Reminder: Quiz 1 for Section K4
This Friday 5:30pm-6:50pm Adelaide time

- **Join on Zoom with your video on; we will take attendance**
- The quiz is 80 minutes long (same as with Pittsburgh sections)
- **You produce a Jupyter notebook and submit it on Canvas**
- Open notes, open internet, **closed to collaboration**
- You are responsible for making sure your laptop has a compute environment set up appropriately and has working internet
    - Check that you can run all lecture demos without issues
- Late exams will *not* be accepted
    - The Canvas submission system will close at 6:50pm Adelaide time; **we will only grade what is submitted to Canvas**

More on Quiz 1

Coverage:

- Up to and including dimensionality reduction/manifold learning
- Clustering and topic modeling are *not* on Quiz 1; there is no need to study these for the quiz

A note on academic integrity:

- The top of the quiz will have a statement you will agree to regarding academic integrity; **if you do not sign it, we will not grade your quiz — no exceptions**
- The Pittsburgh sections are taking the quiz one week after you; **do not discuss the quiz until after the section Z4 quiz 1 slot**

Violations to academic integrity will result in an F in the course =(

We want the quiz to be as fair as possible to all students. We realize that given the pandemic situation, there's only so much we can do.

At least you can take the quiz remotely
hopefully some place comfortable!

Like the beach

Reminder: Your Quiz 1 review session is today at 7pm-8:30pm Adelaide time

Carnegie Mellon University
Heinz College

Unstructured Data Analysis

Lecture 8: More clustering

George Chen

Learning a GMM

Demo

We really want the quiz to be as fair as possible across all students

Learning a GMM

Demo

A Sketch of How to Interpret Clusters

Demo

Automatically Choosing *k*

For *k* = 2, 3, … up to some user-specified max value:

Fit model using *k*

Compute a score for the model

But what score function should we use?

Use whichever *k* has the best score

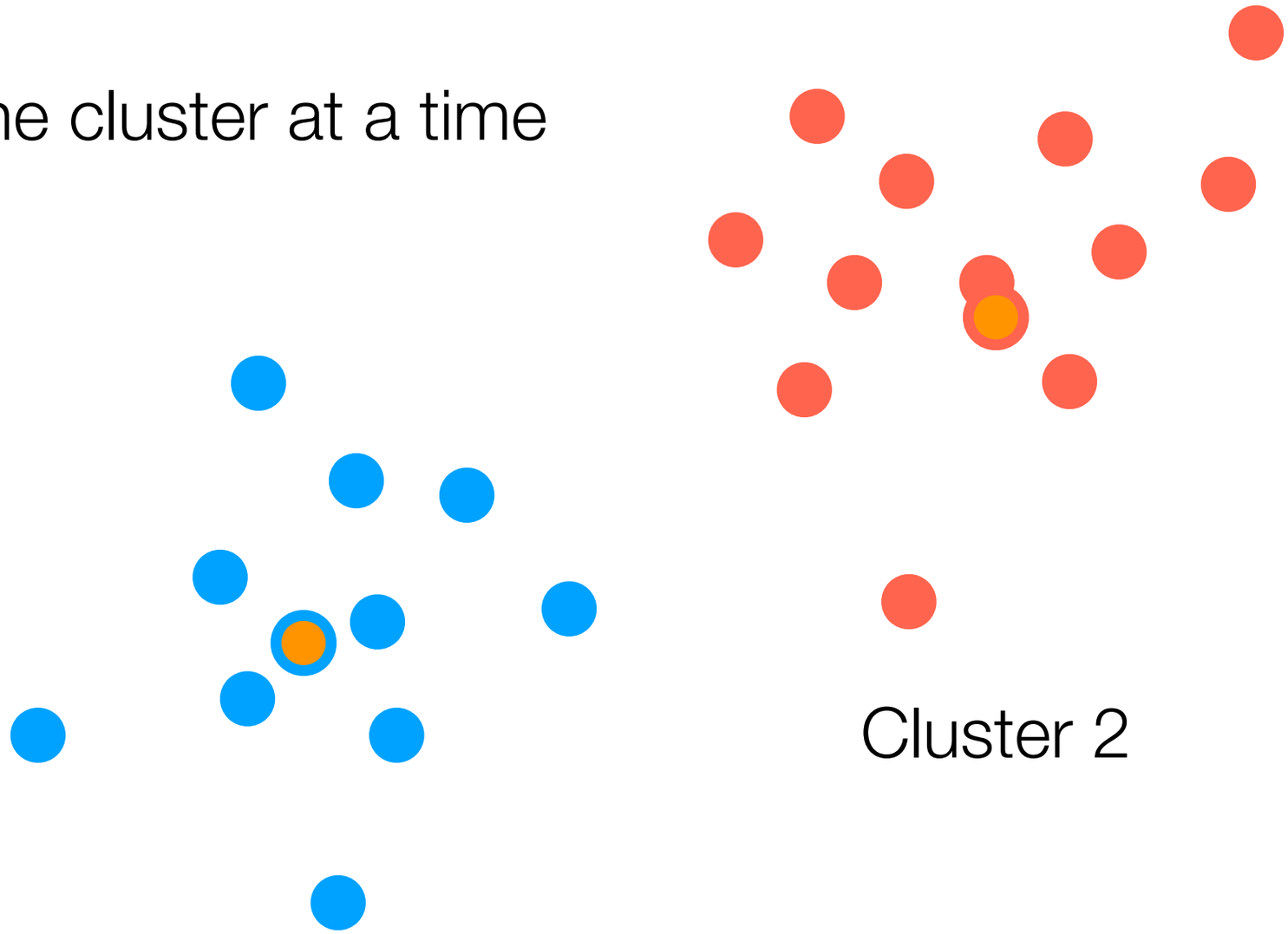
No single way of choosing *k* is the “best” way

Here’s an example of a score function you don’t want to use

But hey it’s worth a shot

Residual Sum of Squares

Look at one cluster at a time



Cluster 1

Cluster 2

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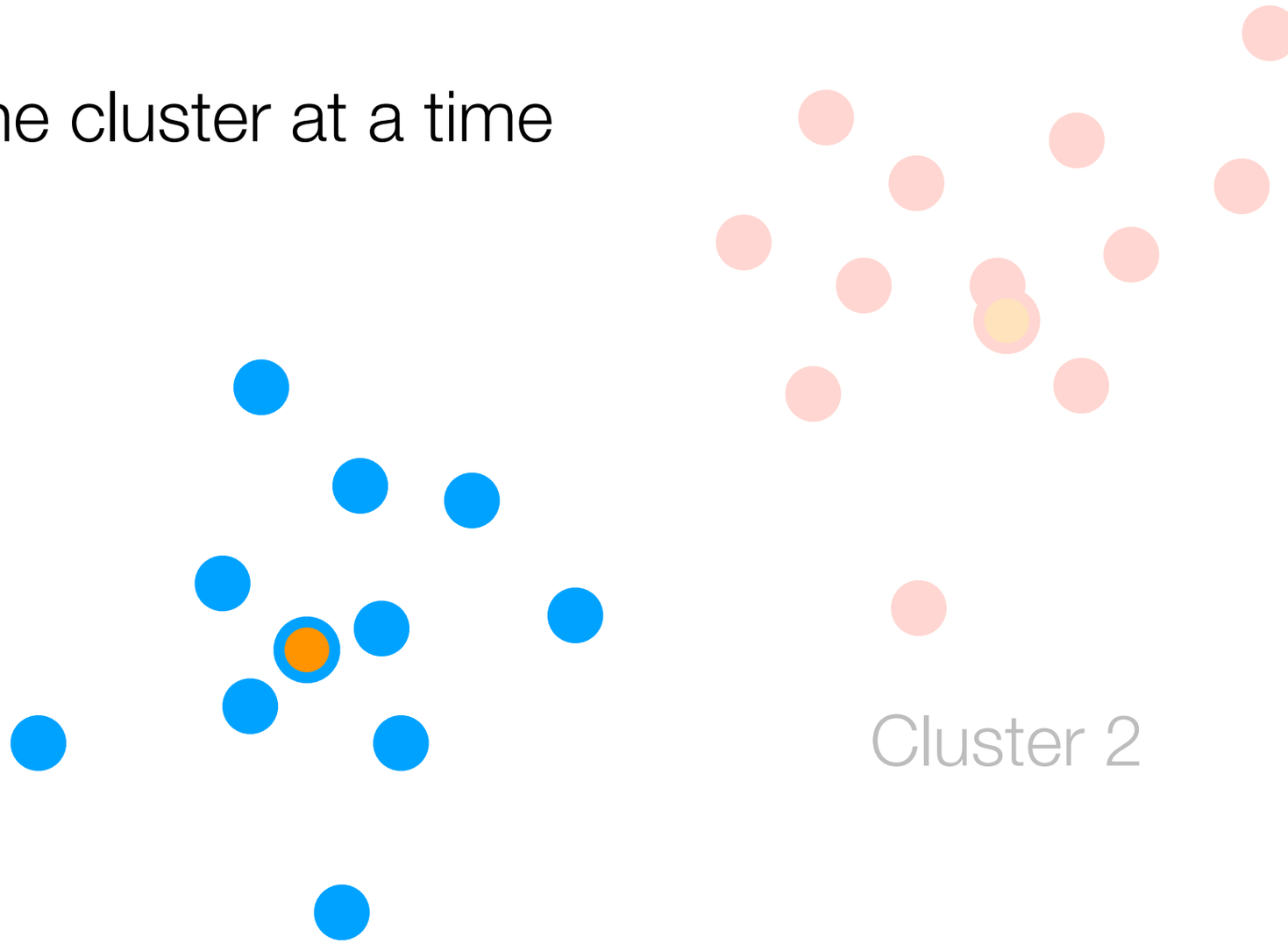

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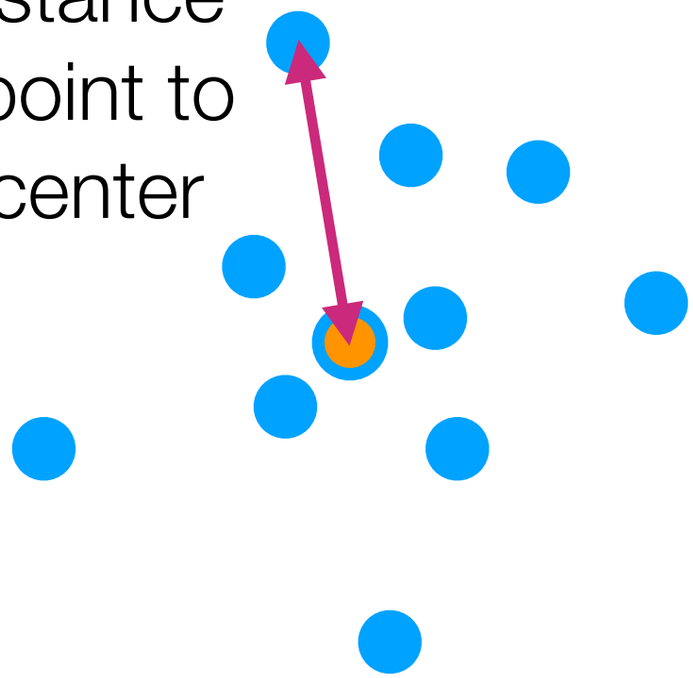

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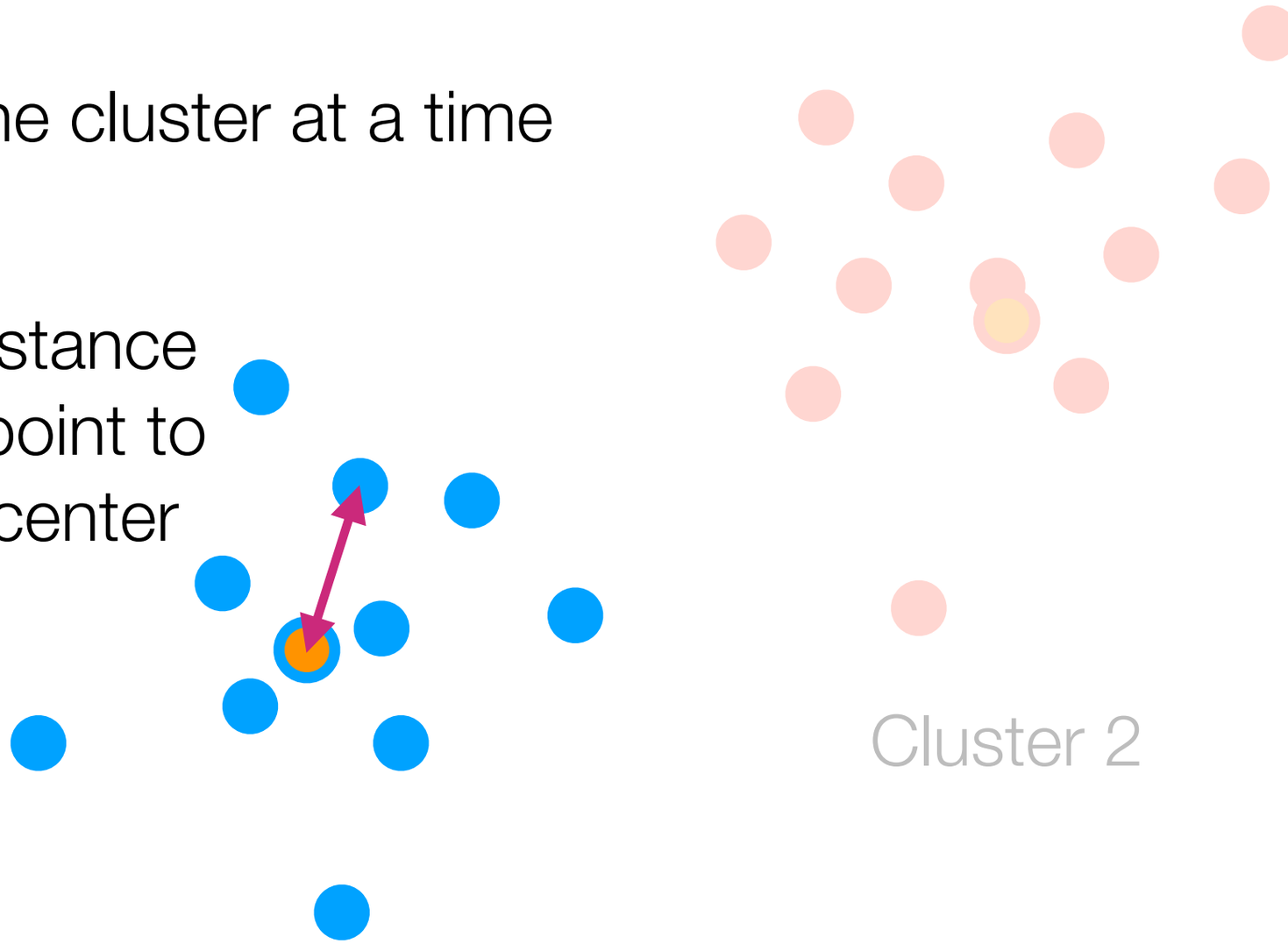

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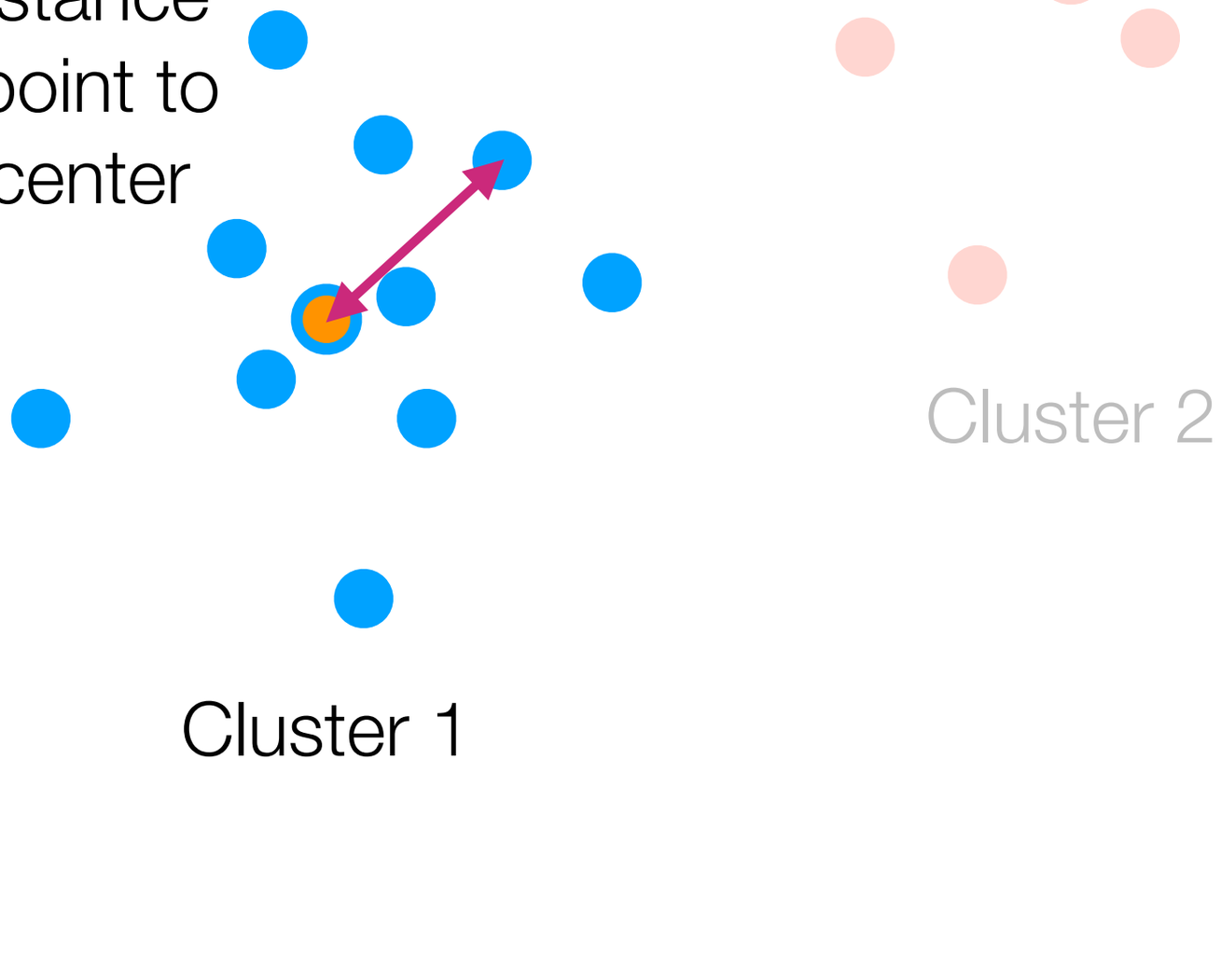

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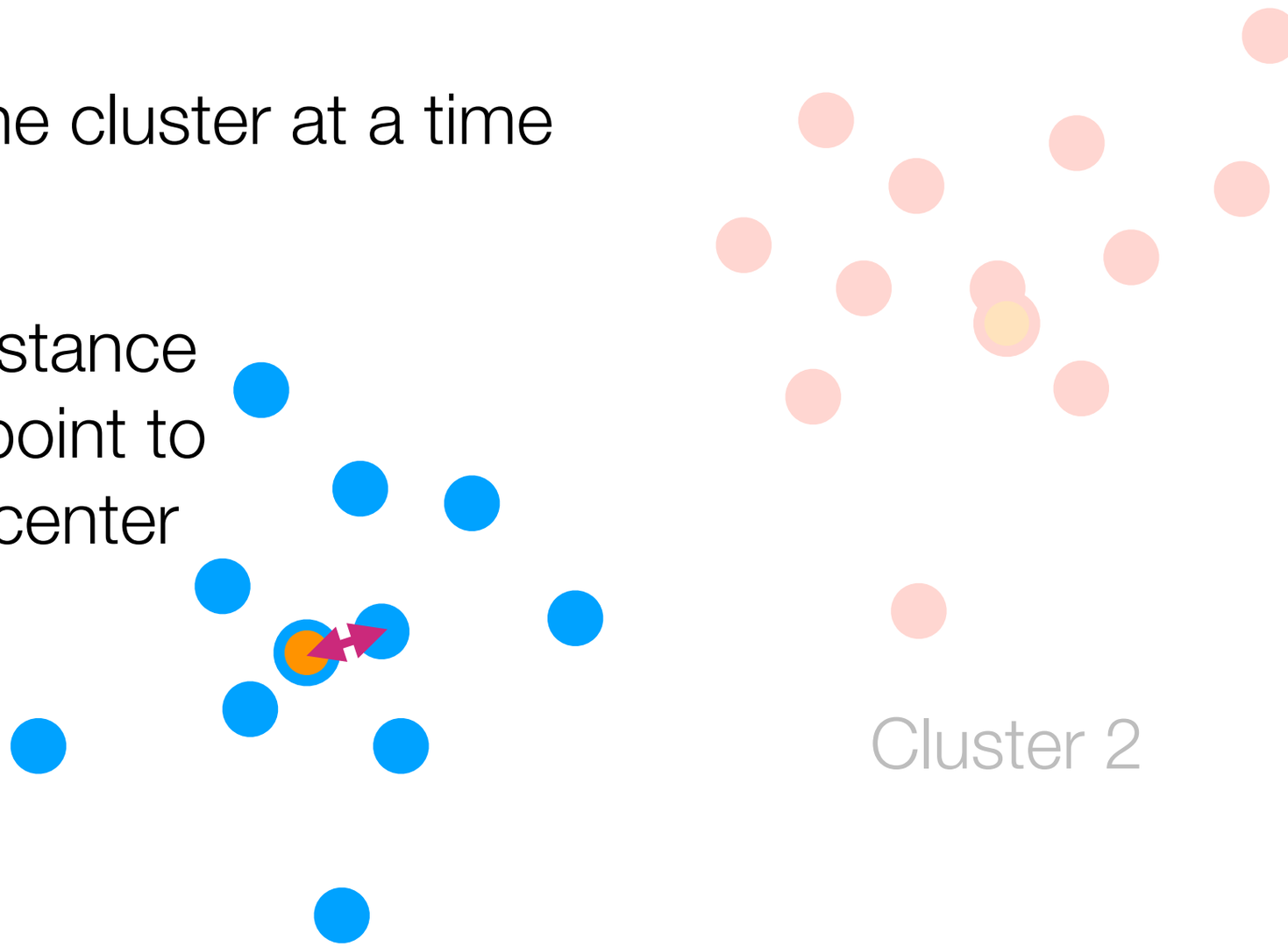

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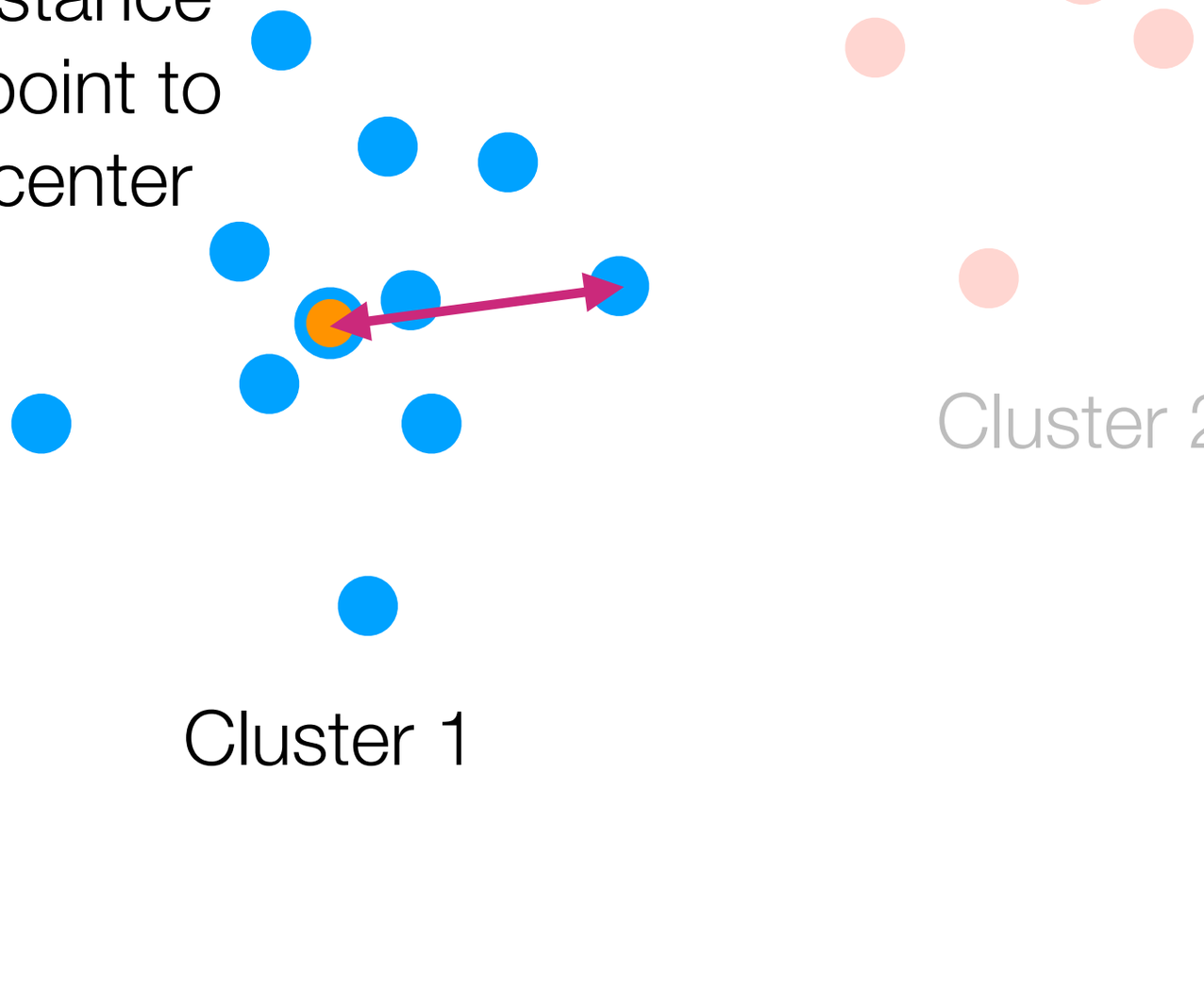

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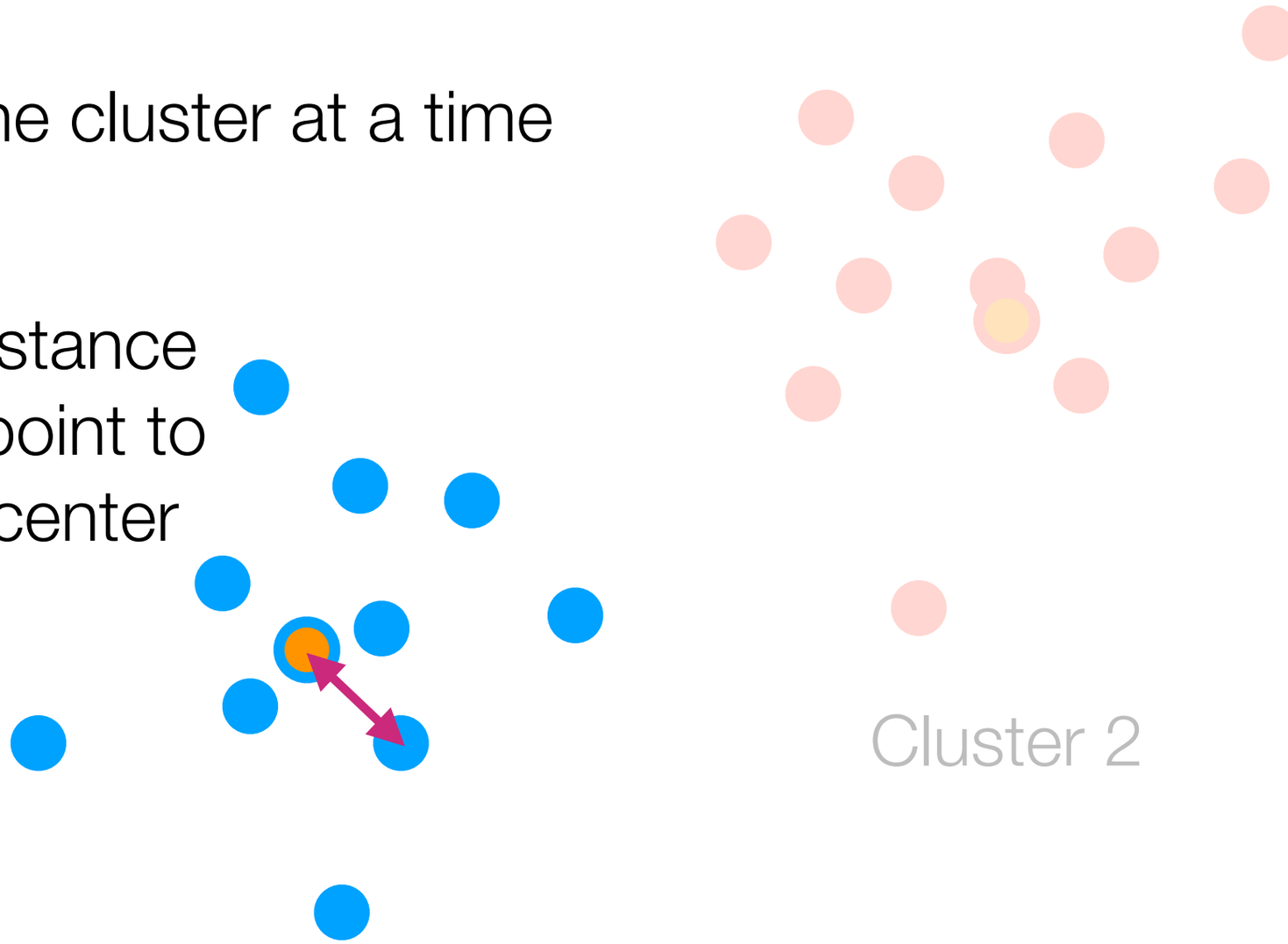

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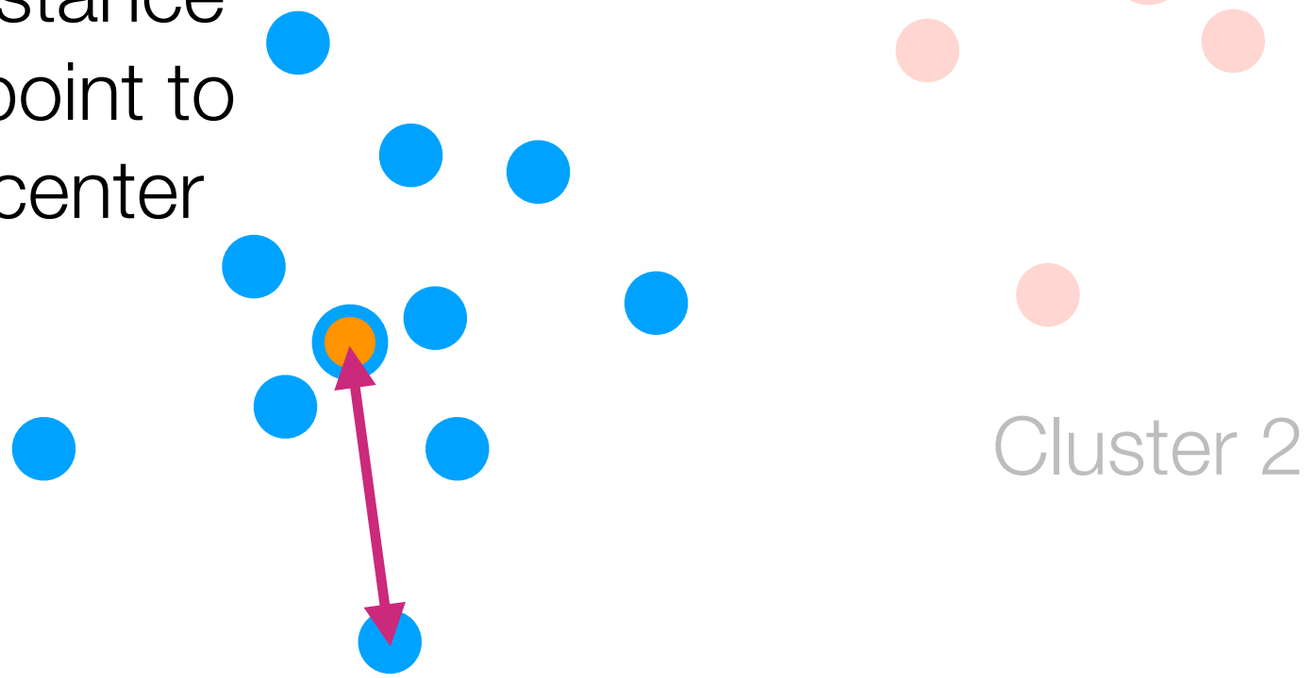

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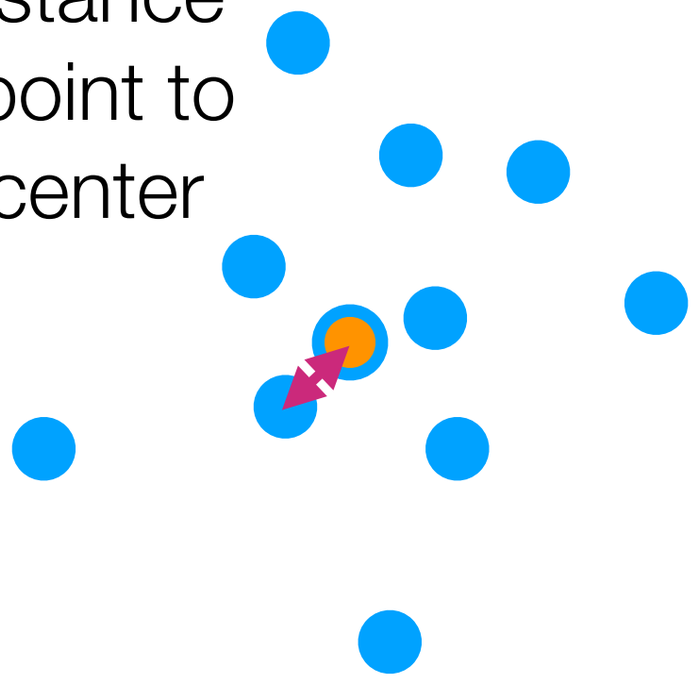

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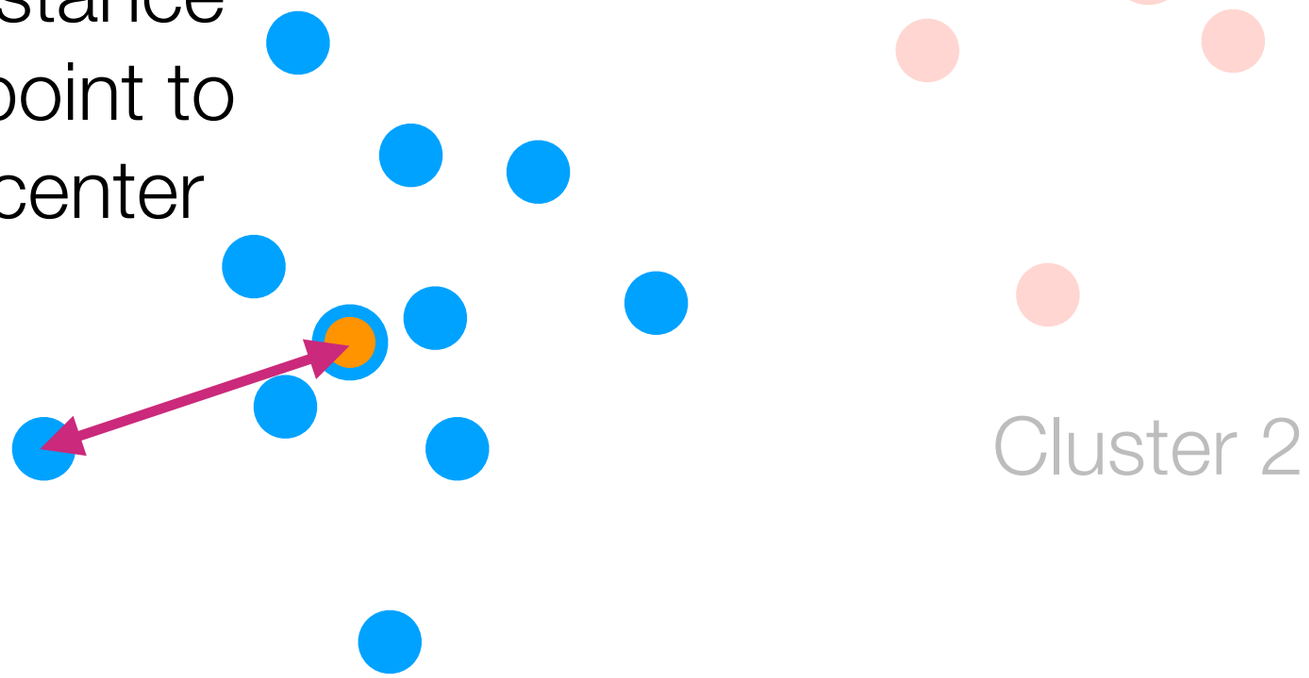

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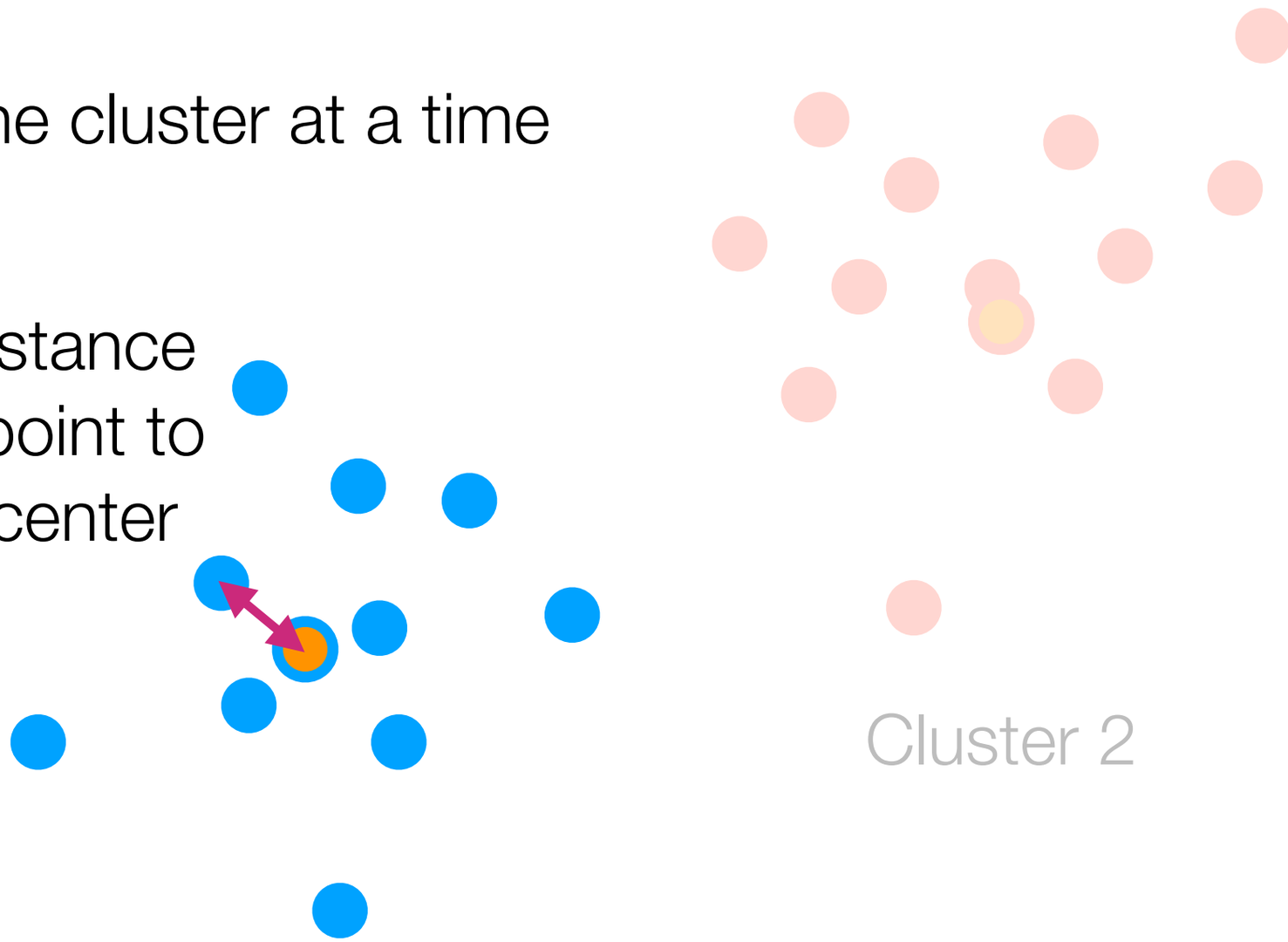

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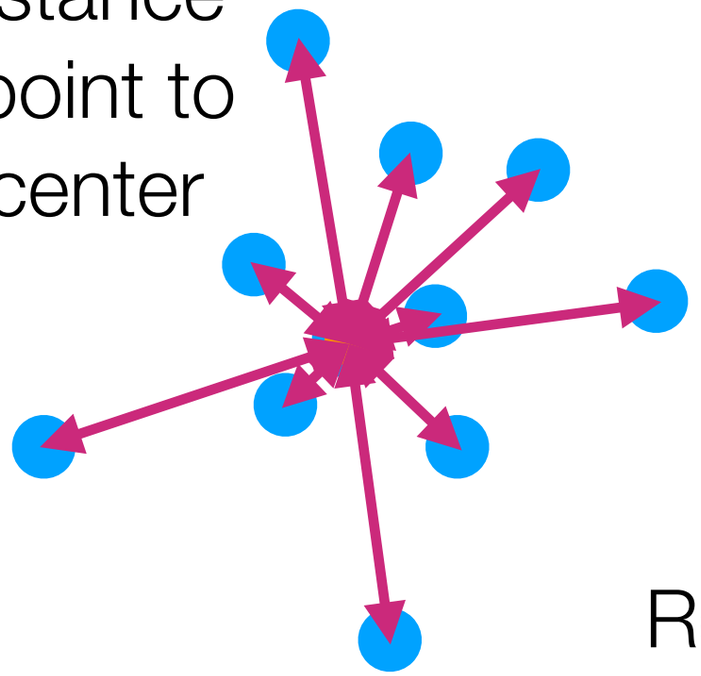


Cluster 1

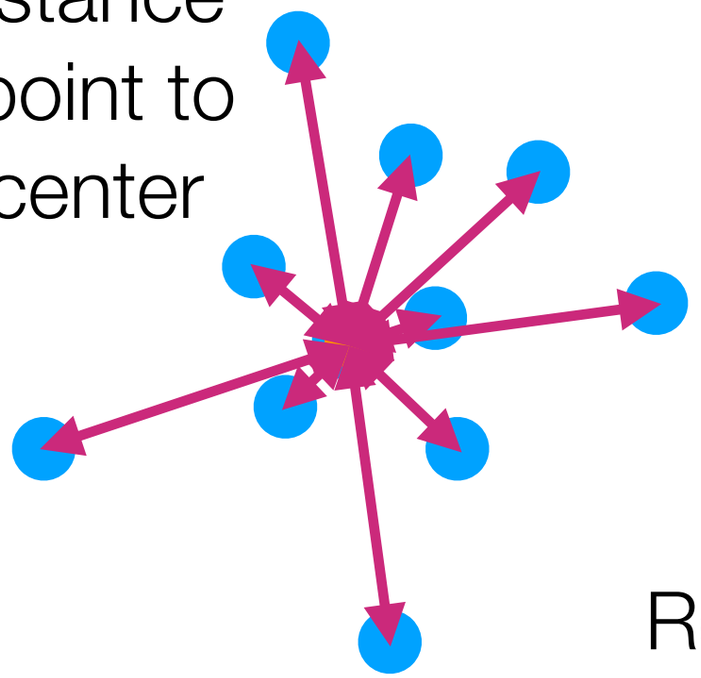
Cluster 2

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

Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



Cluster 1

Cluster 2

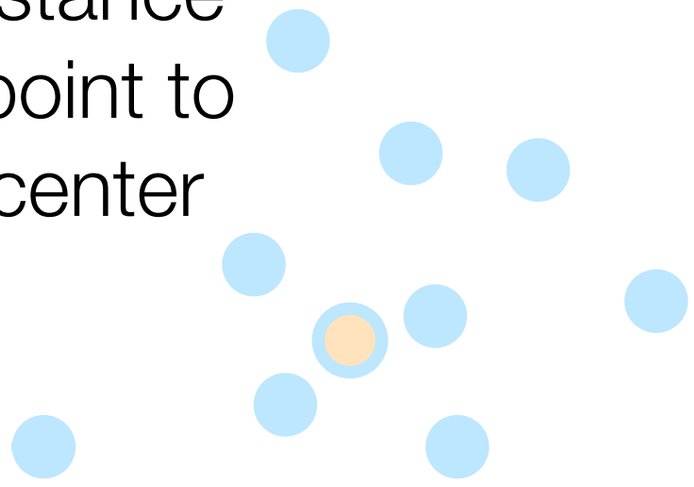
Residual sum of squares for cluster 1:

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

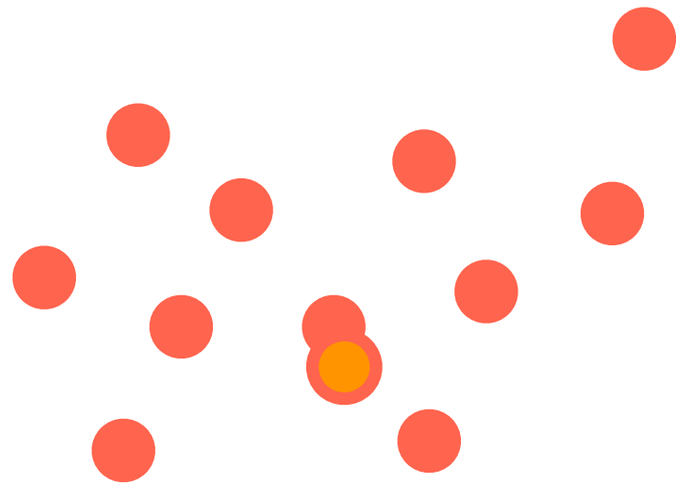
Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



Cluster 1



Repeat similar calculation for other cluster

Cluster 2

Residual sum of squares for cluster 2:

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

Residual Sum of Squares

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

In general if there are k clusters:

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

Remark: k-means *tries* to minimize RSS
(it does so *approximately,* with no guarantee of optimality)

RSS only really makes sense for clusters that look like circles

Why is minimizing RSS a bad way to choose *k*?

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

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*

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

μ: 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)

Automatically Choosing *k*

Demo

More on 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 how large clusters are

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	…
Gaussian mean = μ_1	μ_2	μ_3	It goes on forever!
Gaussian covariance = Σ_1	Σ_2	Σ_3	

There is a parameter that controls how these π values roughly decay

There are an infinite number of parameters

(Rough idea) How to generate points from this DP-GMM:

1. Flip biased ∞-sided coin (the sides have probabilities π_1, π_2, π_3, …)
2. Let Z be the side that we got (it is a positive integer)
3. Sample 1 point from Gaussian mean μ_Z, covariance Σ_Z

Remark: For any given dataset, when learning the DP-GMM, there aren't going to be an infinite number of clusters found

More on 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 how large clusters are

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

Learning a DP-GMM

Common approach: finite approximation where you specify some maximum number of clusters (the algorithm will find up to that many clusters)

- Algorithm is somewhat similar to ***k***-means/EM for GMMs

- Algorithm output: very similar to regular GMM fitting

Learning a DP-GMM

Demo

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

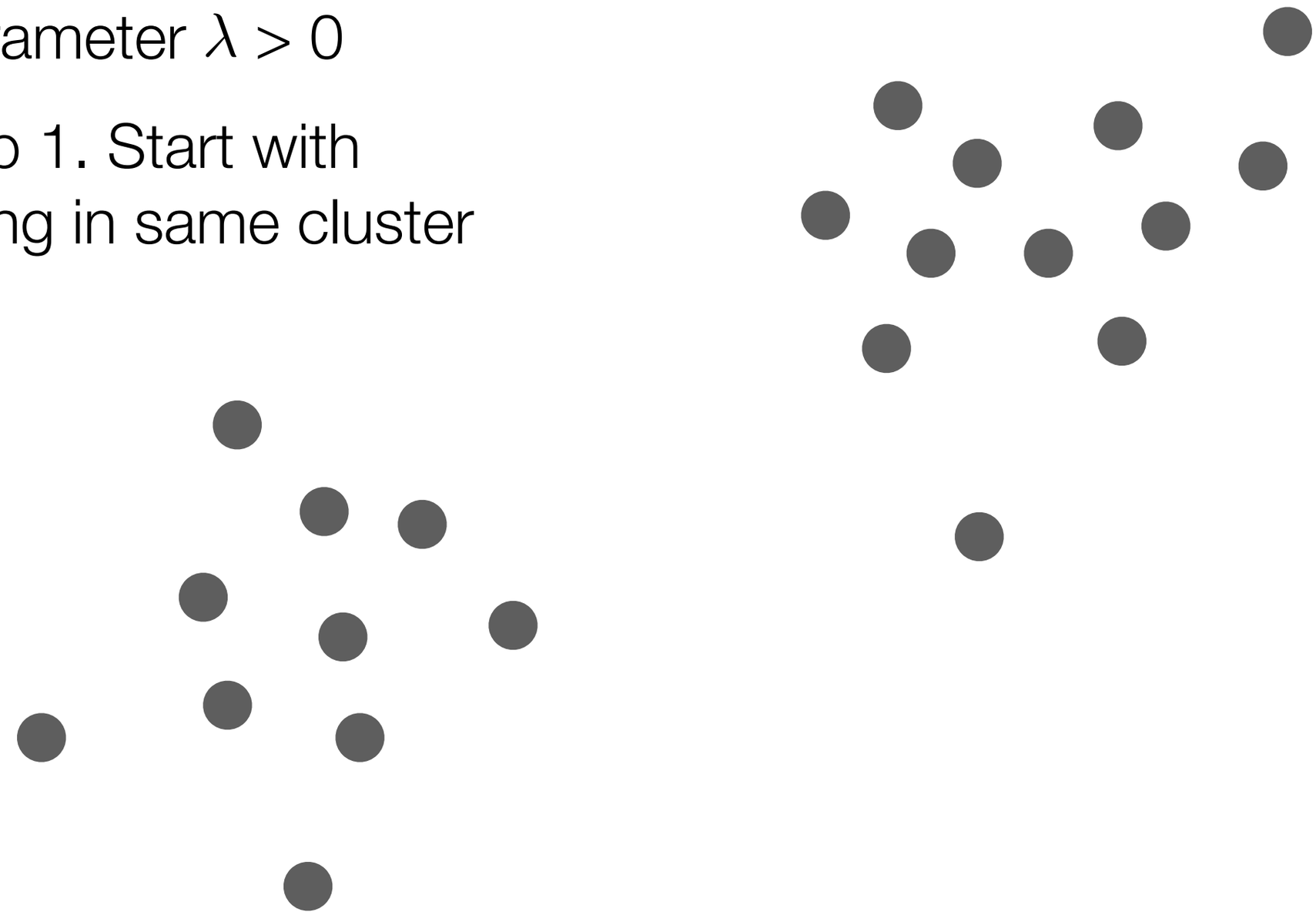
What approximates learning DP-GMMs?

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

DP-means

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

Step 1. Start with everything in same cluster



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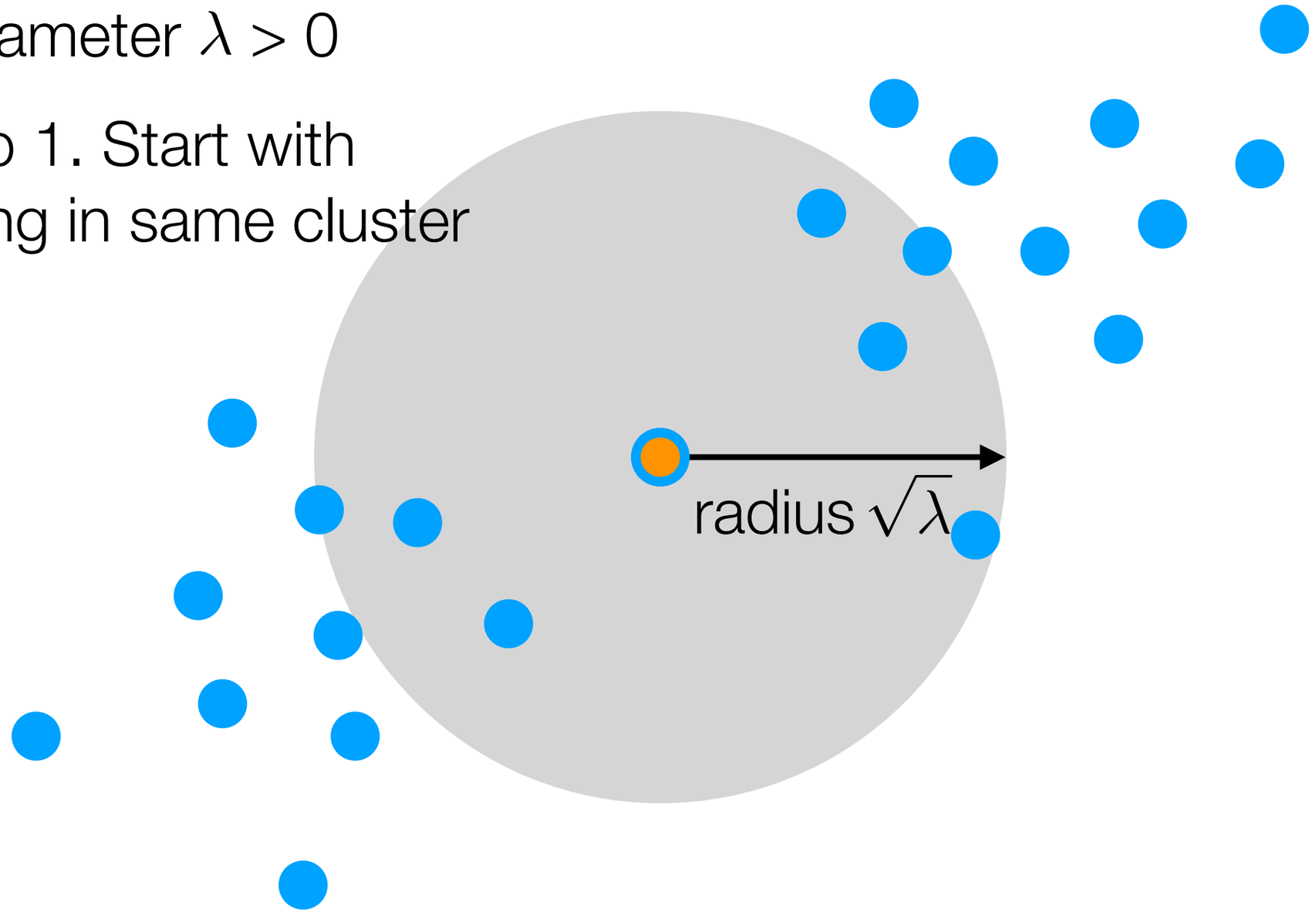

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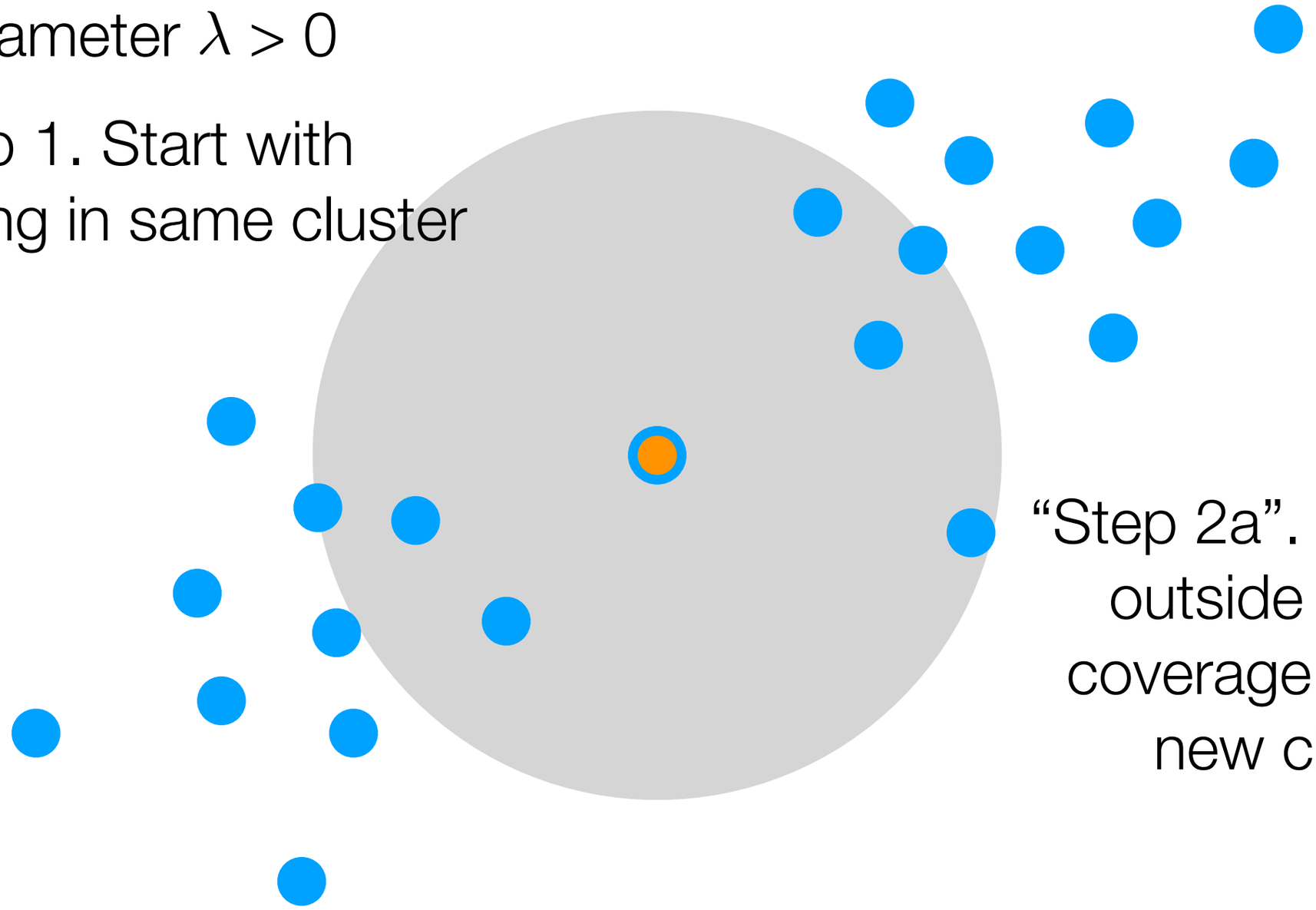

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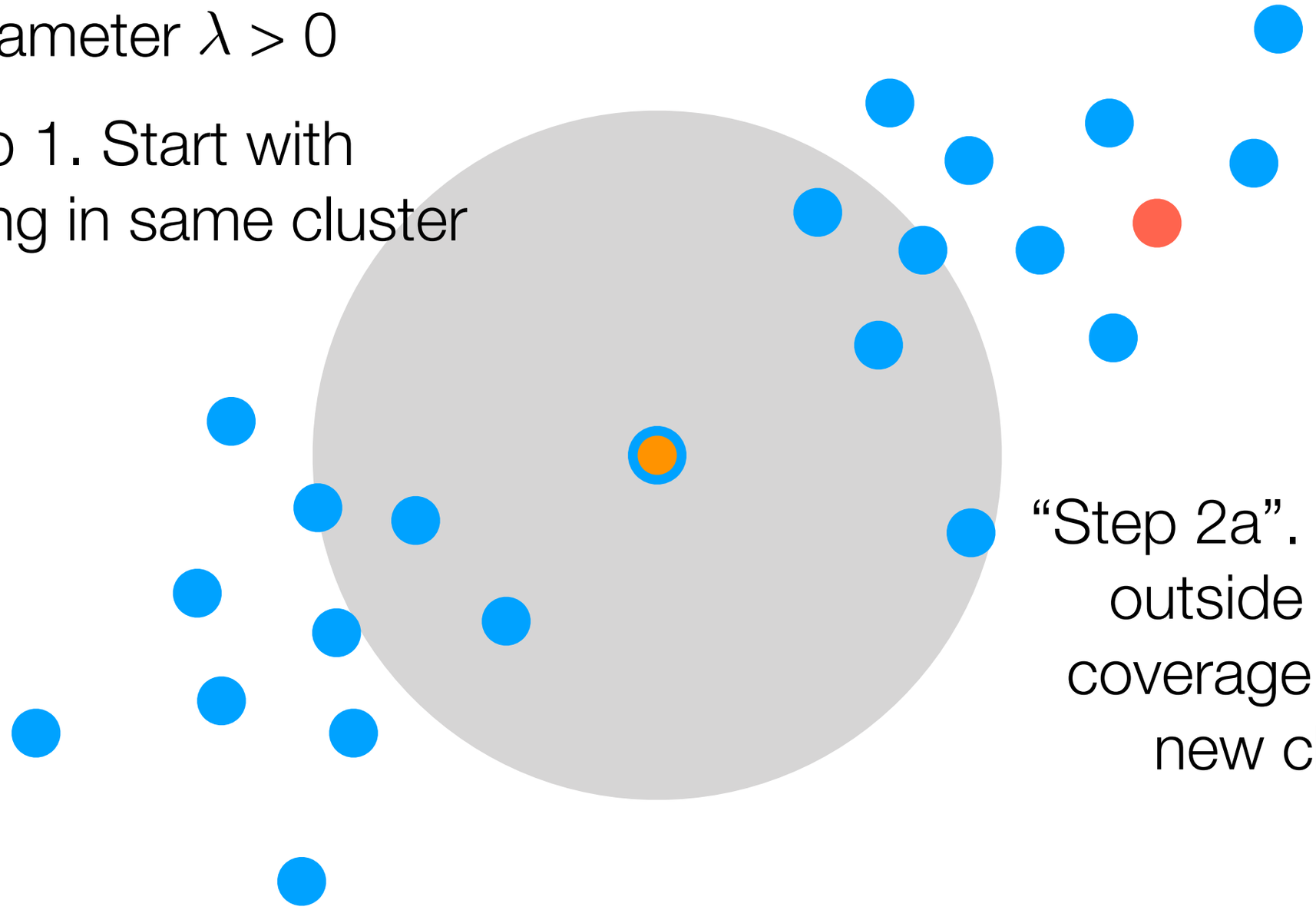

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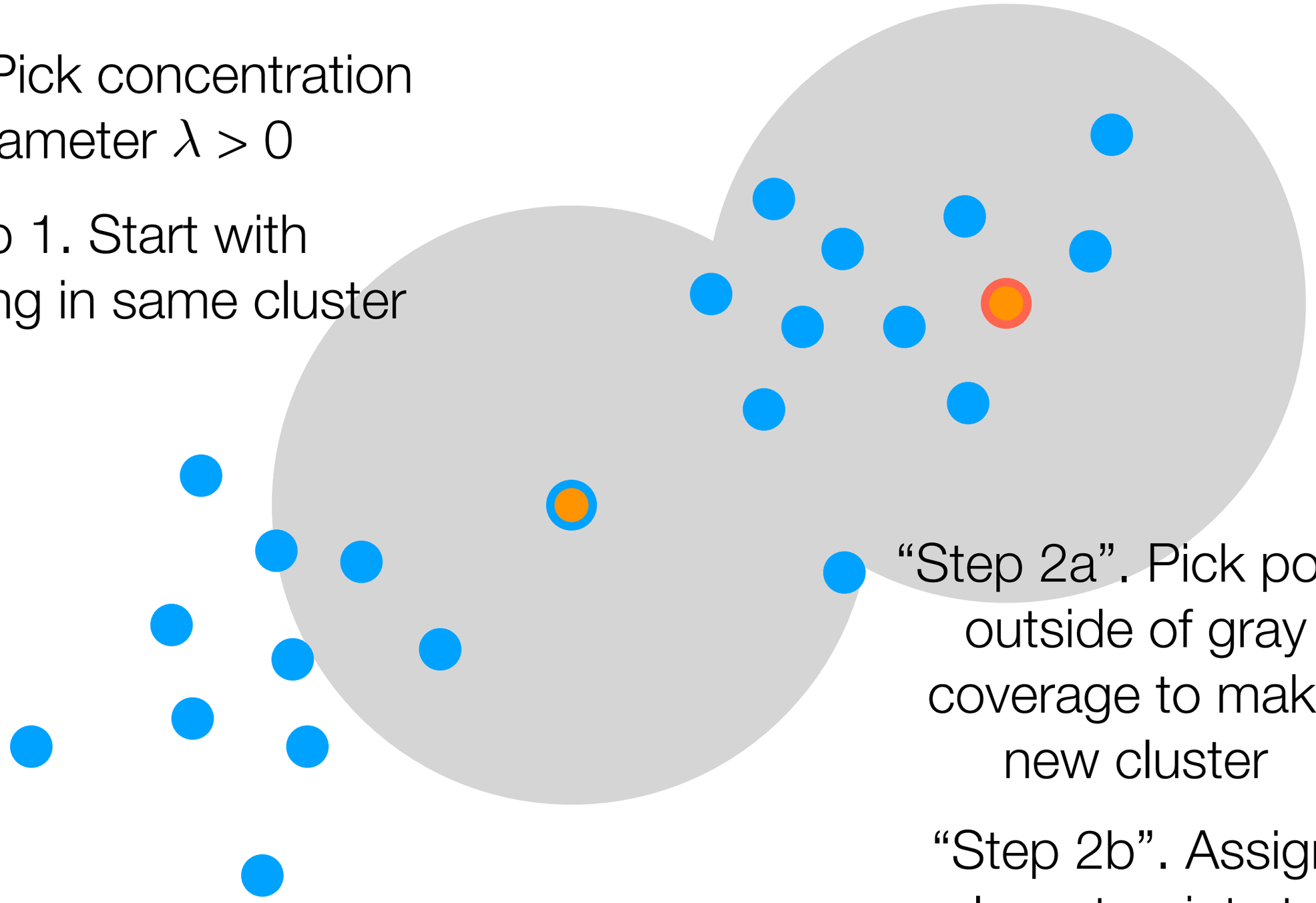

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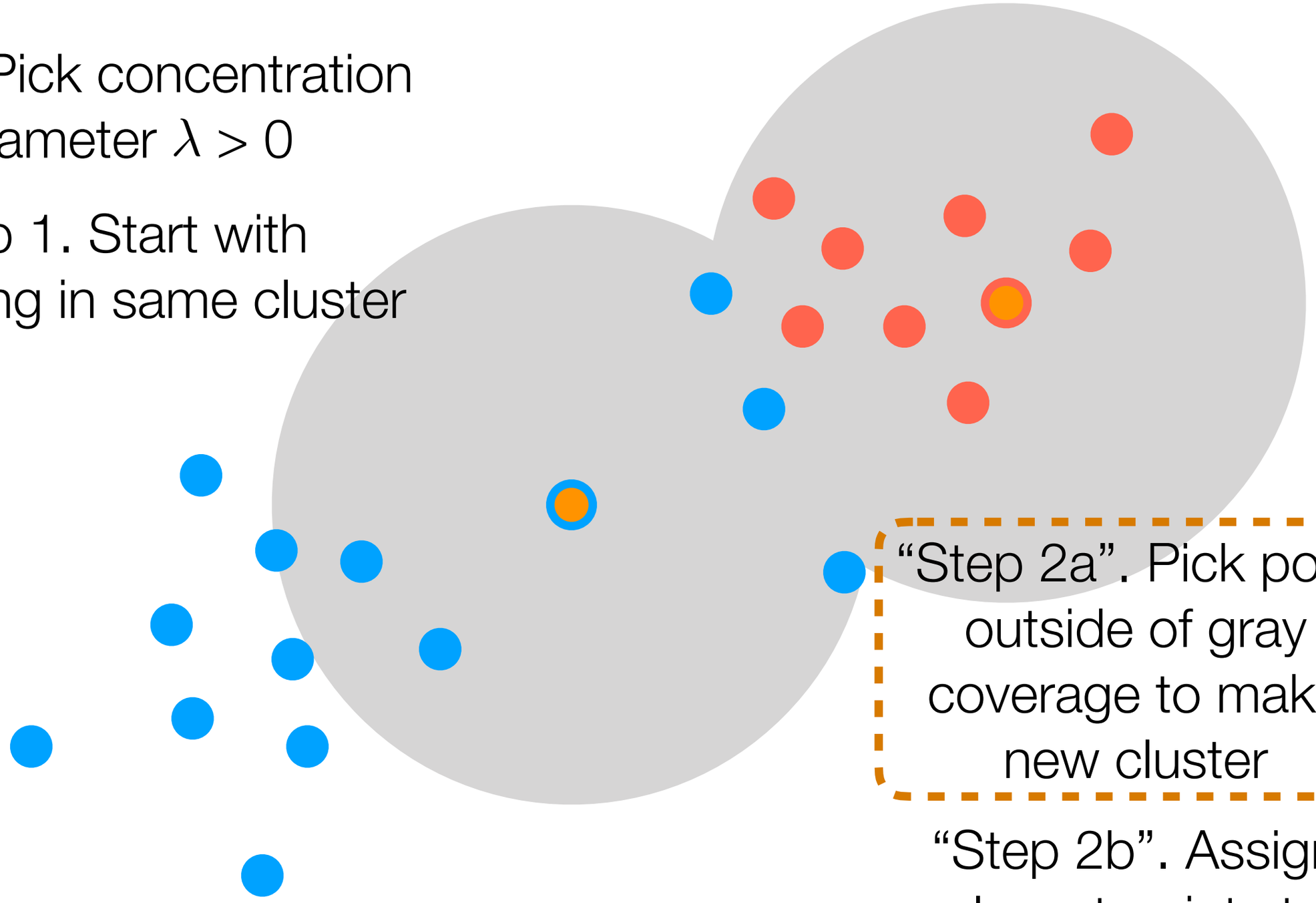

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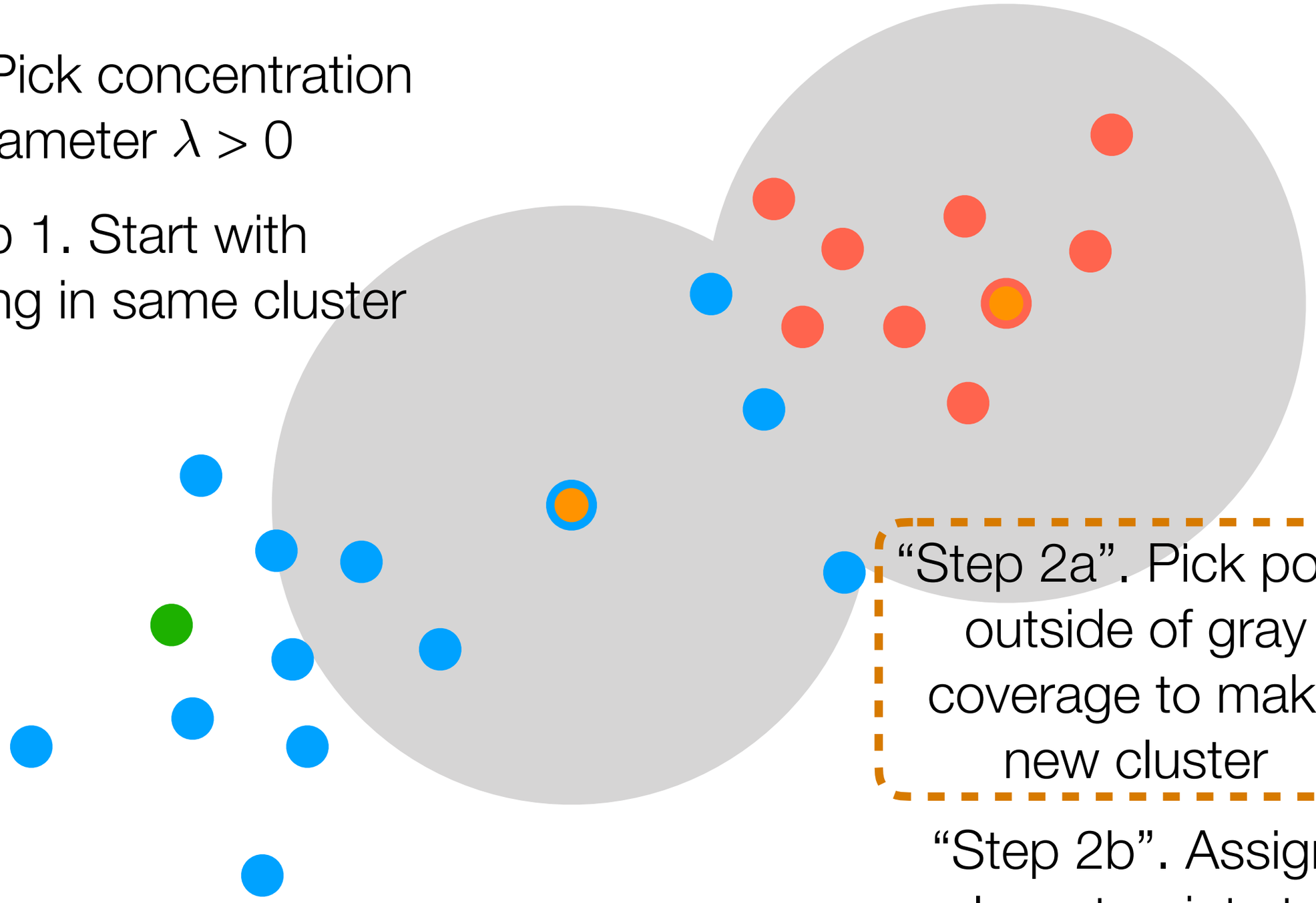

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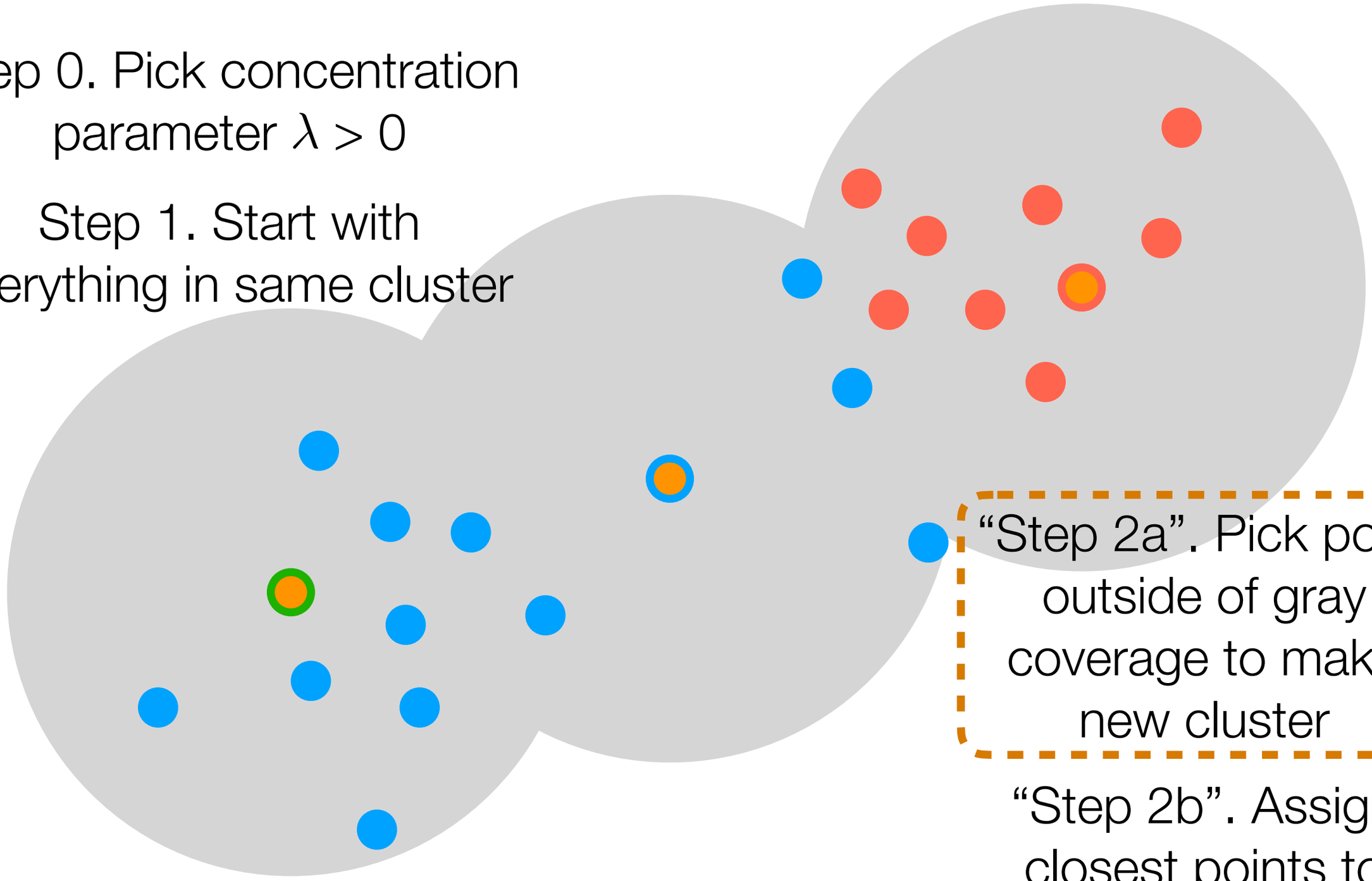

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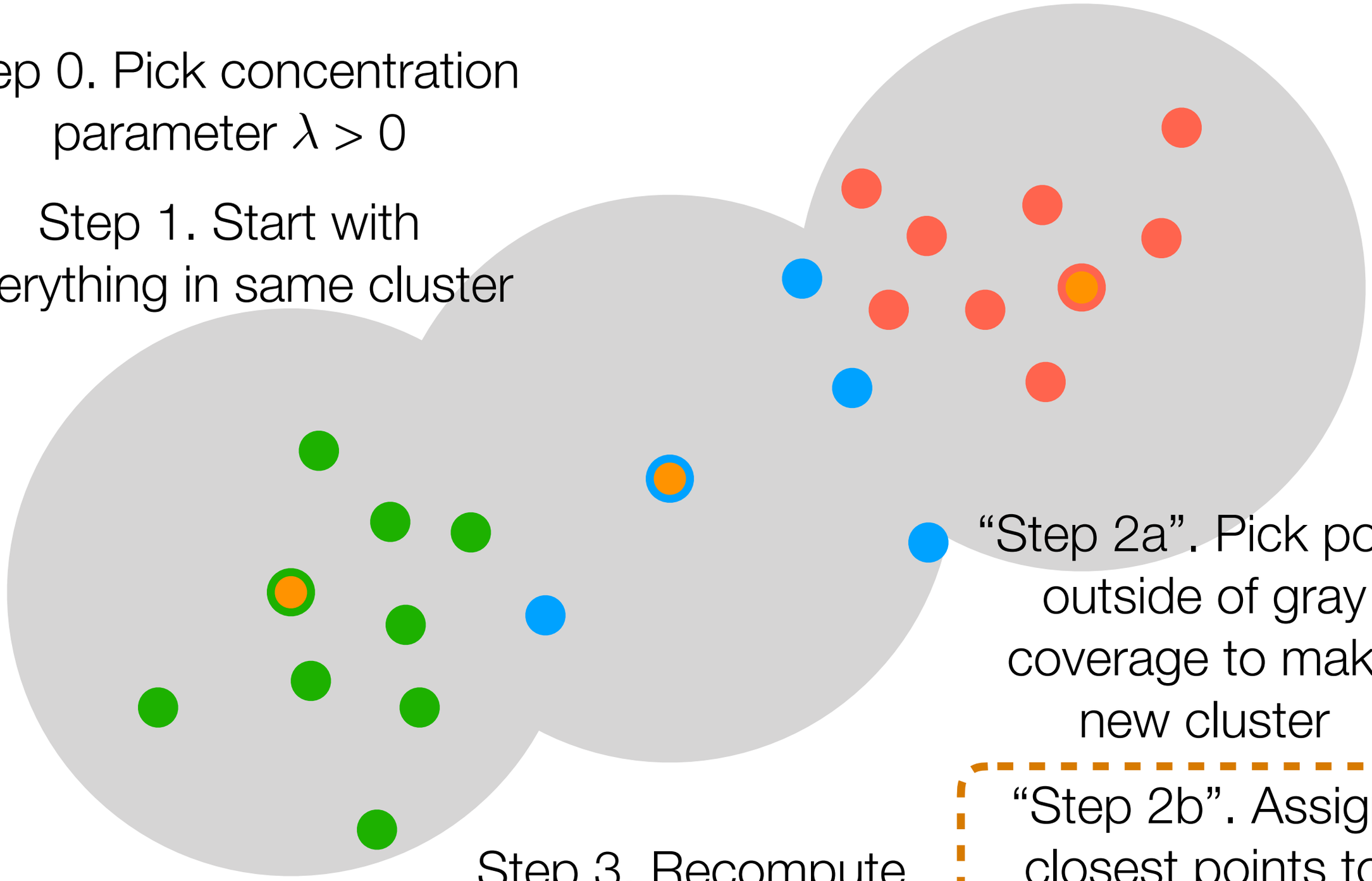

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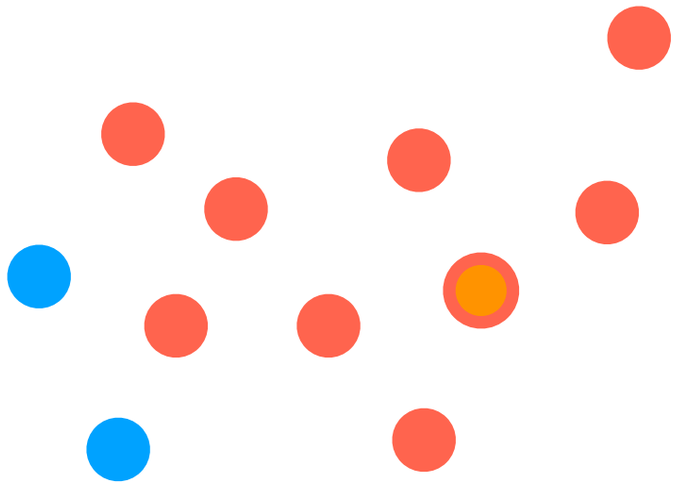

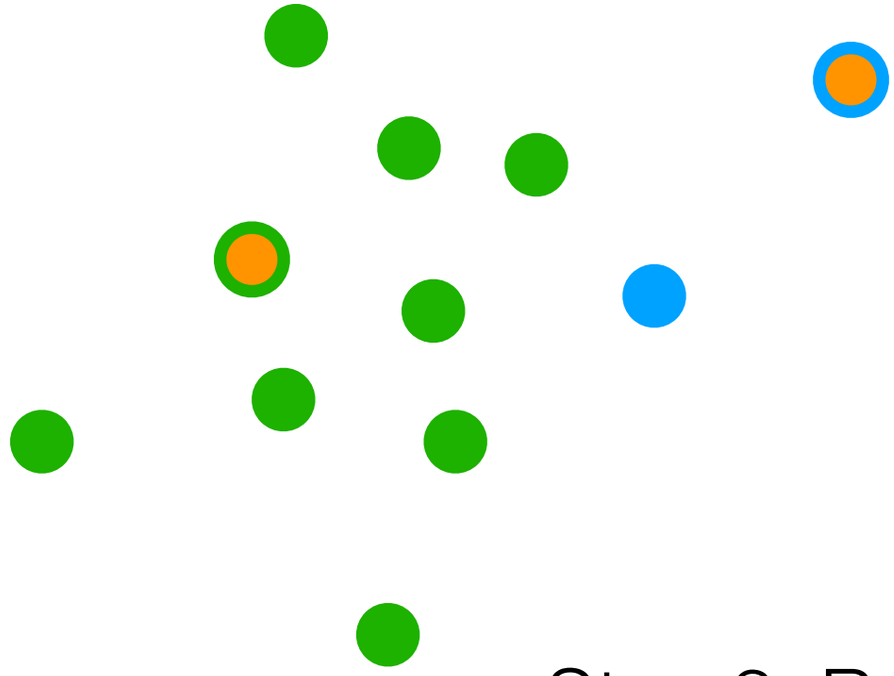

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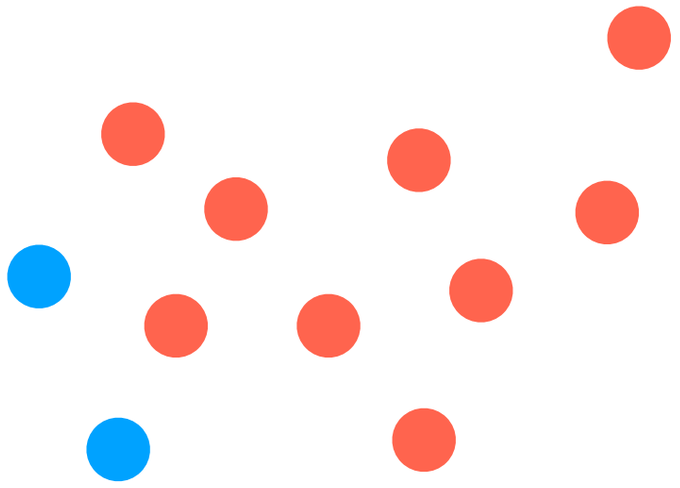

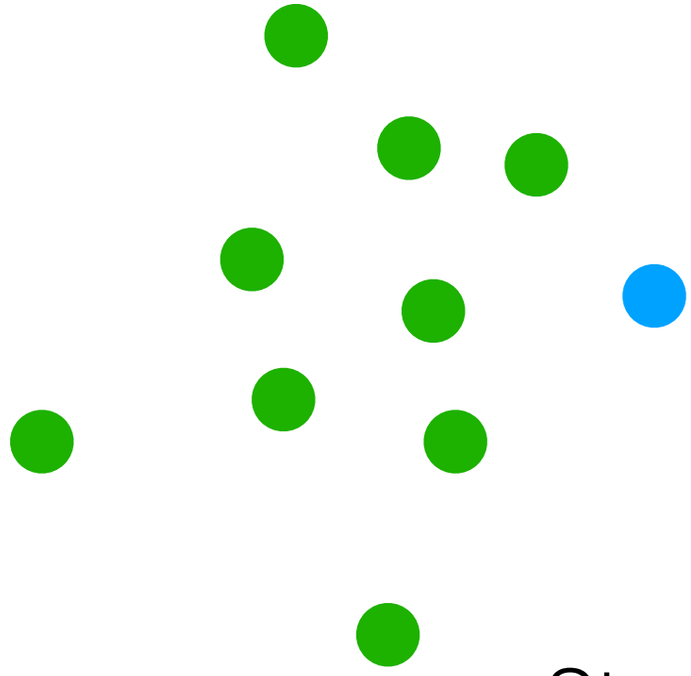

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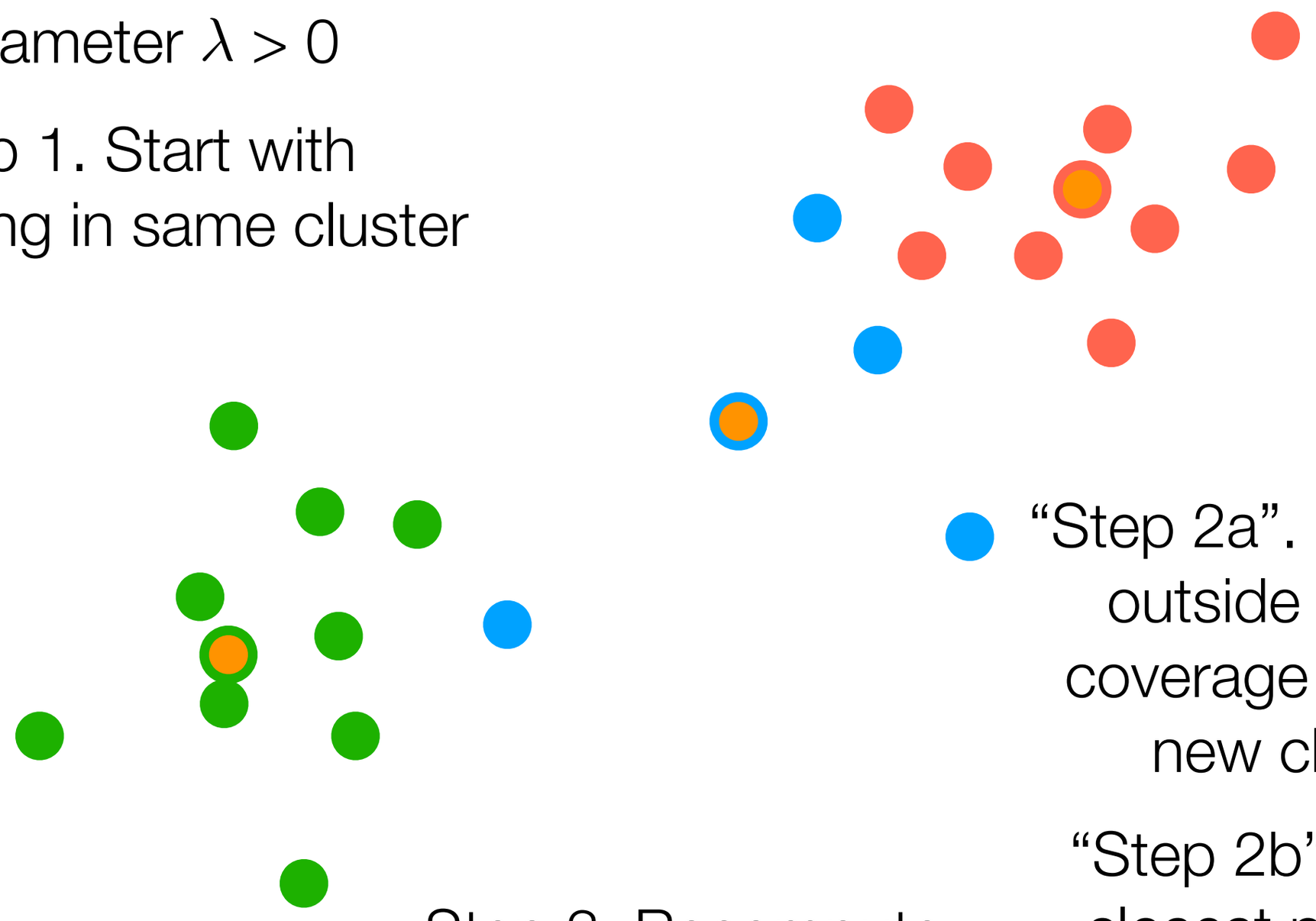

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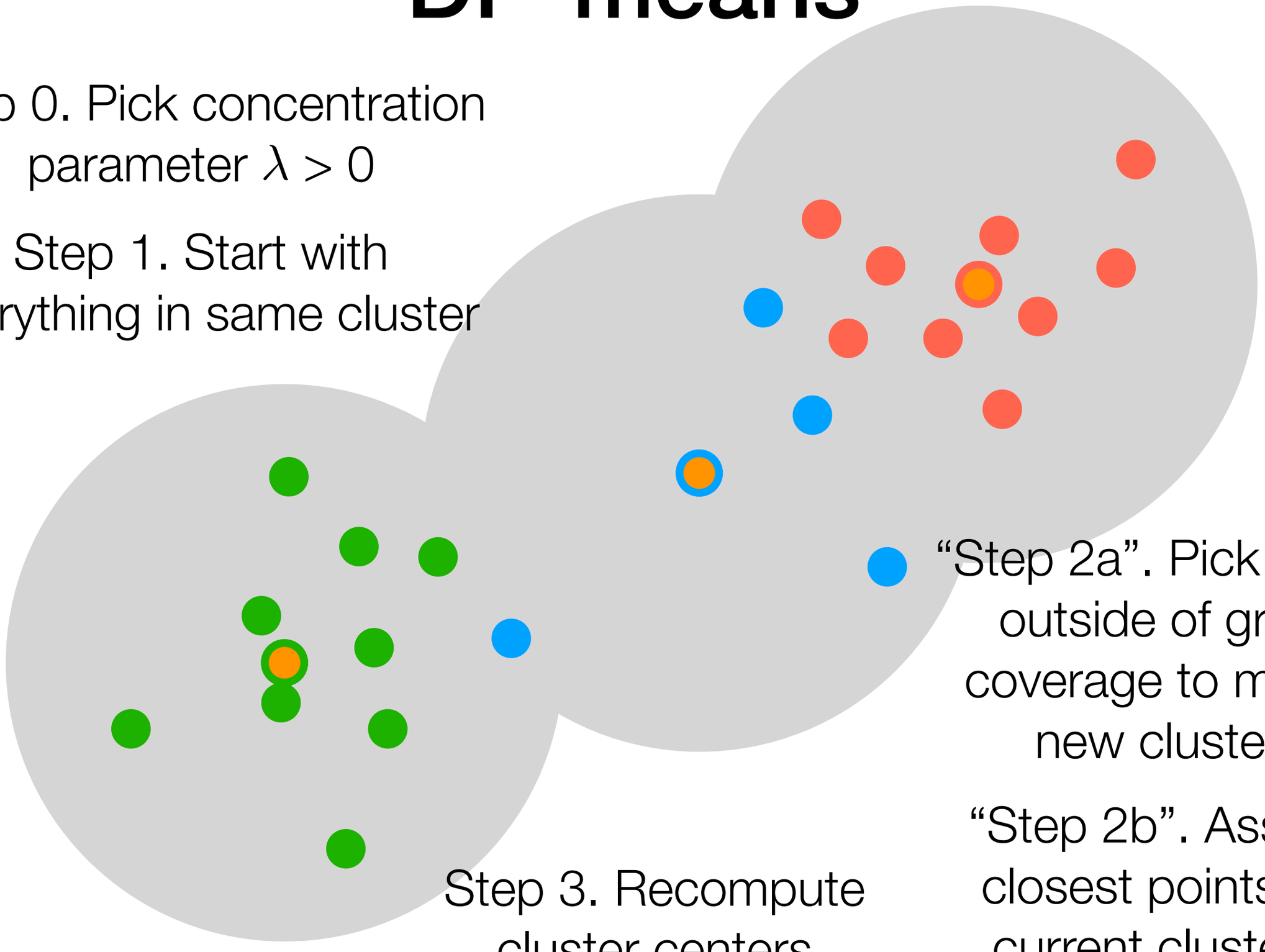

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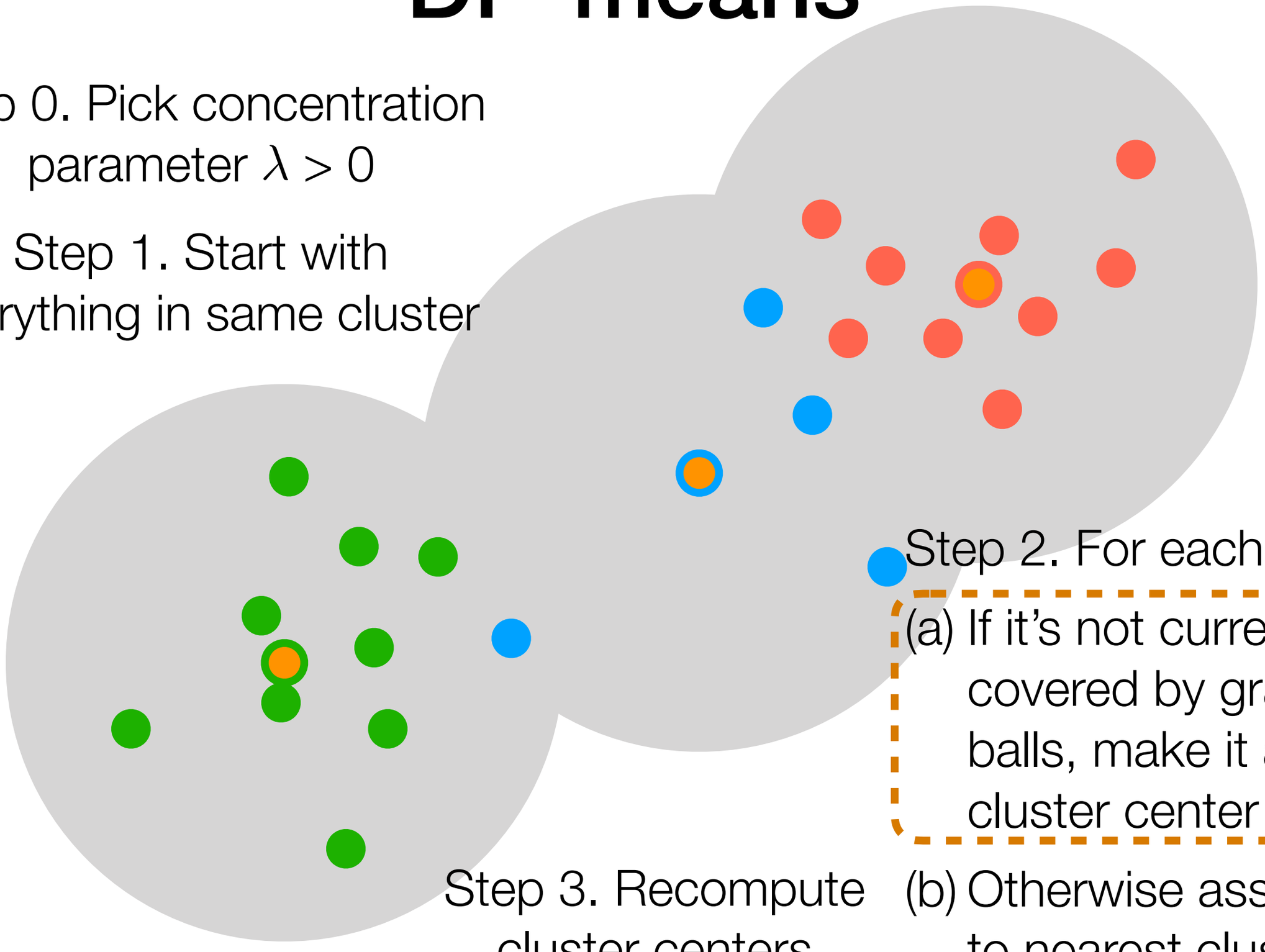

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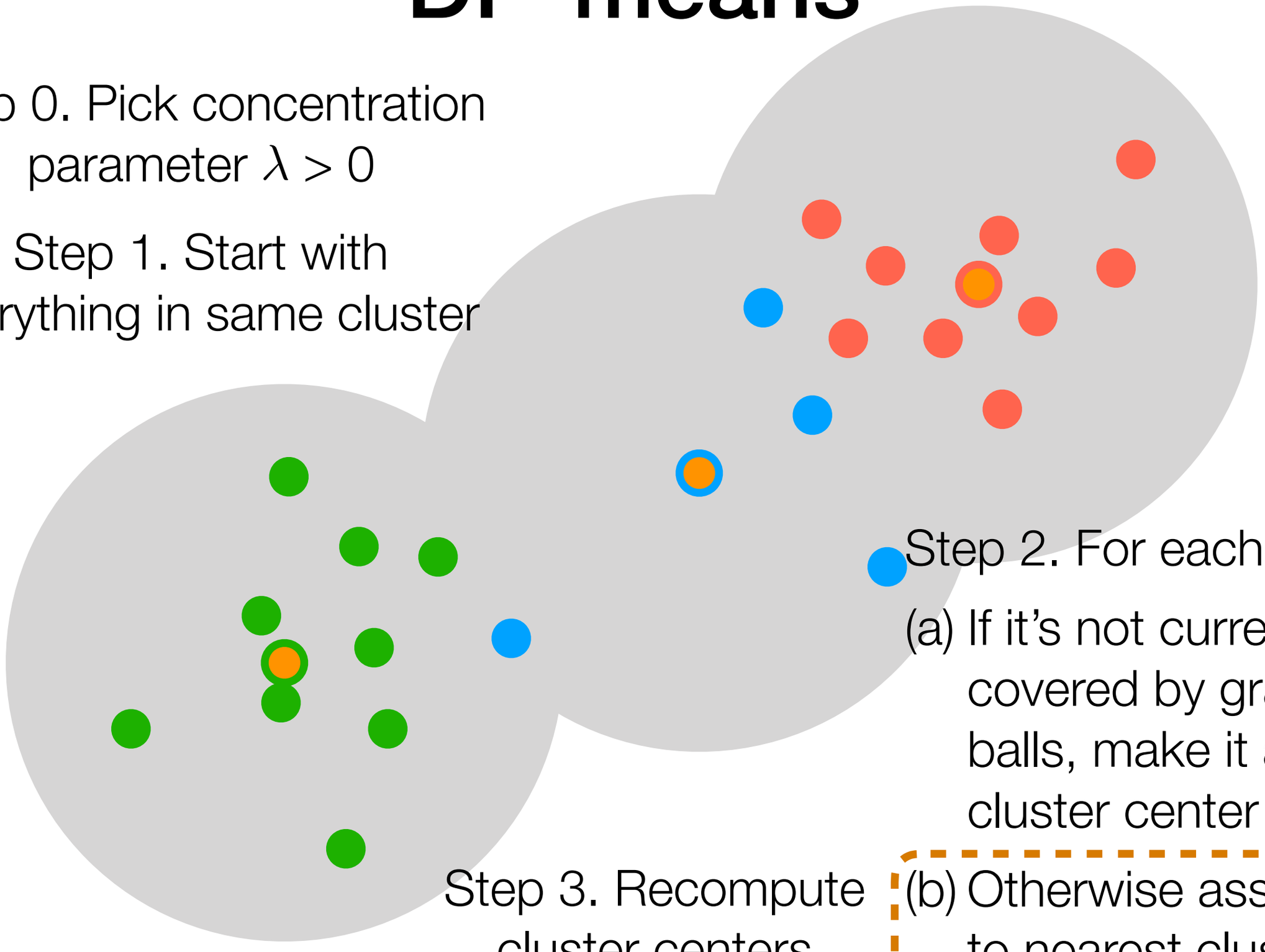

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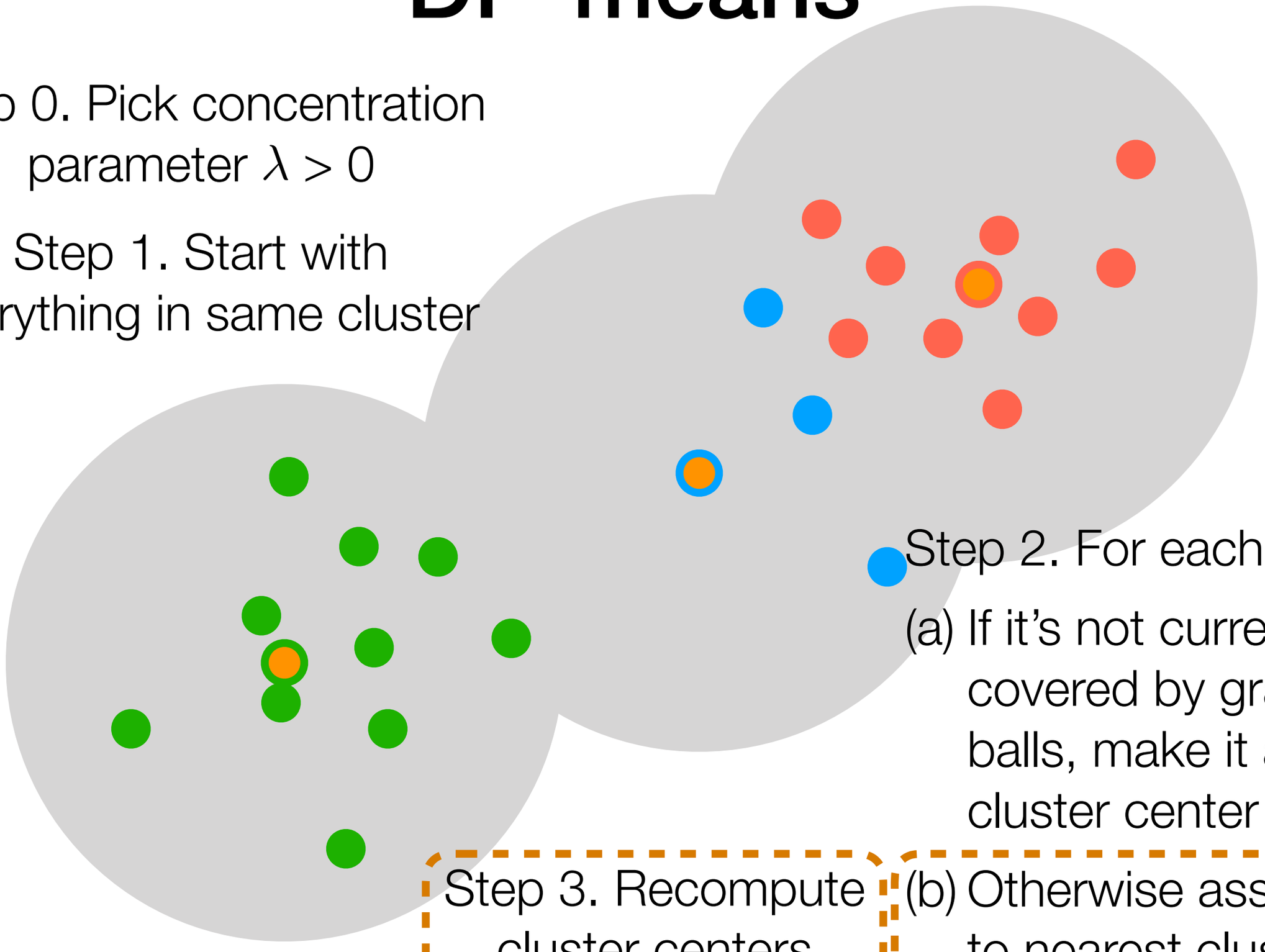

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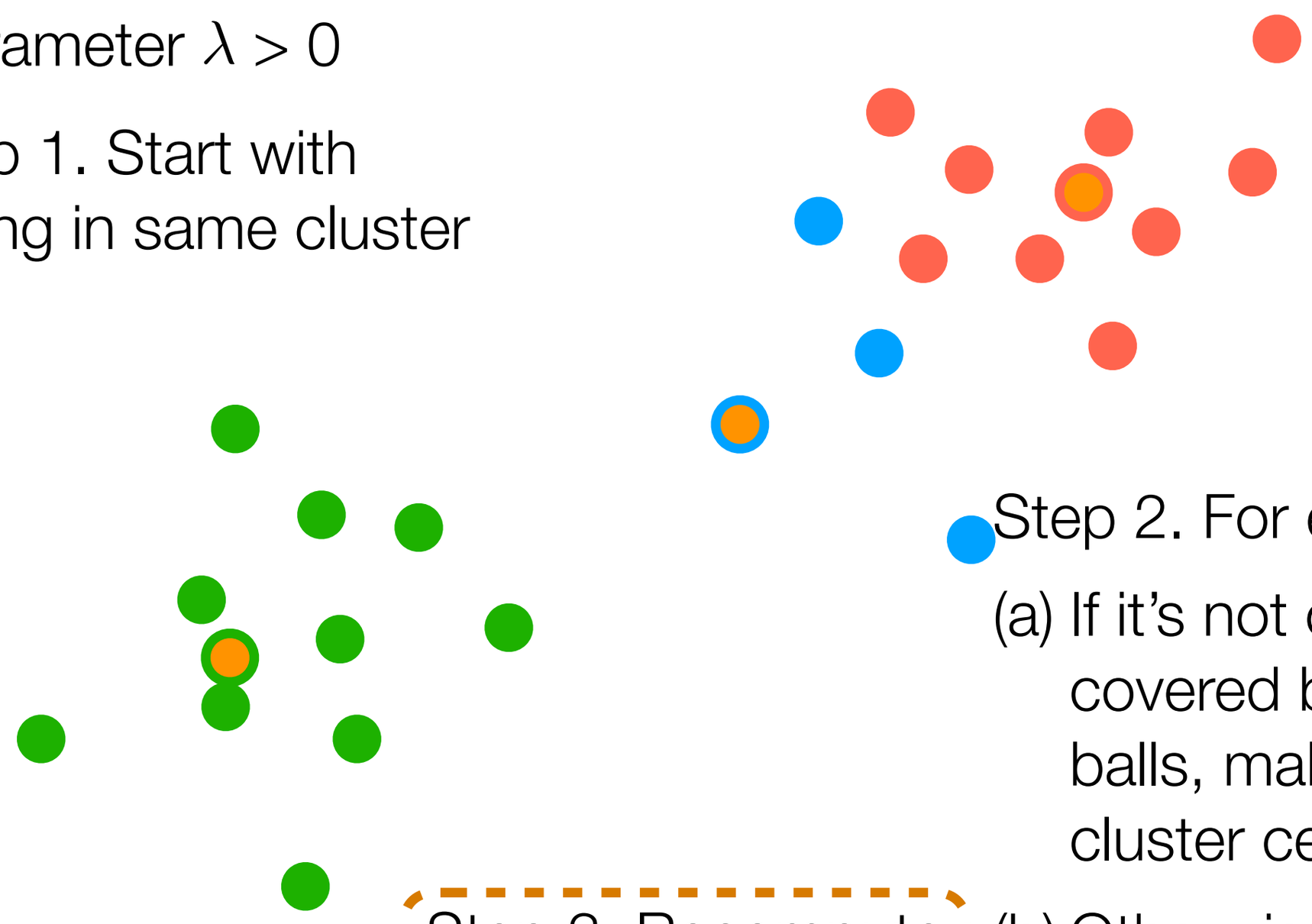

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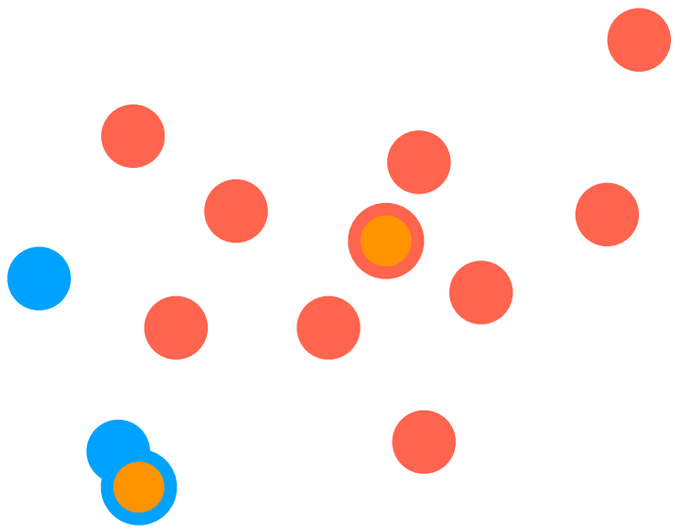

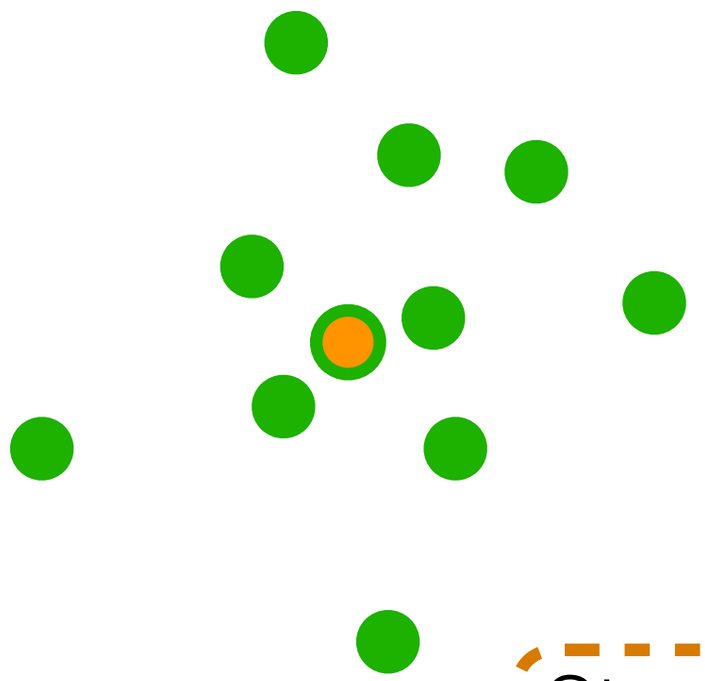

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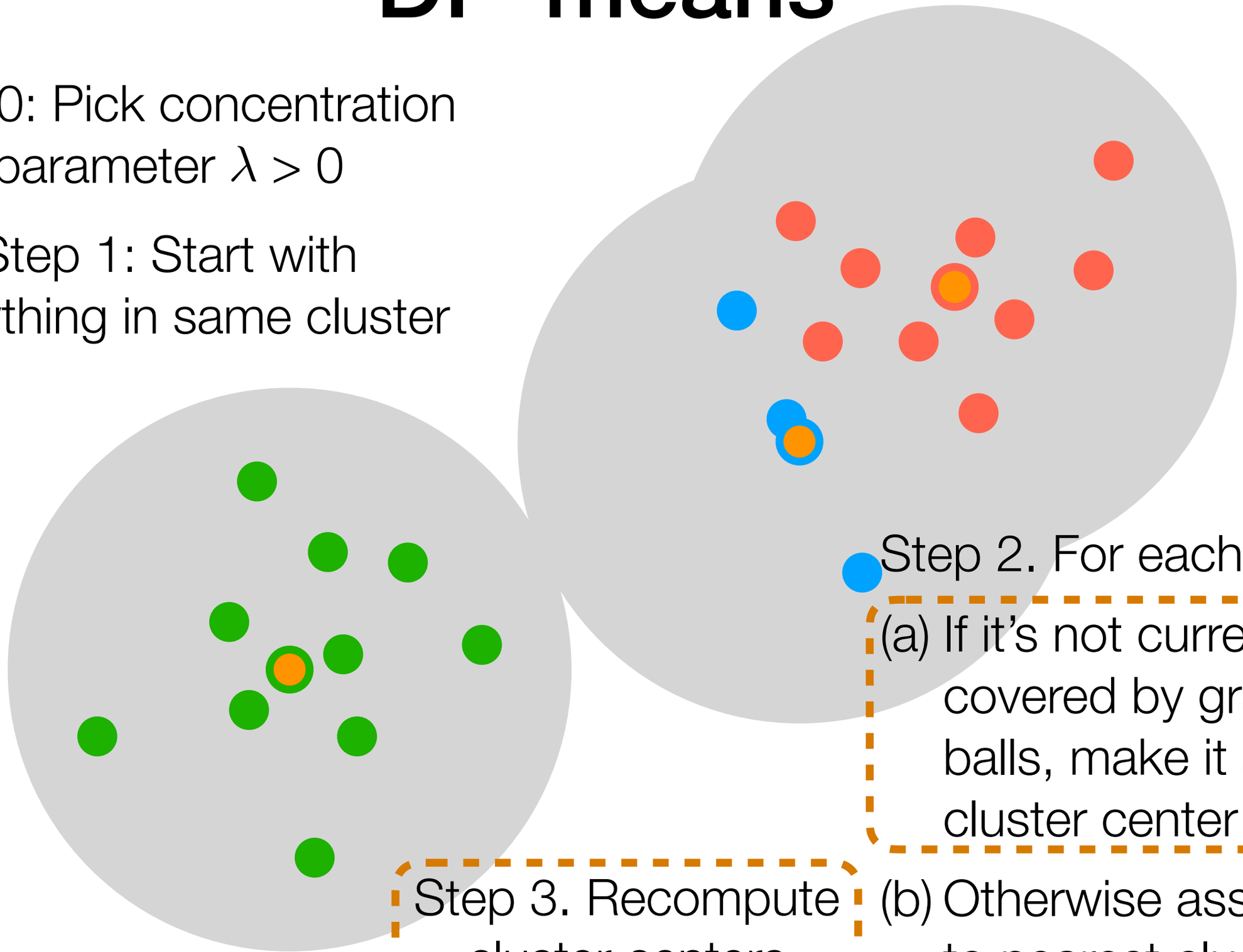
Step 0: Pick concentration parameter $\lambda > 0$

Step 1: Start with everything in same cluster



Step 2. For each point:

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

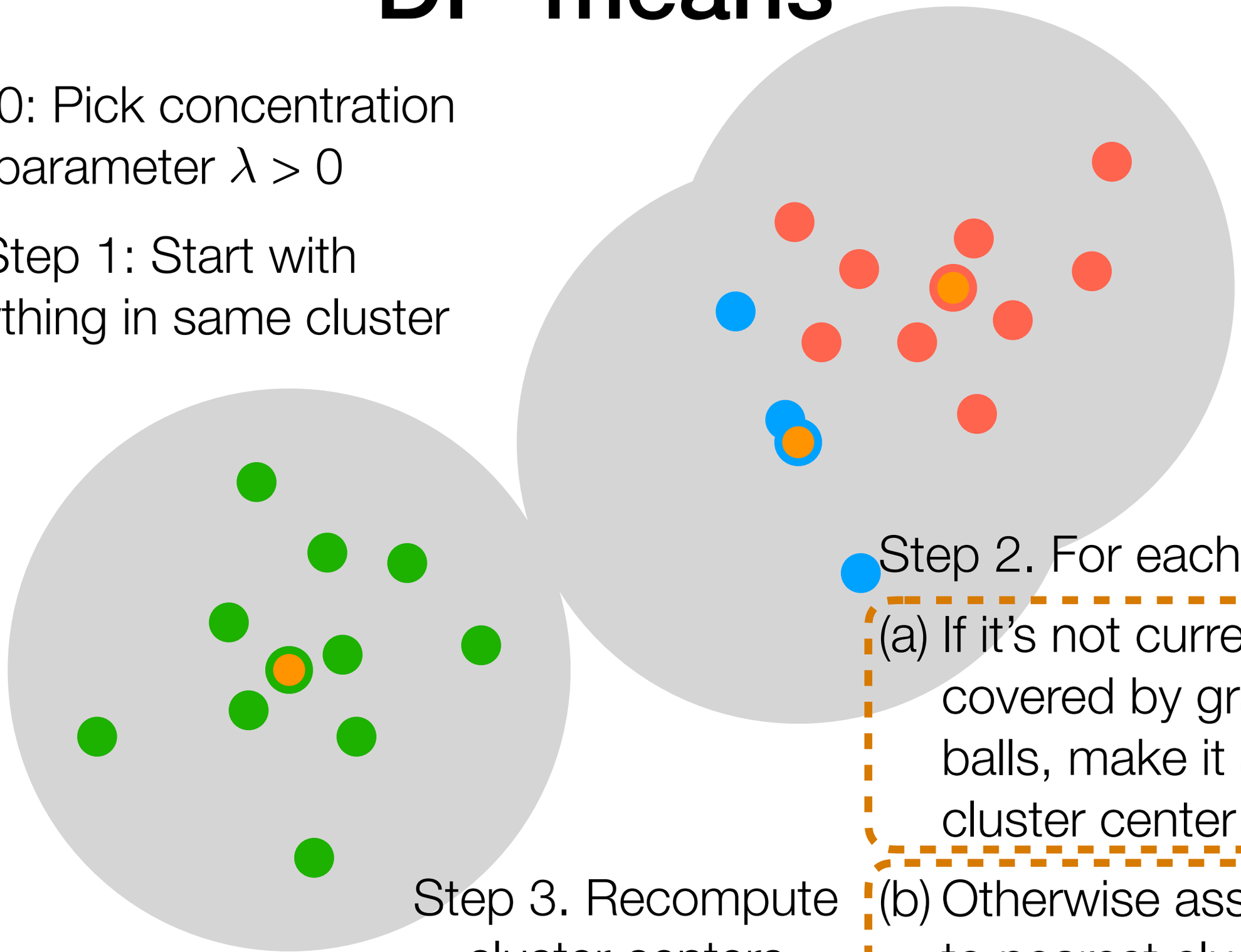
(b) Otherwise assign it to nearest cluster

Step 3. Recompute cluster centers

DP-means

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

Step 1: Start with everything in same cluster



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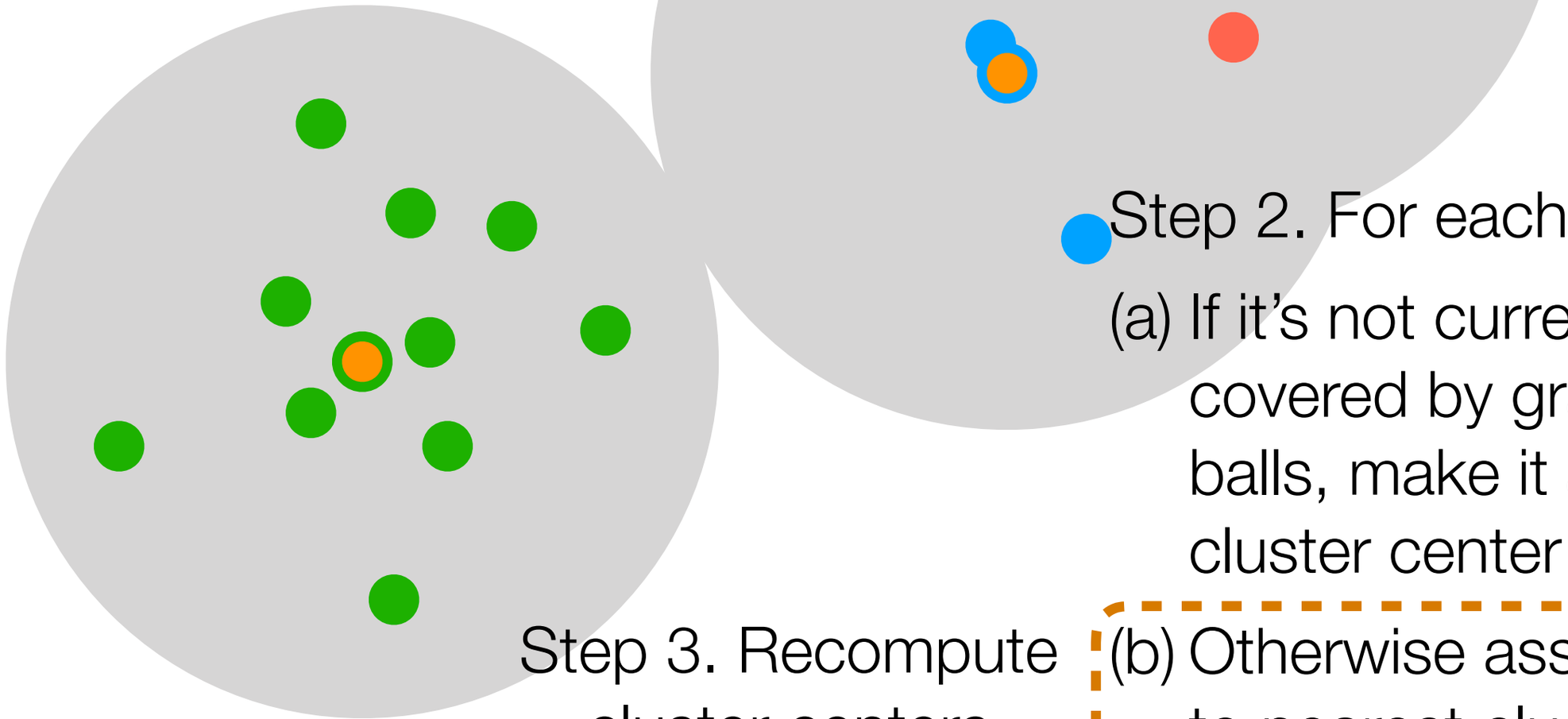

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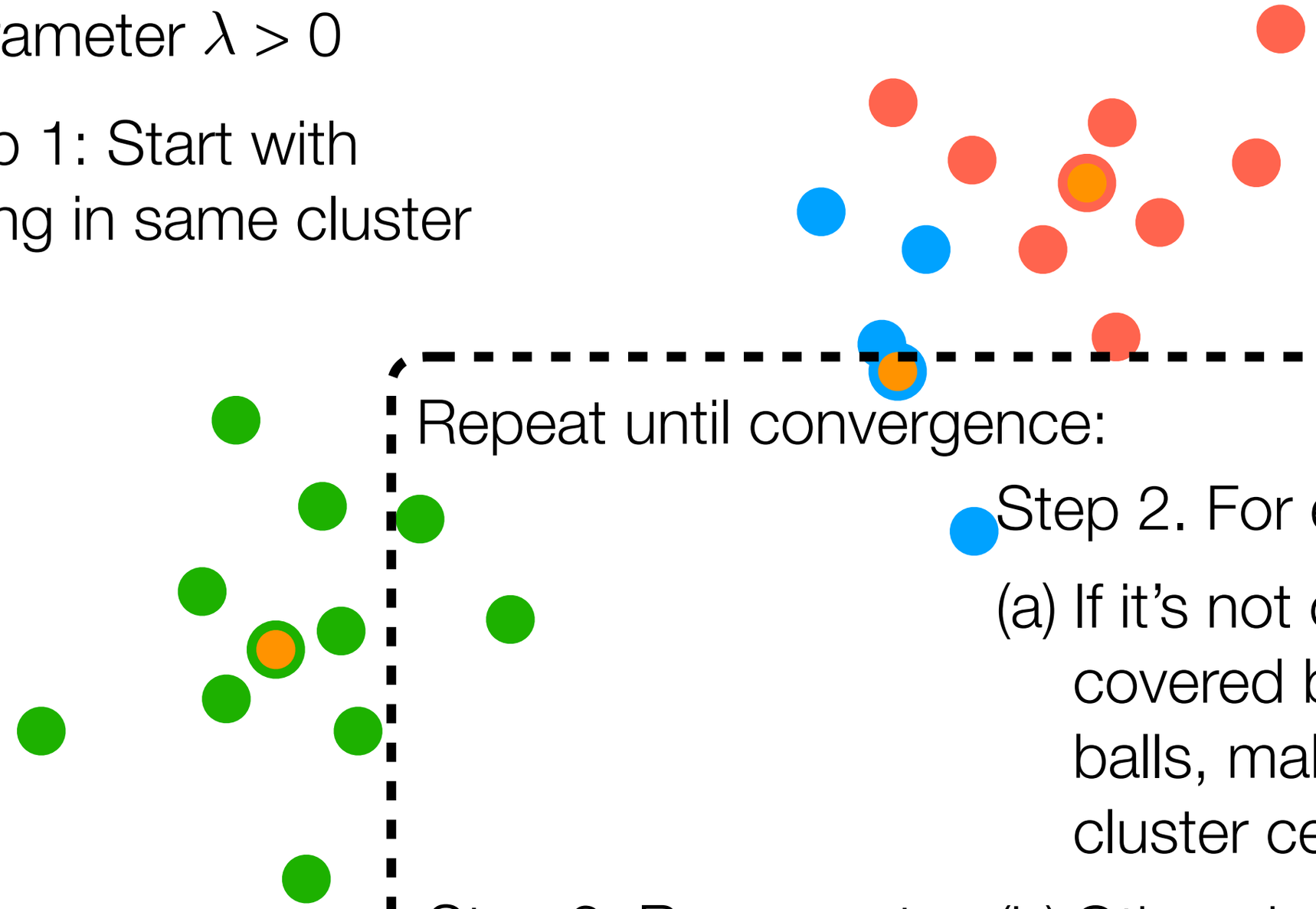


Repeat until convergence:

Step 2. For each point:

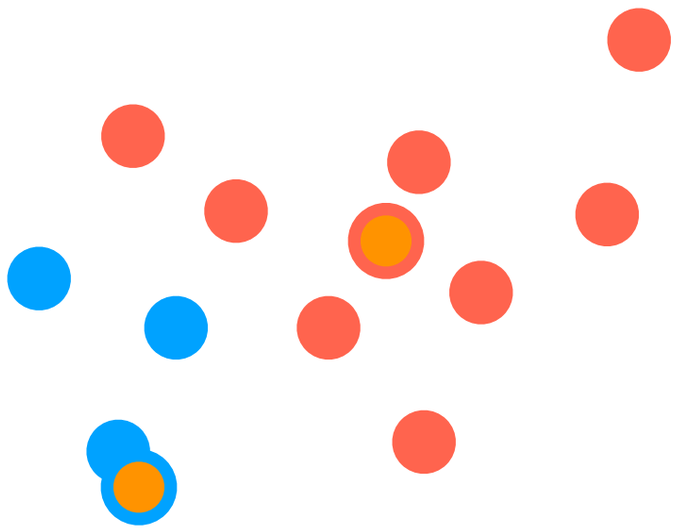
(a) If it's not currently covered by gray balls, make it a new cluster center

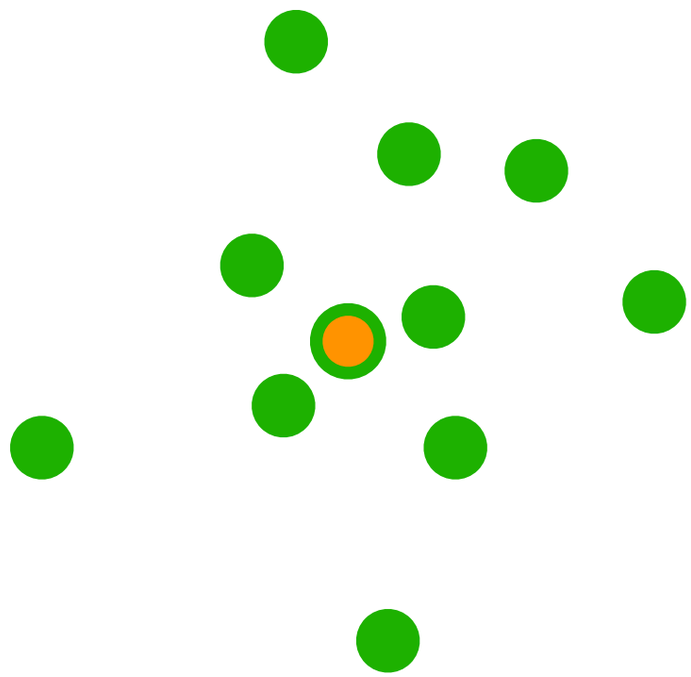
(b) Otherwise assign it to nearest cluster

Step 3. Recompute cluster centers

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





In practice: can reassign points in small clusters to bigger clusters

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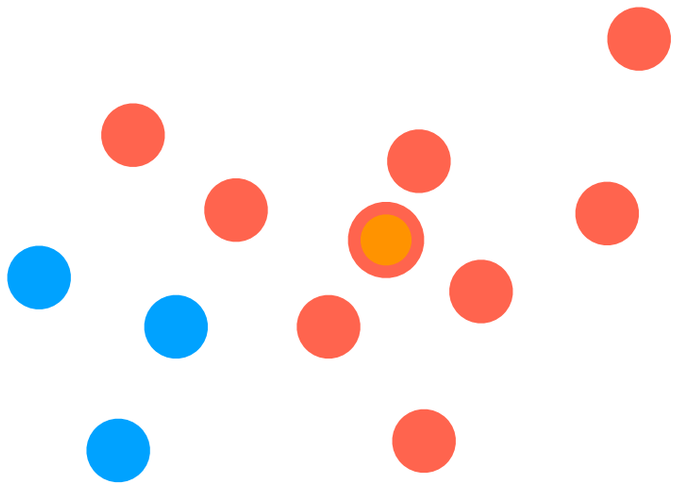

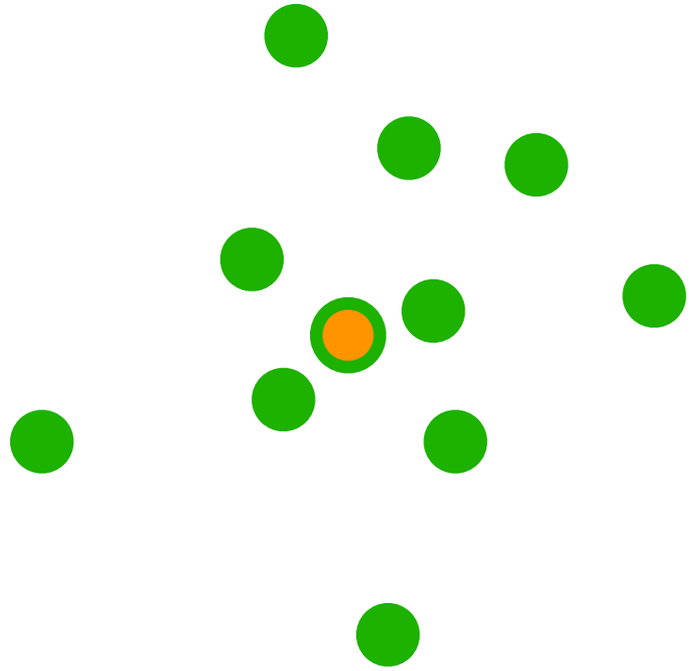

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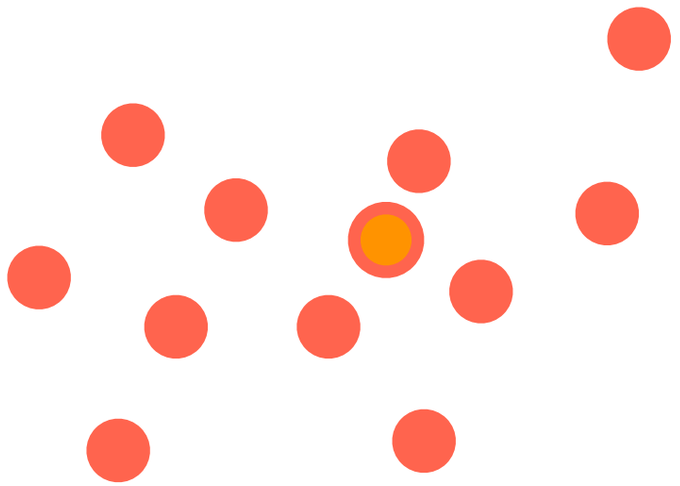

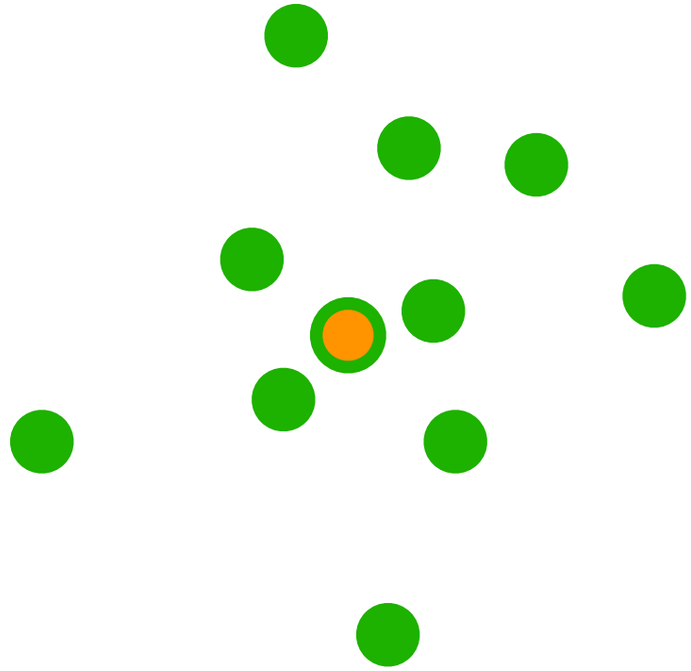

In practice: can reassign points in small clusters to bigger clusters

Can recompute cluster centers

DP-means

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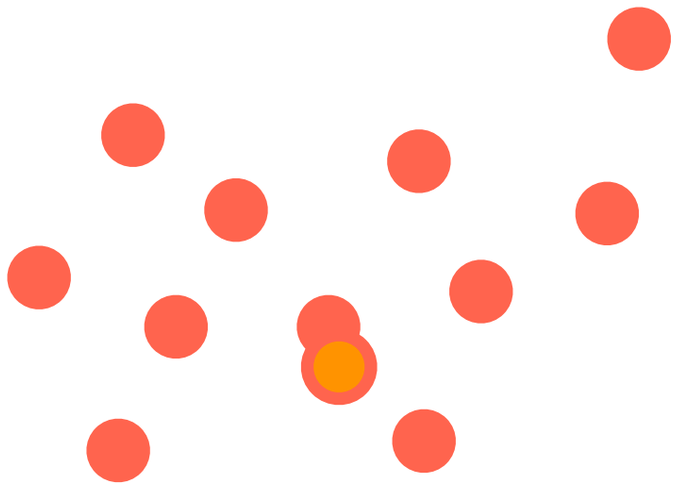

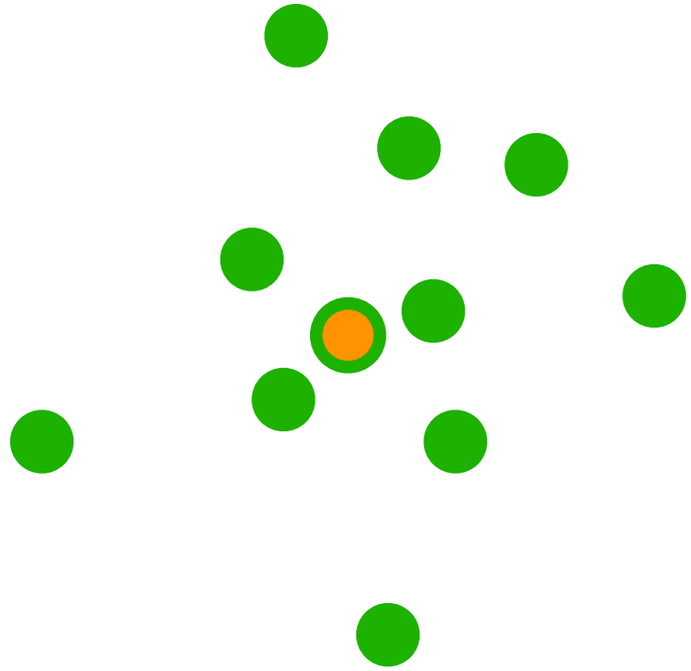

In practice: can reassign points in small clusters to bigger clusters

Can recompute cluster centers

Big picture: DP-means & DP-GMM have a parameter roughly controlling *size* of clusters rather than *number* of clusters

If your problem can more naturally be thought of as having cluster sizes that should not be too large, can use DP-means/DP-GMM instead of k-means/GMM

Real example. *Satellite image analysis of rural India to find villages*

Each cluster is a village: don't know how many villages there are total but rough upper bound on radius of village can be specified

➔ DP-means can provide a decent solution!