Automatically Choosing the Number of Clusters

DP-GMMs, DP-means, CH index
(see also: gap statistic)

slides by
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GMM with *k* Clusters

<u>Cluster 1</u>

Probability of generating a point from cluster 1 = π_1

Gaussian mean = μ_1

Gaussian covariance = Σ_1

…

<u>Cluster *k*</u>

Probability of generating a point from cluster k = π_k

Gaussian mean = μ_k

Gaussian covariance = Σ_k

How to generate points from this GMM:

1. Flip biased k-sided coin (the sides have probabilities $\pi_1, \ldots, \pi_k$)
2. Let Z be the side that we got (it is some value $1, \ldots, k$)
3. Sample 1 point from Gaussian mean μ_Z, covariance Σ_Z

Learning a GMM

Demo

Automatic Selection of *k*

Dirichlet Process Gaussian Mixture Model (DP-GMM):

- Number of clusters is effectively random, and *can grow with the amount of data you have!*

- While you don't have to choose *k*, you have to choose a different parameter which says basically how likely new points are to form new clusters vs join existing clusters

DP-GMM High-Level Idea

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<u>Cluster 1</u>

Probability of generating a point from cluster 1 = π_1

Gaussian mean = μ_1

Gaussian covariance = Σ_1

DP-GMM High-Level Idea

	Cluster 1	Cluster 2
Probability of generating a point from cluster 1	$= \pi_1$	π_2
Gaussian mean	$= \mu_1$	μ_2
Gaussian covariance	$= \Sigma_1$	Σ_2

DP-GMM High-Level Idea

	Cluster 1	Cluster 2	Cluster 3
Probability of generating a point from cluster 1 = π_1		π_2	π_3
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Remark: For any given dataset, when learning the DP-GMM, there aren't going to be an infinite number of clusters found

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- An example of a *Bayesian nonparametric model* (roughly: a generative model with an *infinite number of parameters*, where the *parameters are random*)

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This is what's implemented in R (package *dpmixsim*)

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k-means approximates
(a special case of) learning GMM's.

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What approximates learning DP-GMMs?

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What approximates learning DP-GMMs?

This next algorithm will give you a sense of how we get around specifying the number of clusters directly

DP-means

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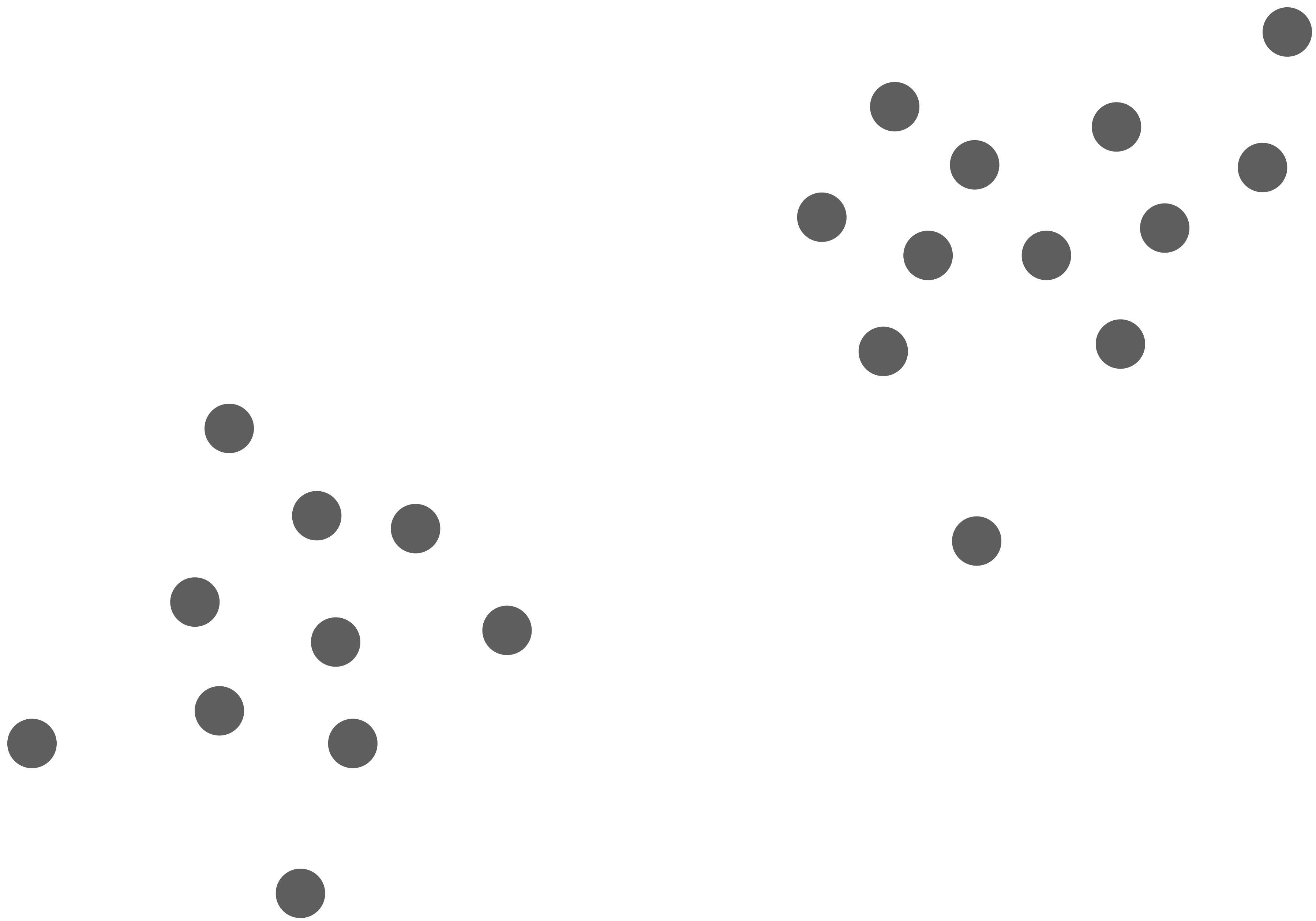
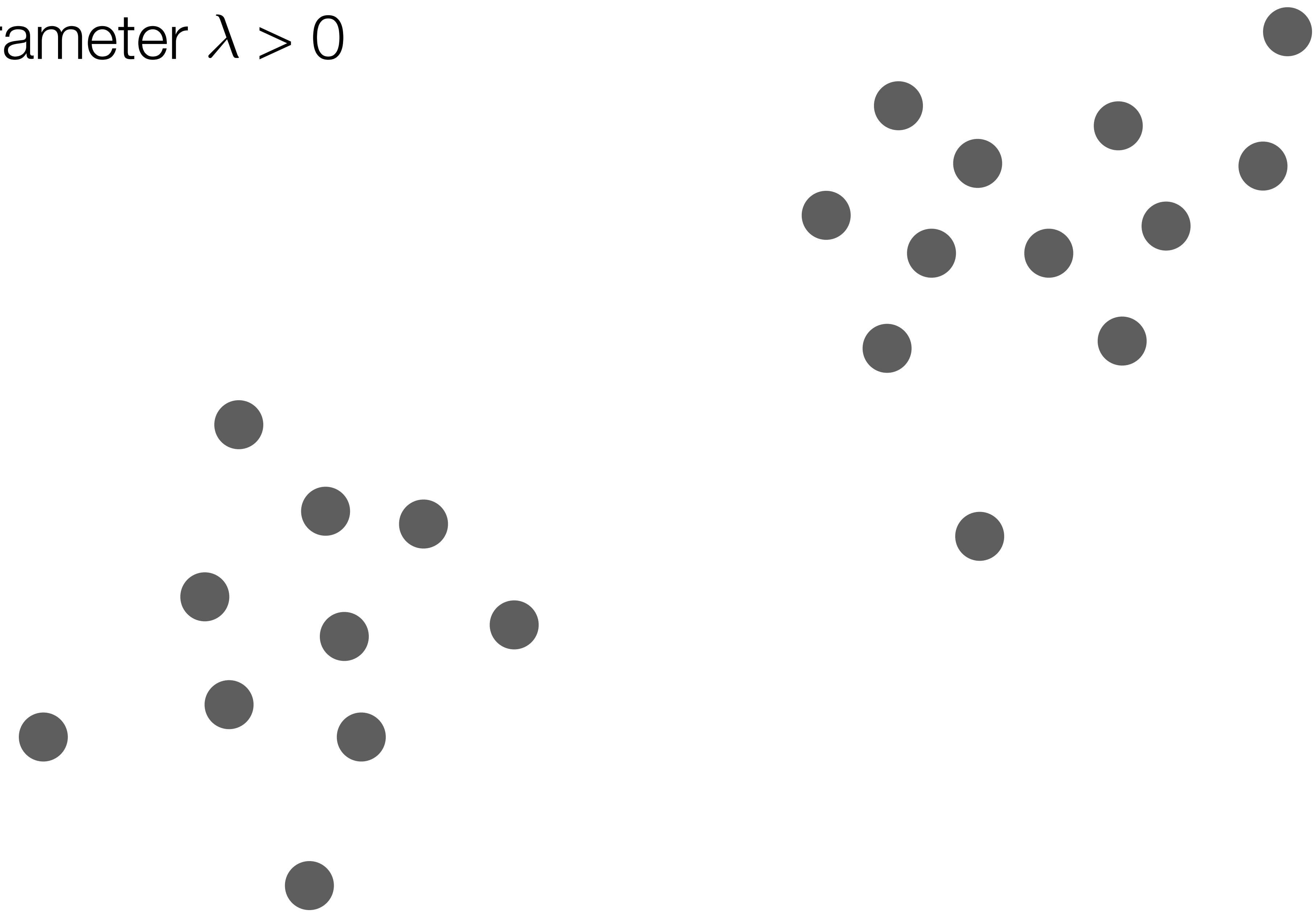


DP-means

Step 0. Pick concentration parameter $\lambda > 0$



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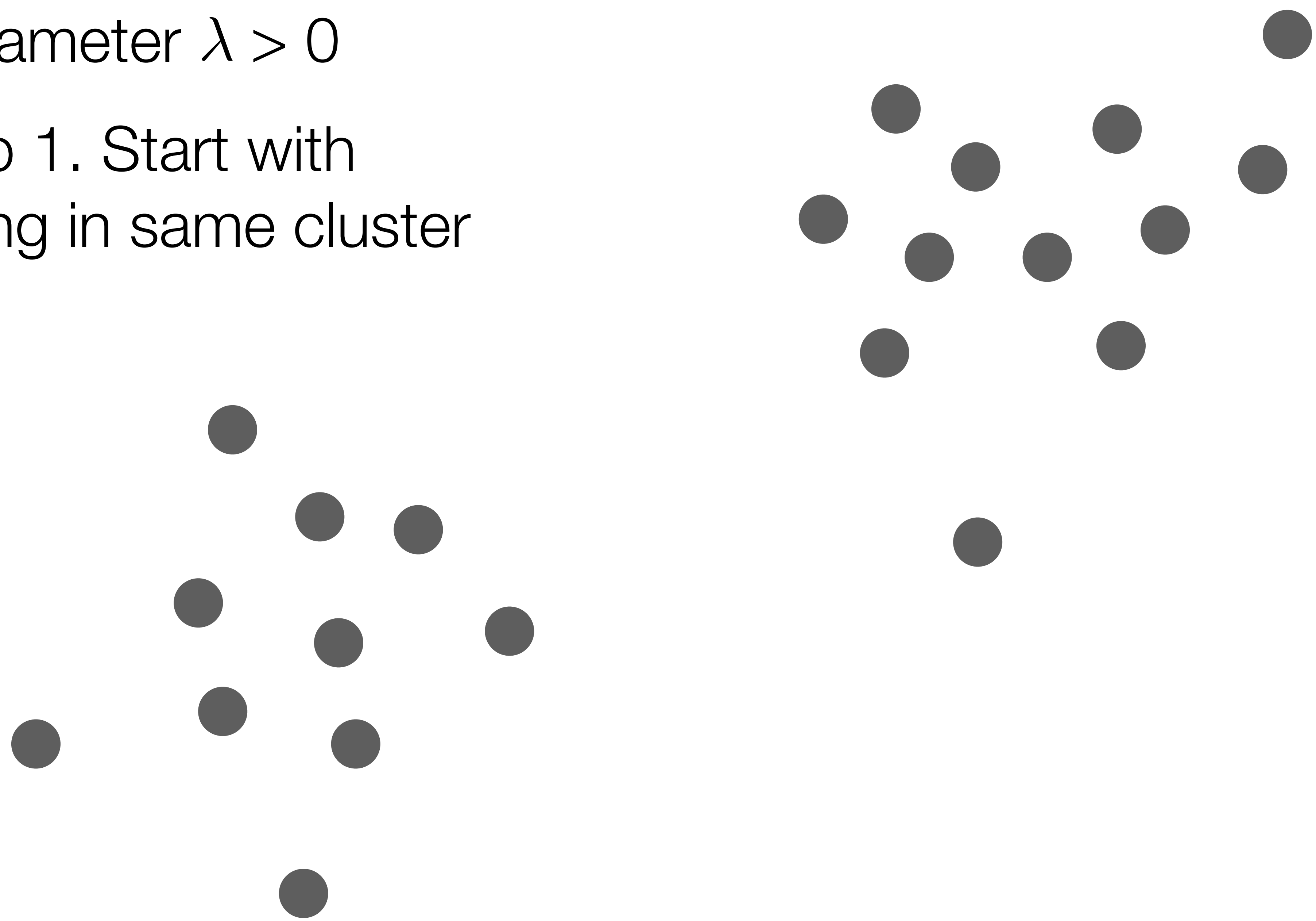

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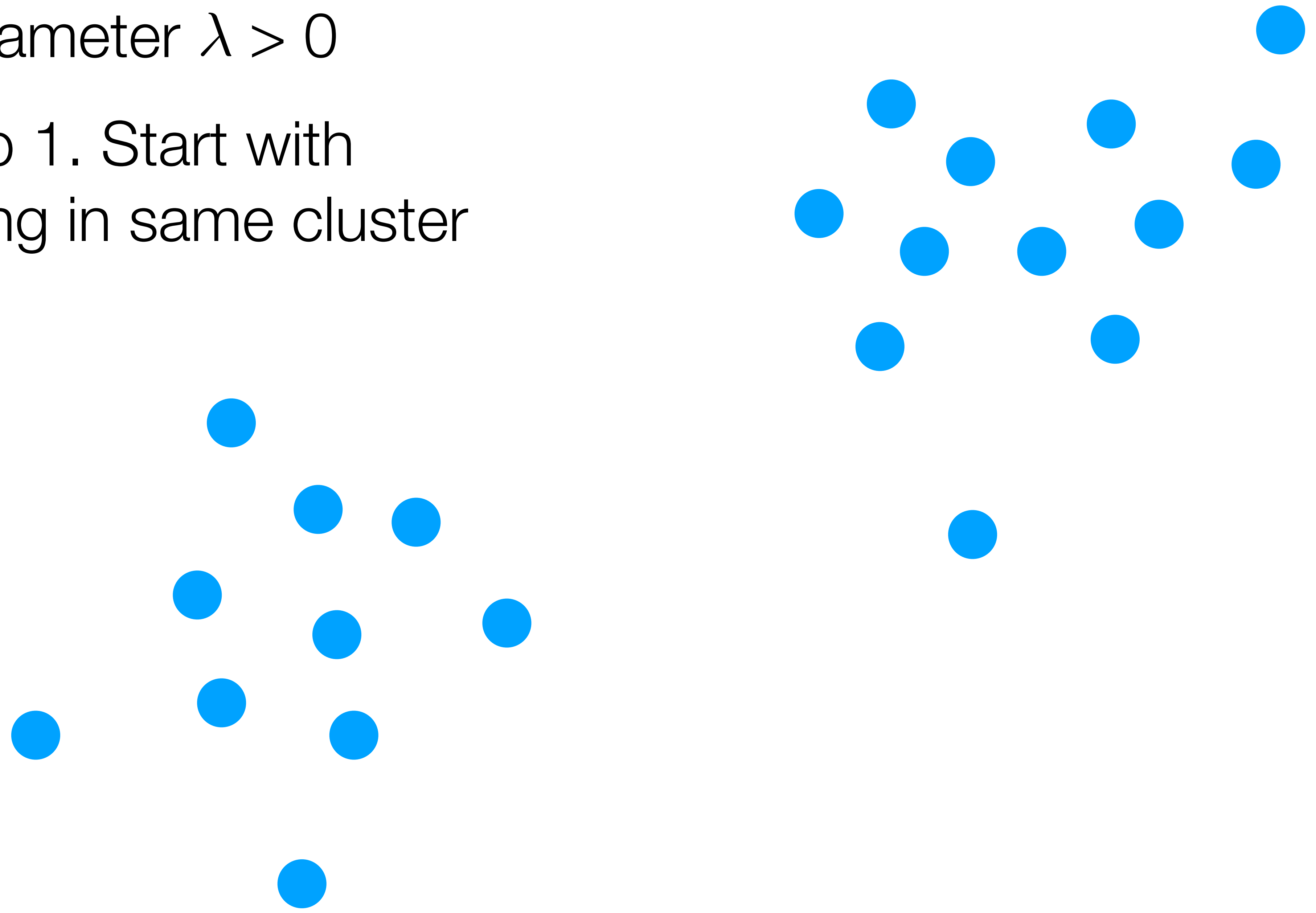

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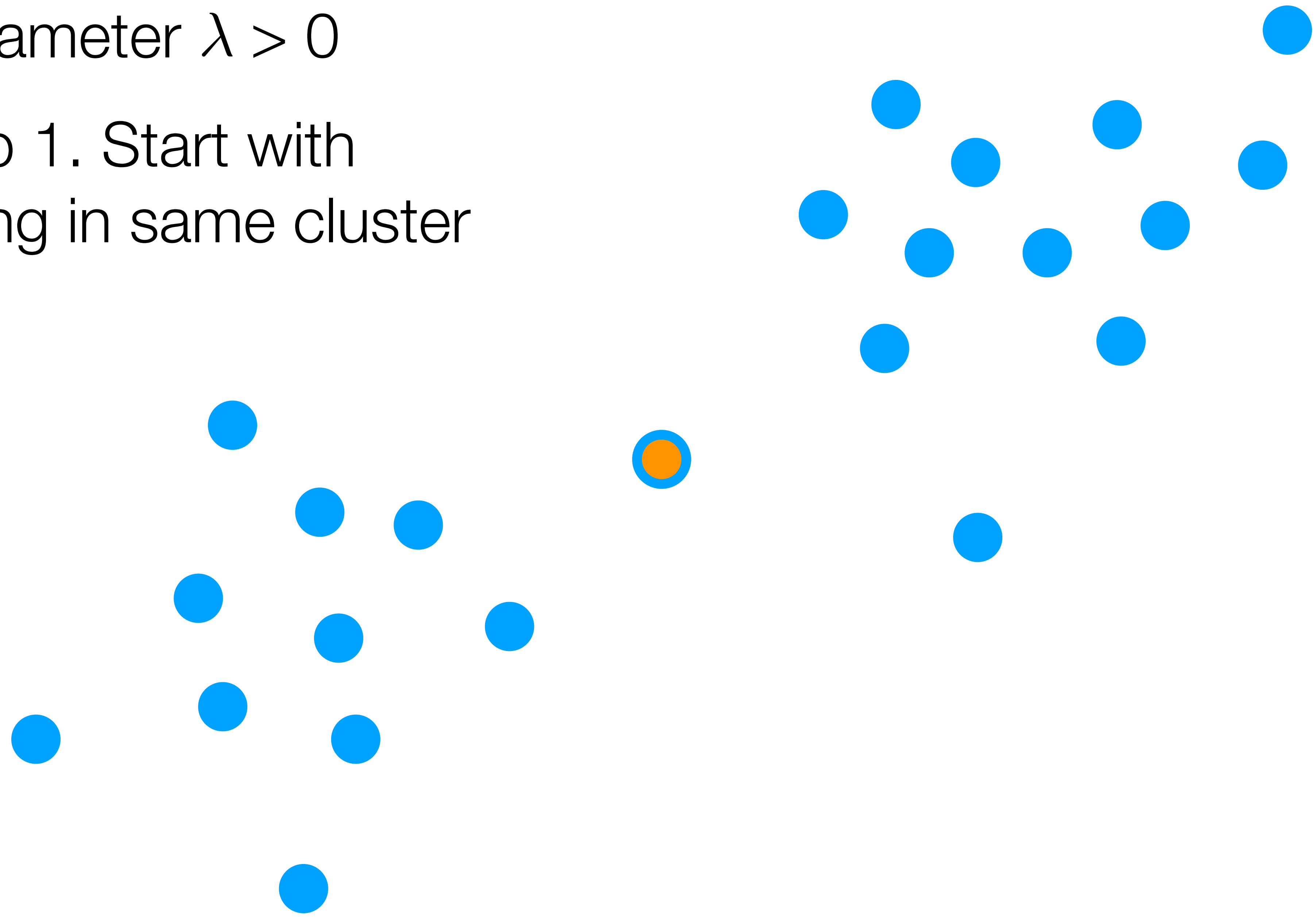

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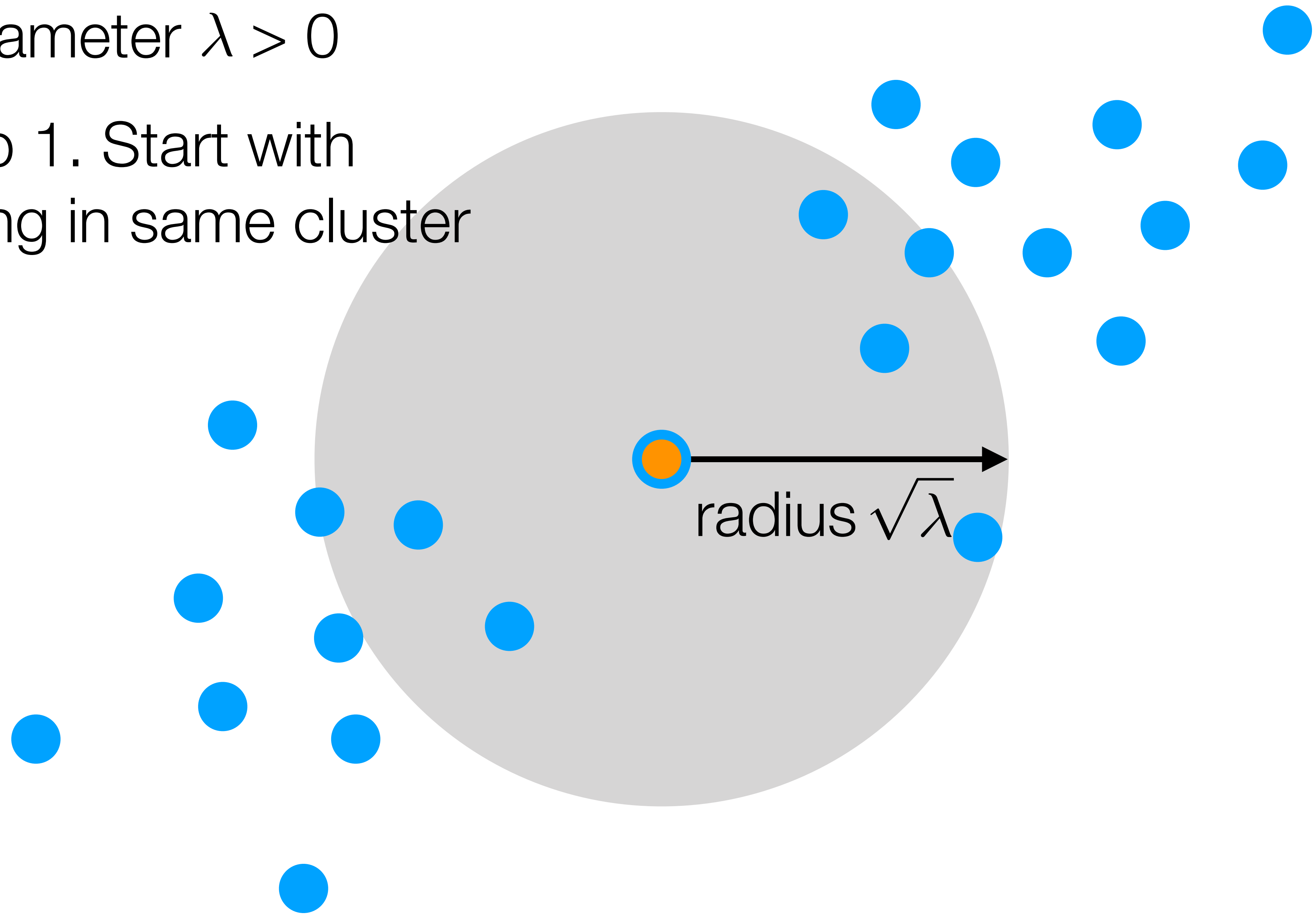

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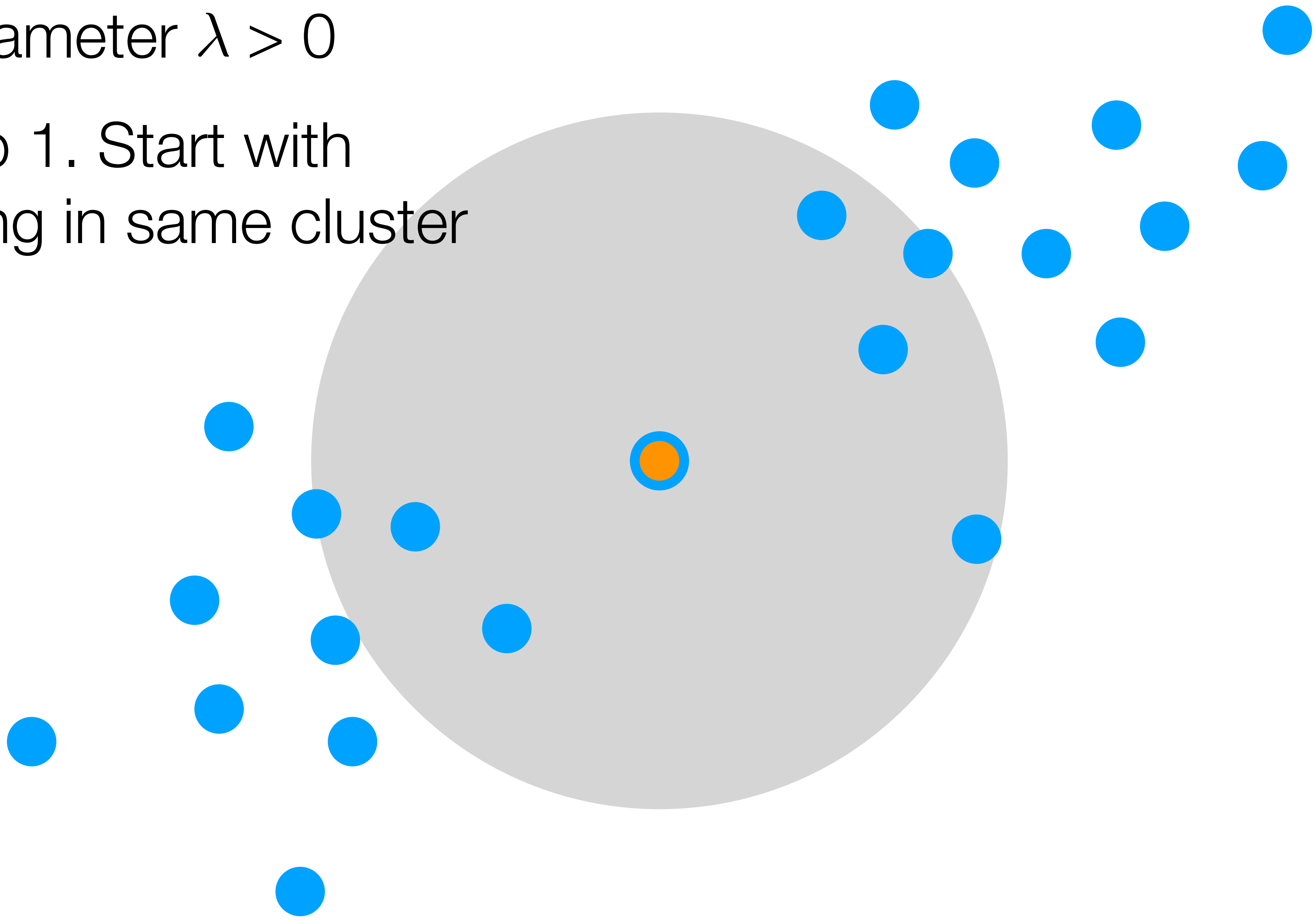

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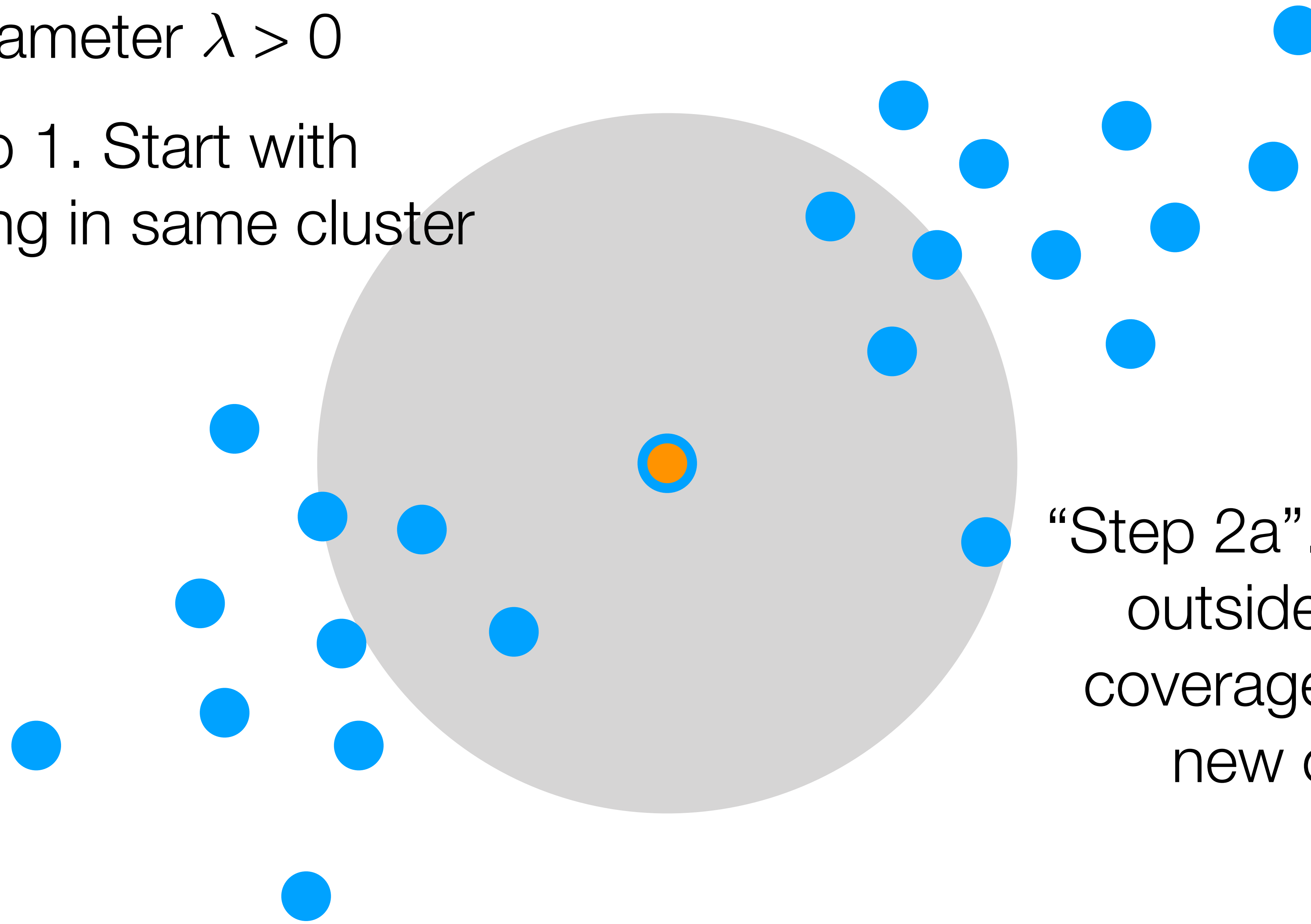

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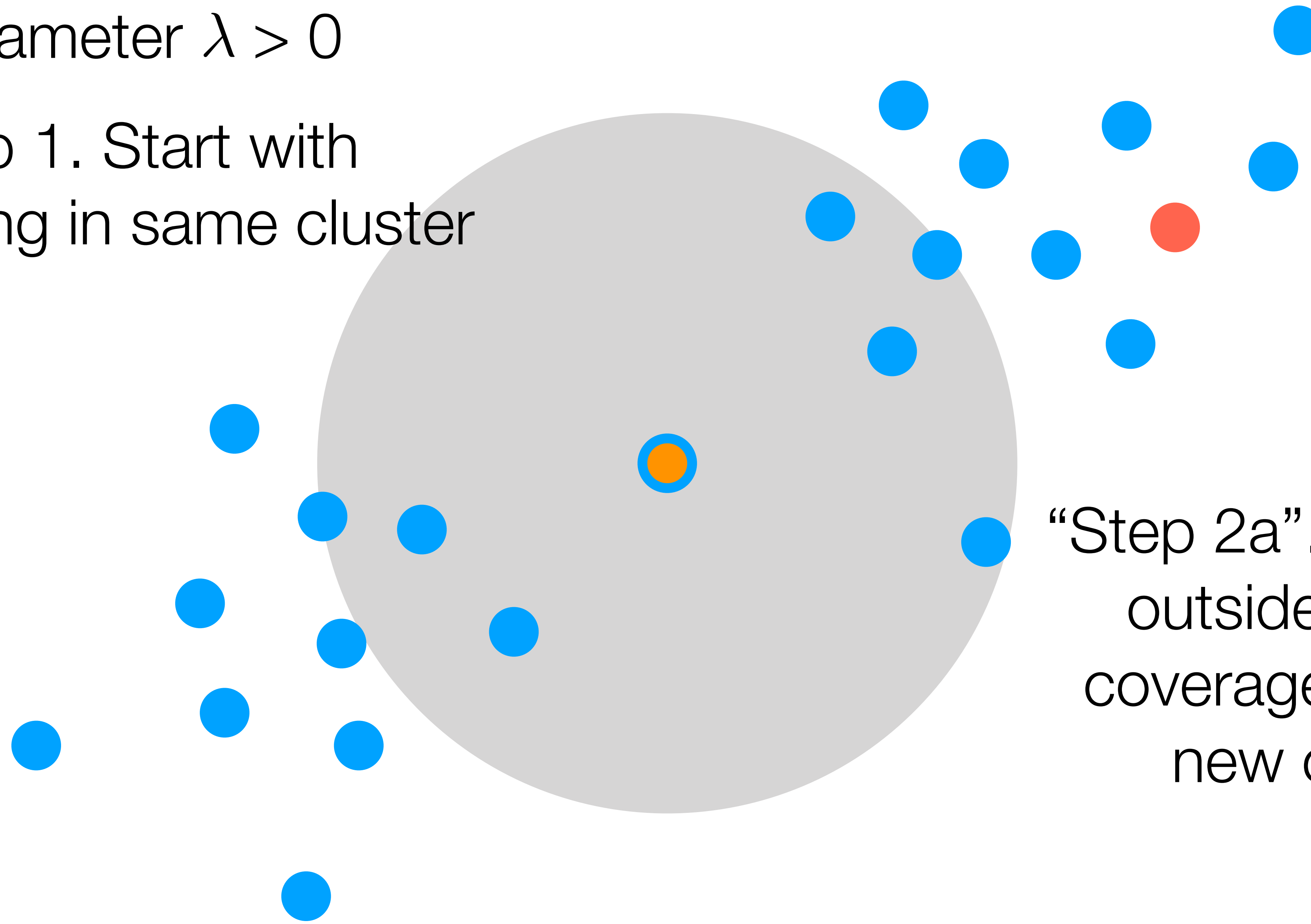

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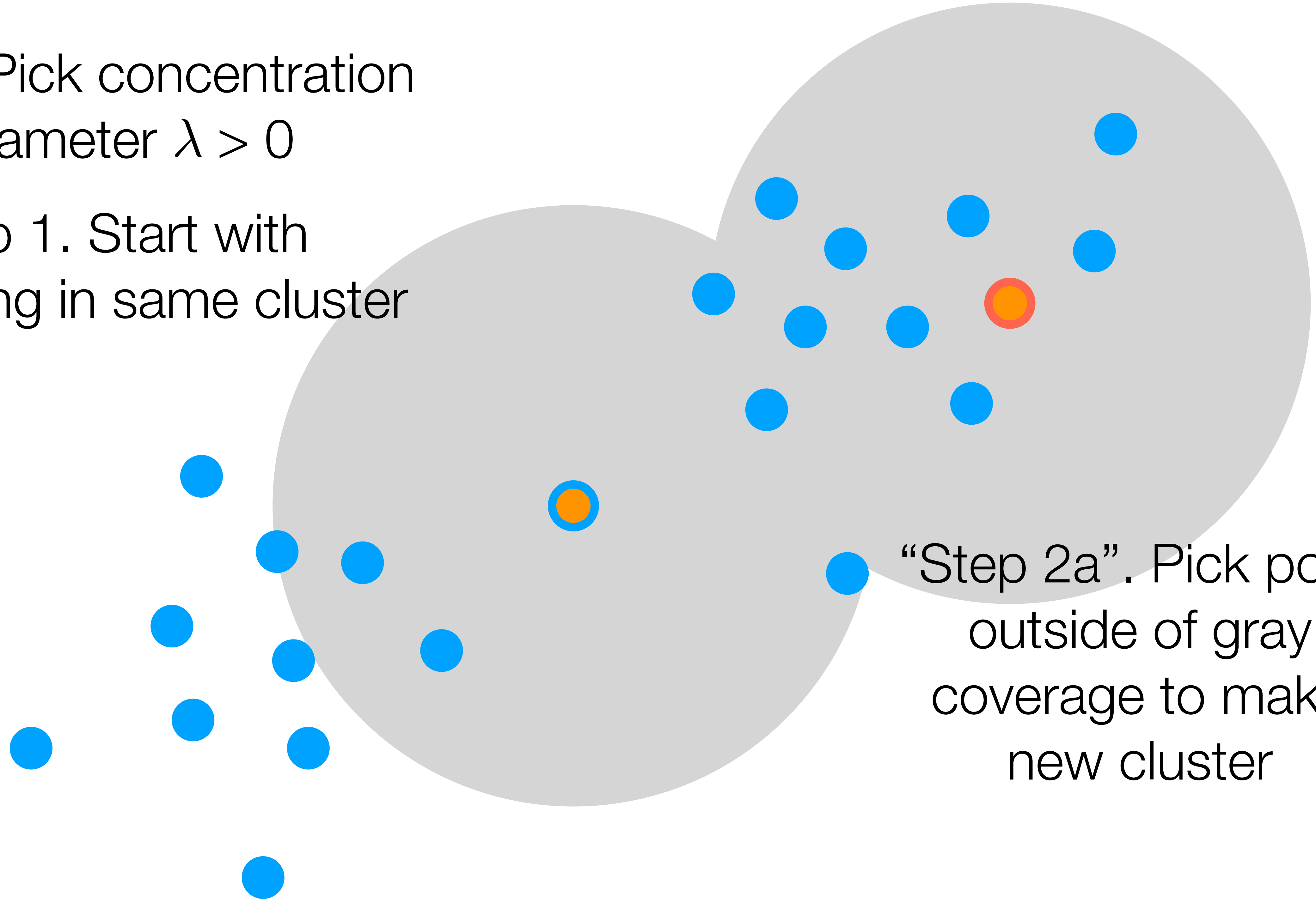

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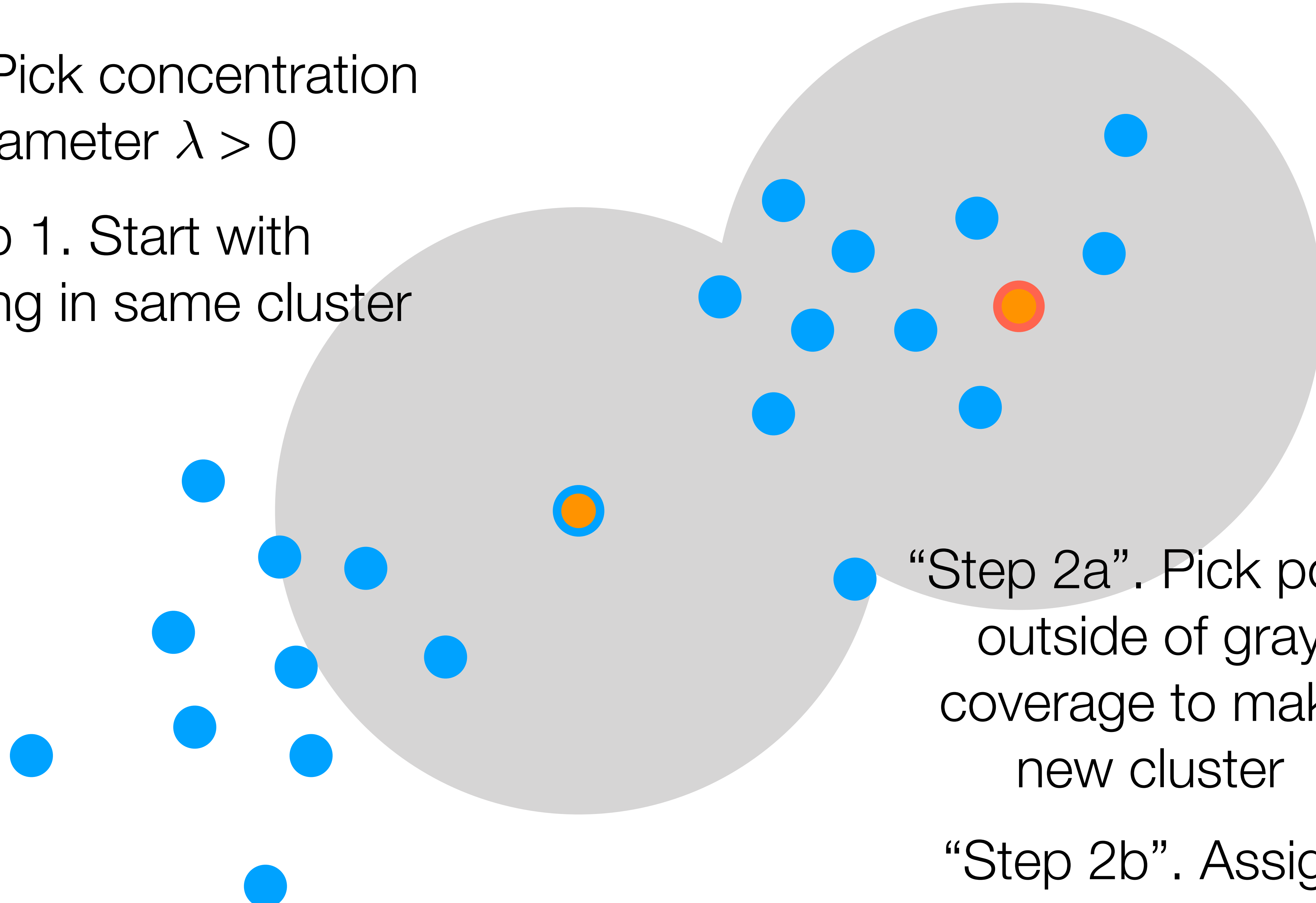

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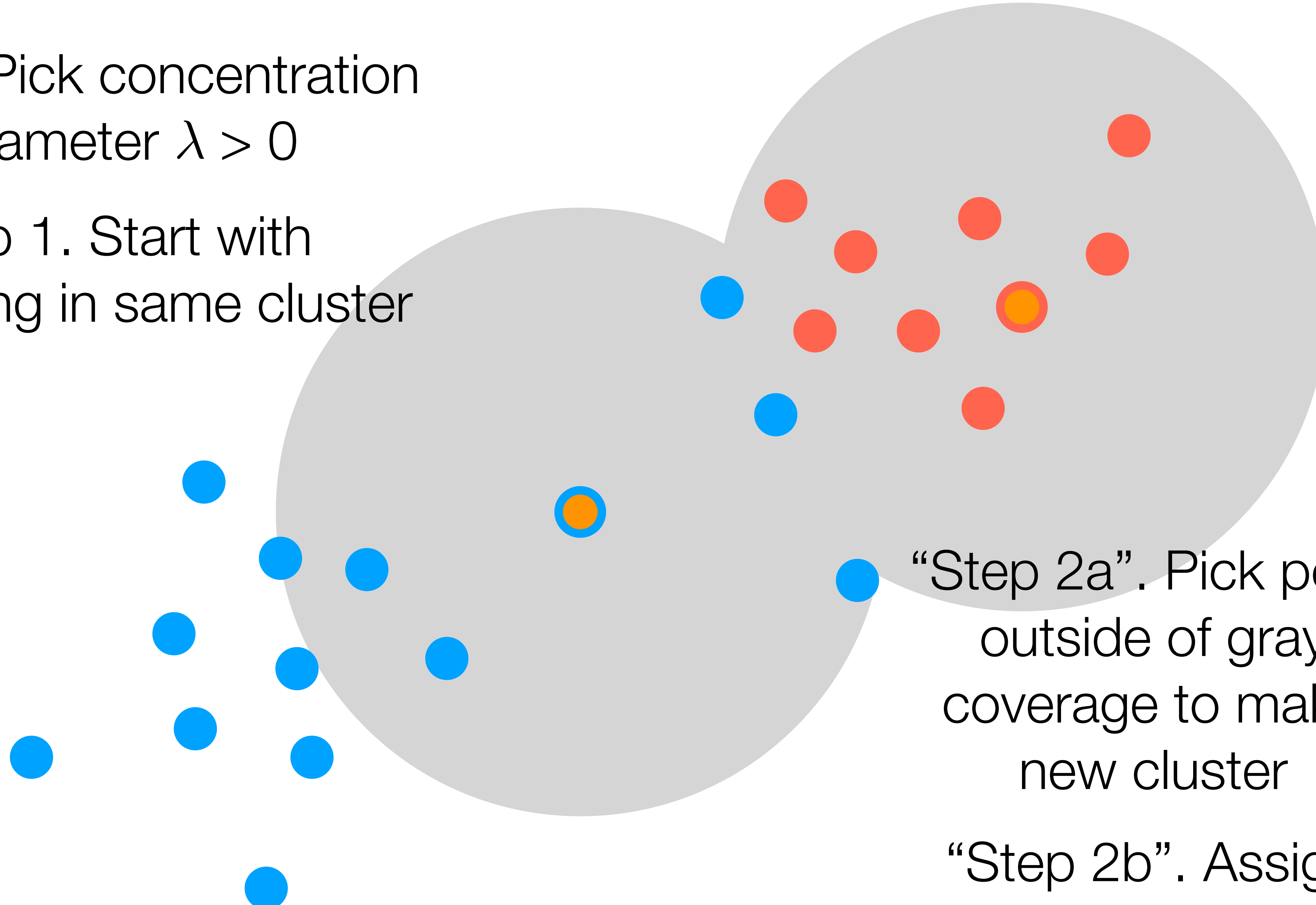

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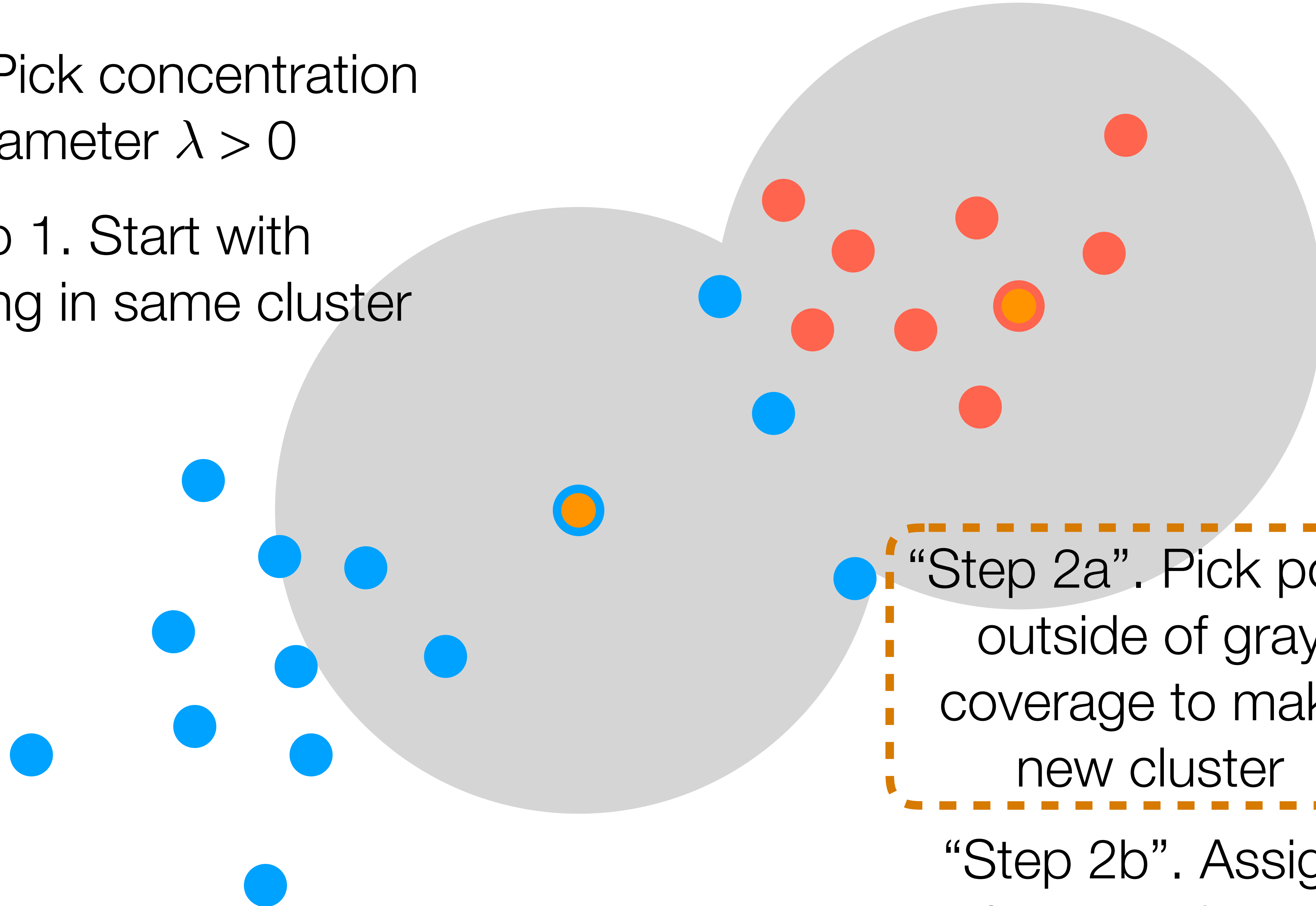

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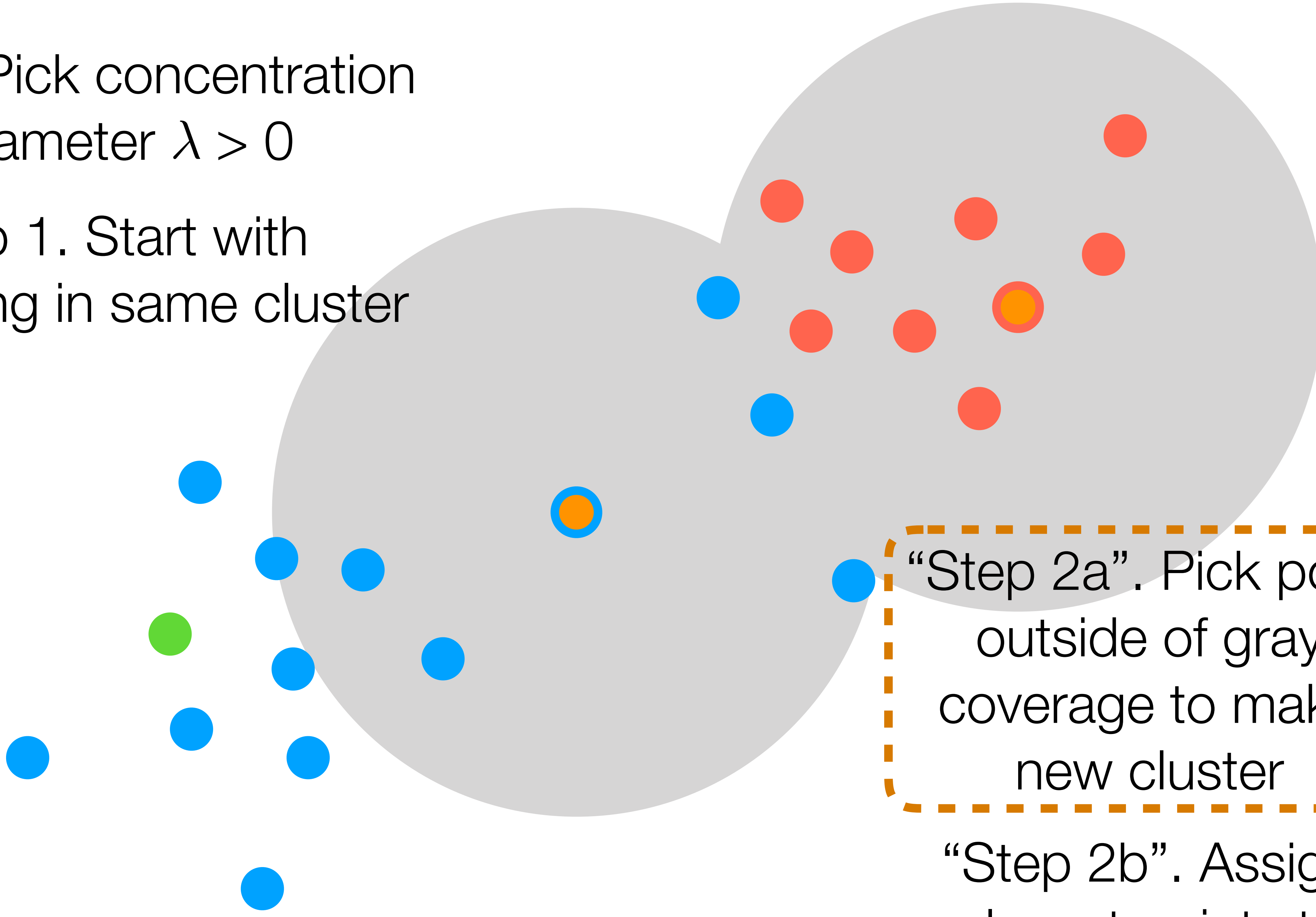

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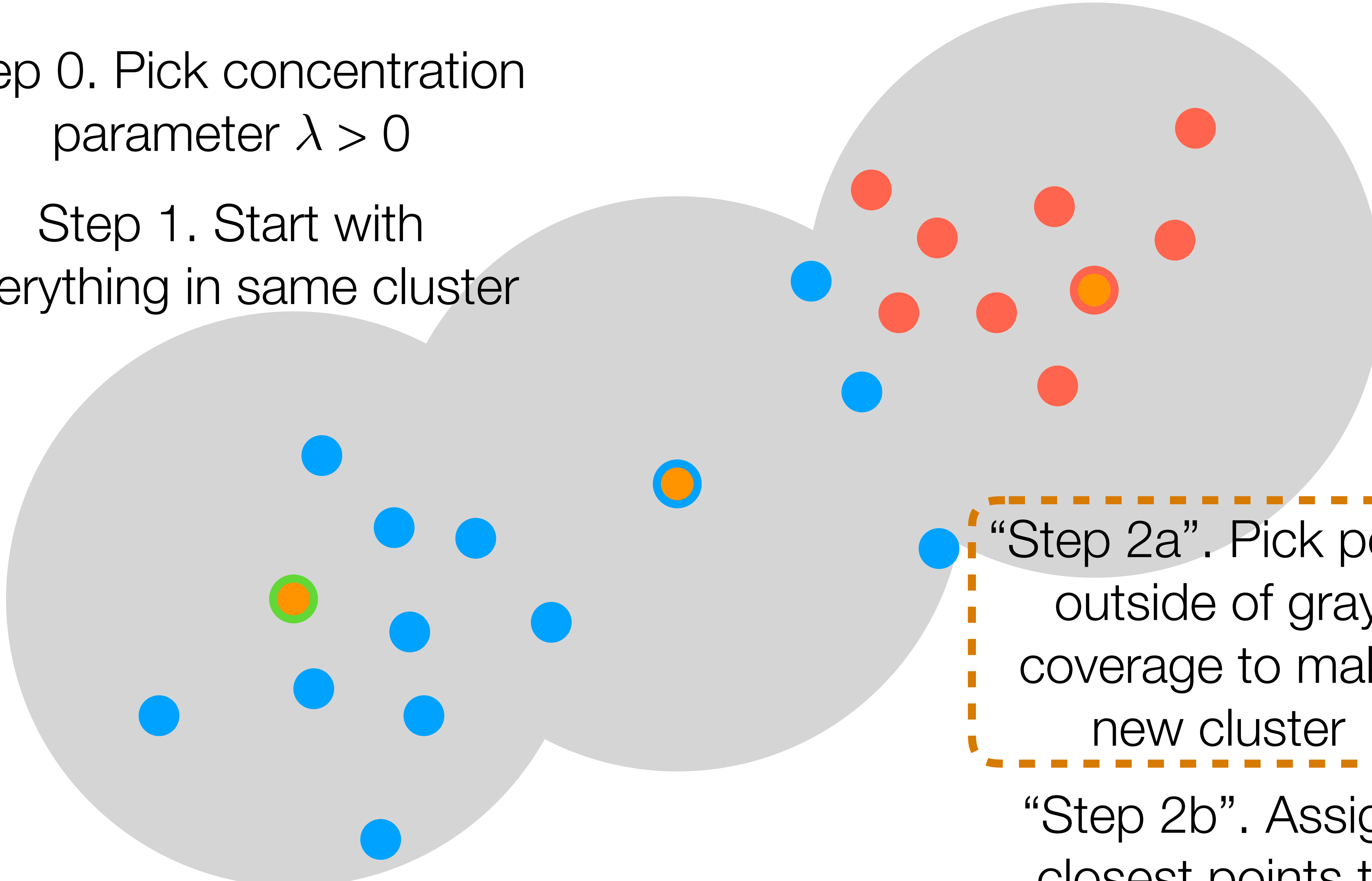

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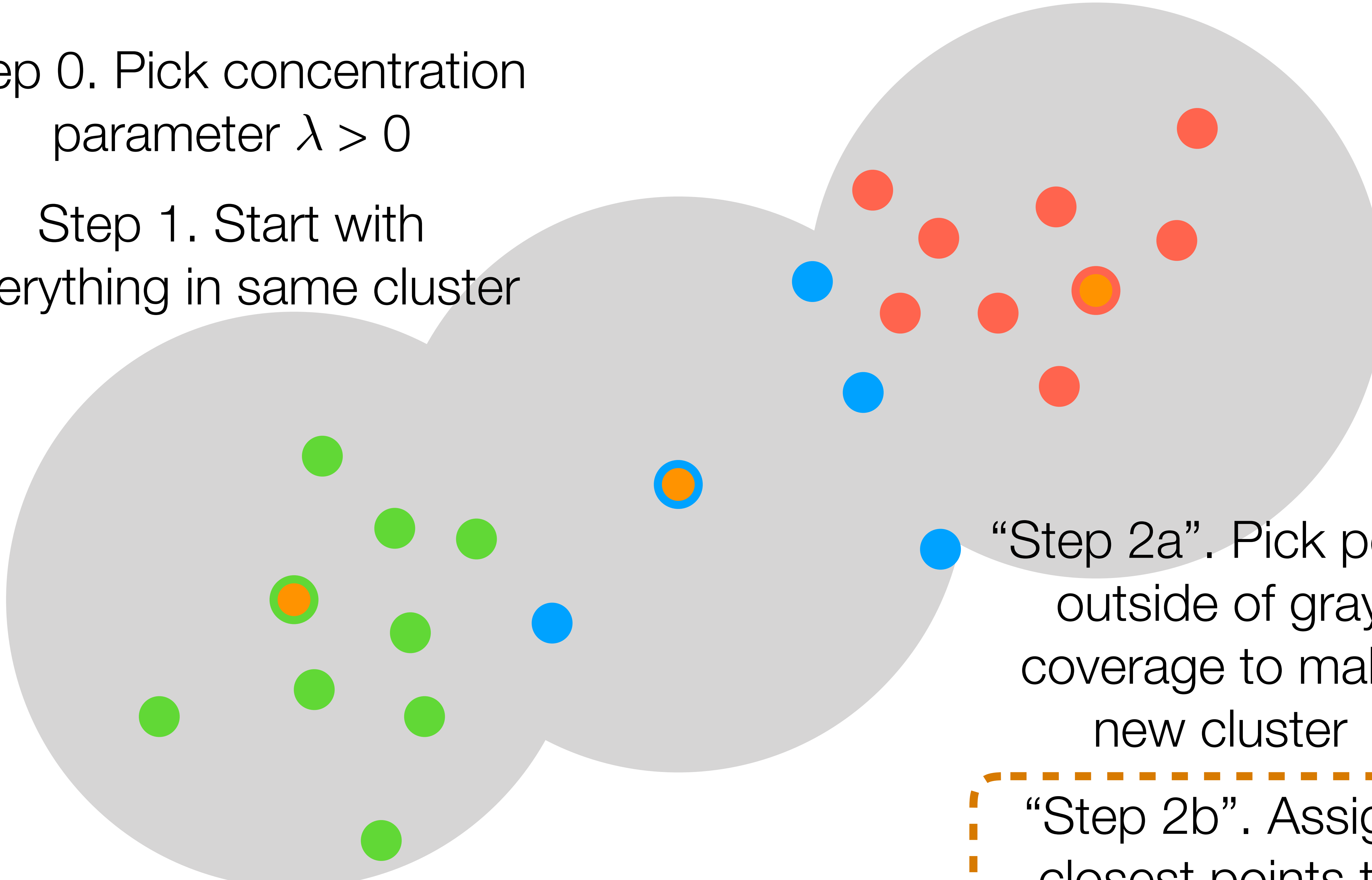

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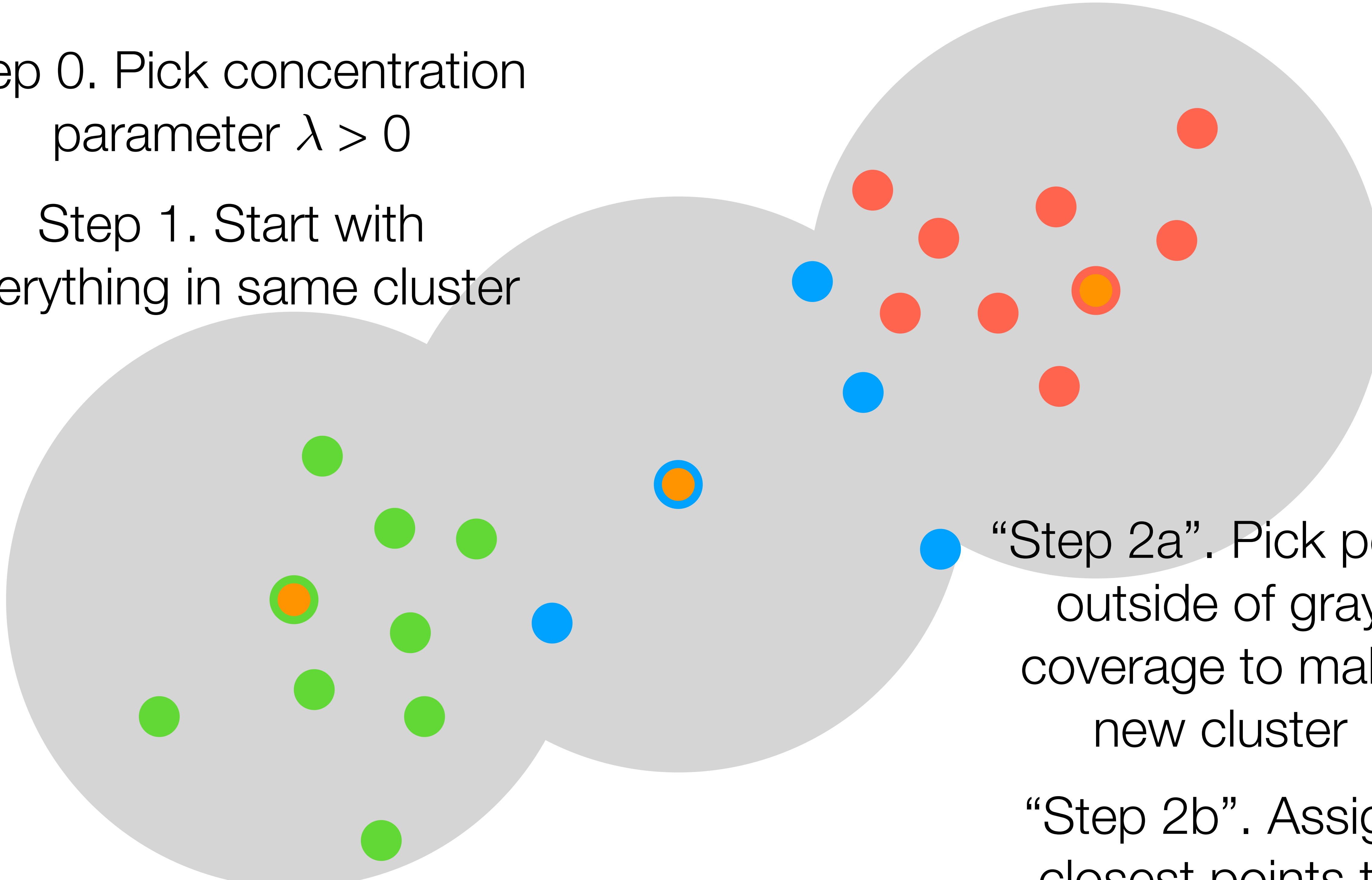

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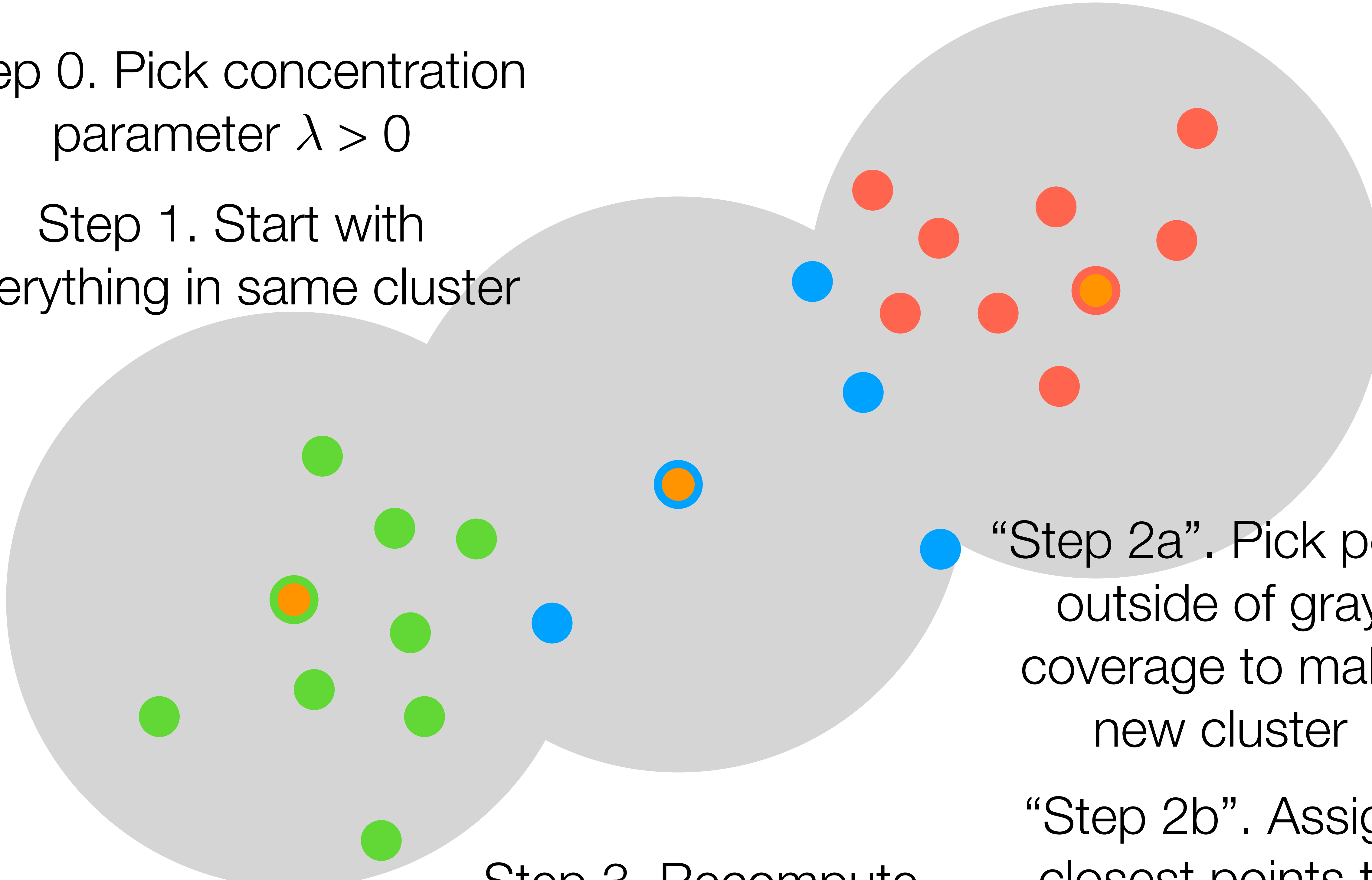

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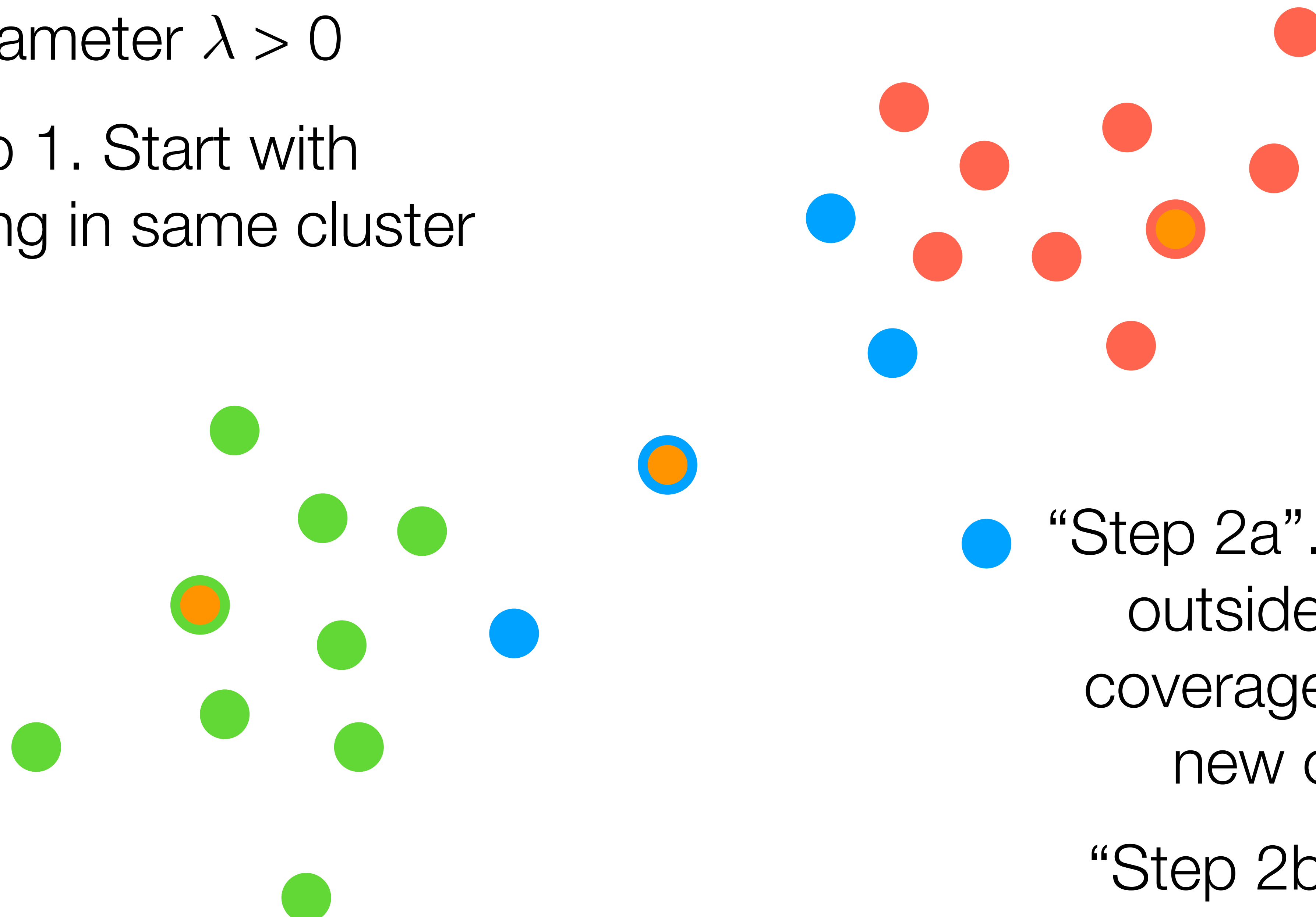

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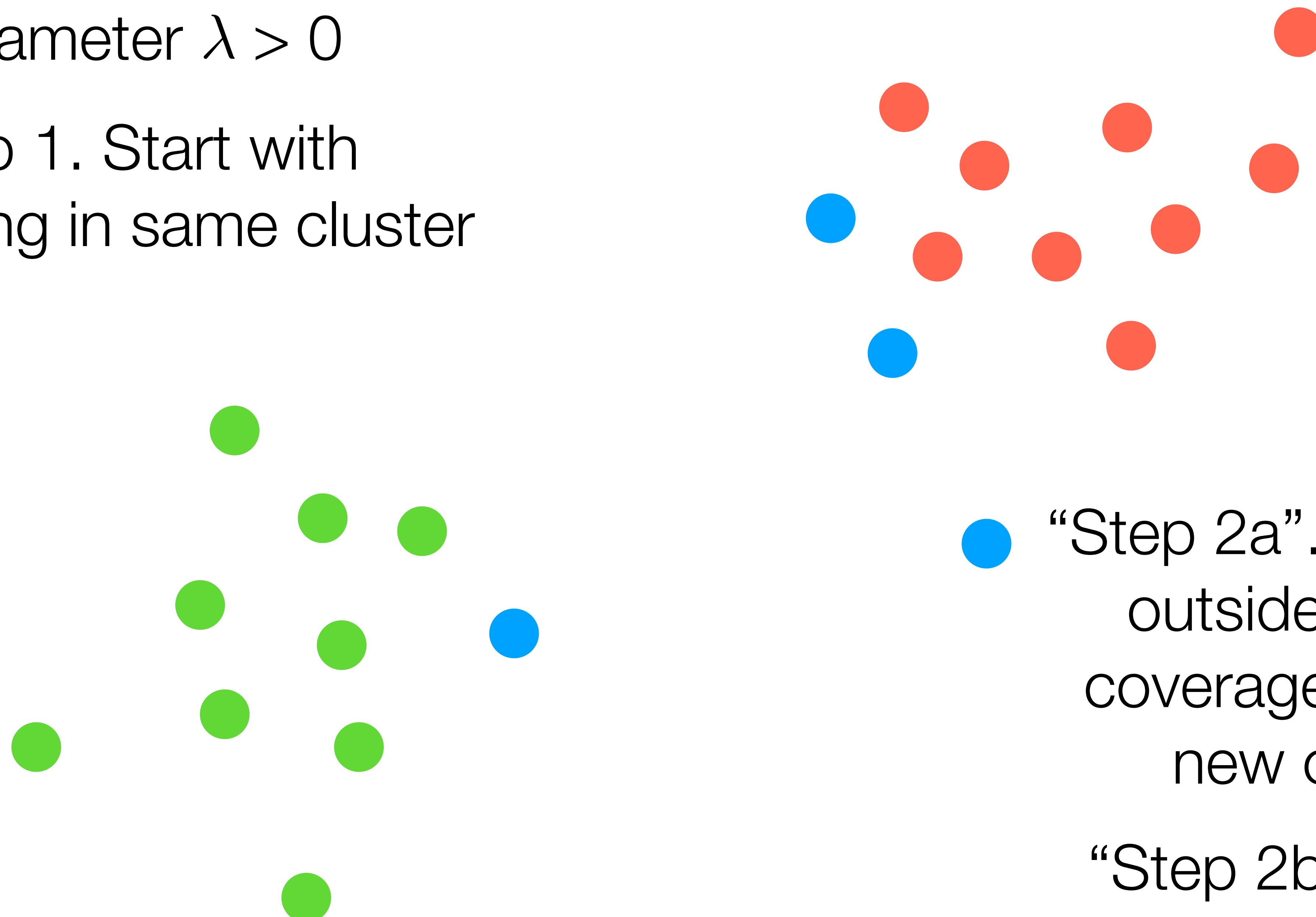

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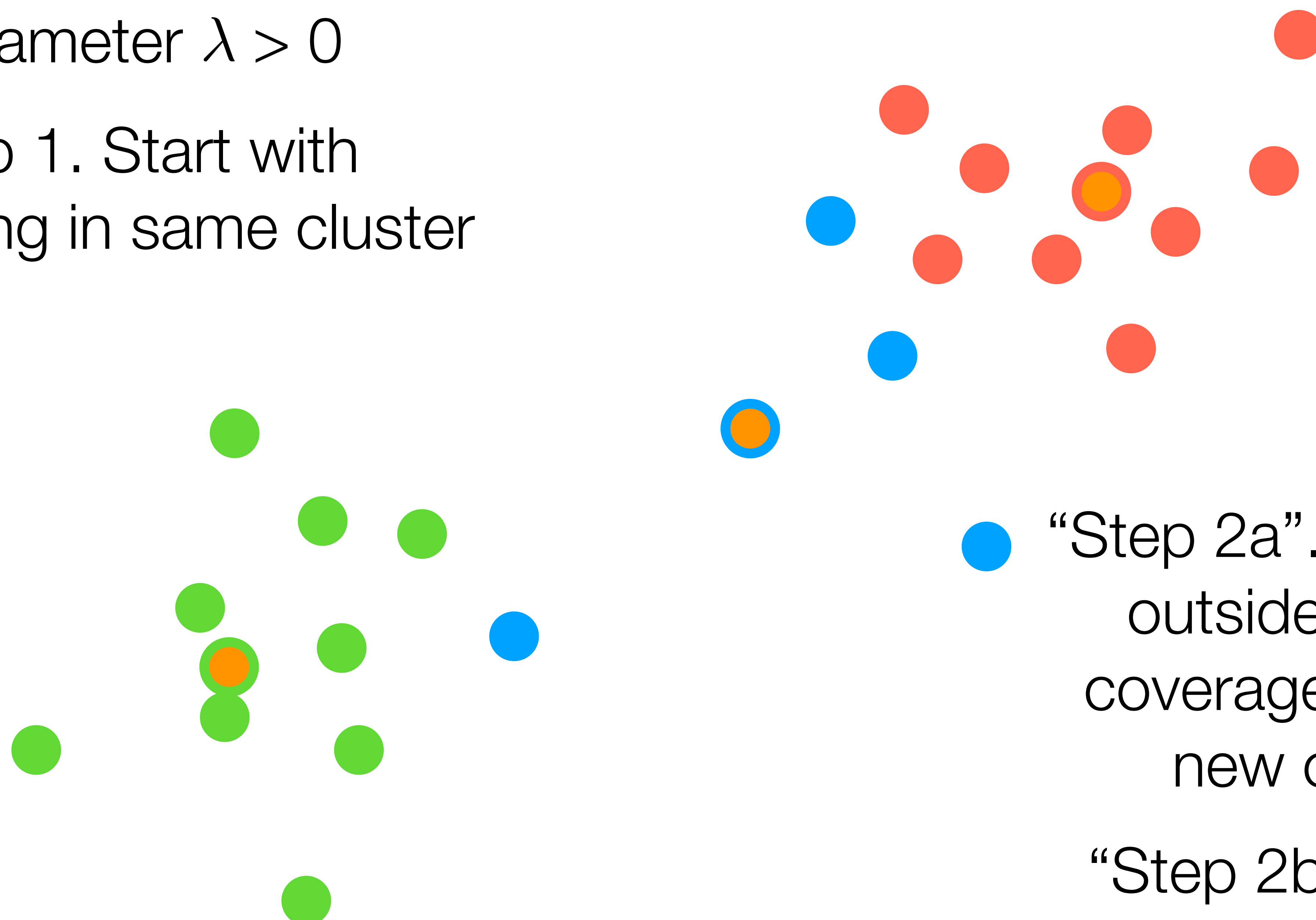

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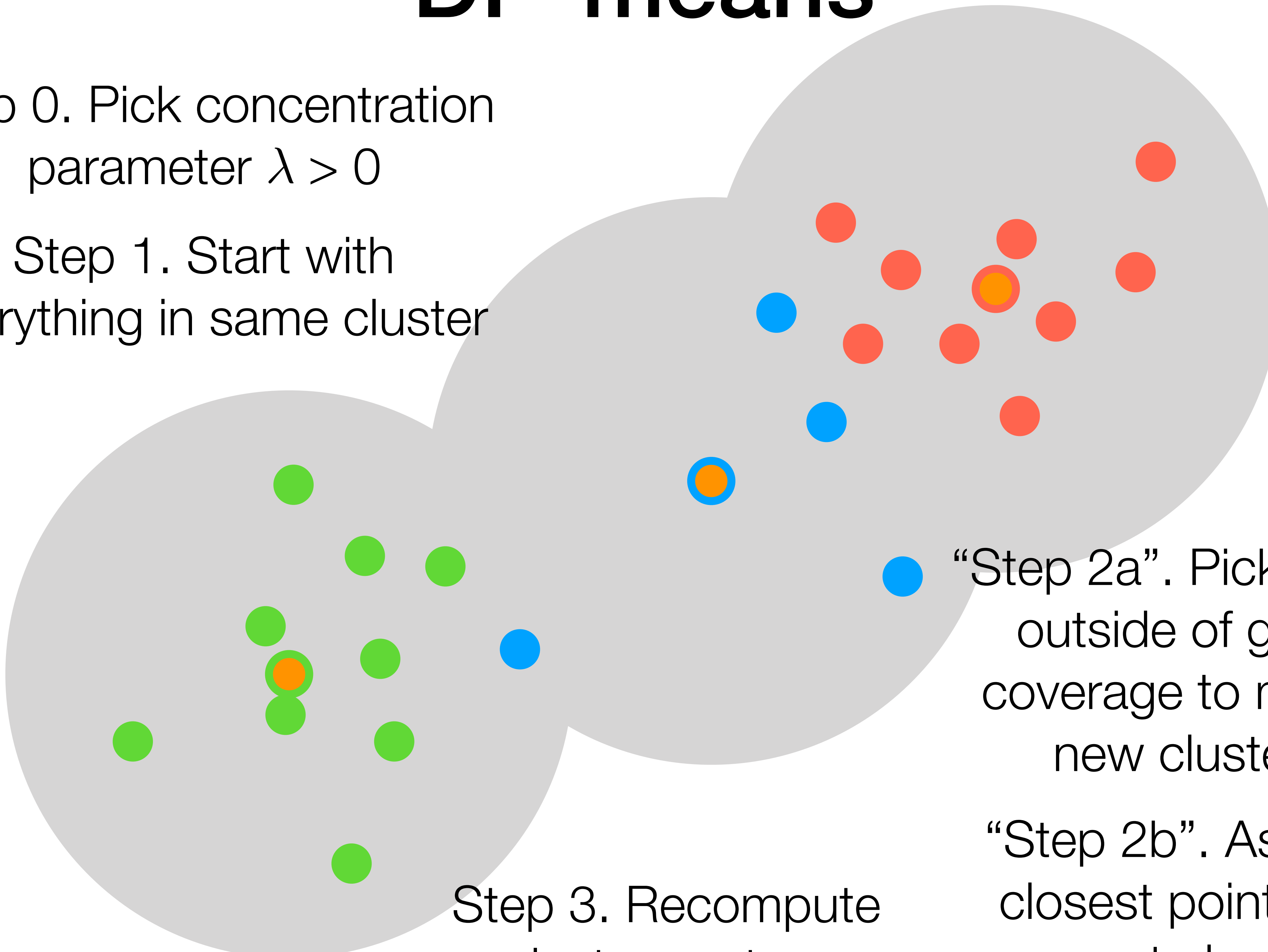

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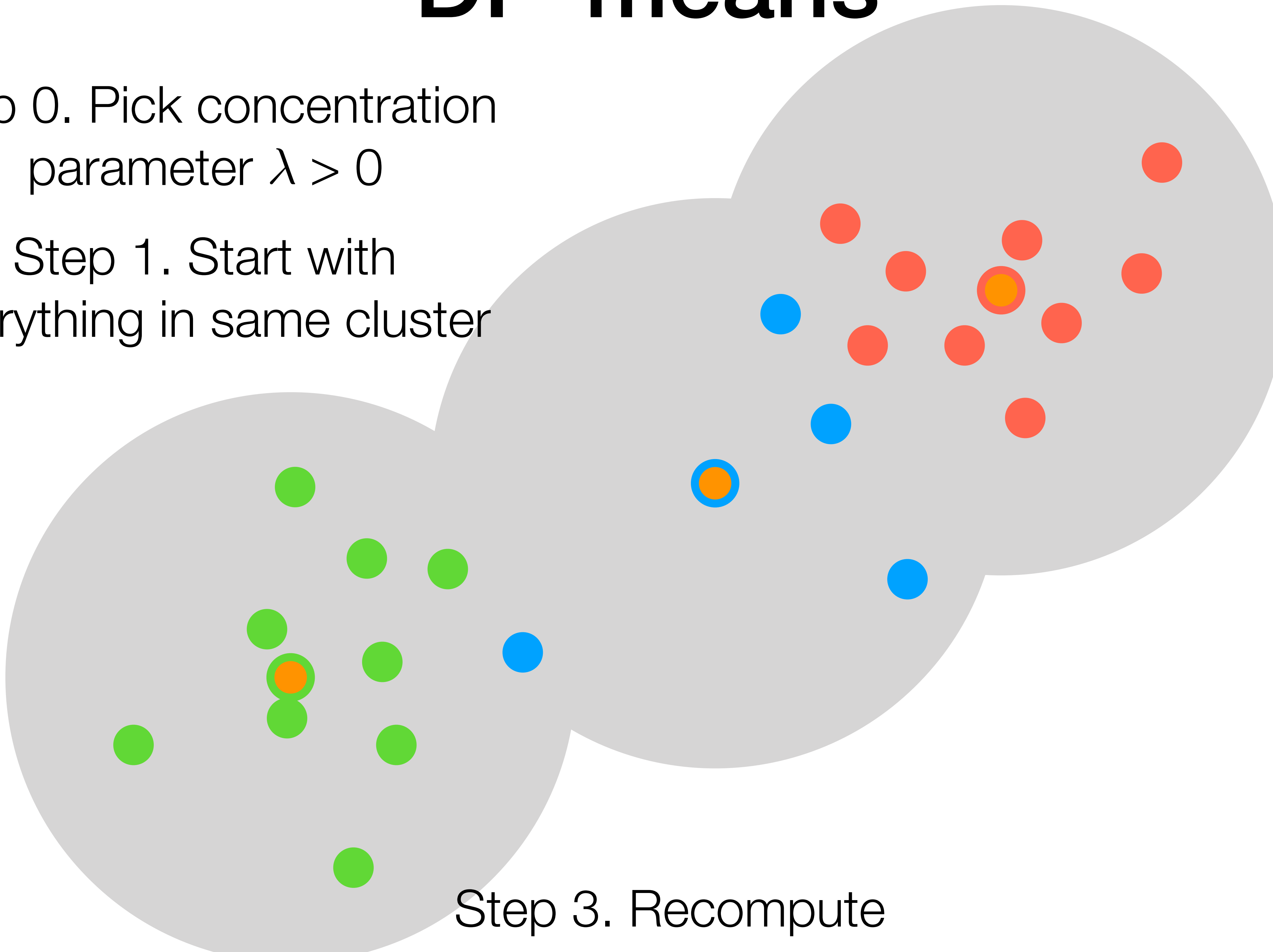

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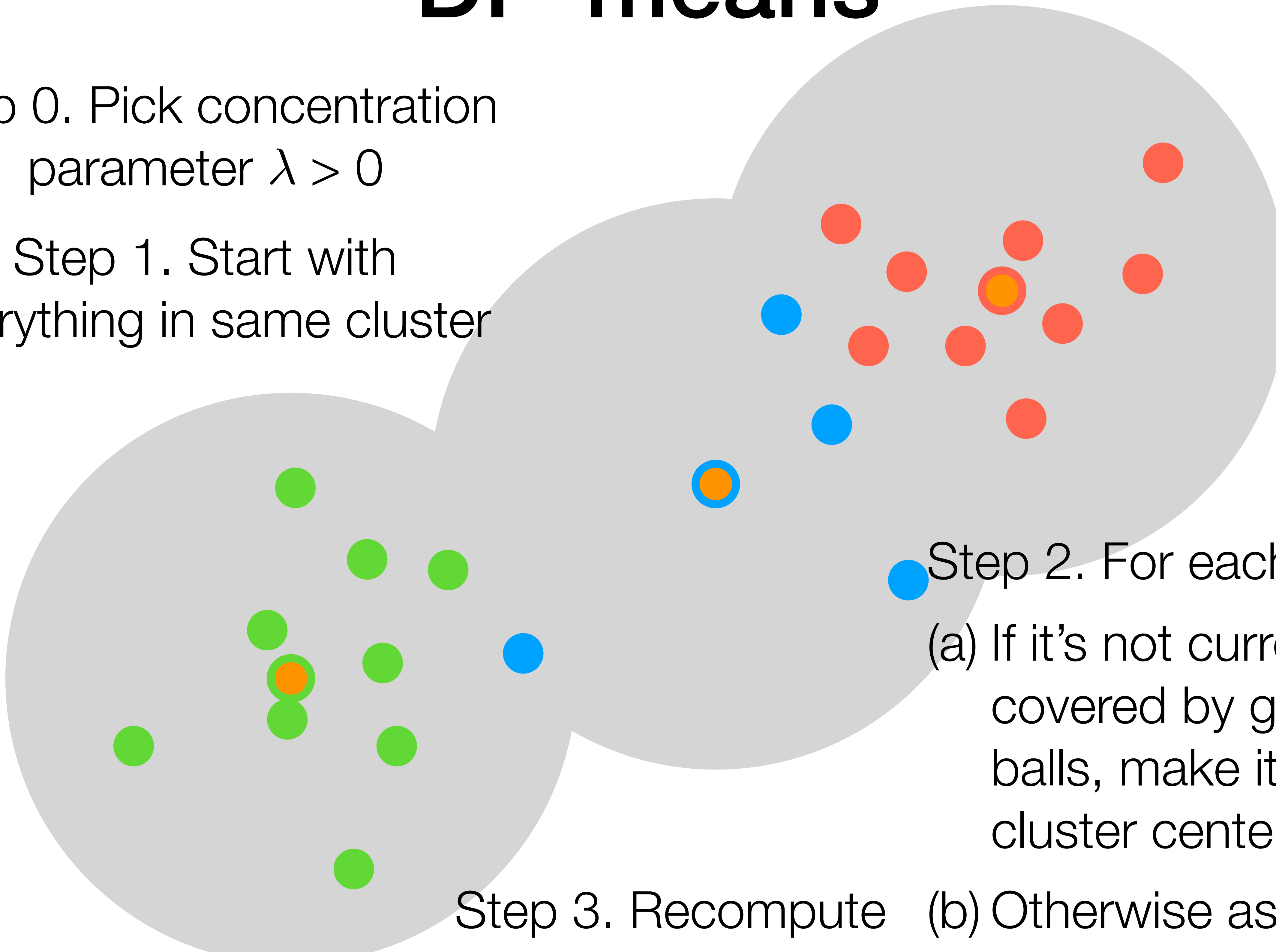

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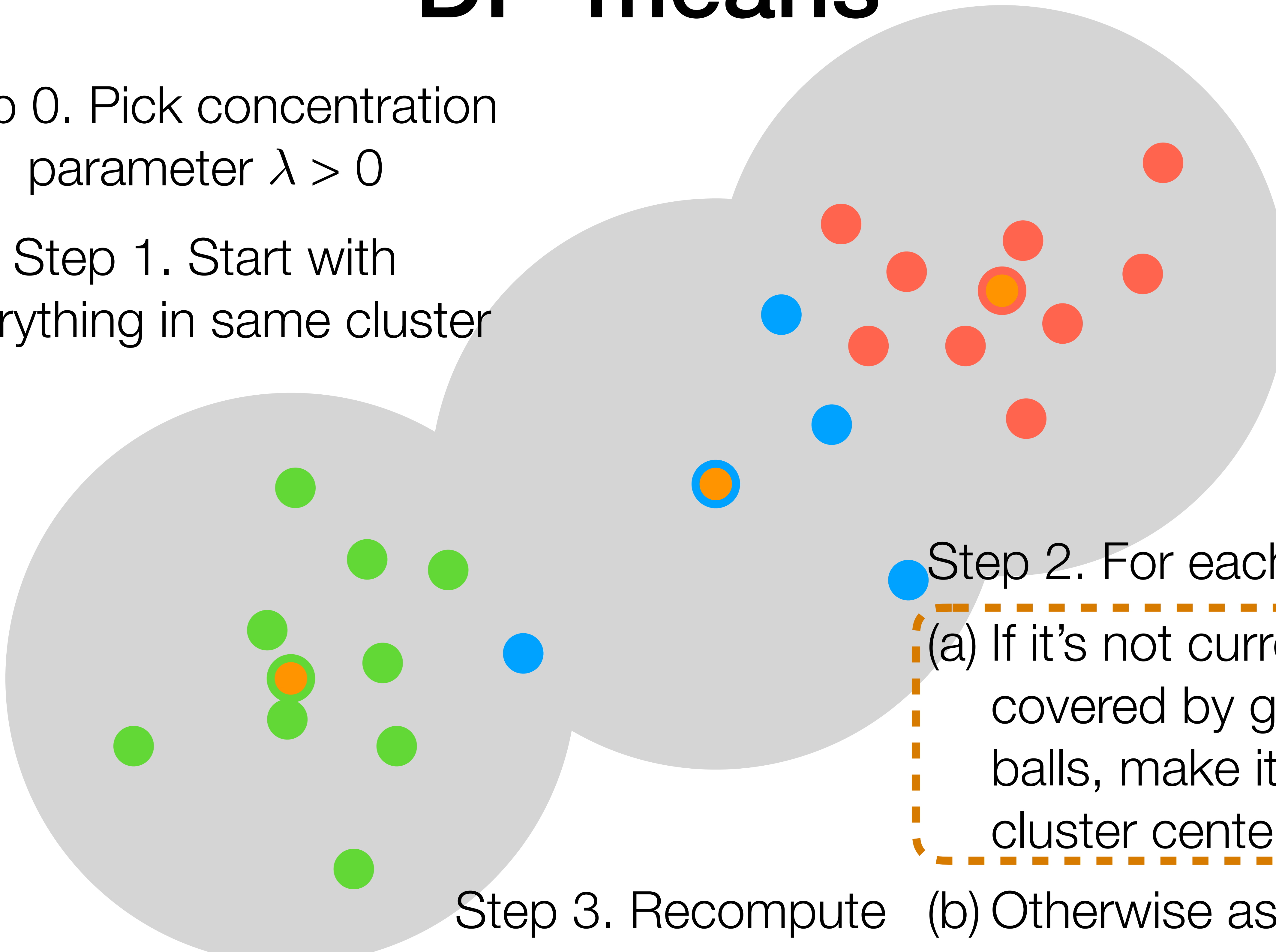

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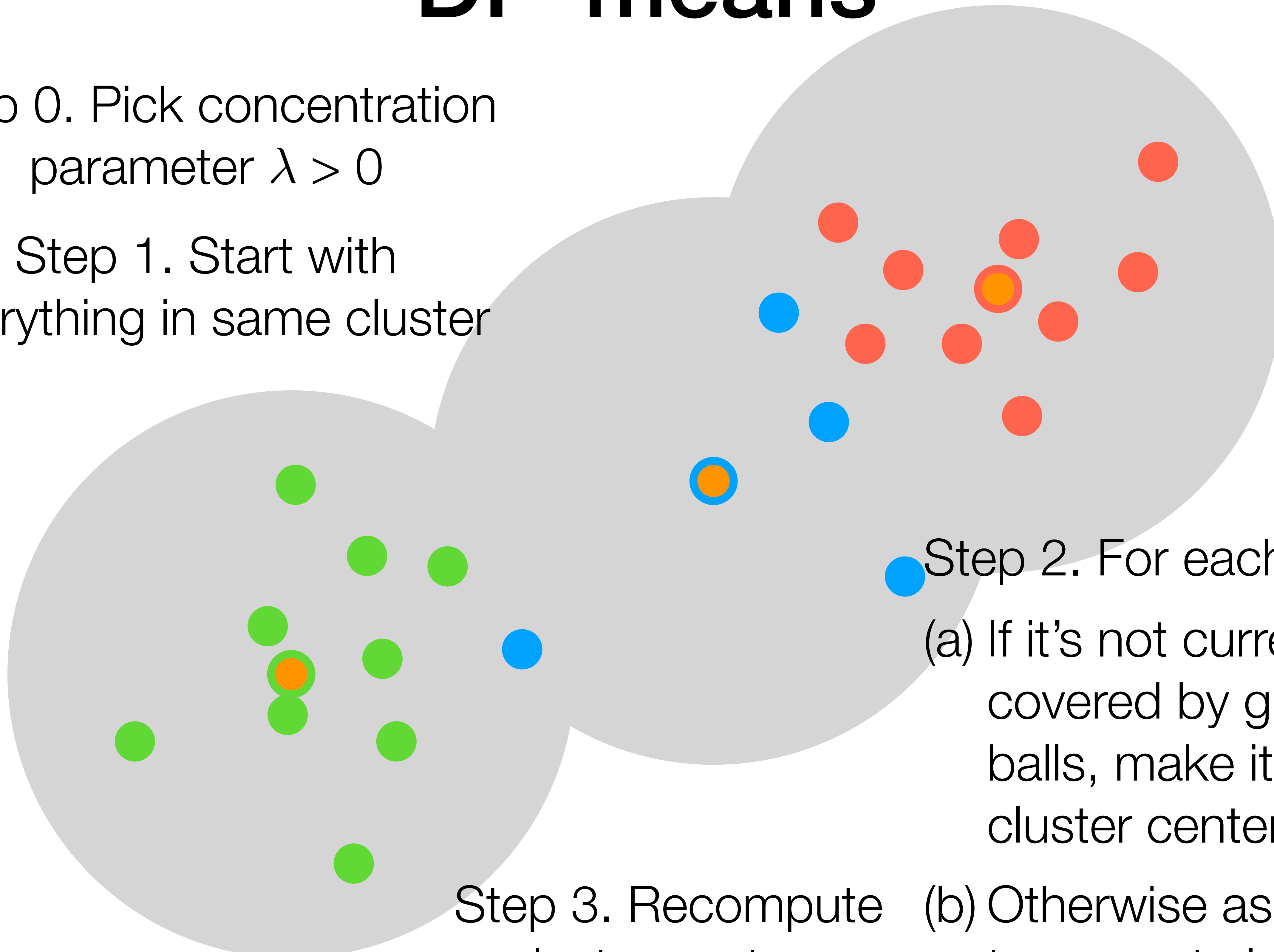

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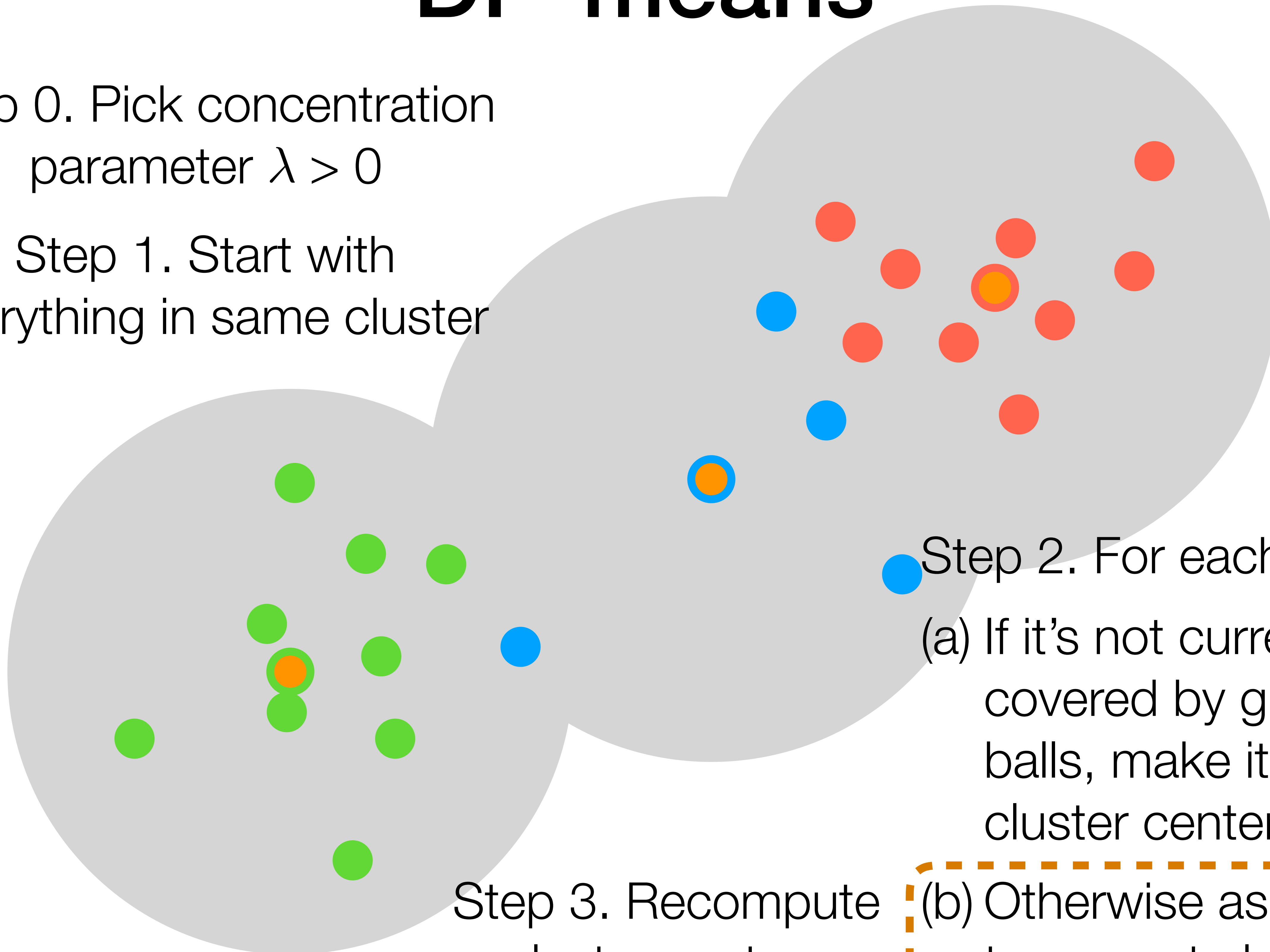

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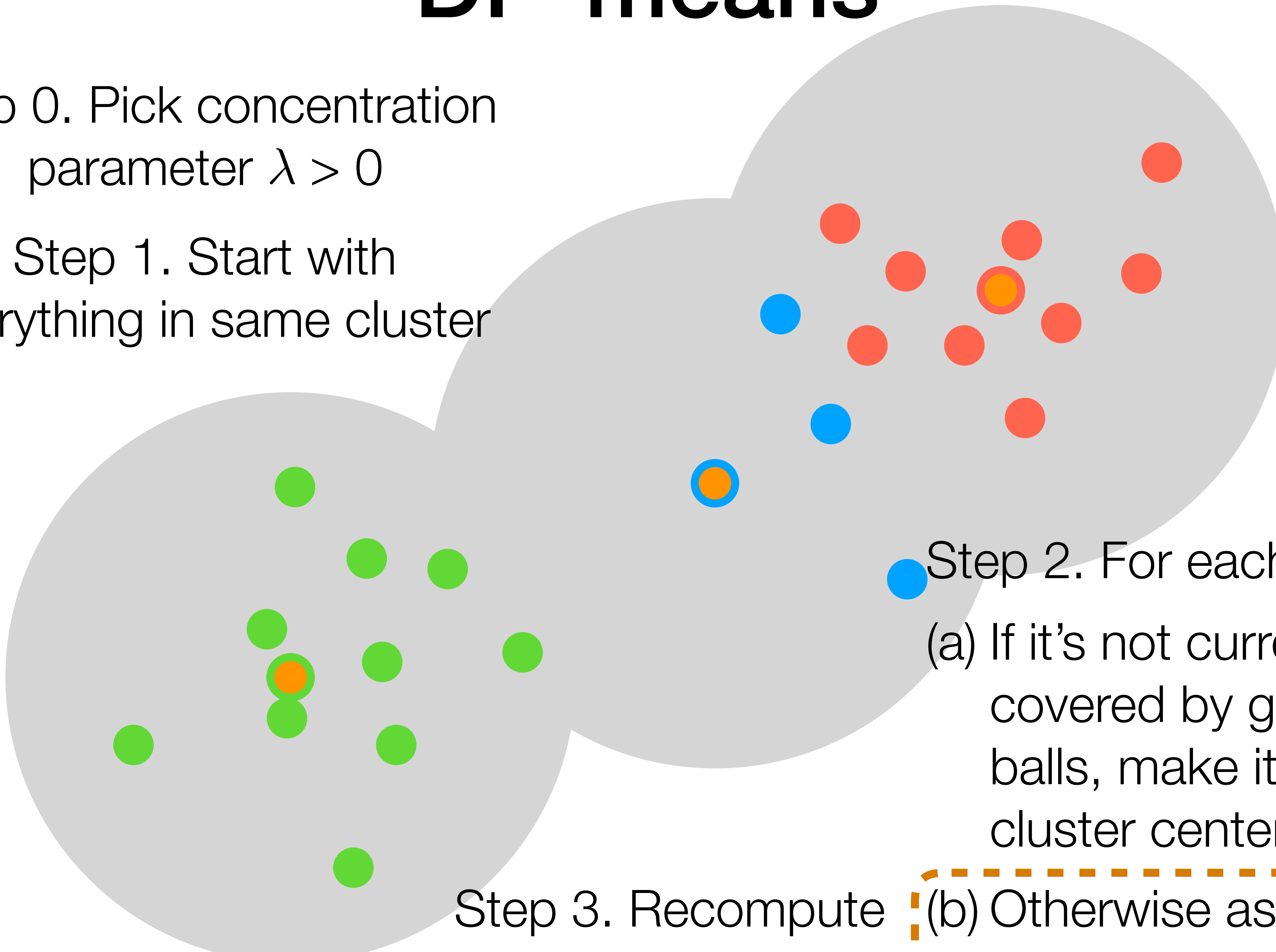

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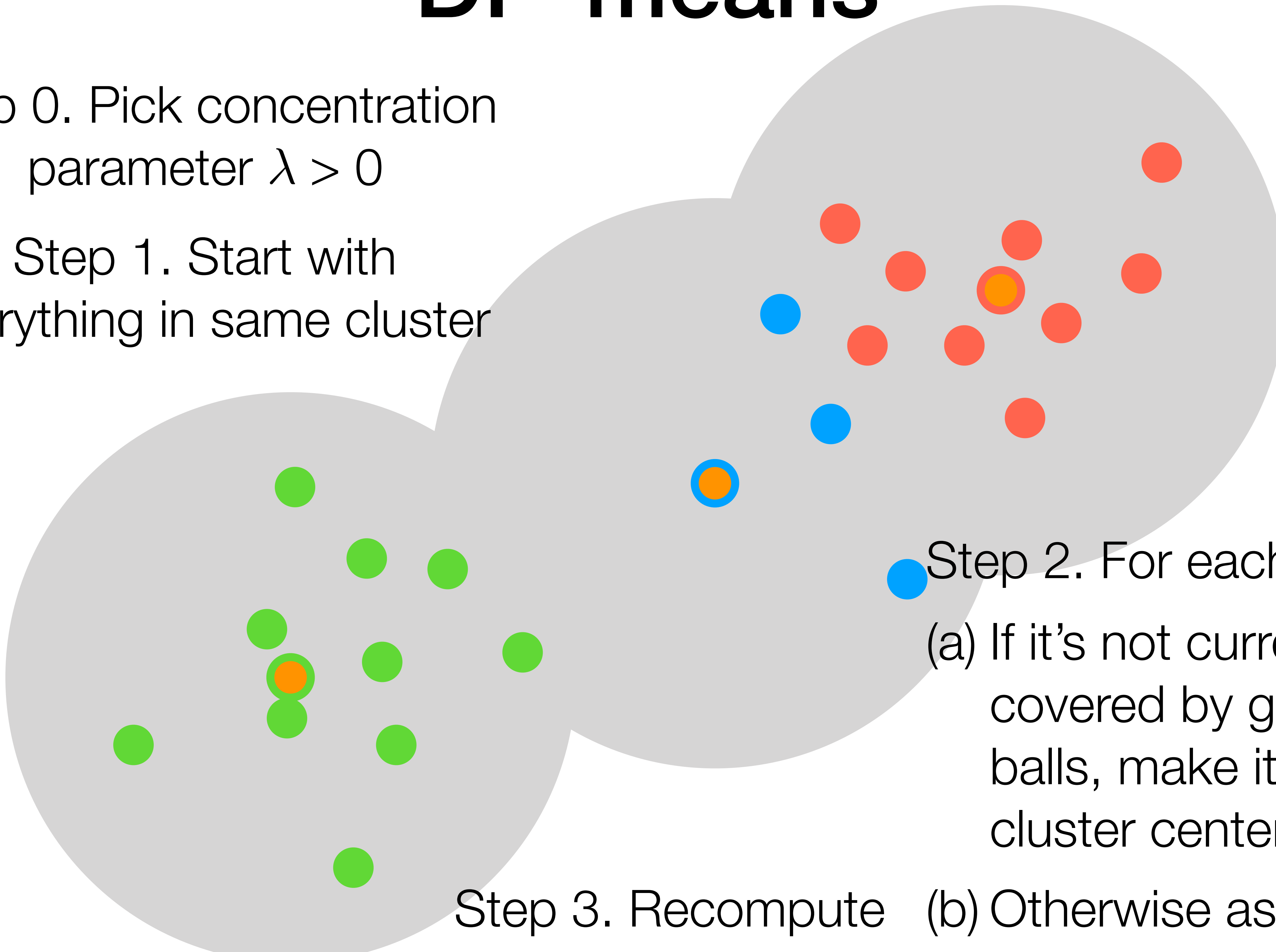

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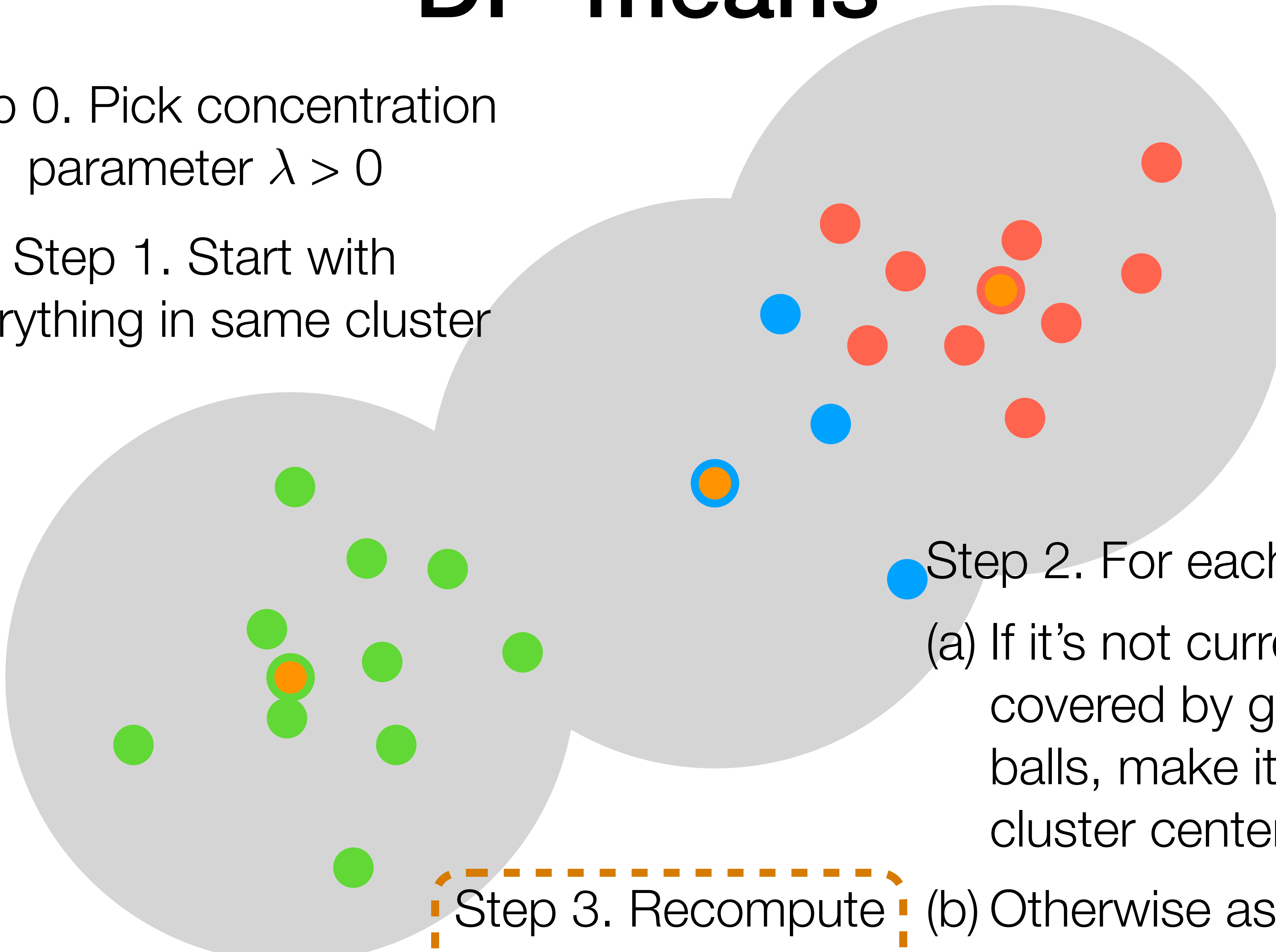

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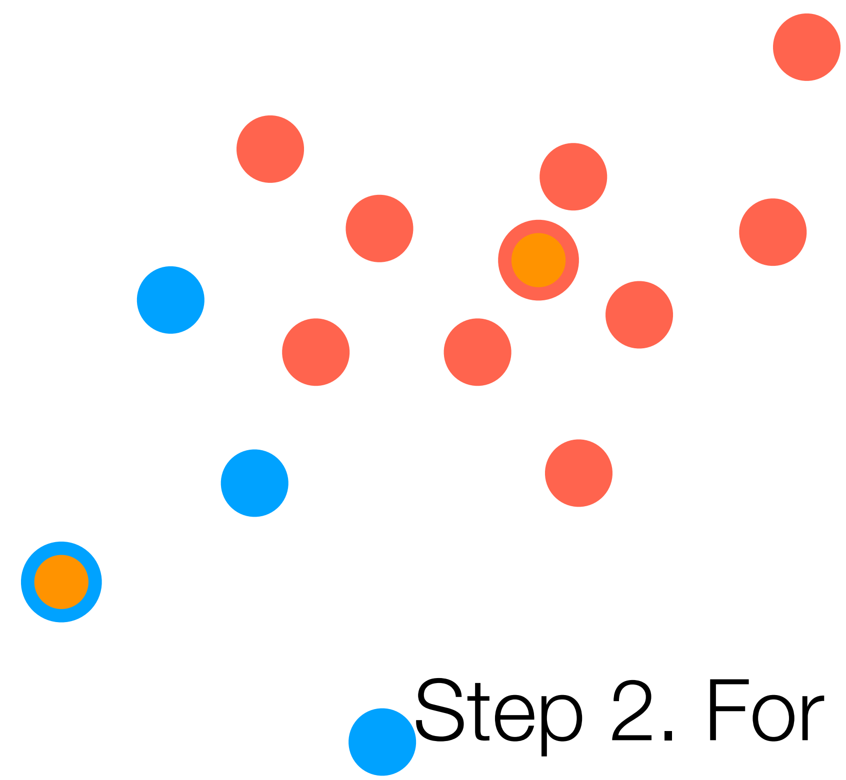

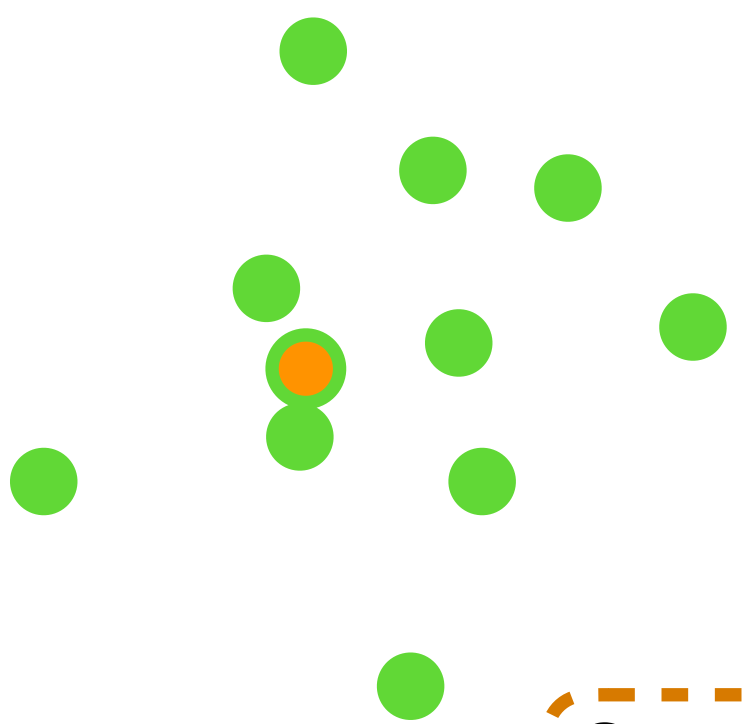

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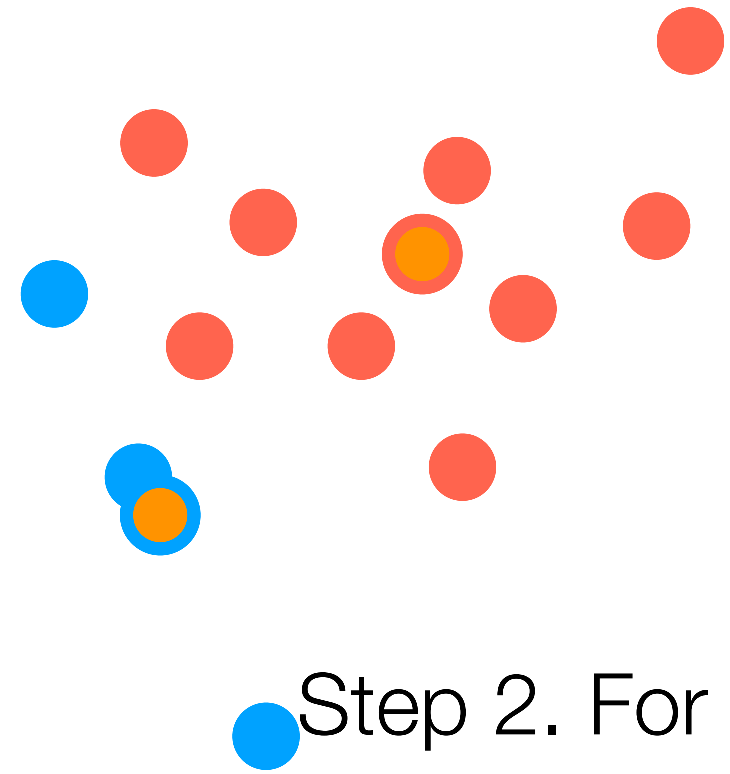

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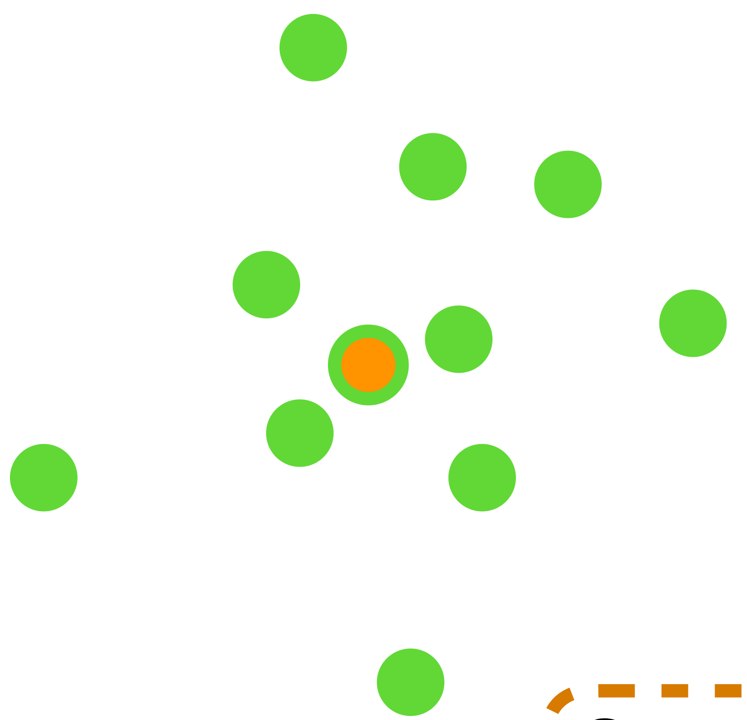

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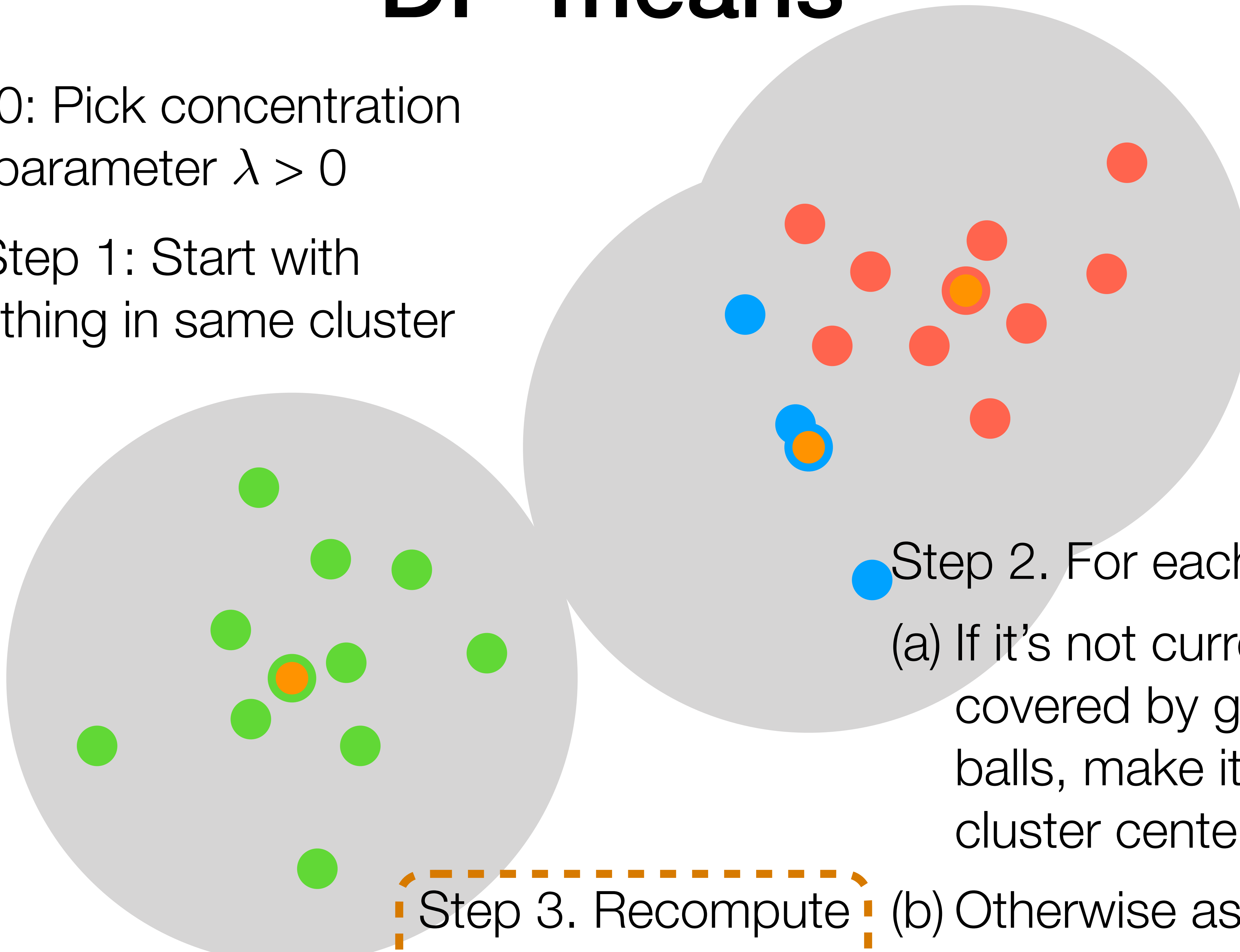

Step 2. For each point:

(a) If it's not currently covered by gray balls, make it a new cluster center

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Step 3. Recompute cluster centers

DP-means

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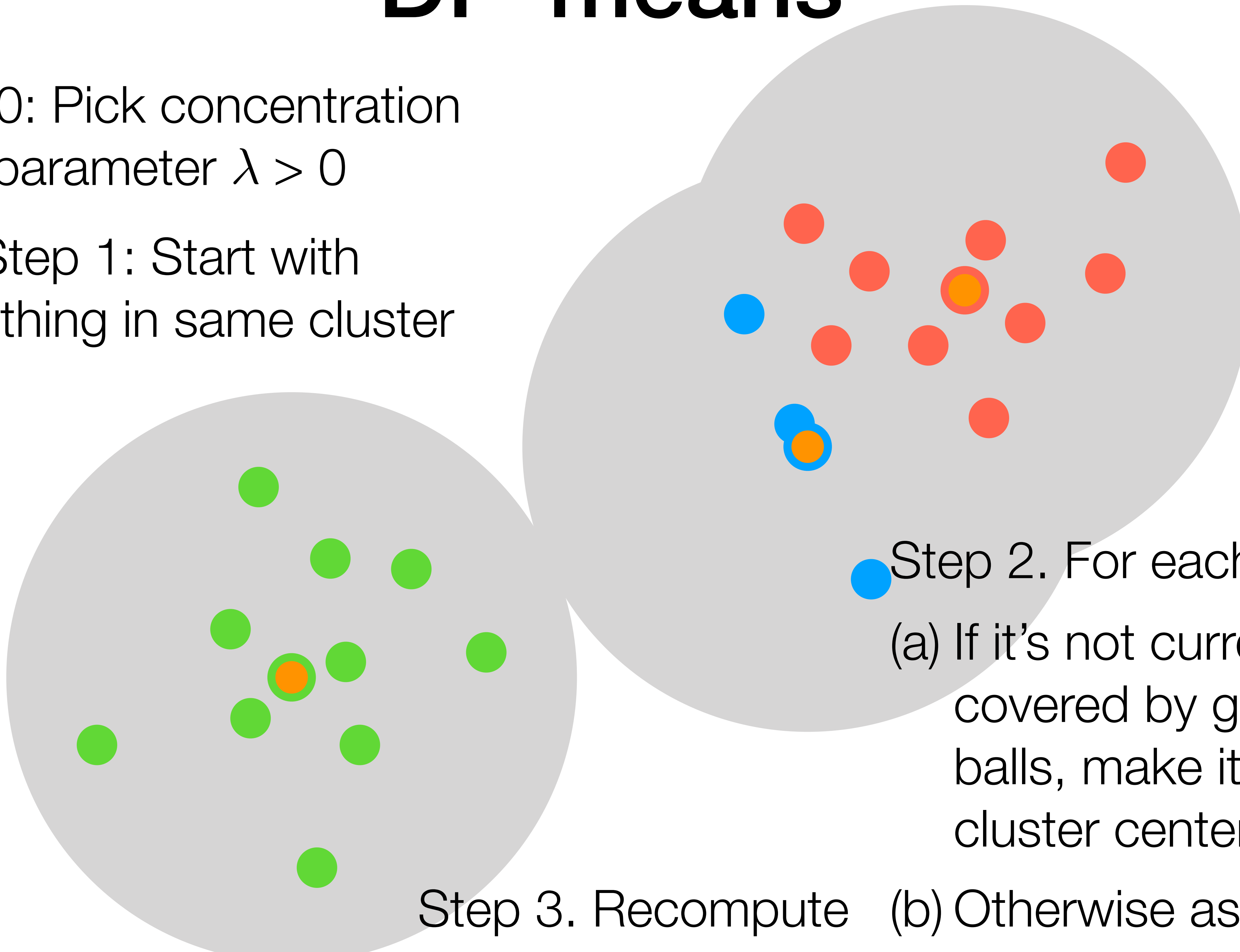

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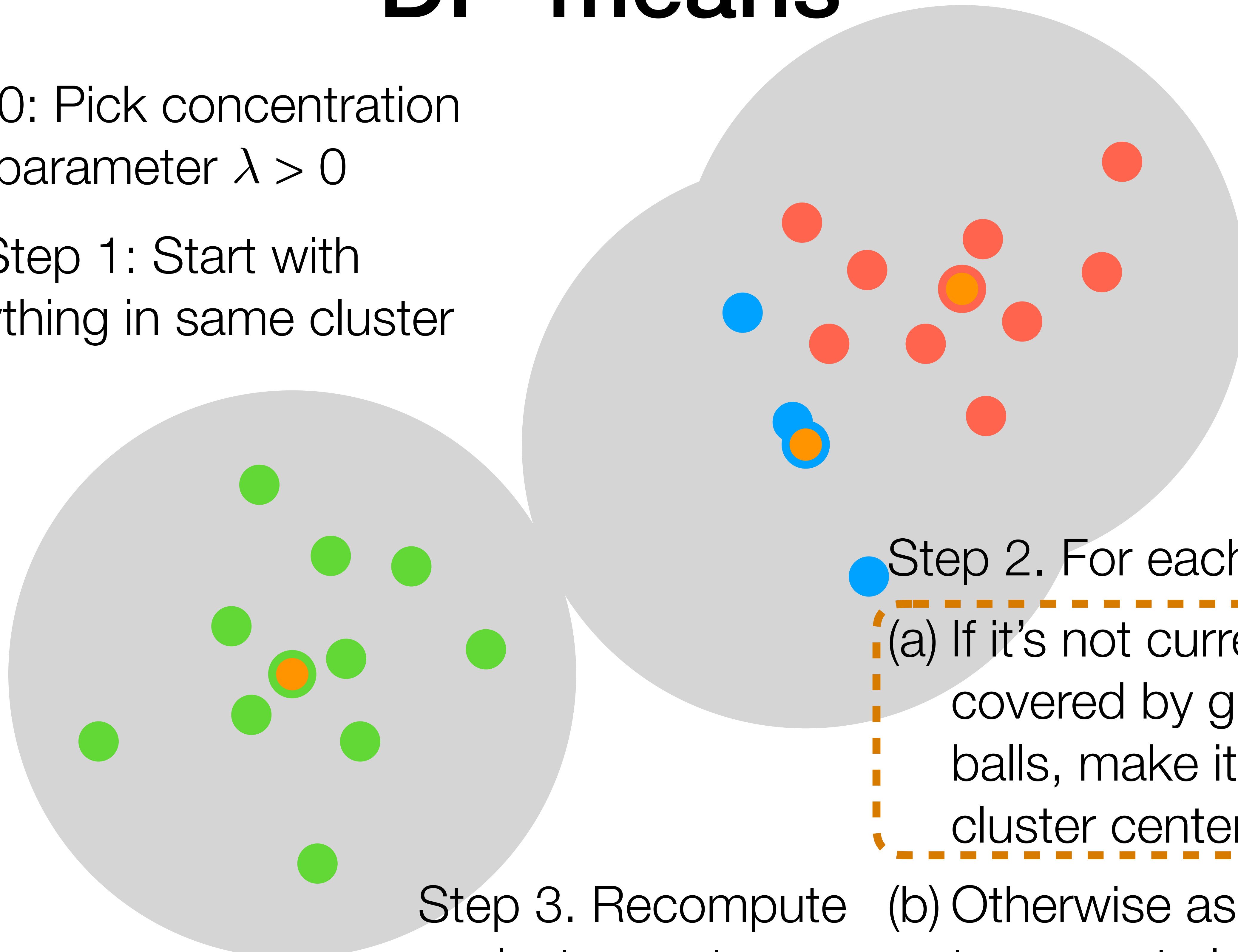

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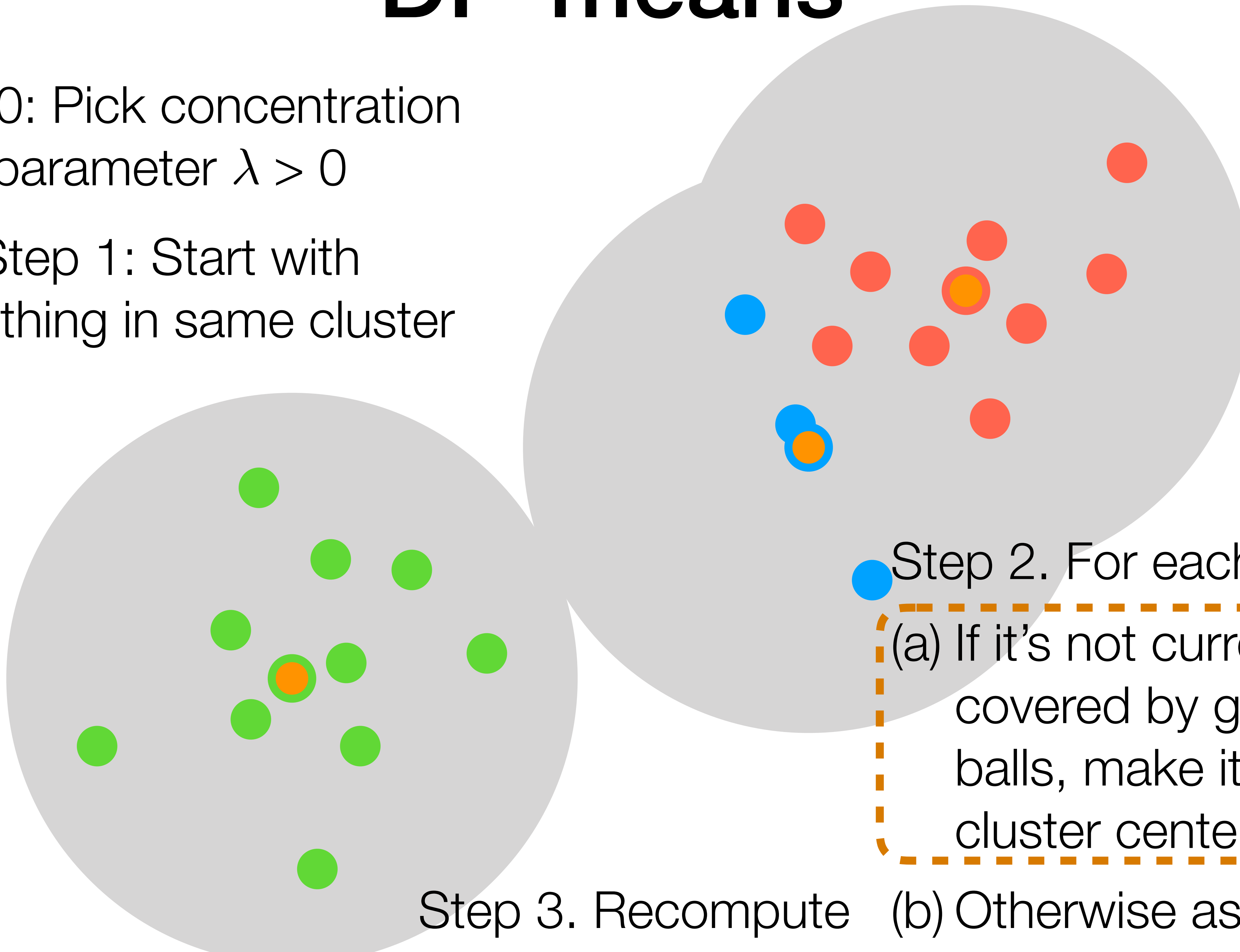

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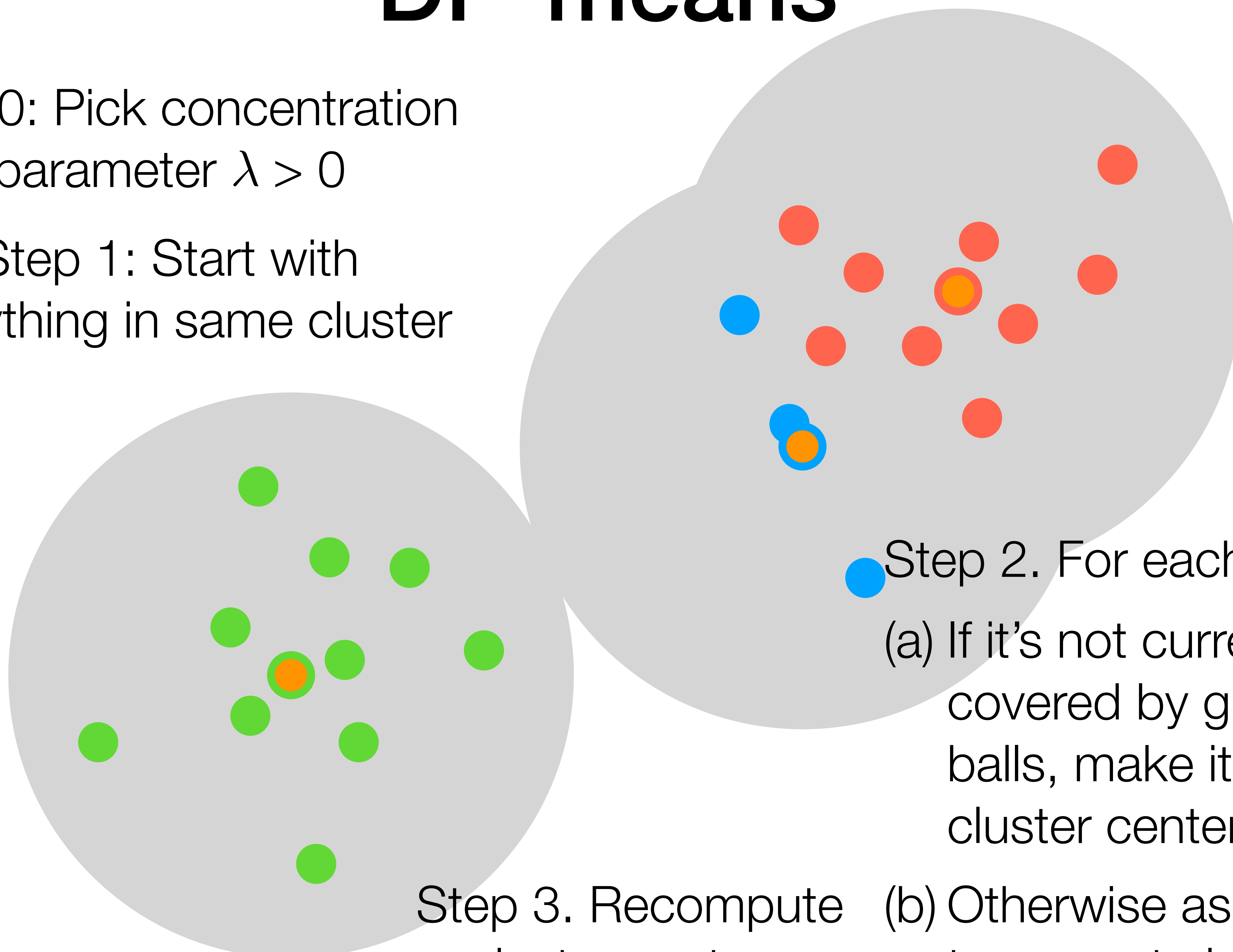

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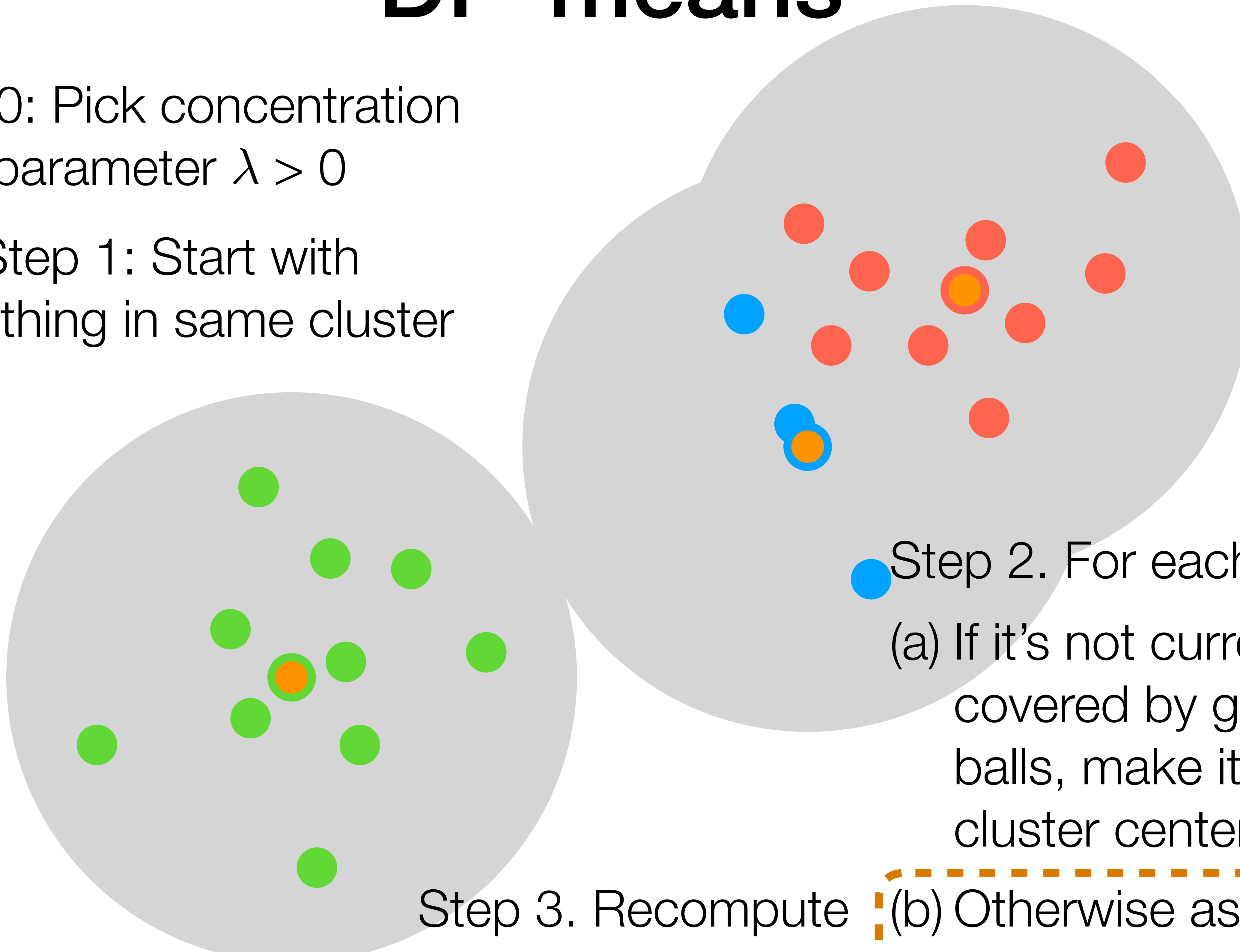

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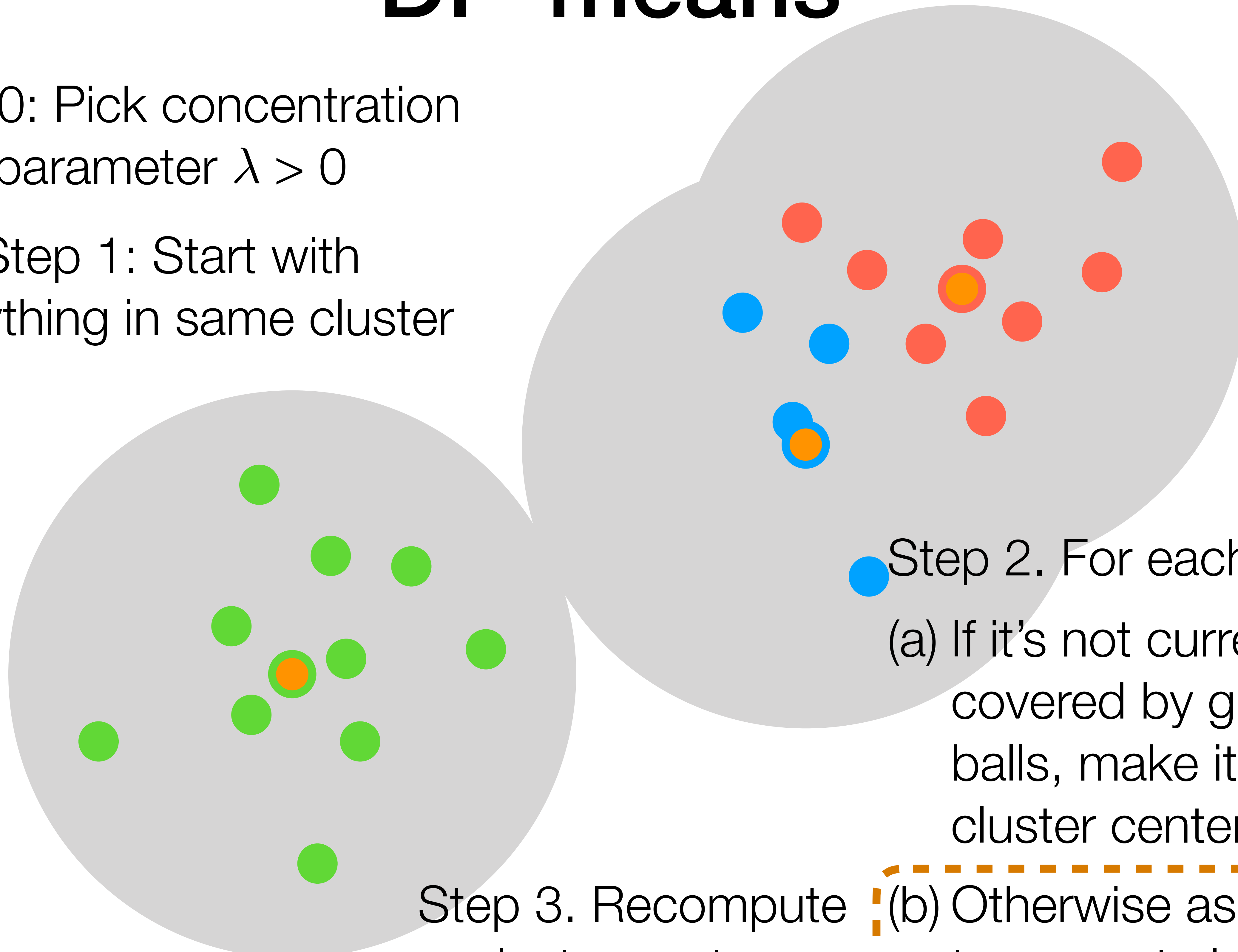

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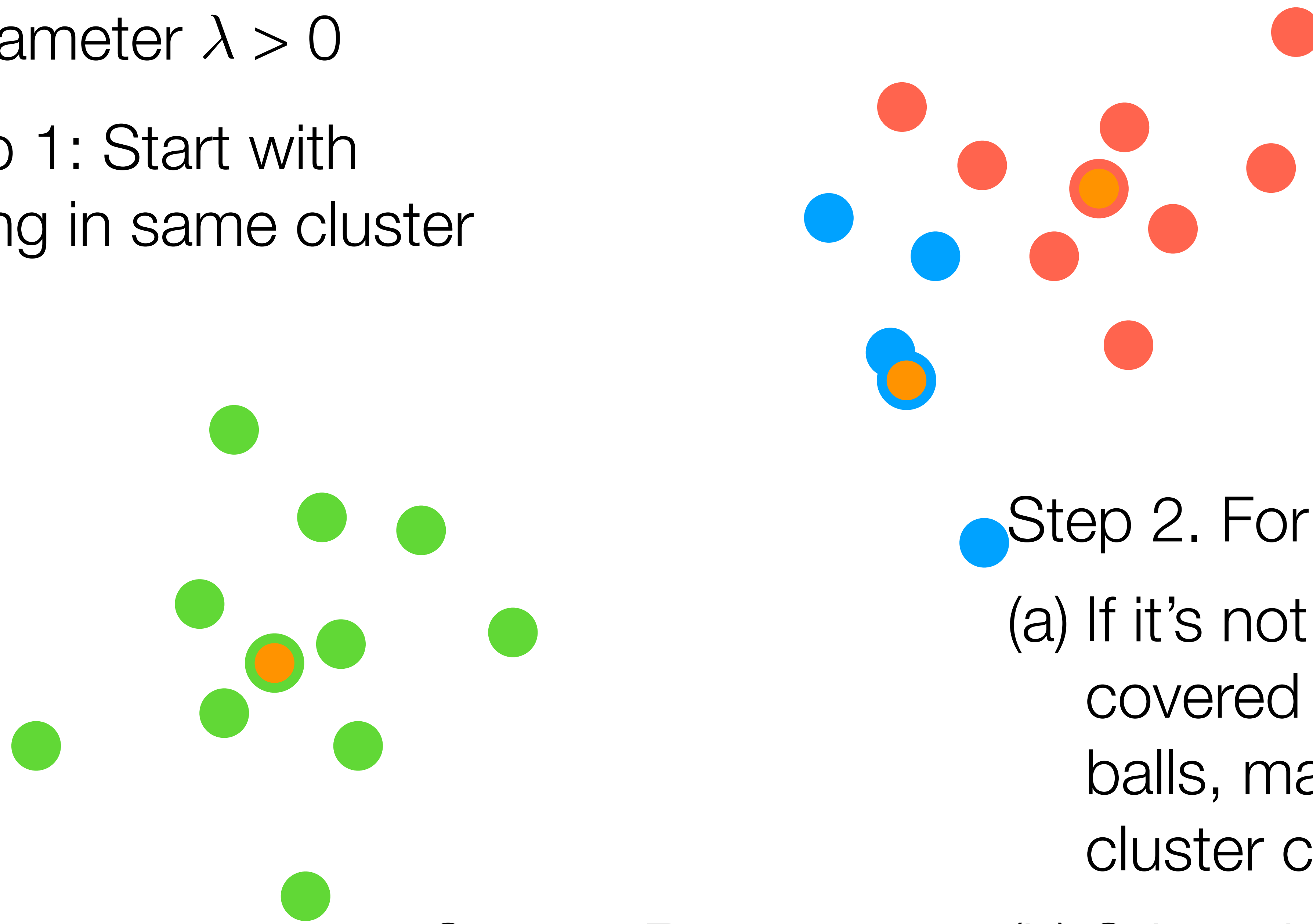

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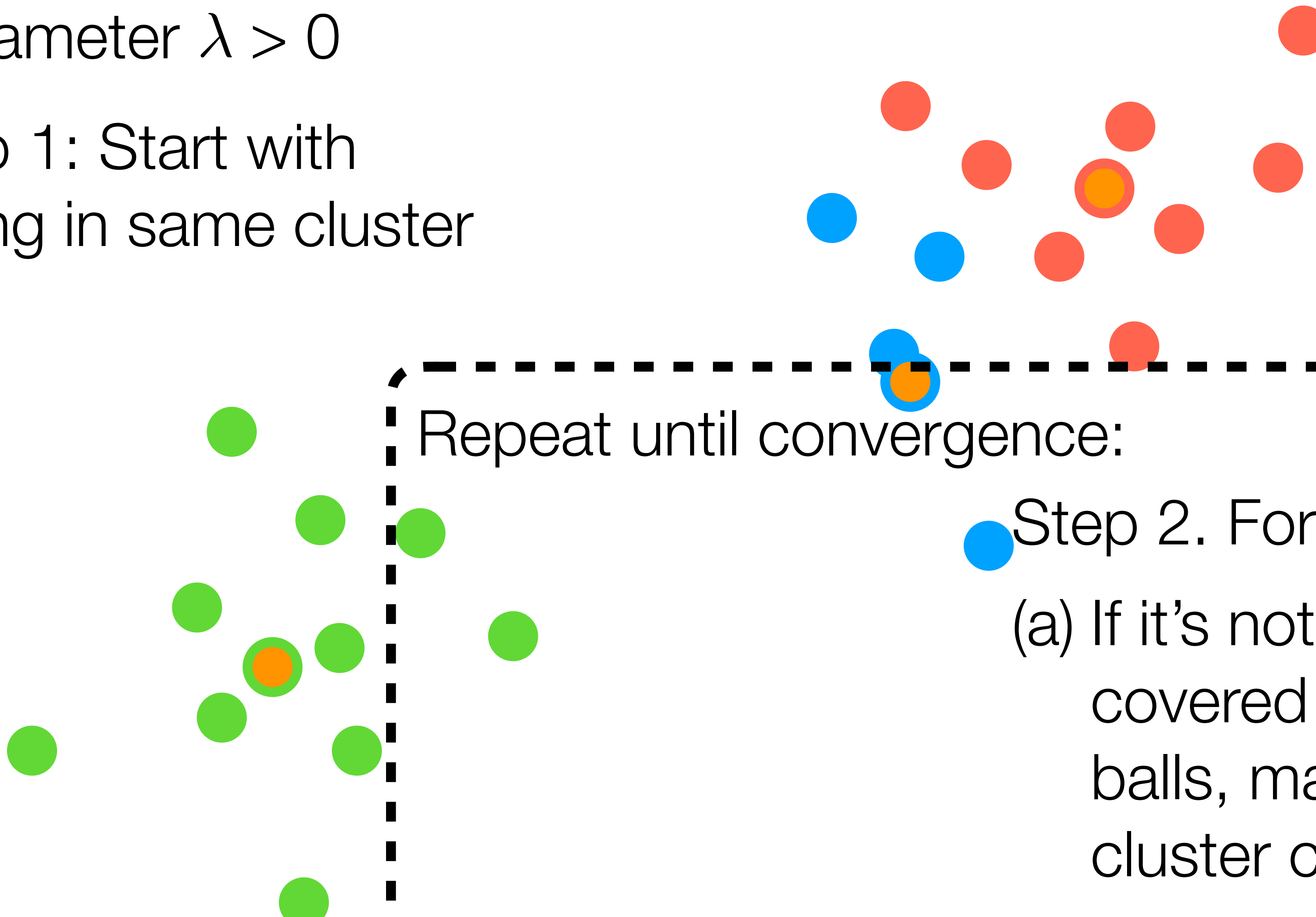

Repeat until convergence:

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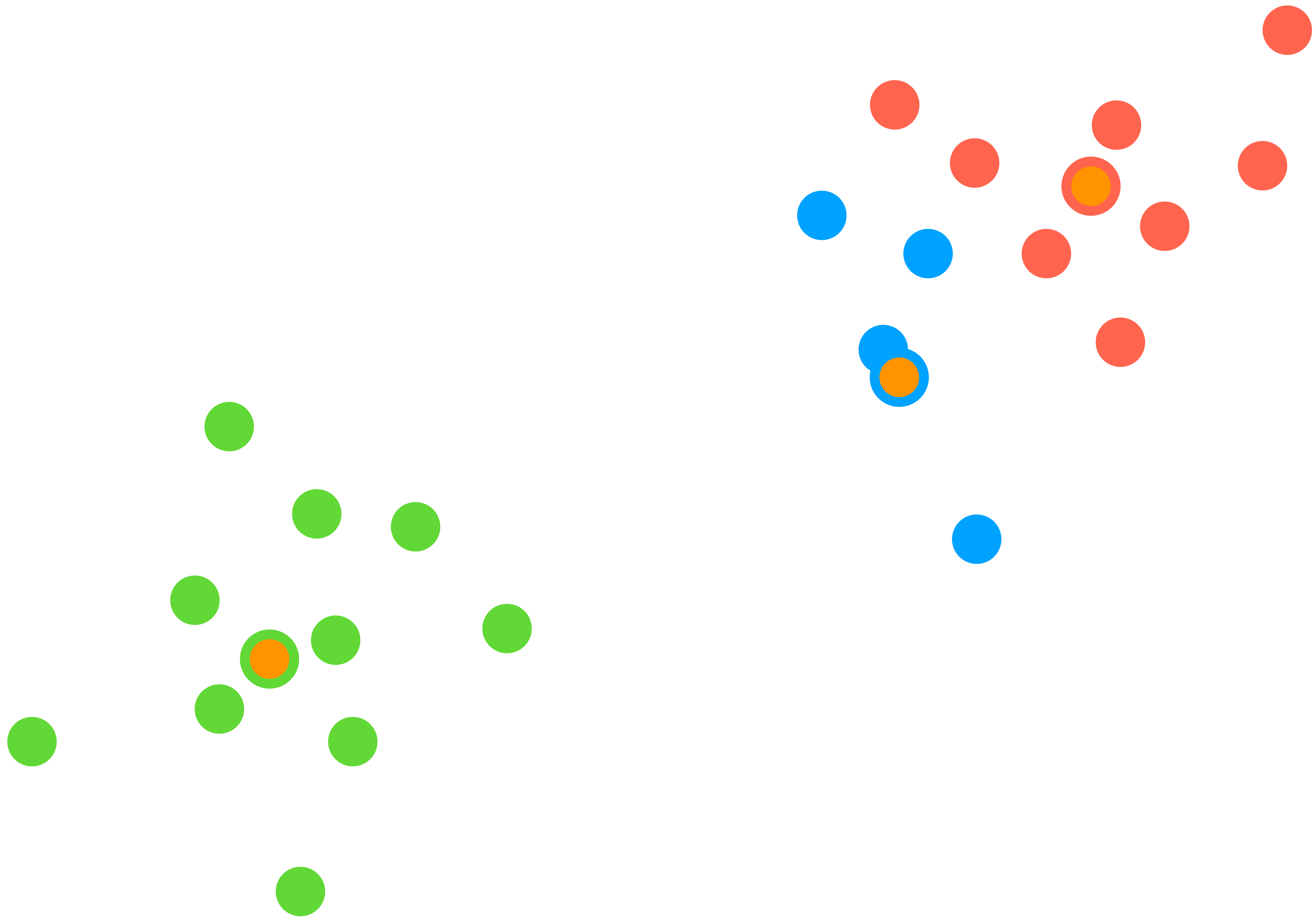
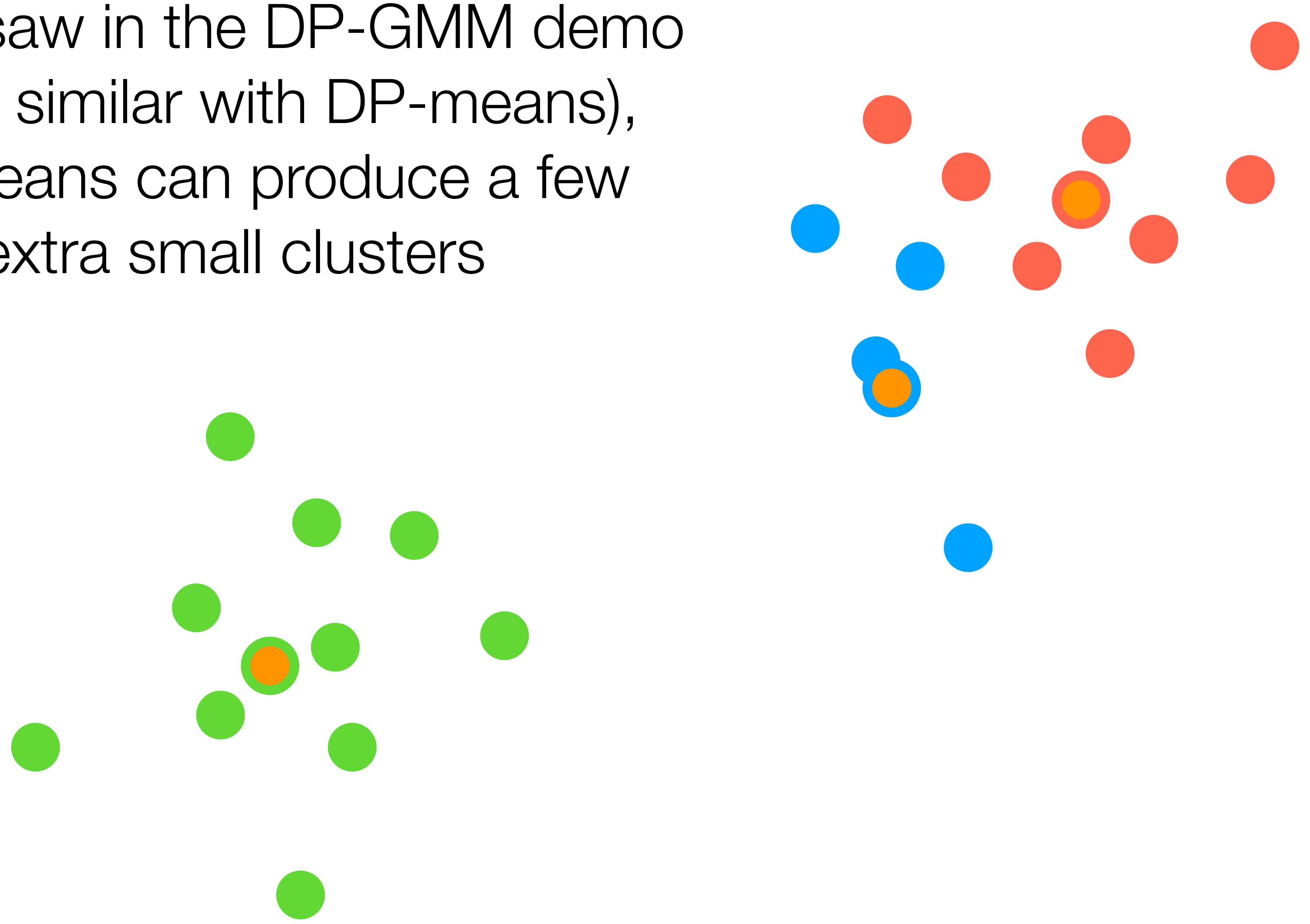
DP-means



DP-means

As you saw in the DP-GMM demo (and is similar with DP-means), DP-means can produce a few extra small clusters



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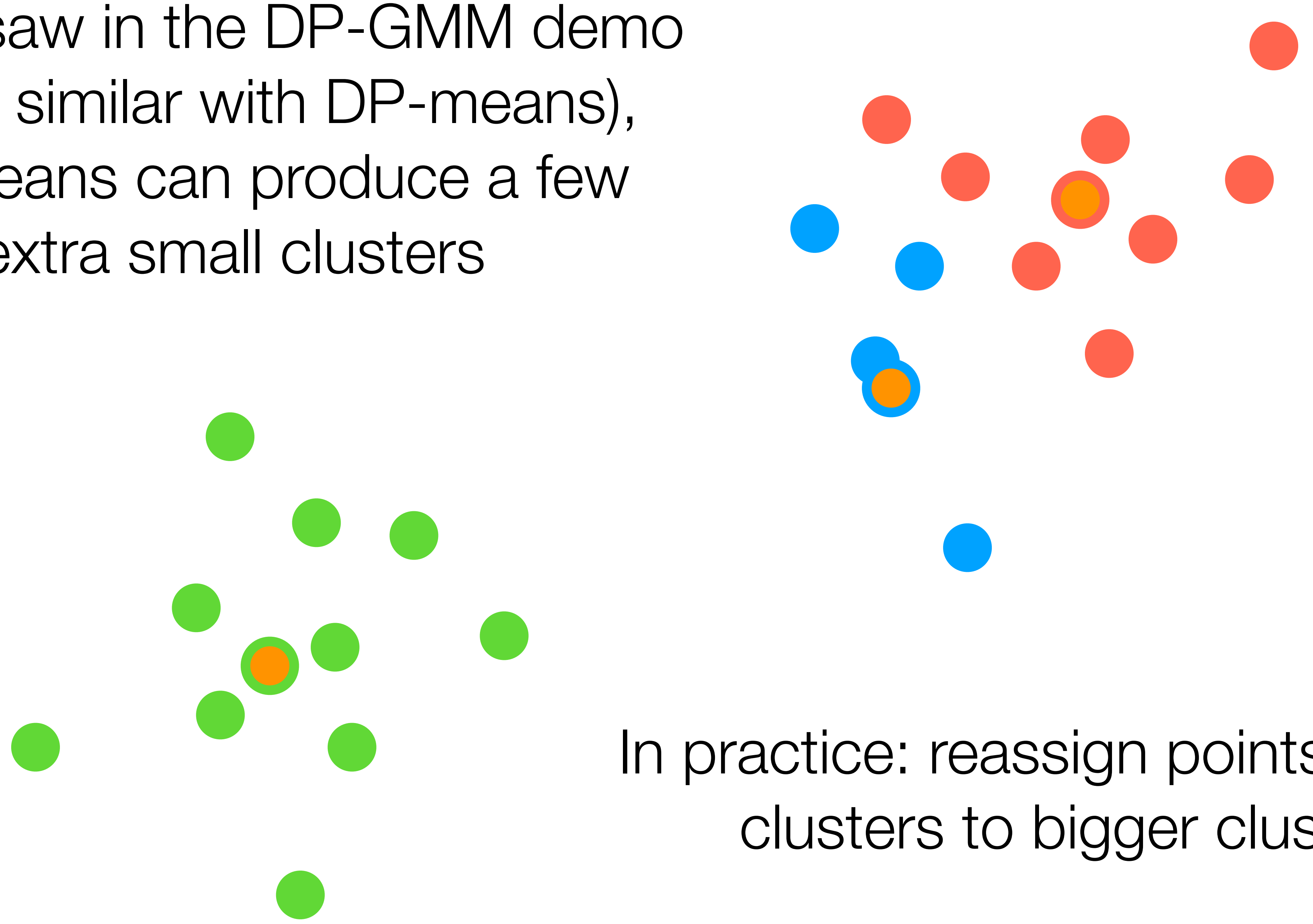

In practice: reassign points in small clusters to bigger clusters

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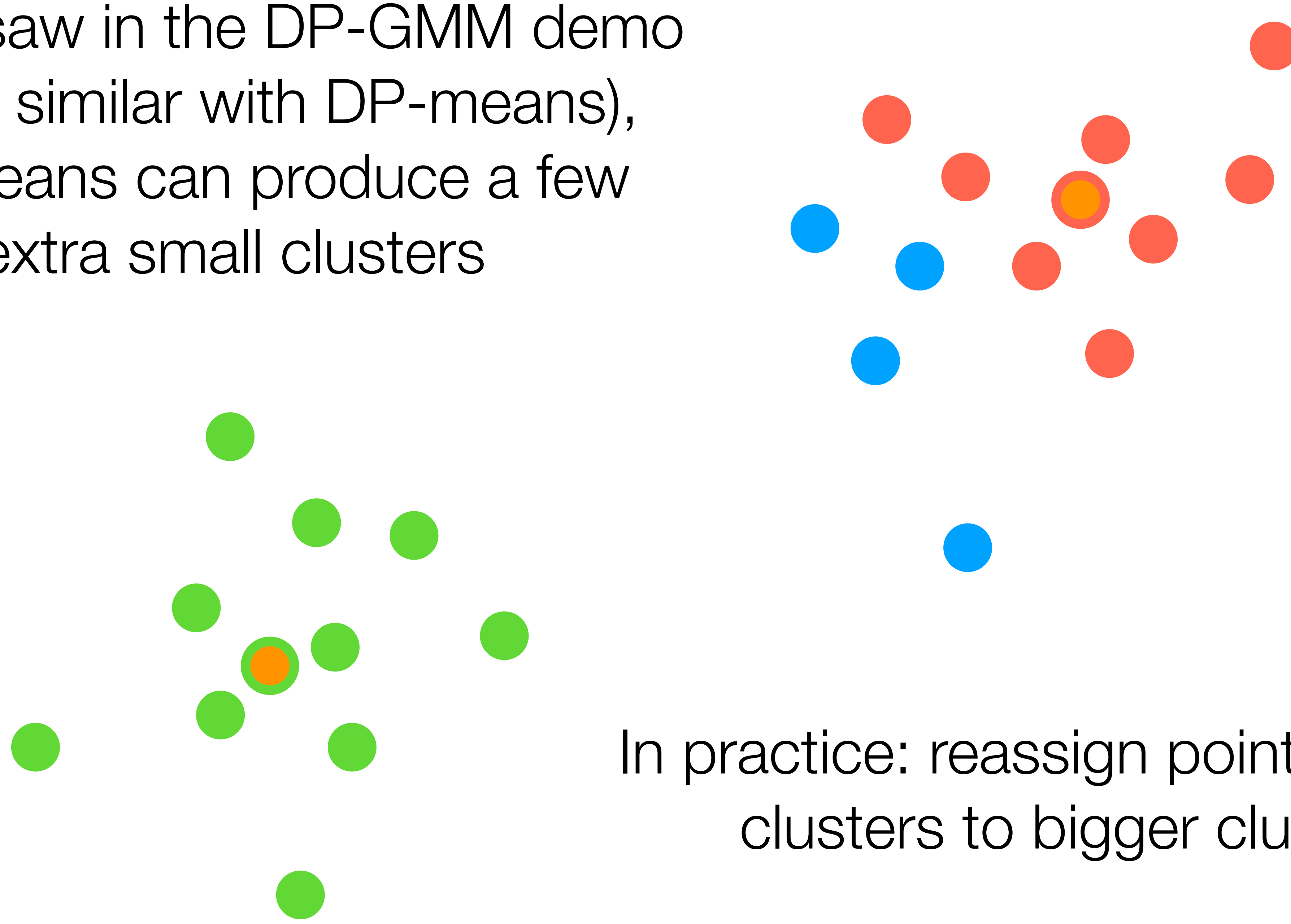

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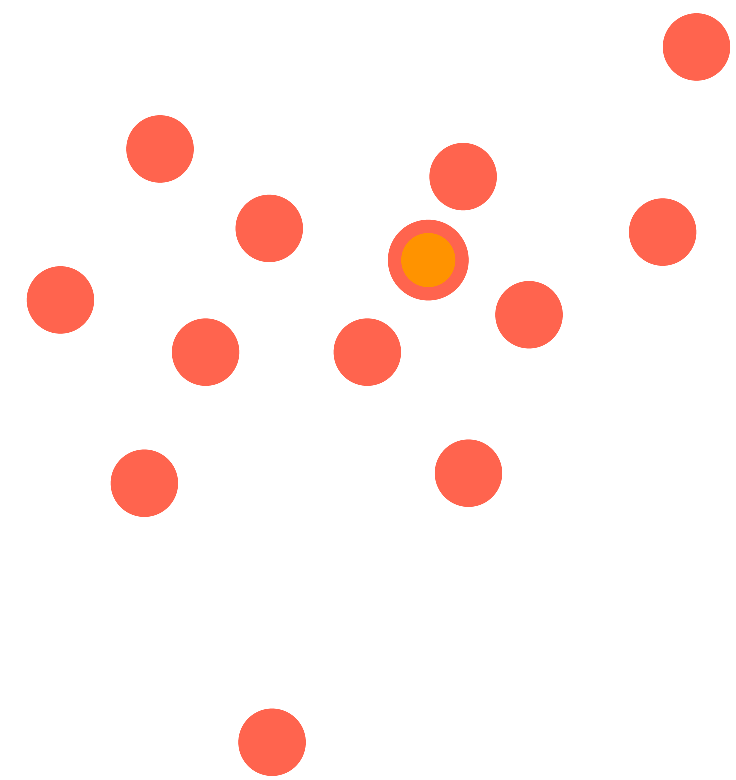

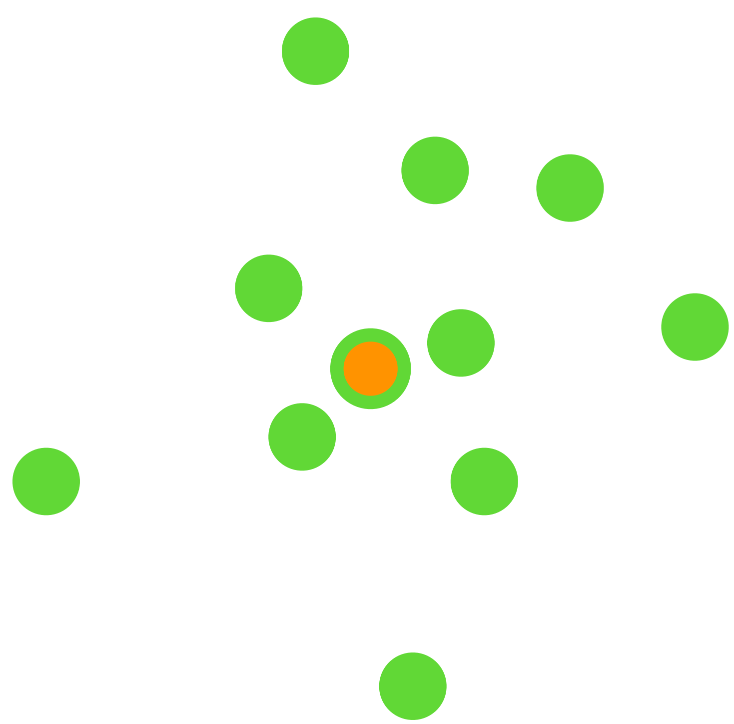

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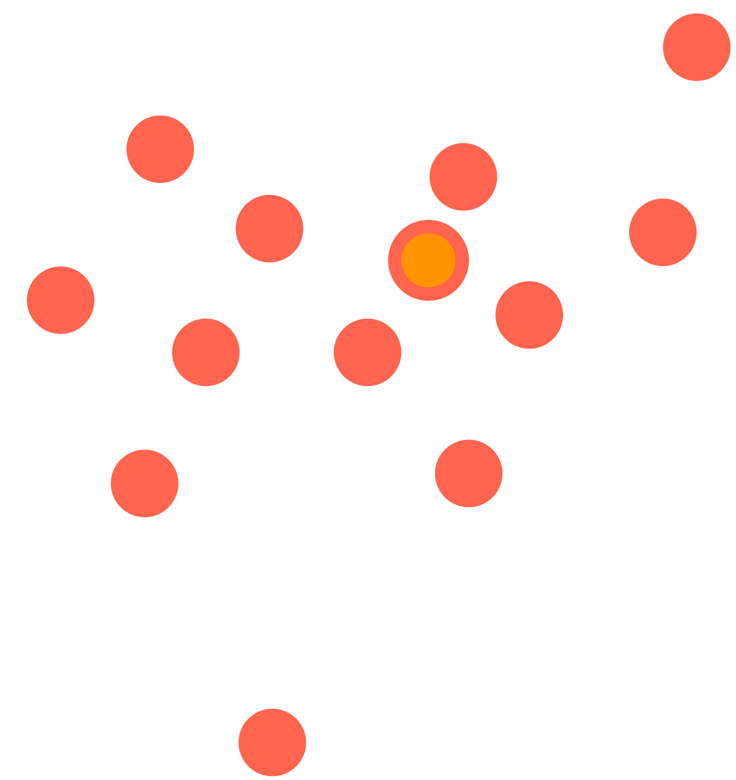

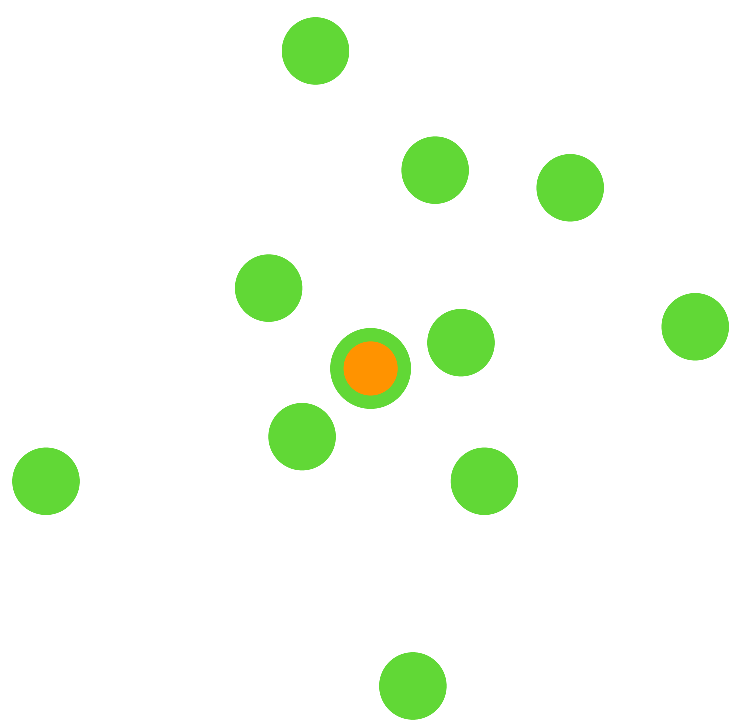

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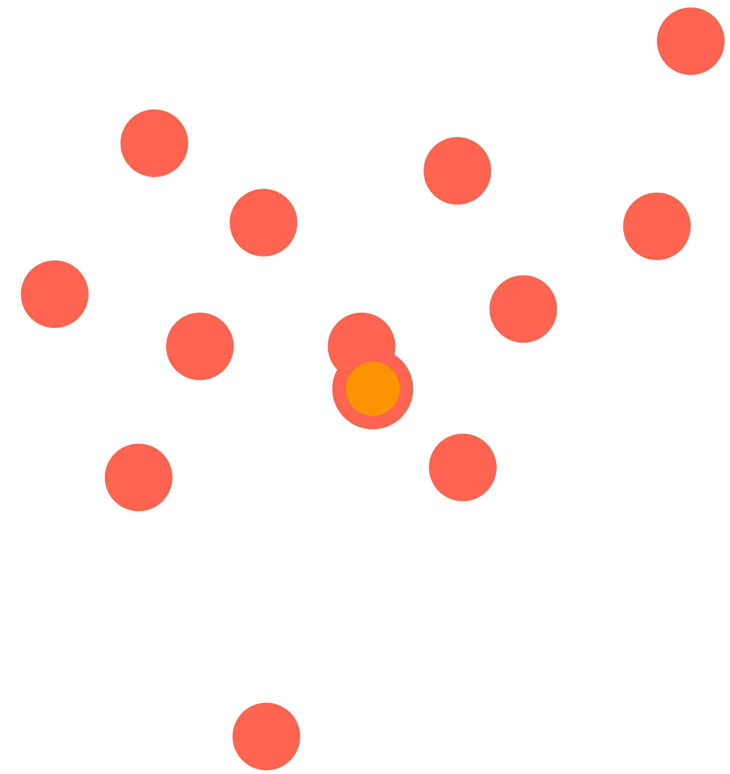

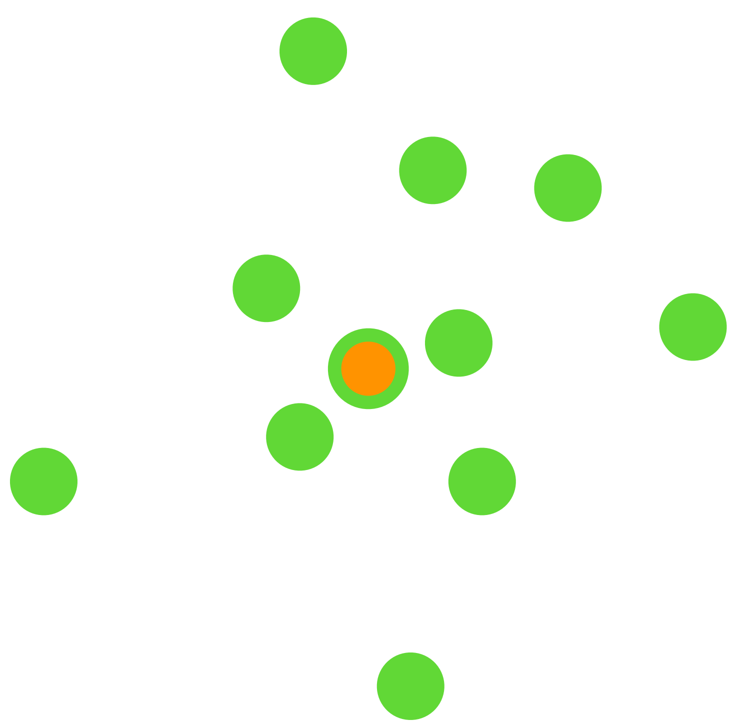

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➔ DP-means provides a decent solution!

Other Ways for Choosing *k*

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- Choose a cost function to compute for different *k*
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    - Ideally: cost function should relate to your application of interest
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Here’s an example of a cost function you don’t want to use

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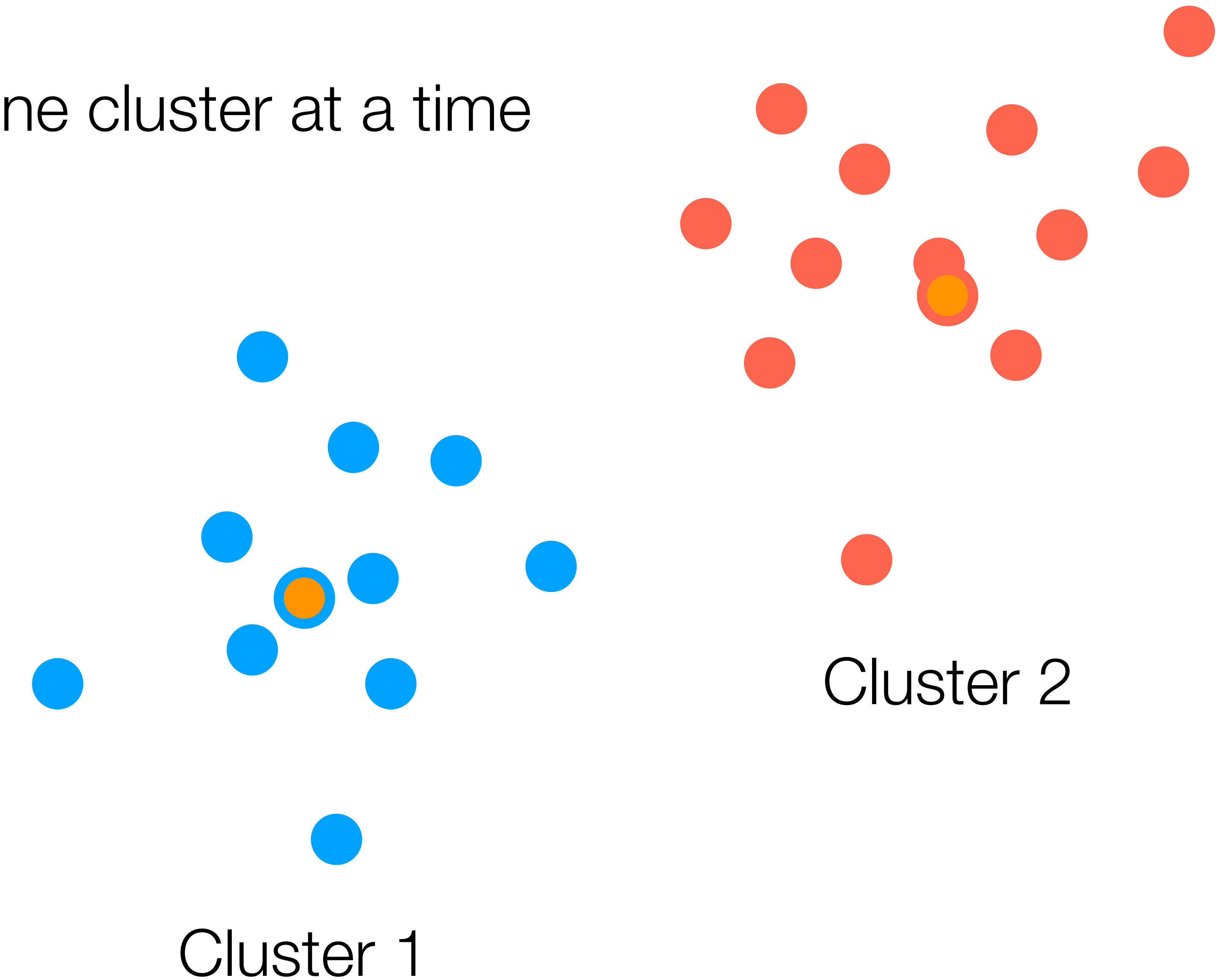
But hey it’s worth a shot

Residual Sum of Squares

Look at one cluster at a time



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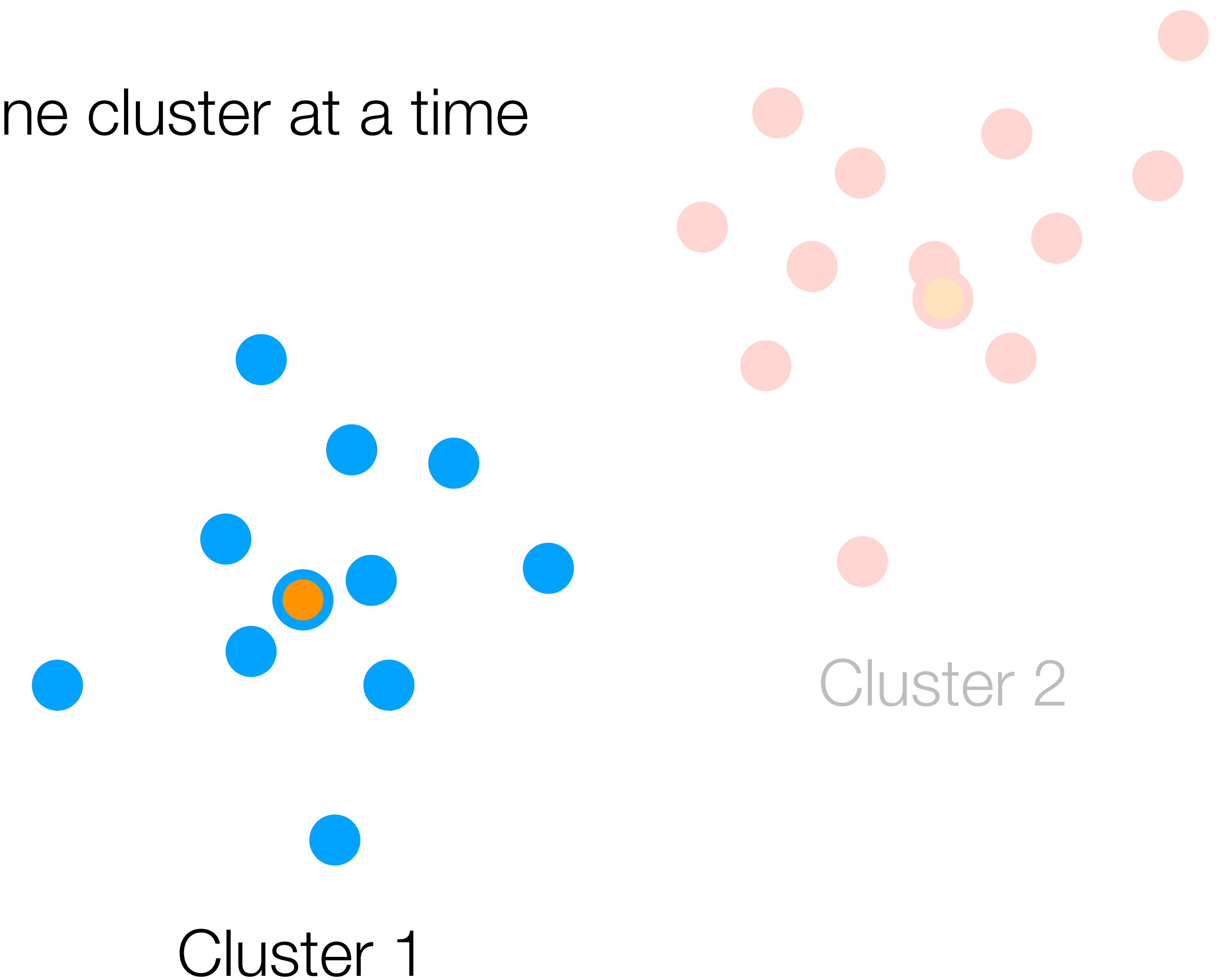

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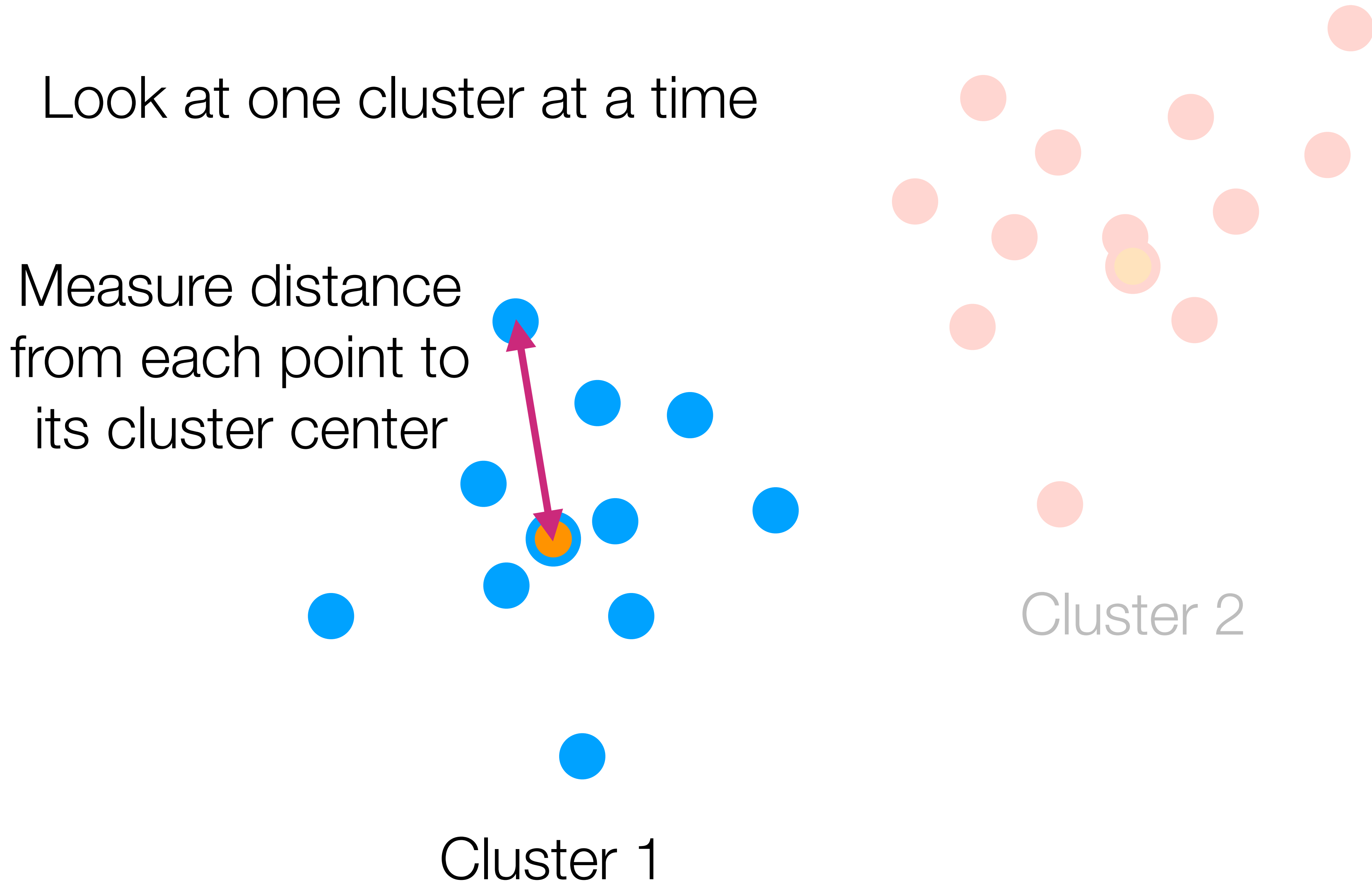
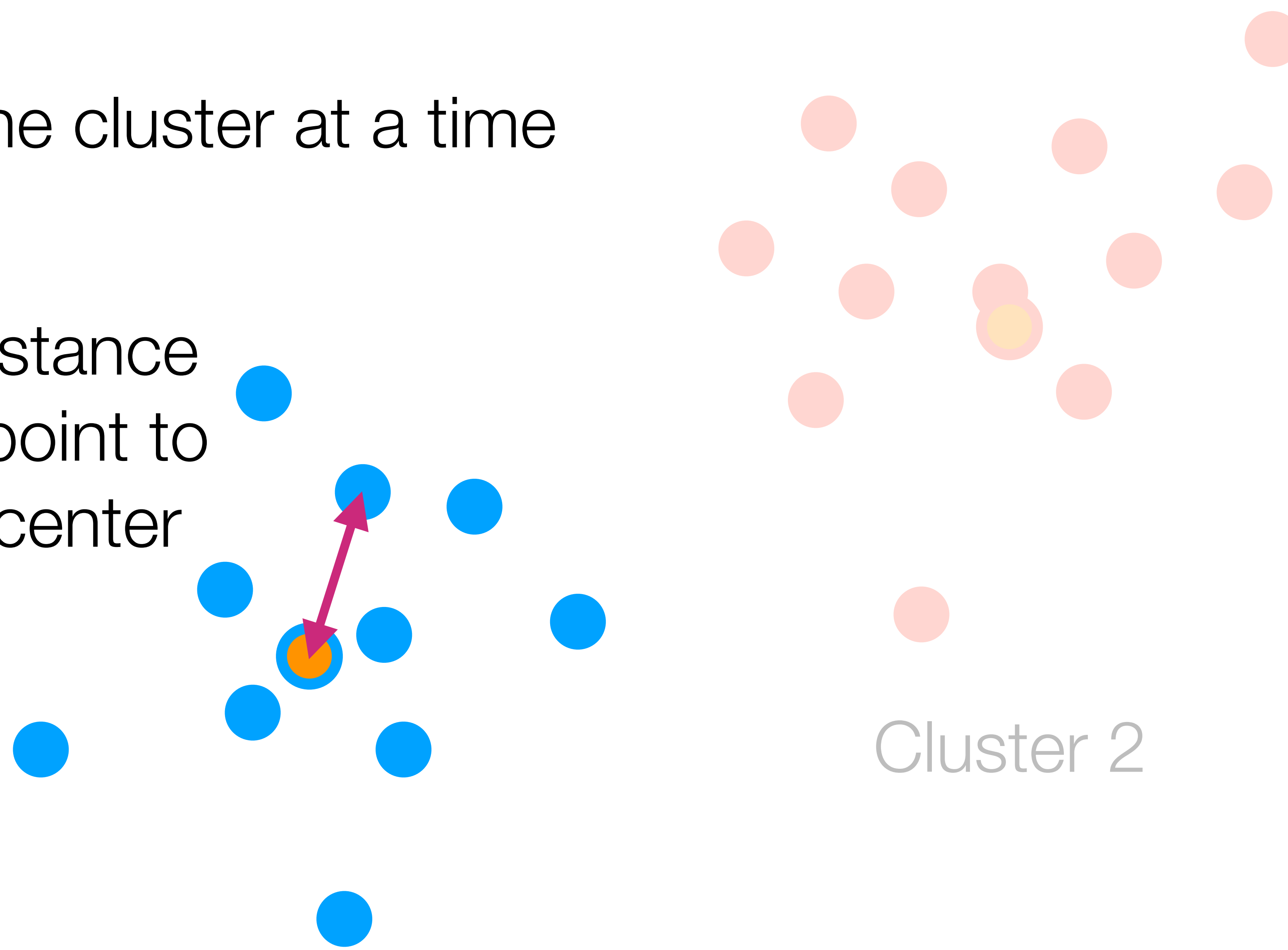


Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



Cluster 2

Cluster 1

Residual Sum of Squares

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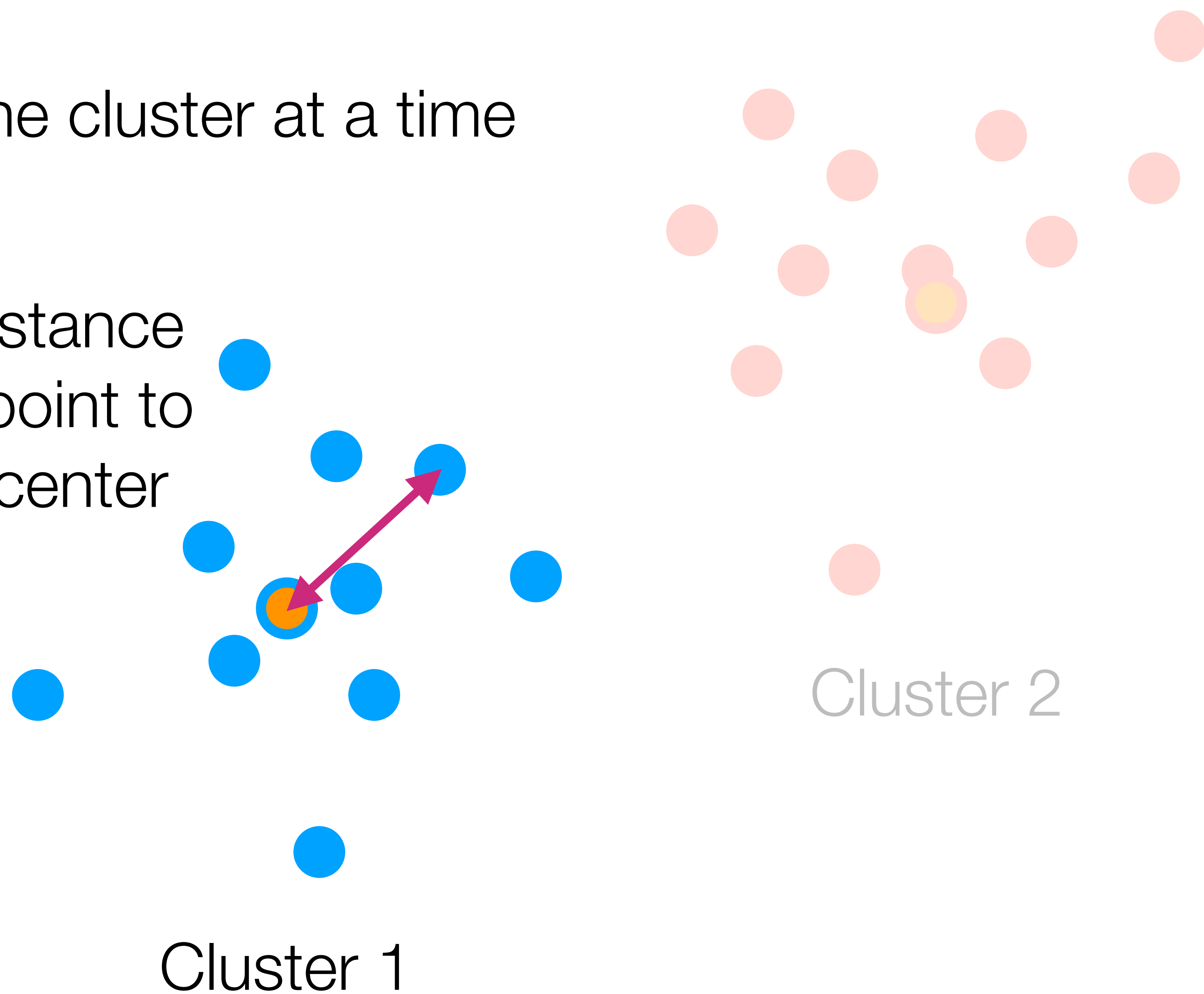

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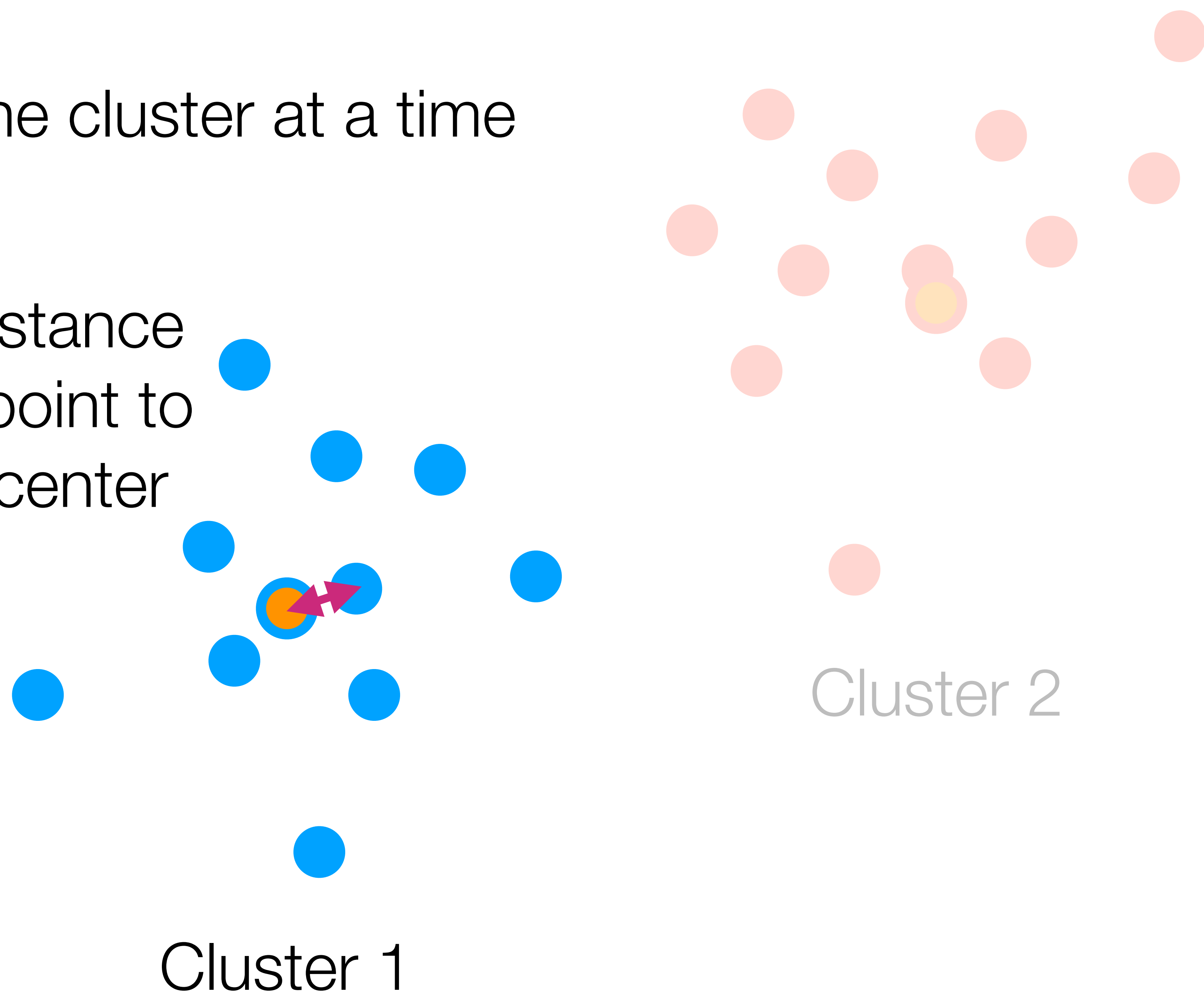

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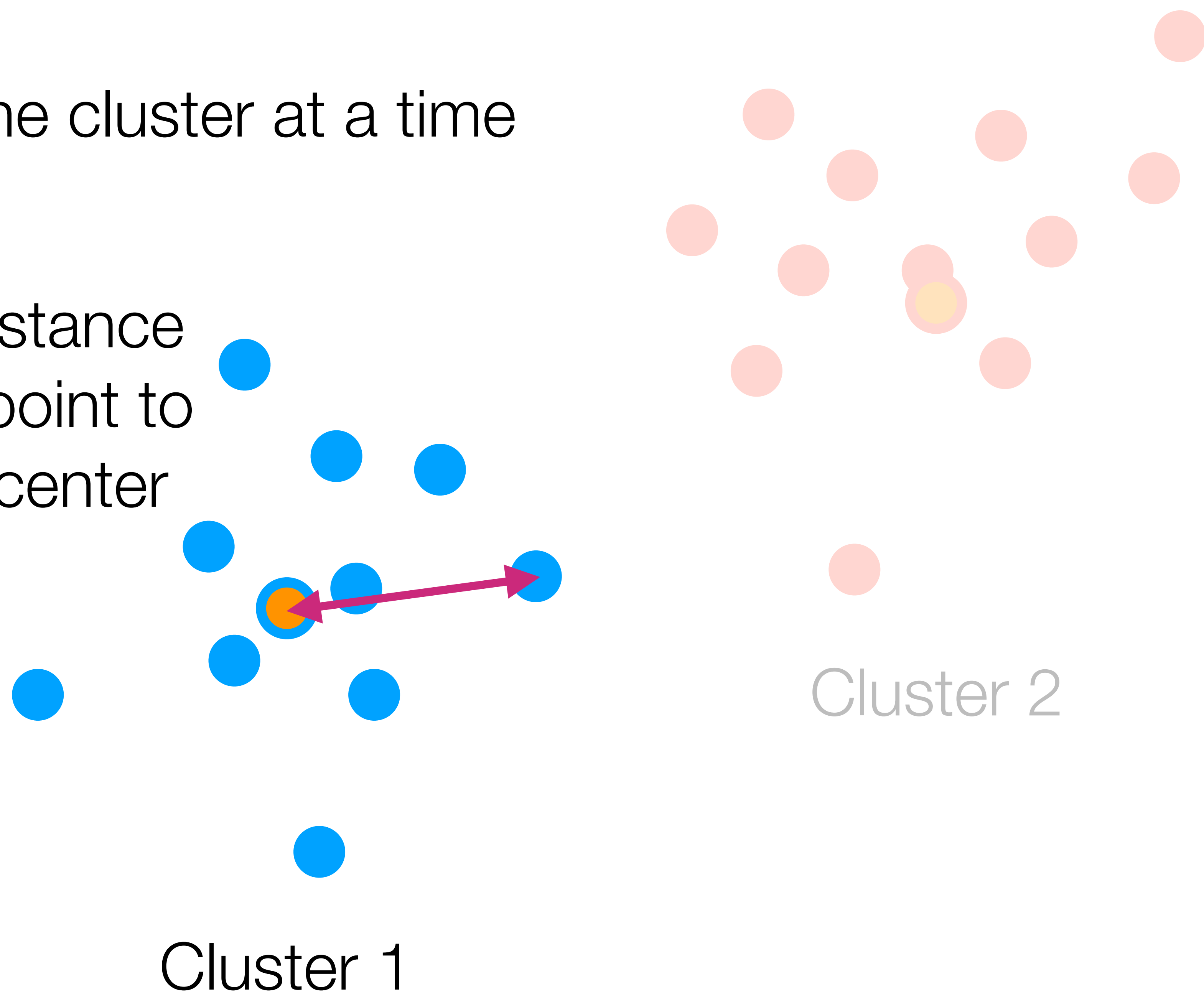

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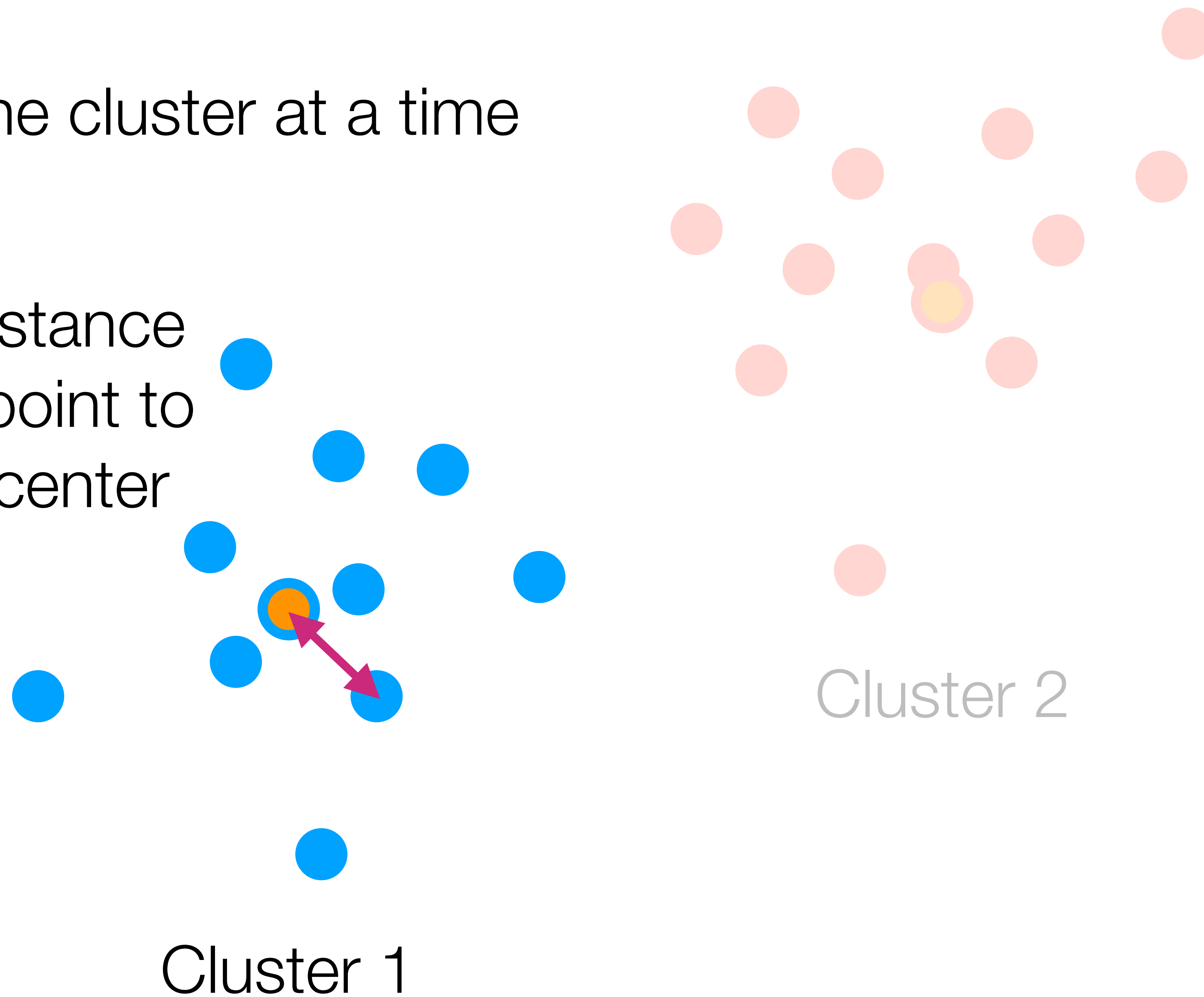

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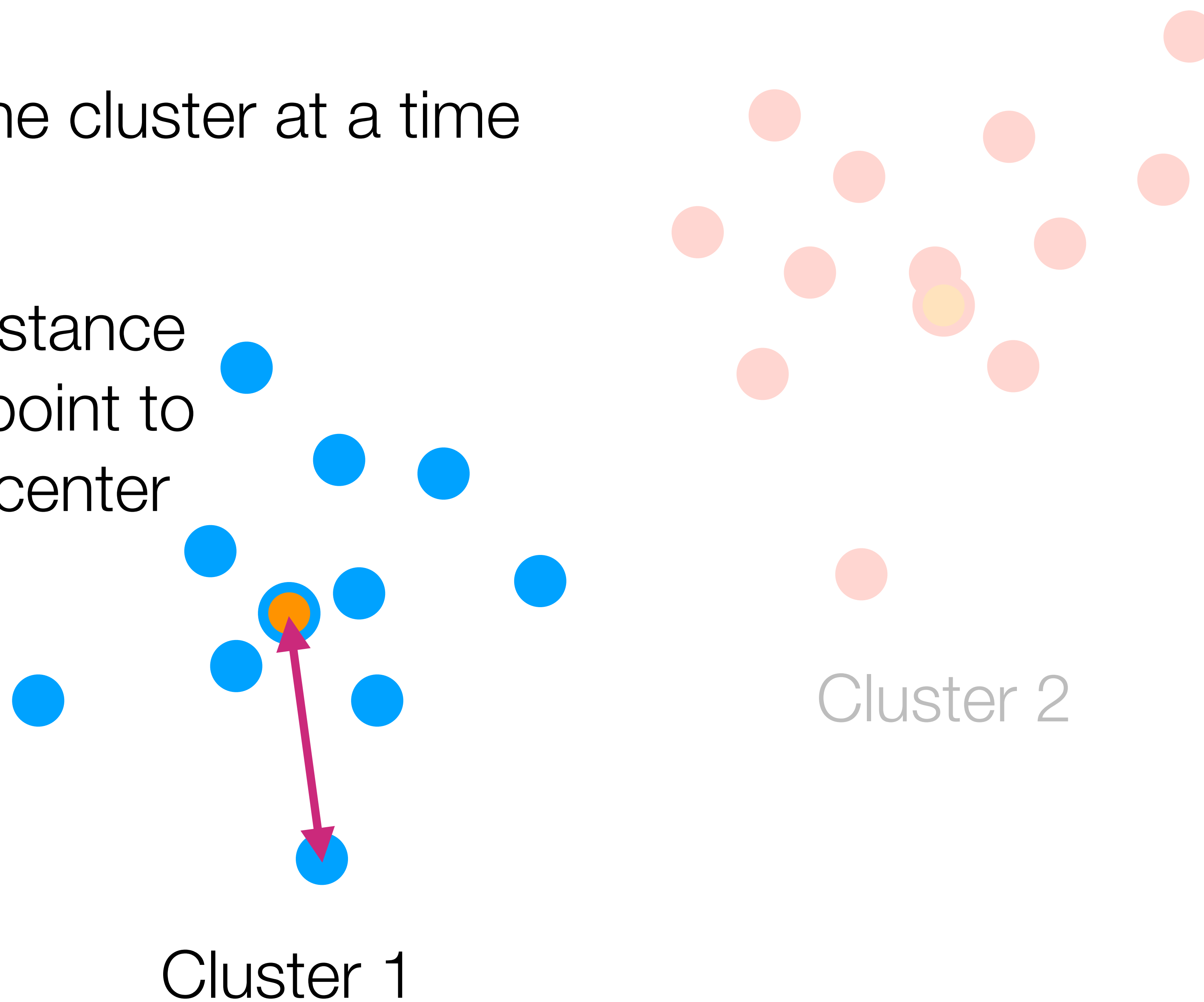

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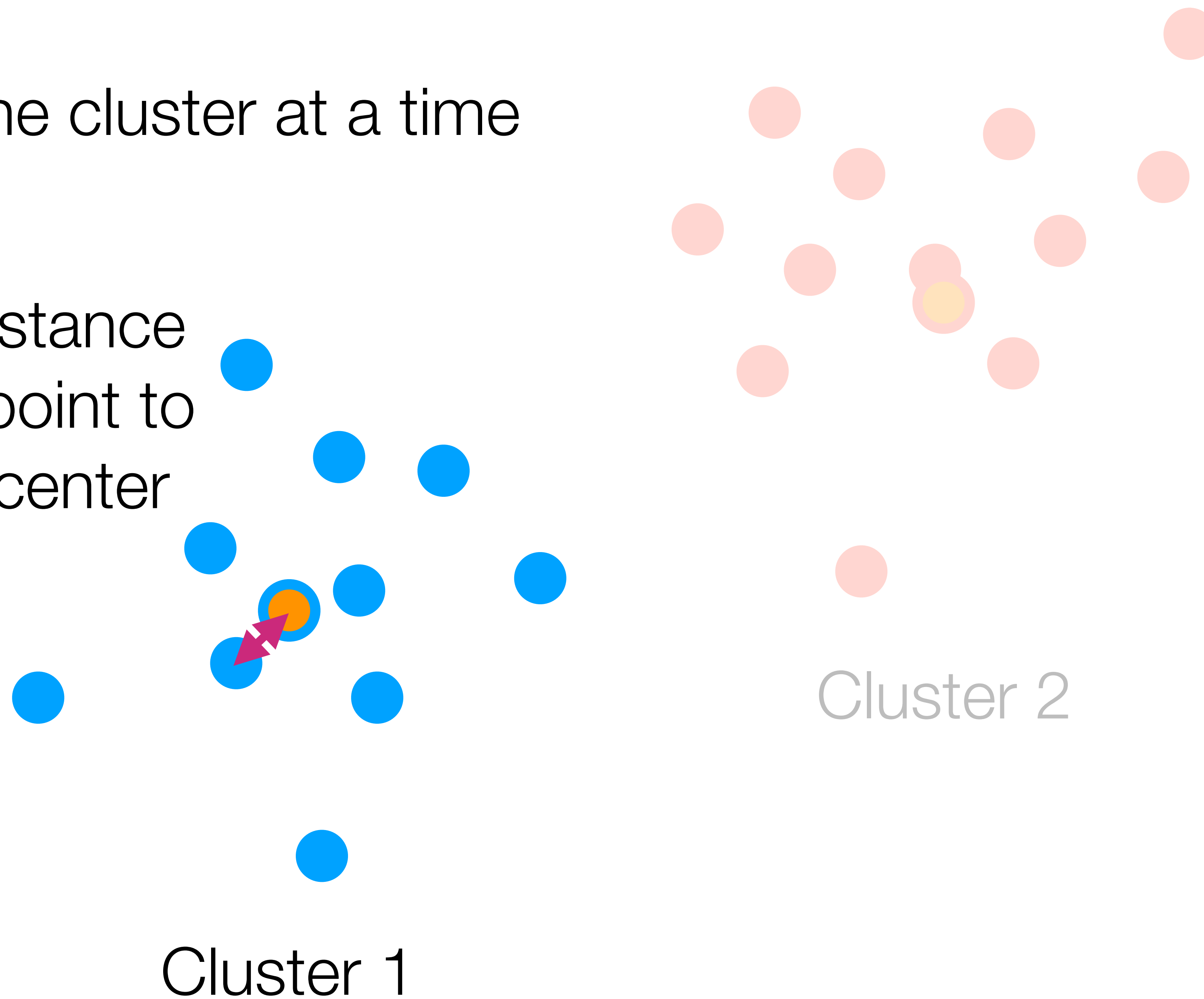

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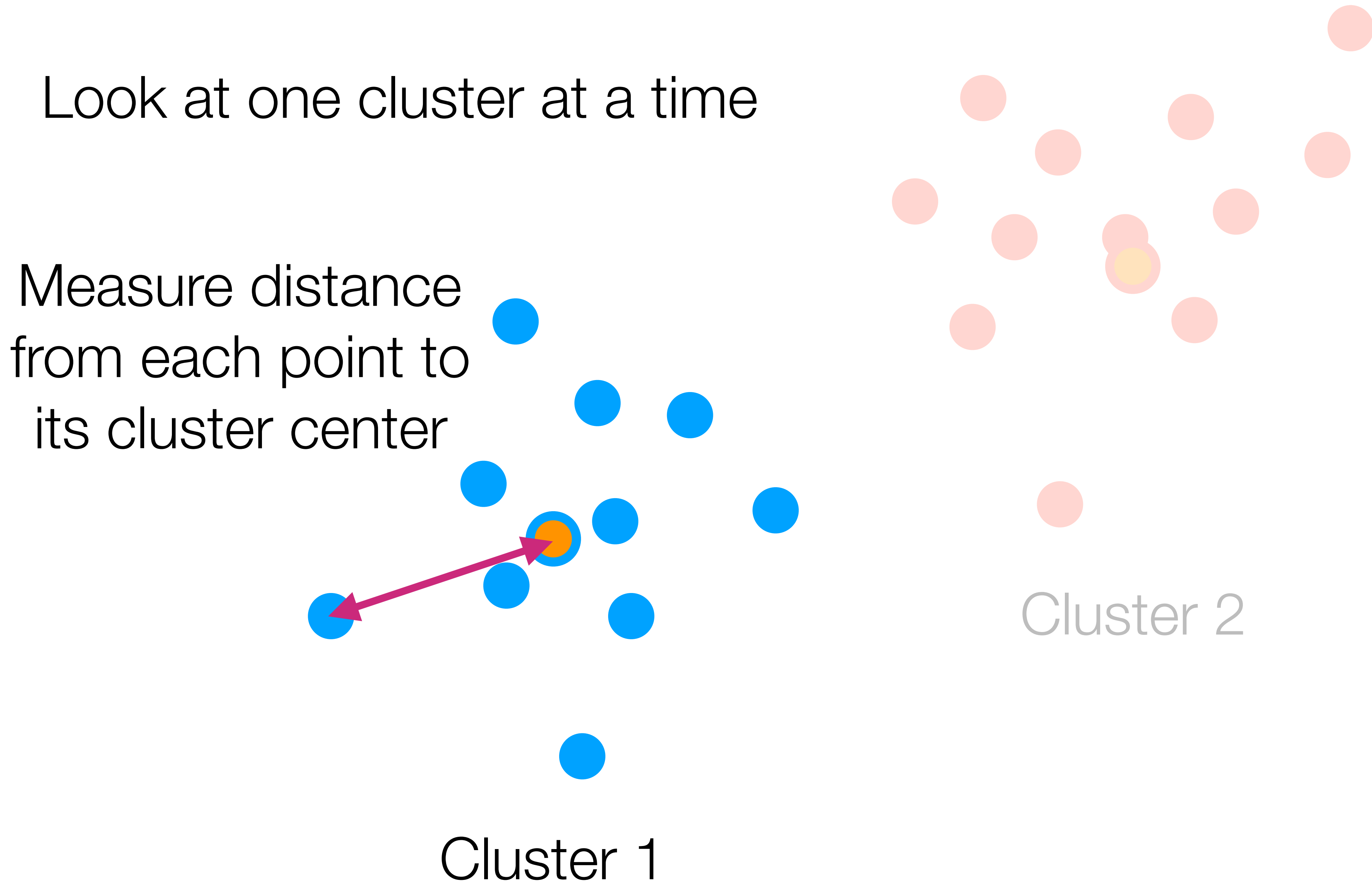

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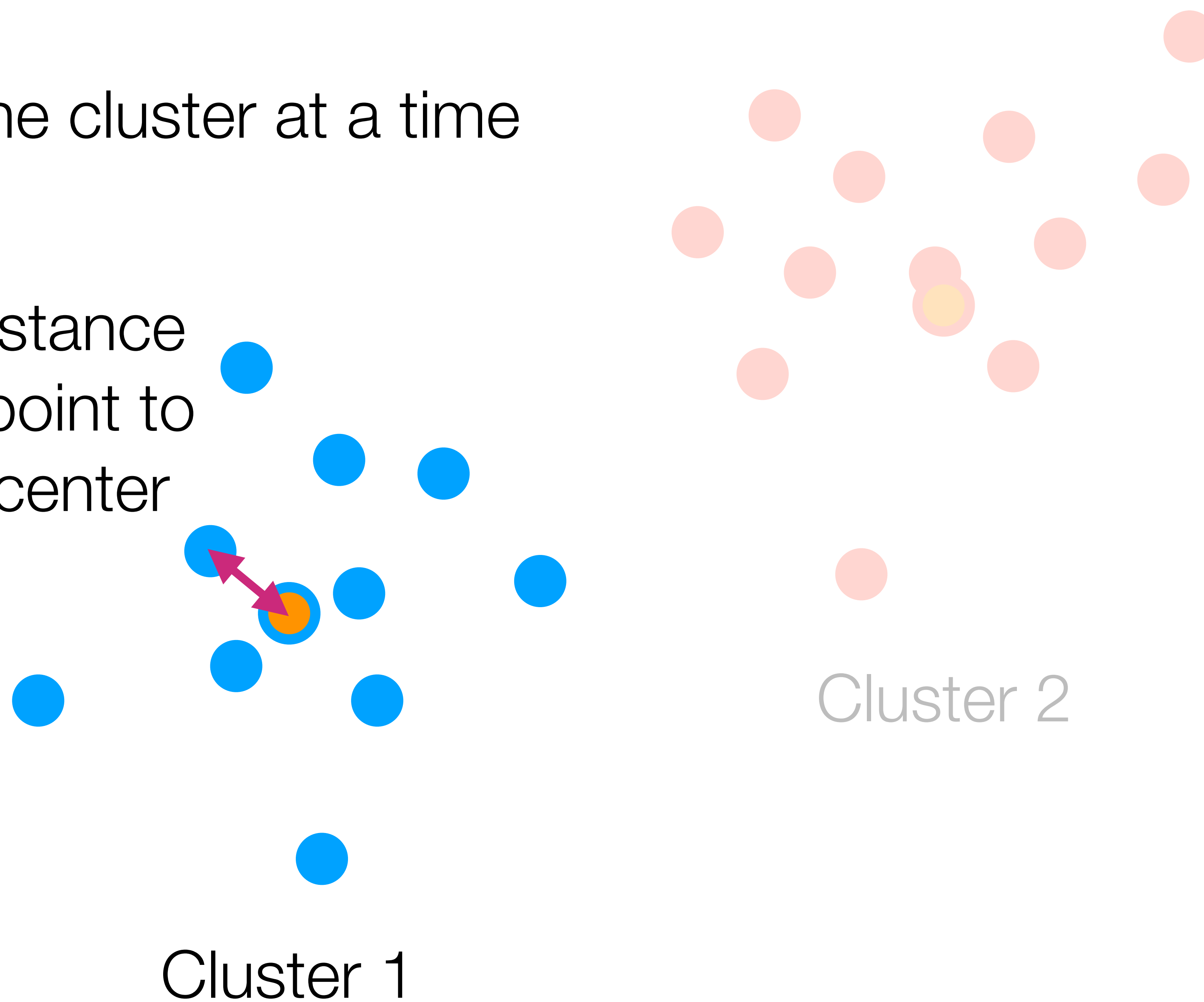

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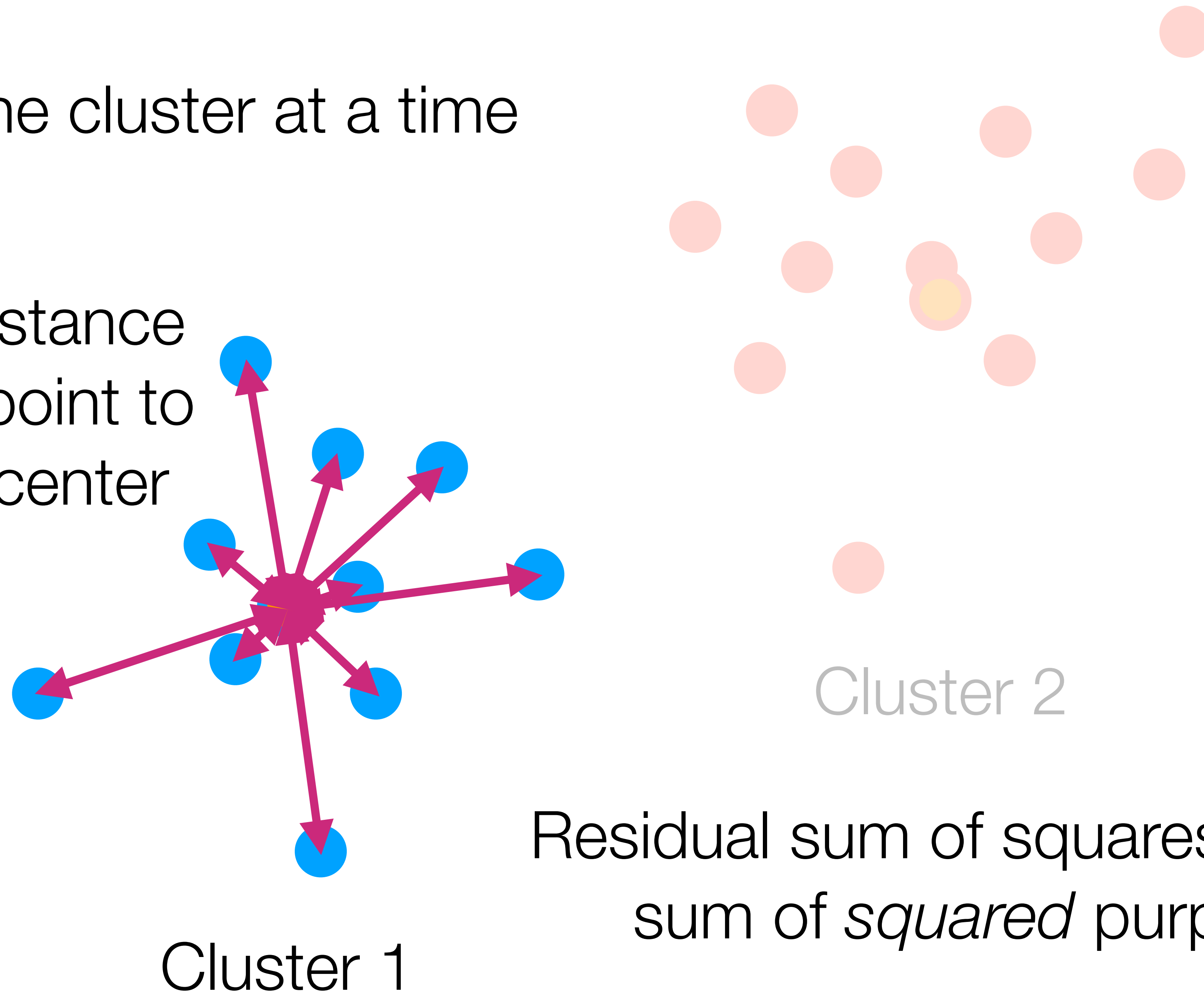

Residual sum of squares for cluster 1: sum of *squared* purple lengths

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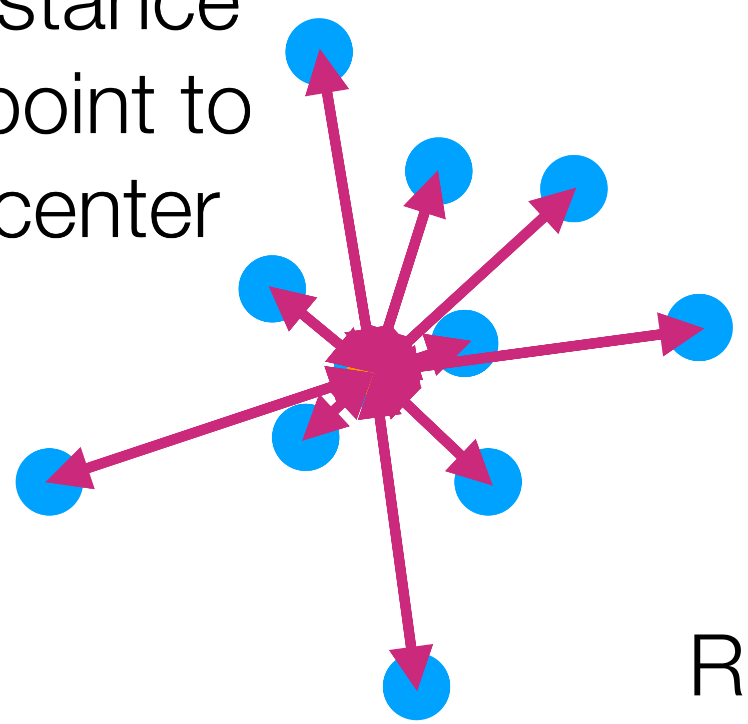

Cluster 1

Cluster 2

Residual sum of squares for cluster 1:

$$\mathrm{RSS}_1 = \sum_{x \in \text{cluster 1}} \|x - \mu_1\|^2$$

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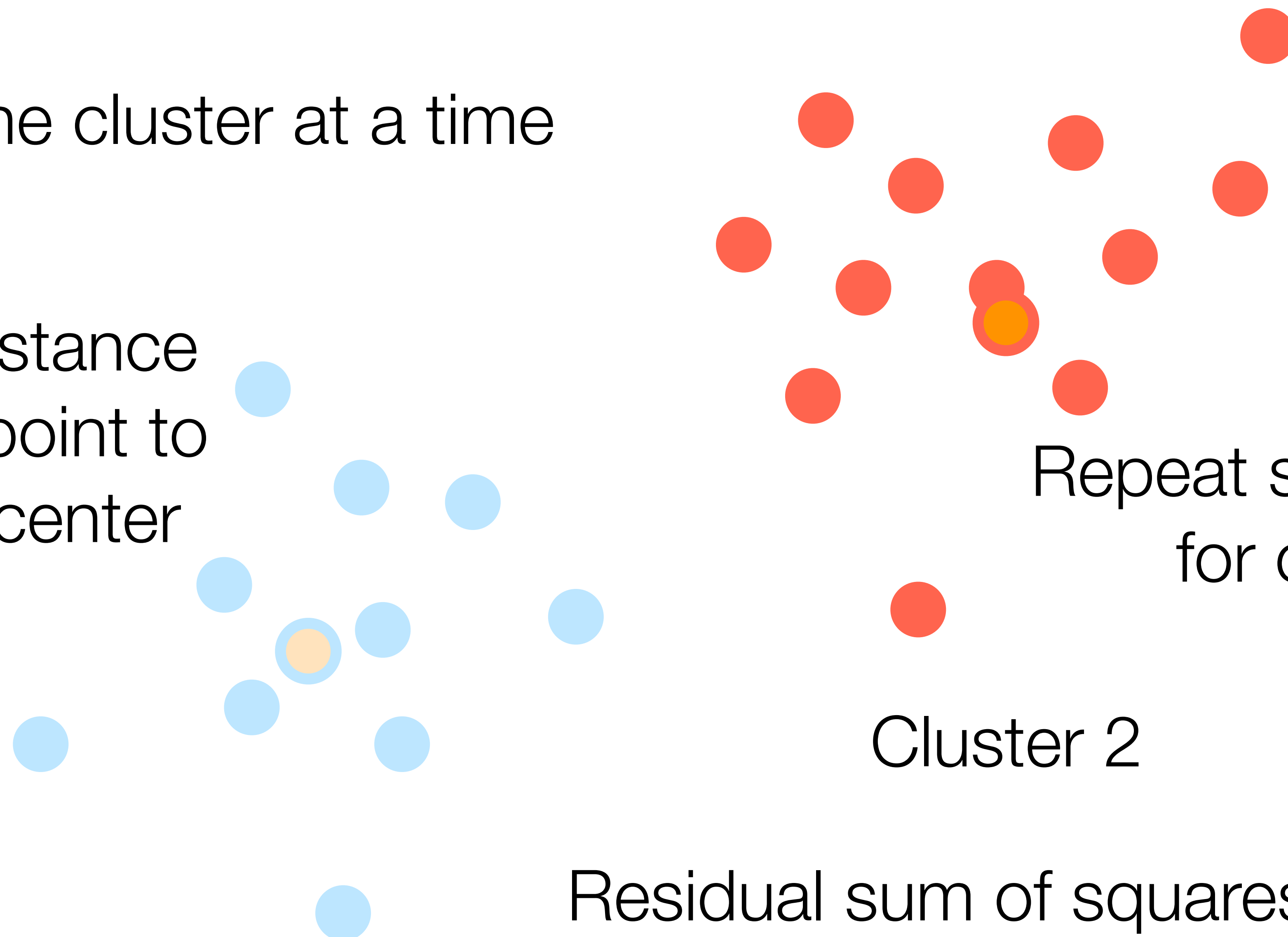

Repeat similar calculation
for other cluster

Cluster 2

Cluster 1

Residual sum of squares for cluster 2:

$$\mathrm{RSS}_2 = \sum_{x \in \text{cluster } 2} \left\| x - \mu_2 \right\|^2$$

Residual Sum of Squares

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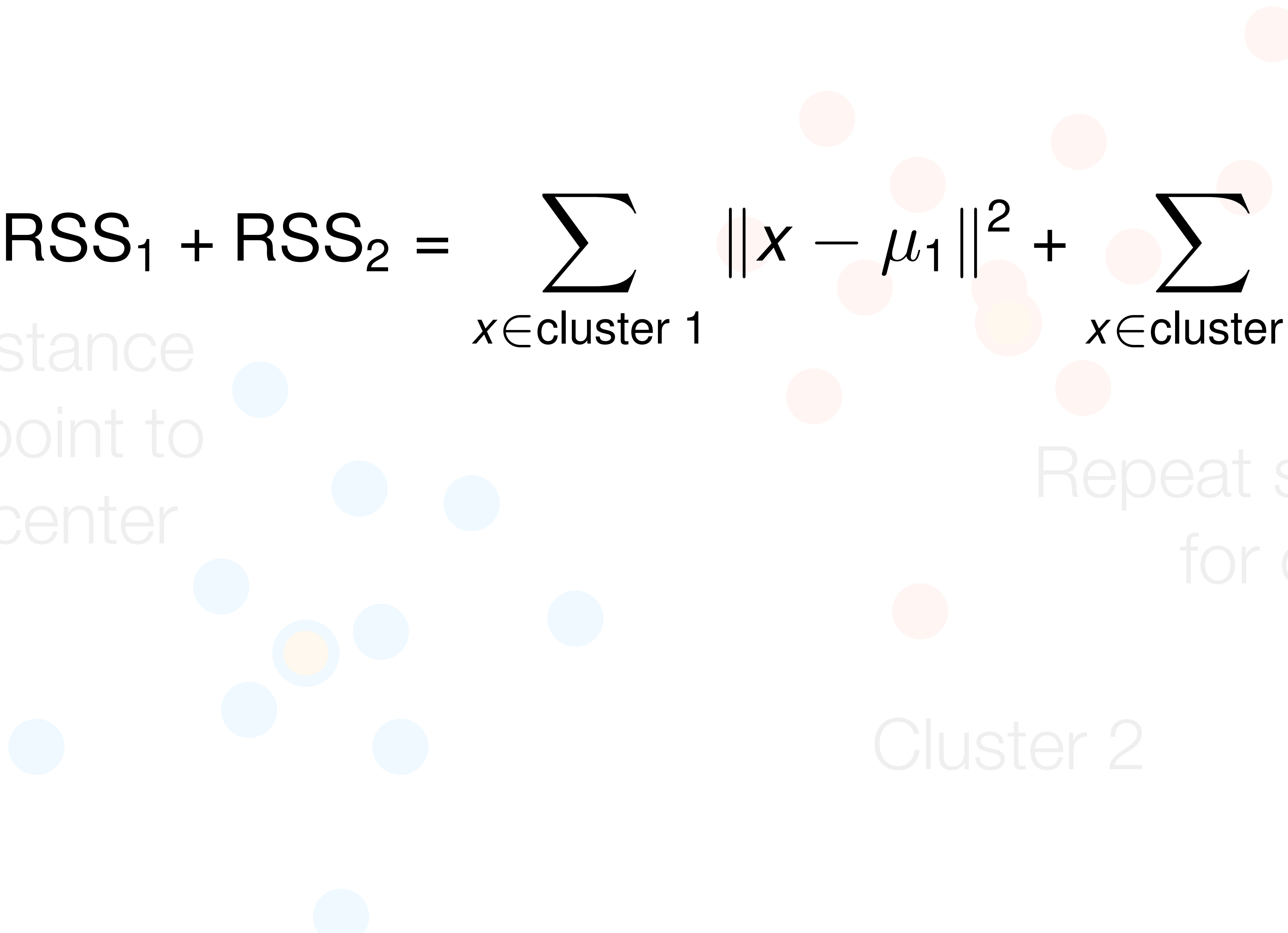
$$\text{RSS} = \text{RSS}_1 + \text{RSS}_2 = \sum_{x \in \text{cluster 1}} \|x - \mu_1\|^2 + \sum_{x \in \text{cluster 2}} \|x - \mu_2\|^2$$



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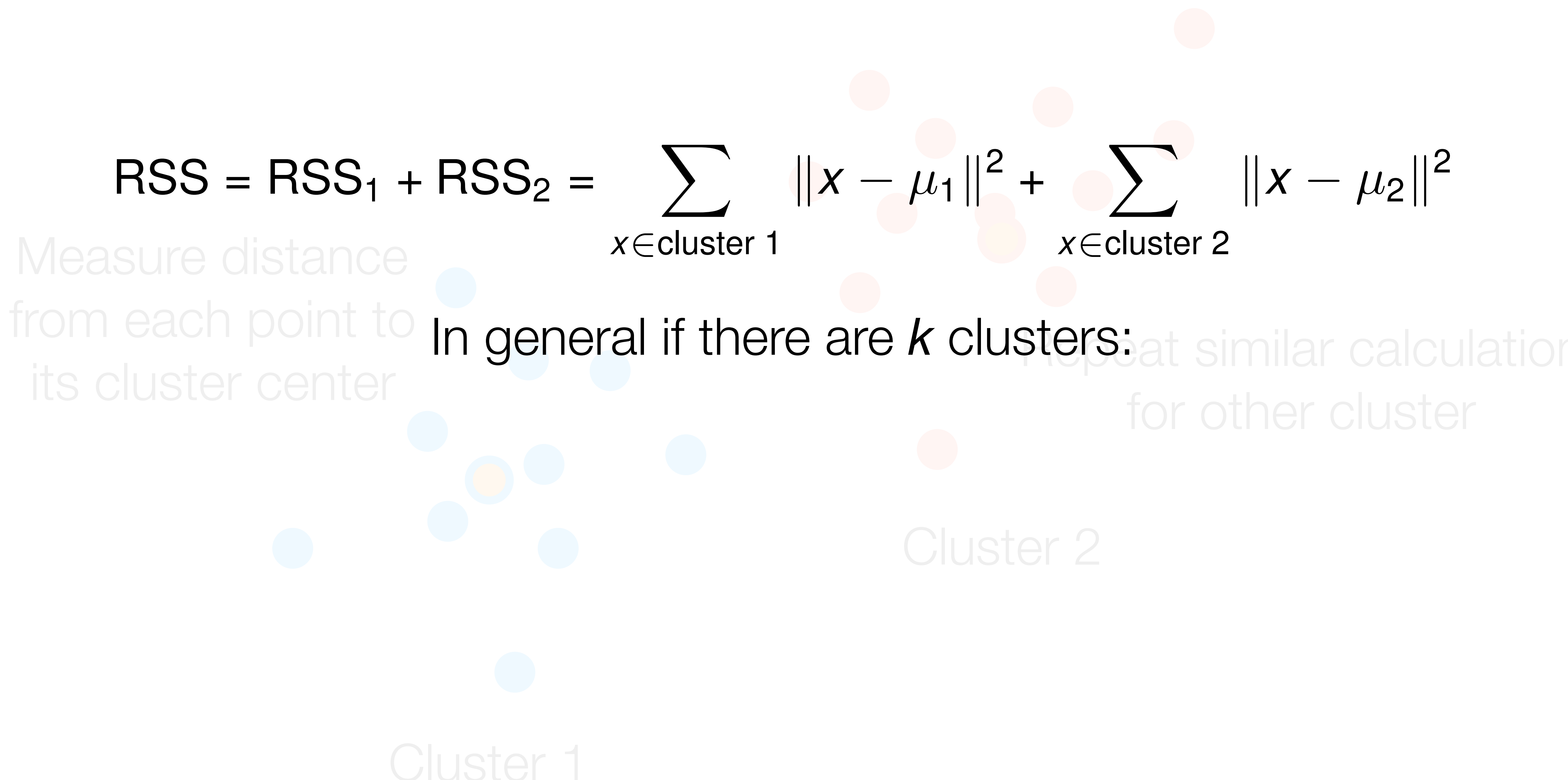

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RSS only really makes sense for clusters that look like circles

Why is RSS not a good way to choose k?

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What is RSS when k is equal to the number of data points?

A Good Way to Choose *k*

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RSS measures *within-cluster variation*

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Want to also measure *between-cluster variation*

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$$\text{CH}(k) = \frac{B \cdot (n-k)}{W \cdot (k-1)}$$

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Pick *k* with highest CH(*k*)

A Good Way to Choose k

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n = total # points

Pick k with highest **CH(*k*)**

(Choose k among 2, 3, … up to pre-specified max)

A Good Way to Choose k

RSS measures *within-cluster variation*

$$W = \text{RSS} = \sum_{g=1}^{k} \text{RSS}_g = \sum_{g=1}^{k} \sum_{x \in \text{cluster } g} \|x - \mu_g\|^2$$

Want to also measure *between-cluster variation*

$$B = \sum_{g=1}^{k} (\text{\# points in cluster } g) \|\mu_g - \mu\|^2$$

mean of *all* points

Called the **CH index**
[Calinski and Harabasz 1974]

A good score function to use for choosing k:

$$\text{CH}(k) = \frac{B \cdot (n - k)}{W \cdot (k - 1)}$$

n = total # points

Pick k with highest **CH(**k**)**

(Choose k among 2, 3, … up to pre-specified max)

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Another good way is called the **gap statistic** [Tibshirani et al 2001]