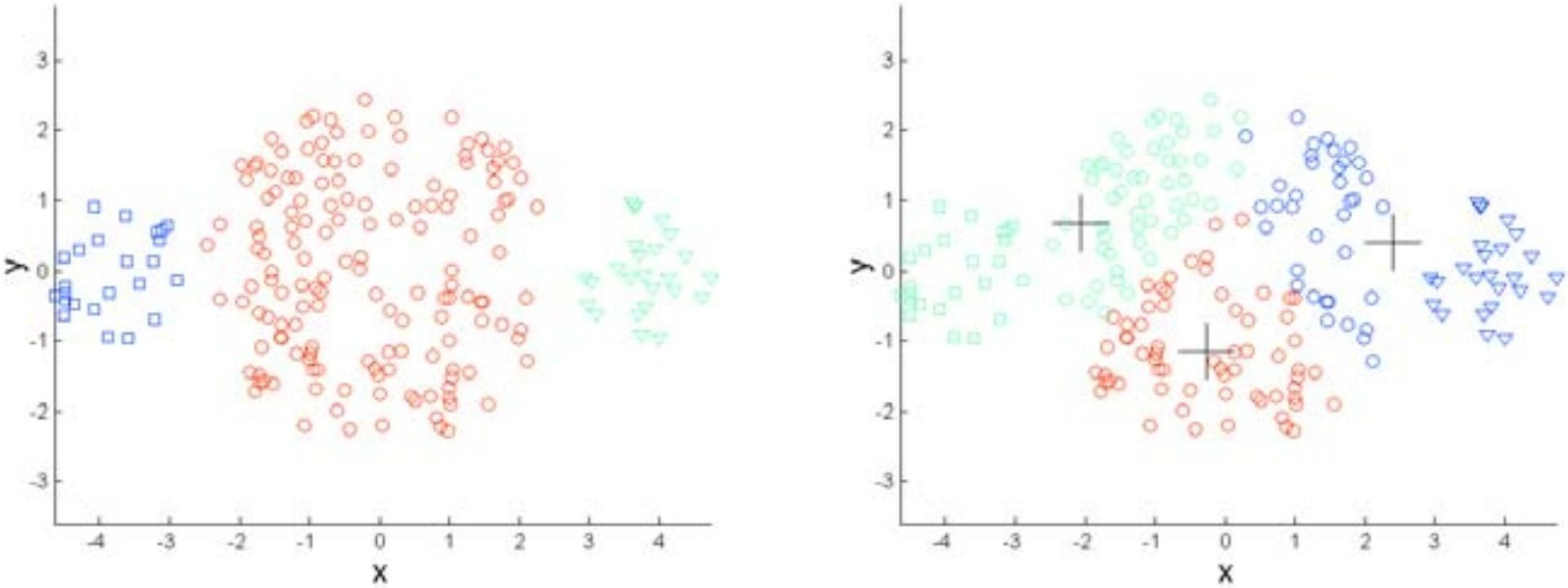
Q4: the black box returns “4” as the random number generated. Which point do we choose for the next center (x, y, or z) ?



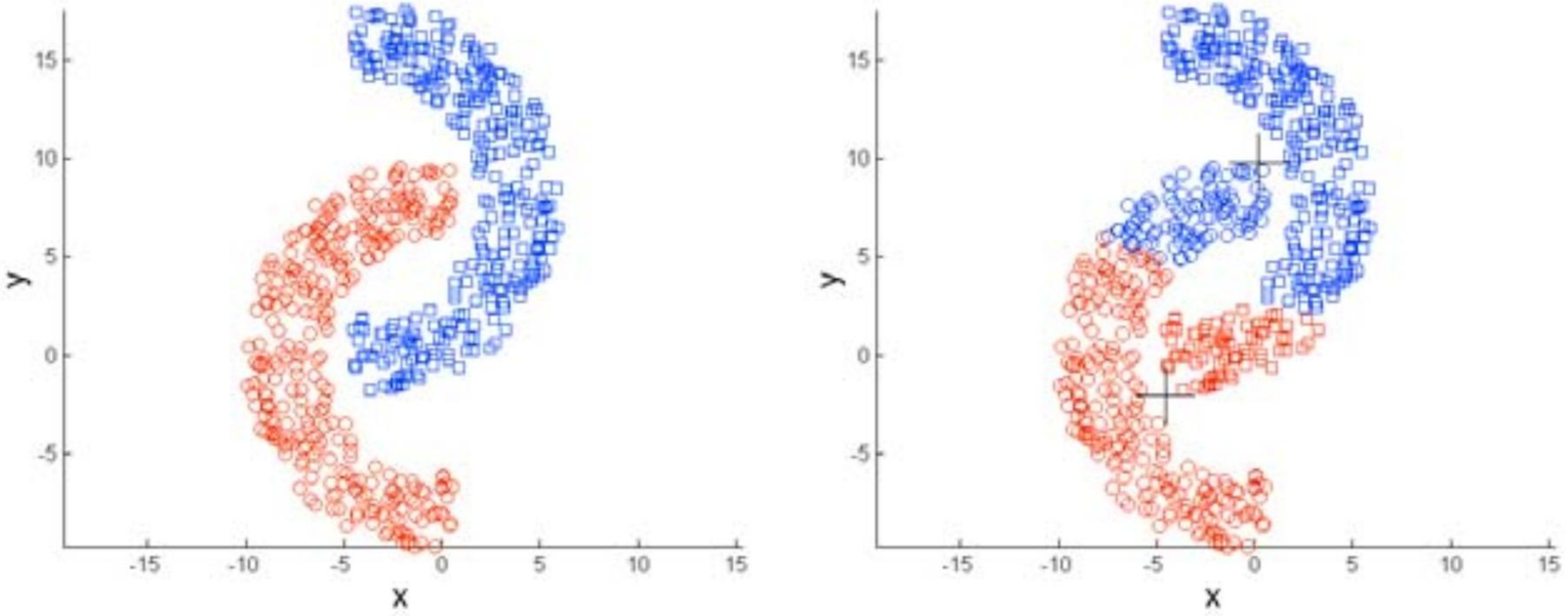
# K-means++

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

# K-means / K-means++ Limitations

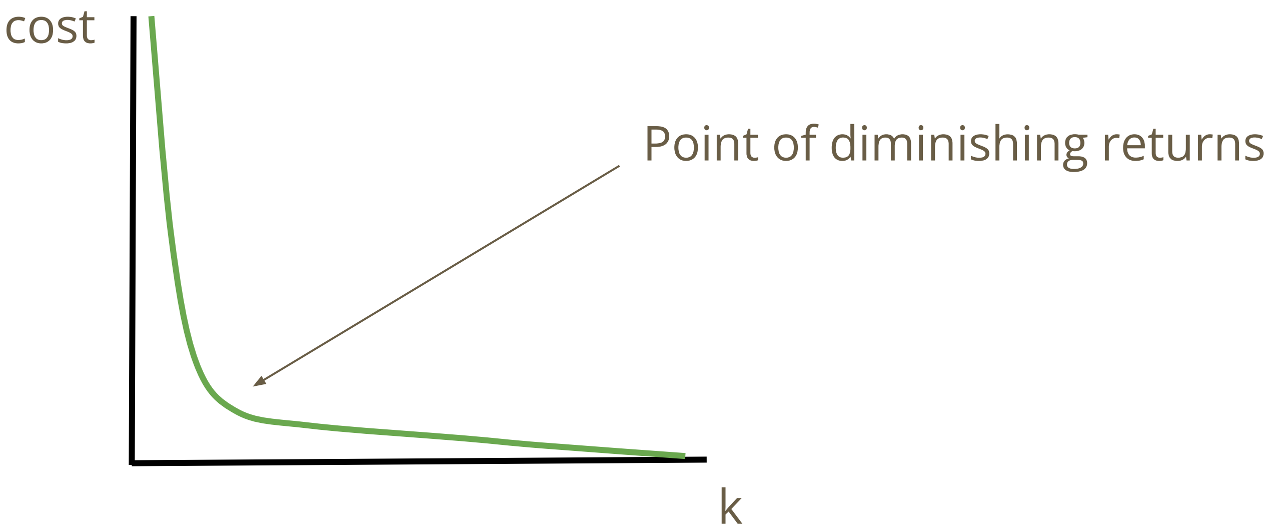


# K-means / K-means++ Limitations



# 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

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- **Similar** data points are in the **same cluster** ✅
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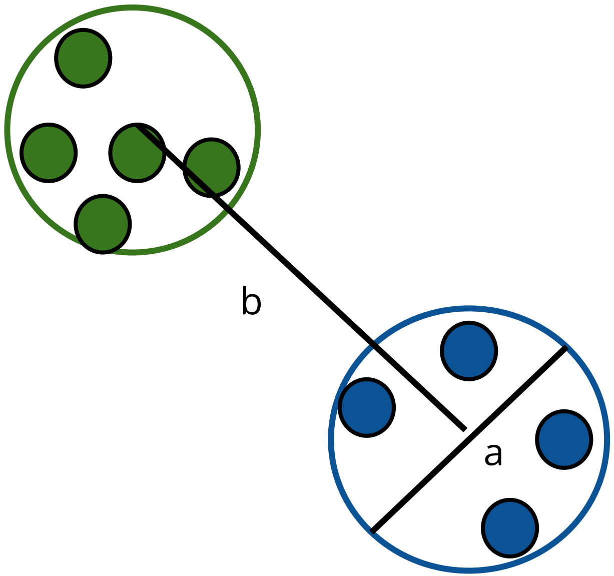
# Evaluation

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?

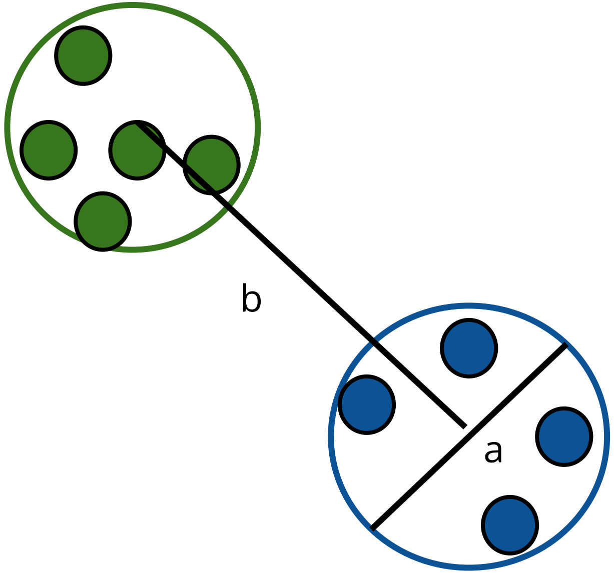
# Discuss - 5min

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

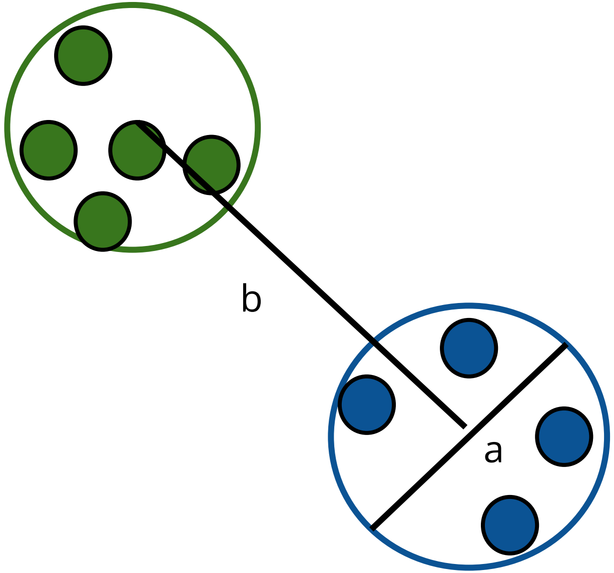



a: average within-cluster distance

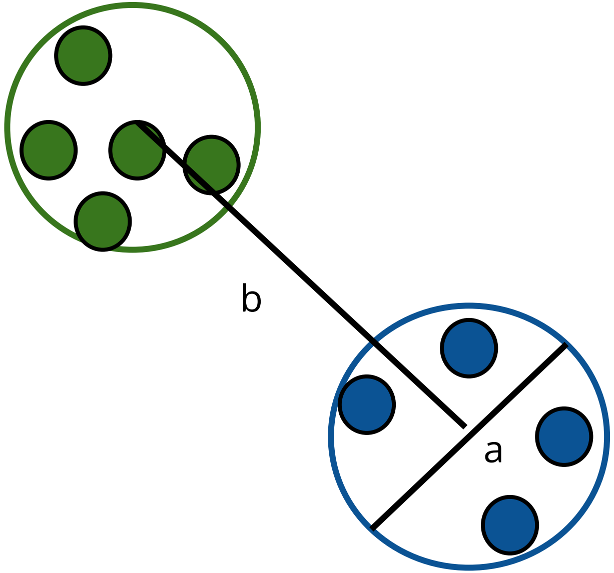
b: average intra-cluster distance



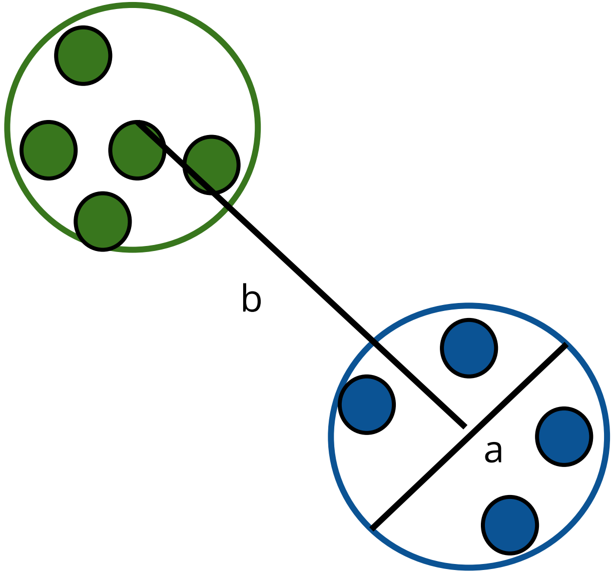

What does it mean for (b - a) to be 0?



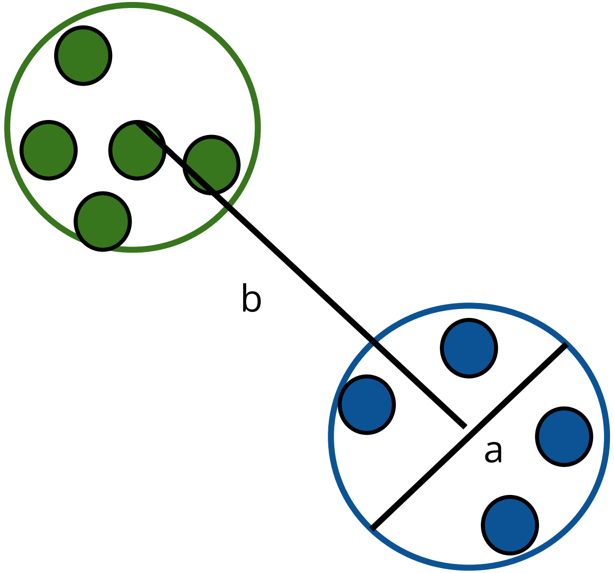

What does it mean for (b - a) to be large?



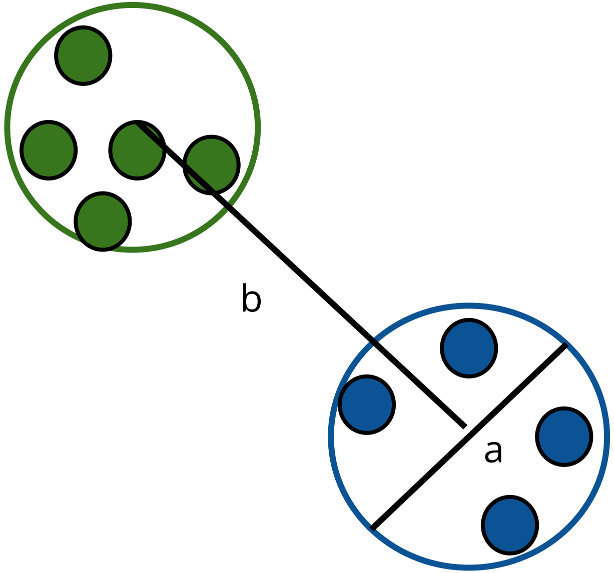

The value of (b-a) doesn't mean much by itself. Can we compare it to something so that the ratio becomes a value between 0 and 1?




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

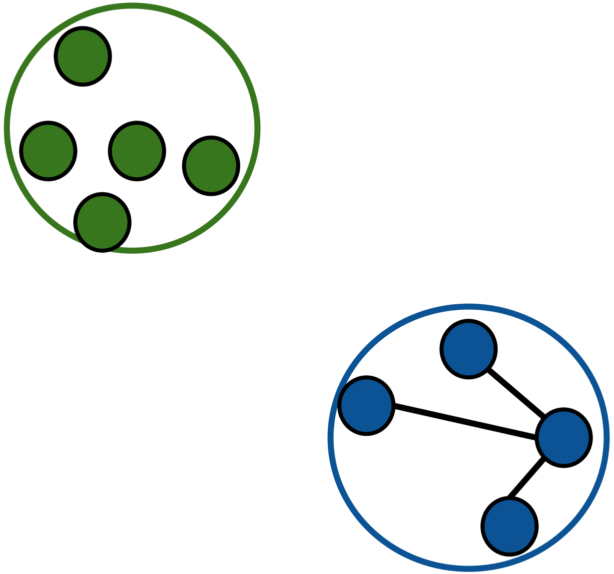



What does it mean for (b - a) / max(a, b) to be close to 1?



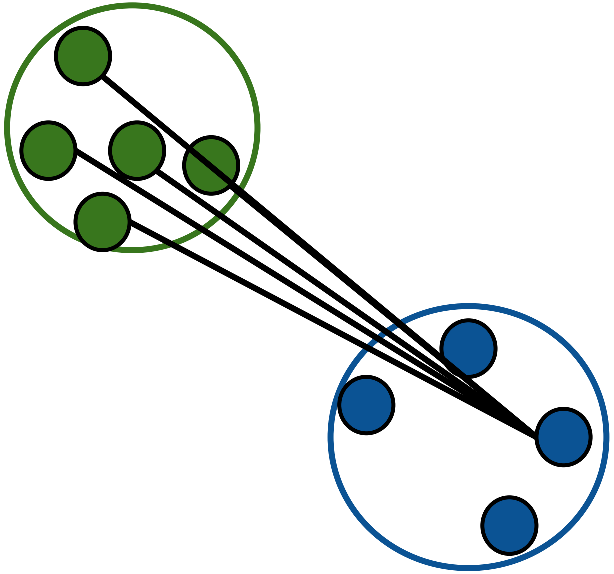

What does it mean for (b - a) / max(a, b) to be close to 0?

# Silhouette Scores



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

# Silhouette Scores

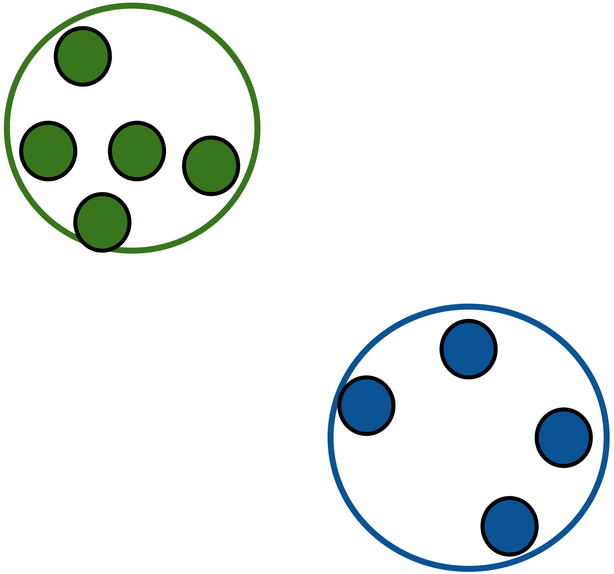


For each data point i:

$a_i$ : 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

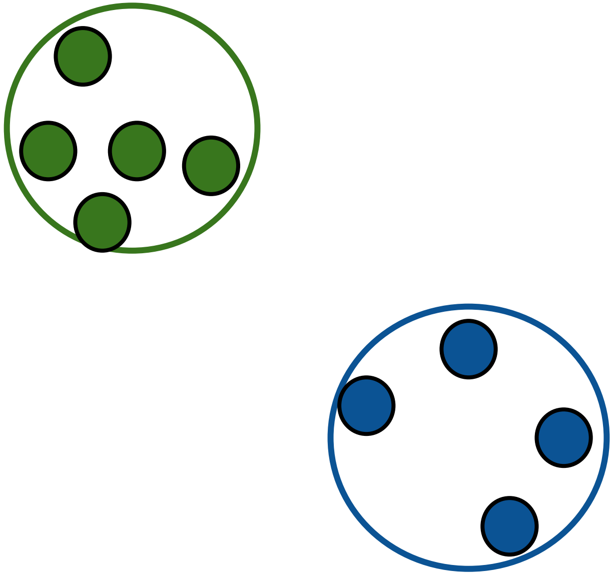
# Silhouette Scores



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



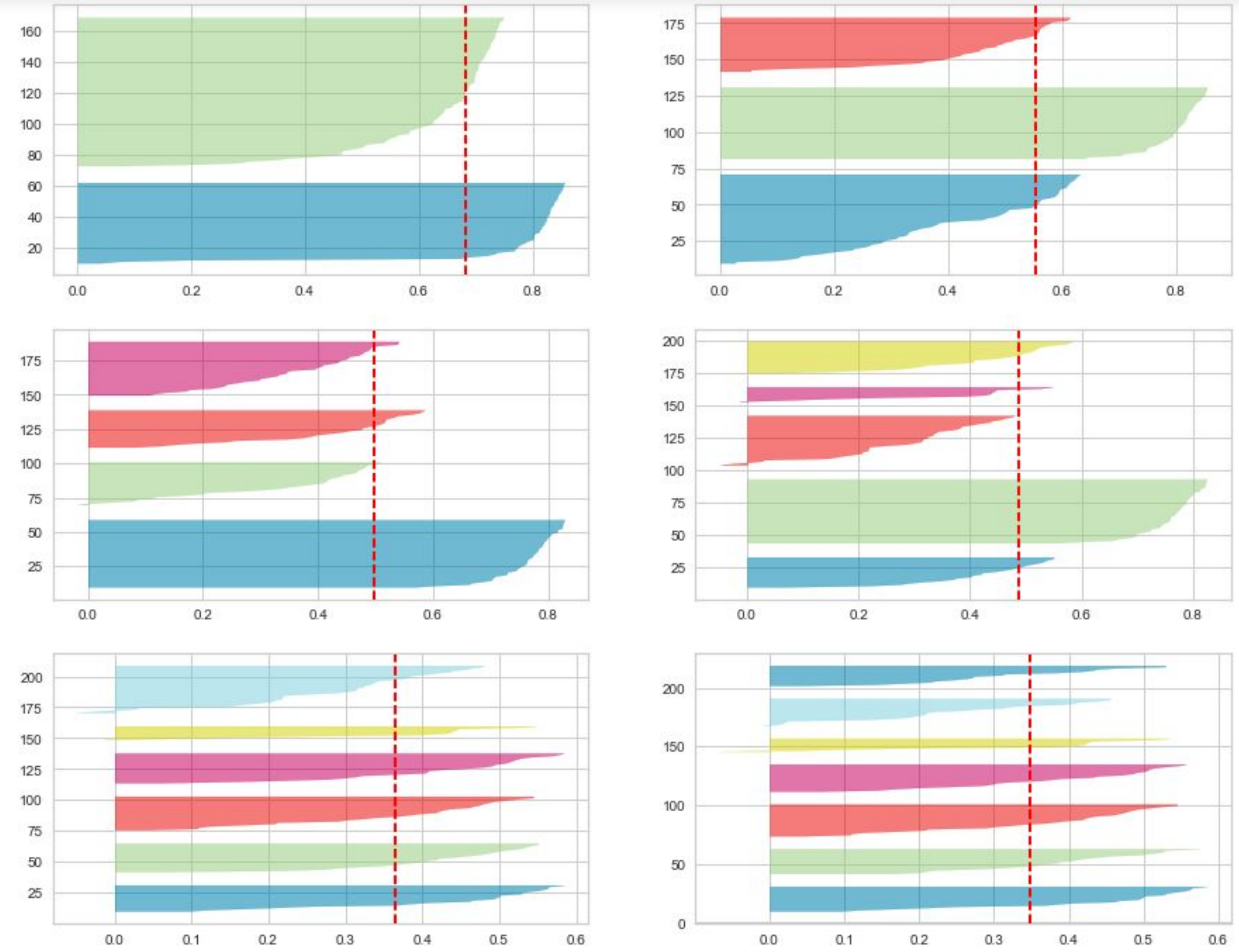
$s_i = (b_i - a_i) / \max(a_i, b_i)$

Silhouette score plot

OR

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

# Q5



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
200
0.1
0.3
0.5
0

# 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)