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

Cluster 1

Probability of generating a point from cluster 1 = π_1

Gaussian mean = μ_1

Gaussian covariance = Σ_1

…

Cluster k

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

	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

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 you are to form new clusters vs try to stick to already existing clusters

- 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

Two main approaches:

- Finite approximation where you specify some maximum number of possible clusters (the algorithm will find up to that many clusters) This is what's implemented in *sklearn*
  - Algorithm is somewhat similar to *k*-means/EM for GMMs
  - Algorithm output: very similar to regular GMM fitting
- Random sampling approach (no finite approximation needed!)
  - Algorithm output: a bunch of samples of different cluster assignments (can pick one with highest probability)

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

Learning a DP-GMM

Demo

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

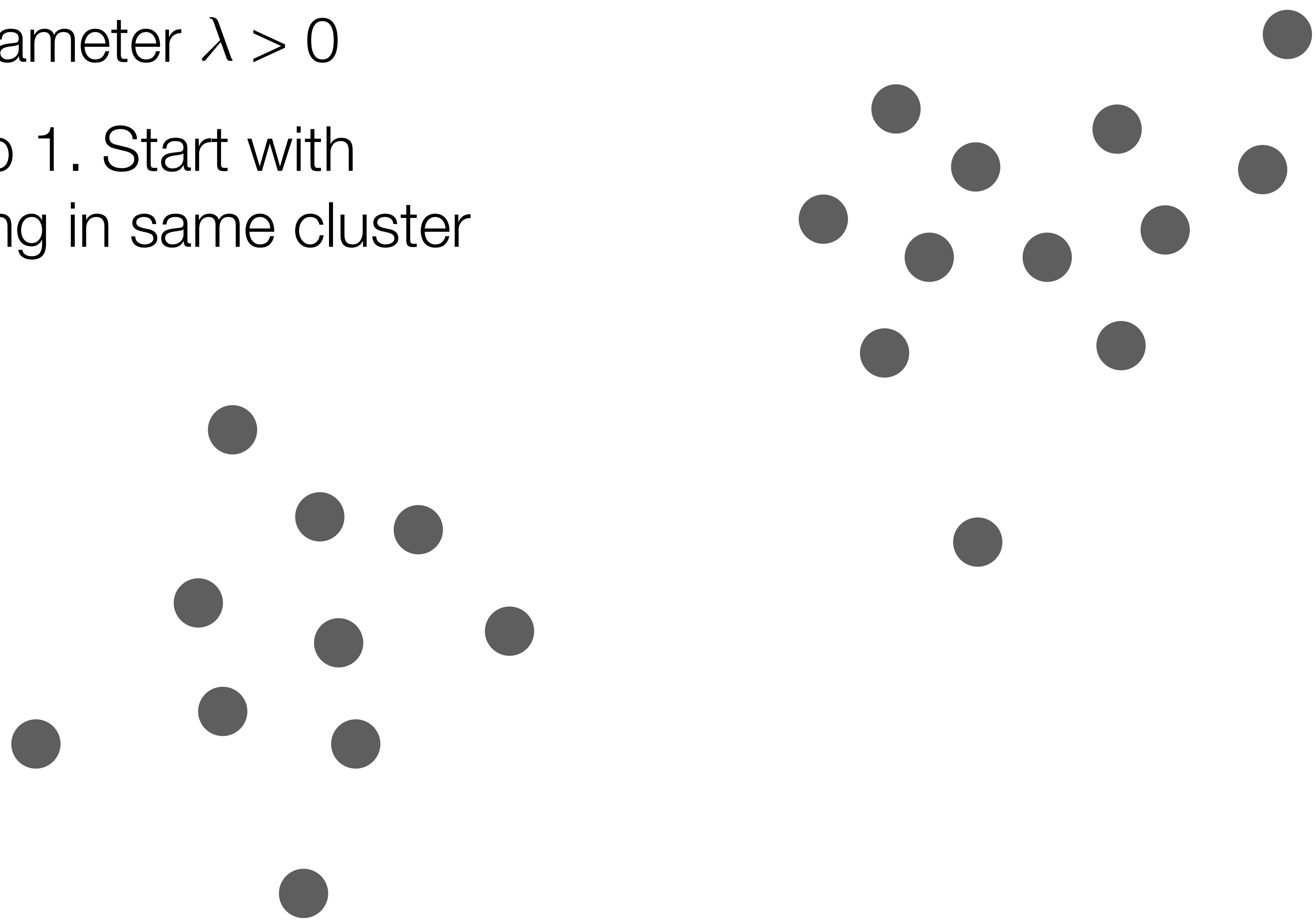
What approximates learning DP-GMMs?

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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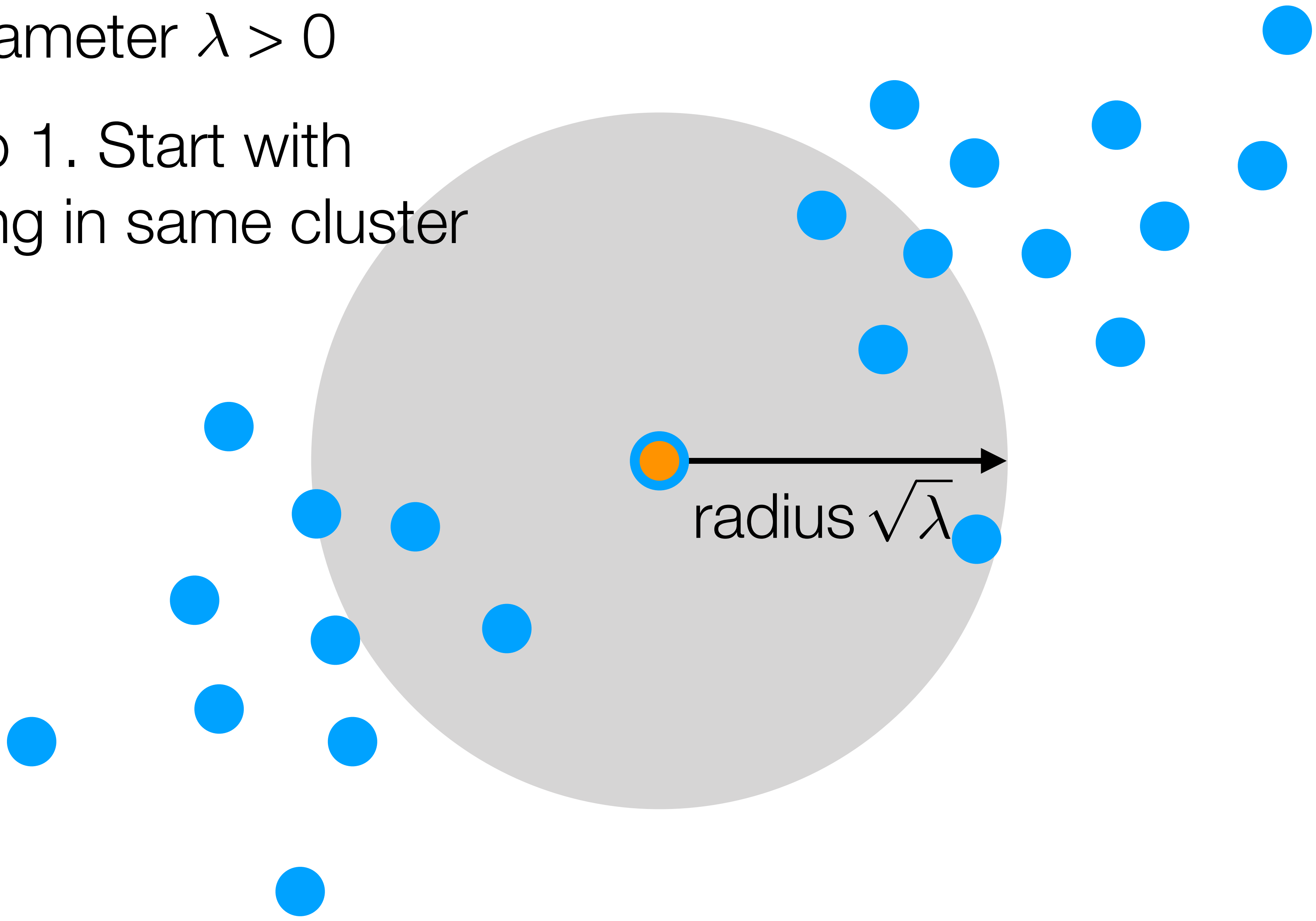

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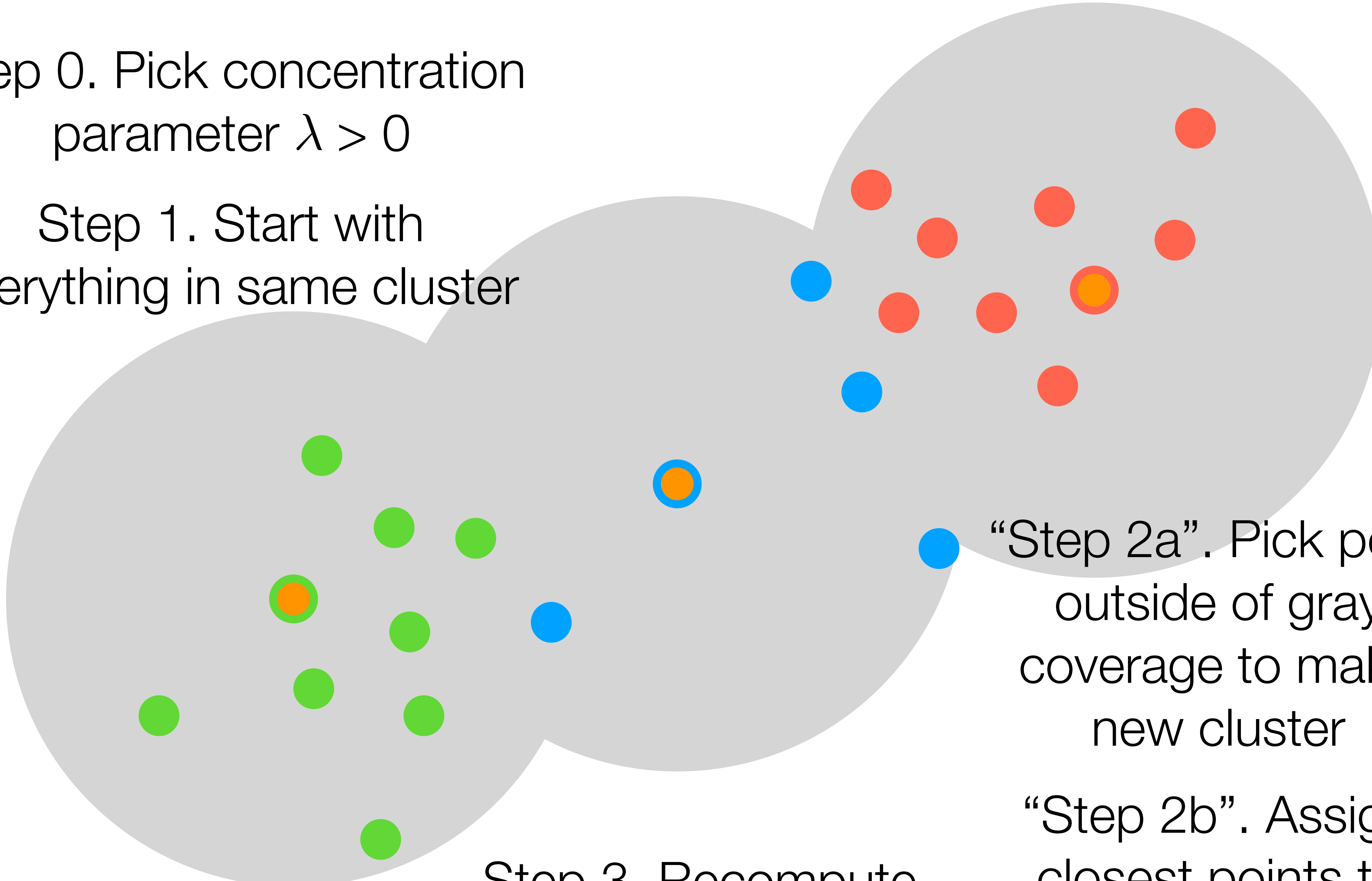

"Step 2a". Pick point outside of gray coverage to make new cluster

"Step 2b". Assign closest points to current clusters

Step 3. Recompute cluster centers

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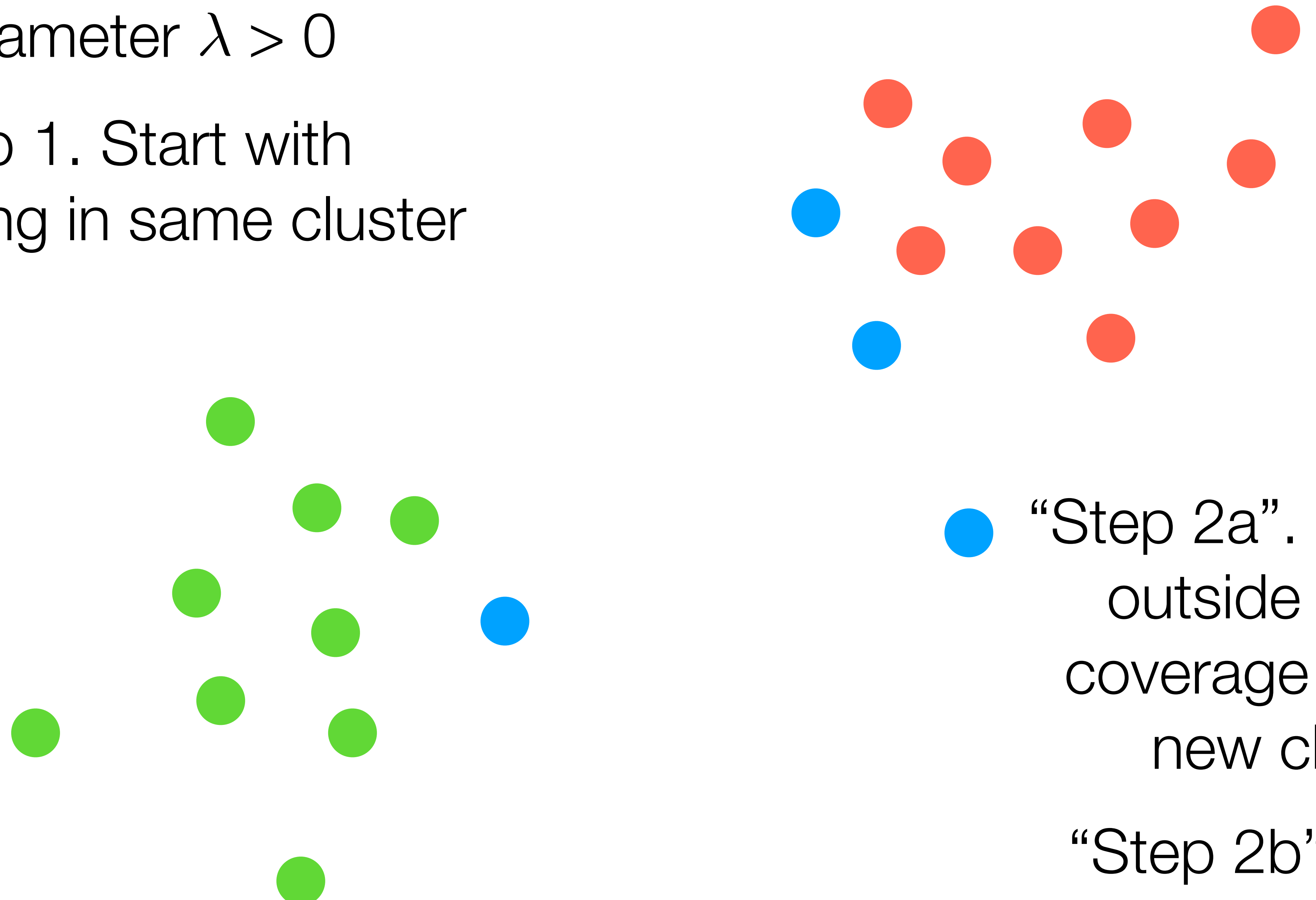

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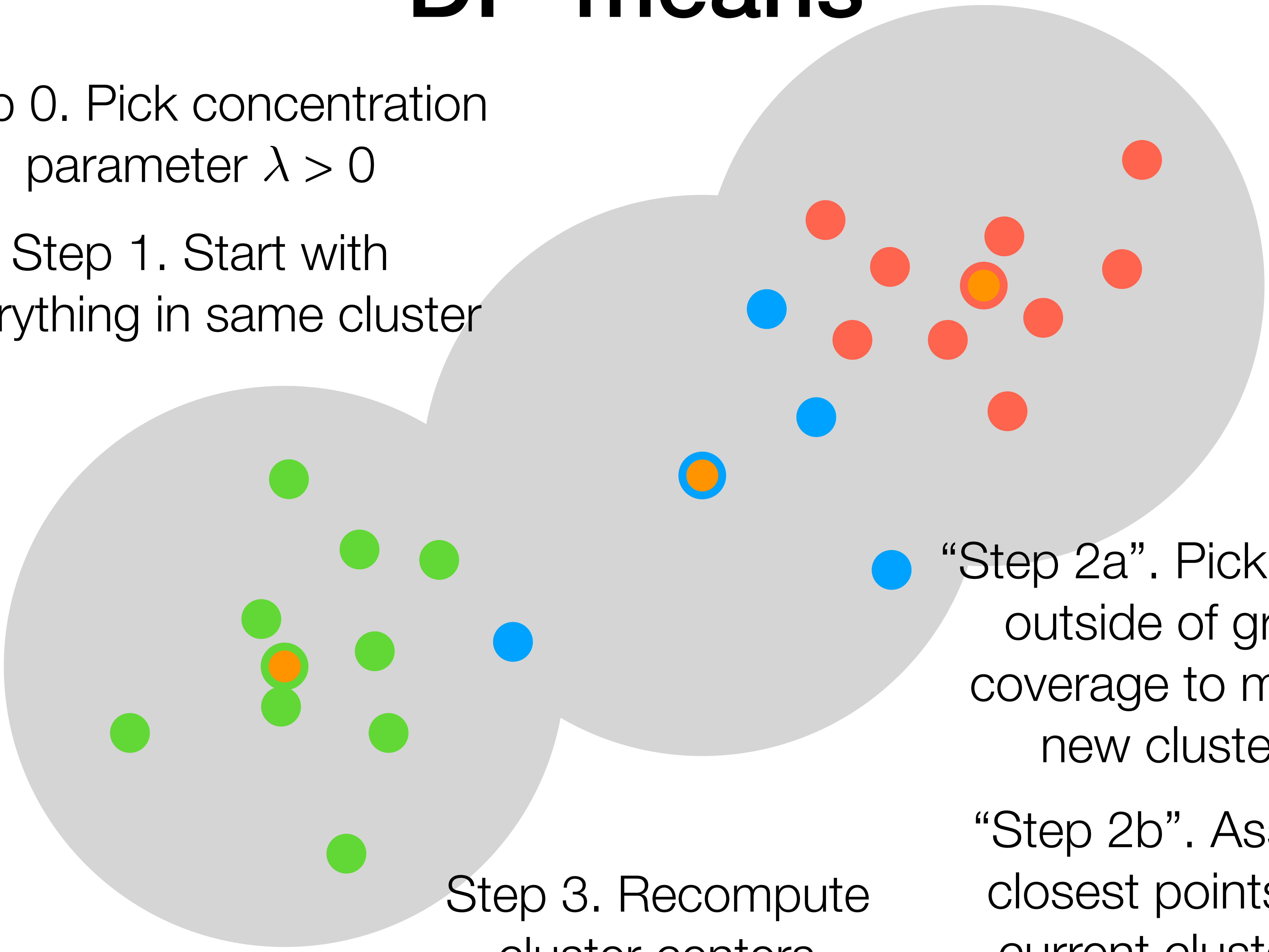

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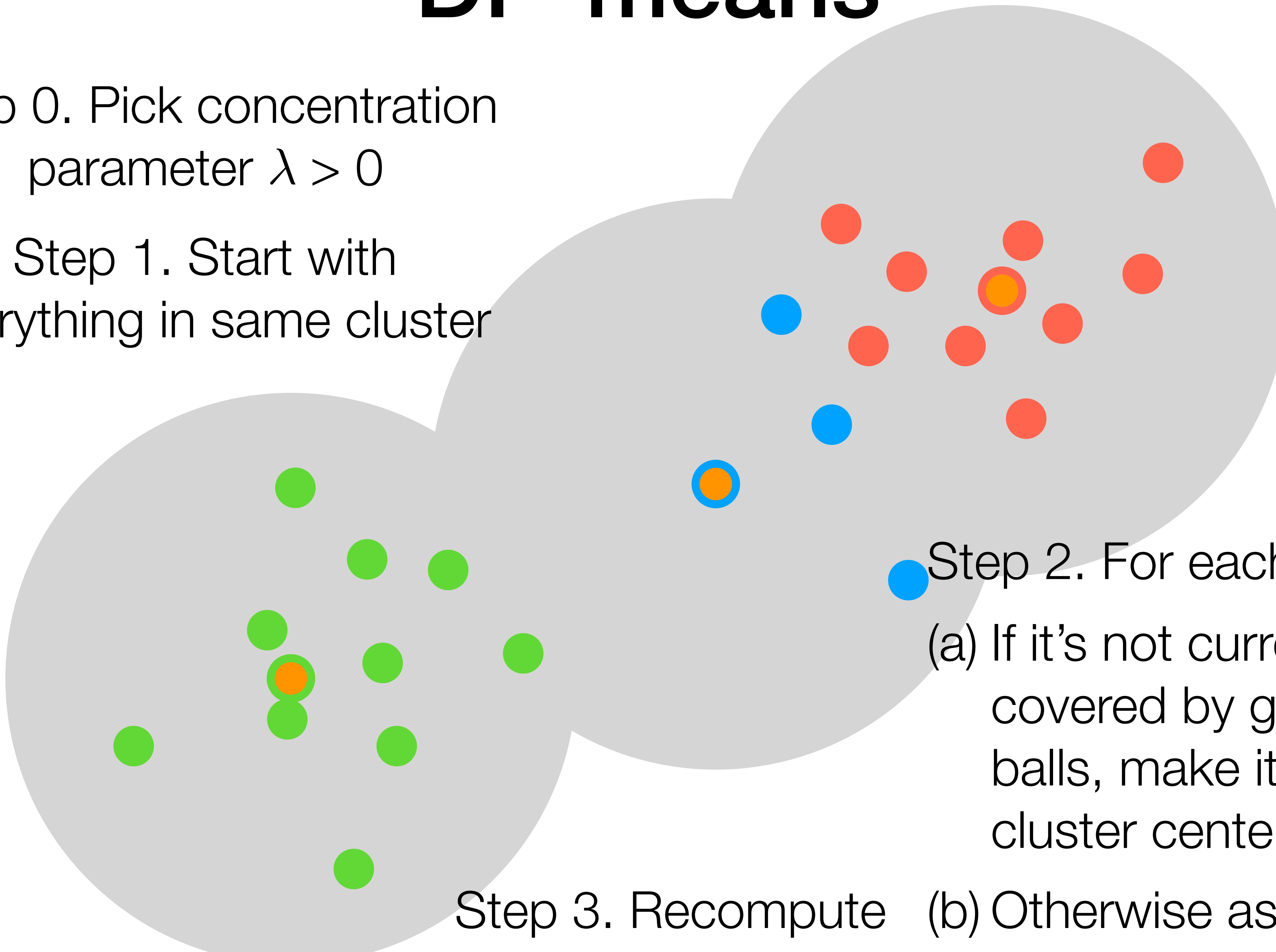

Step 2. For each point:

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

(b) Otherwise assign it to nearest cluster

Step 3. Recompute cluster centers

DP-means

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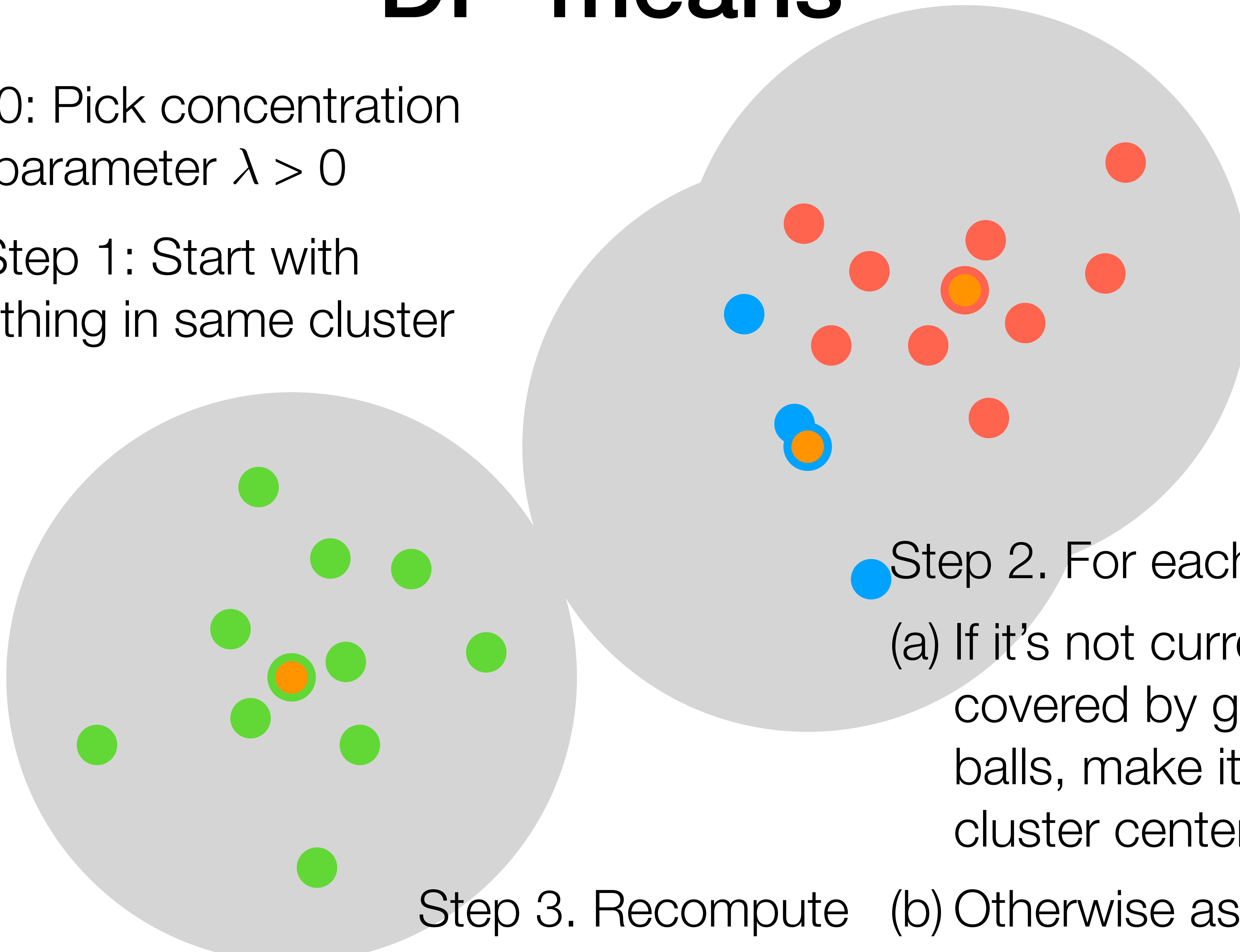

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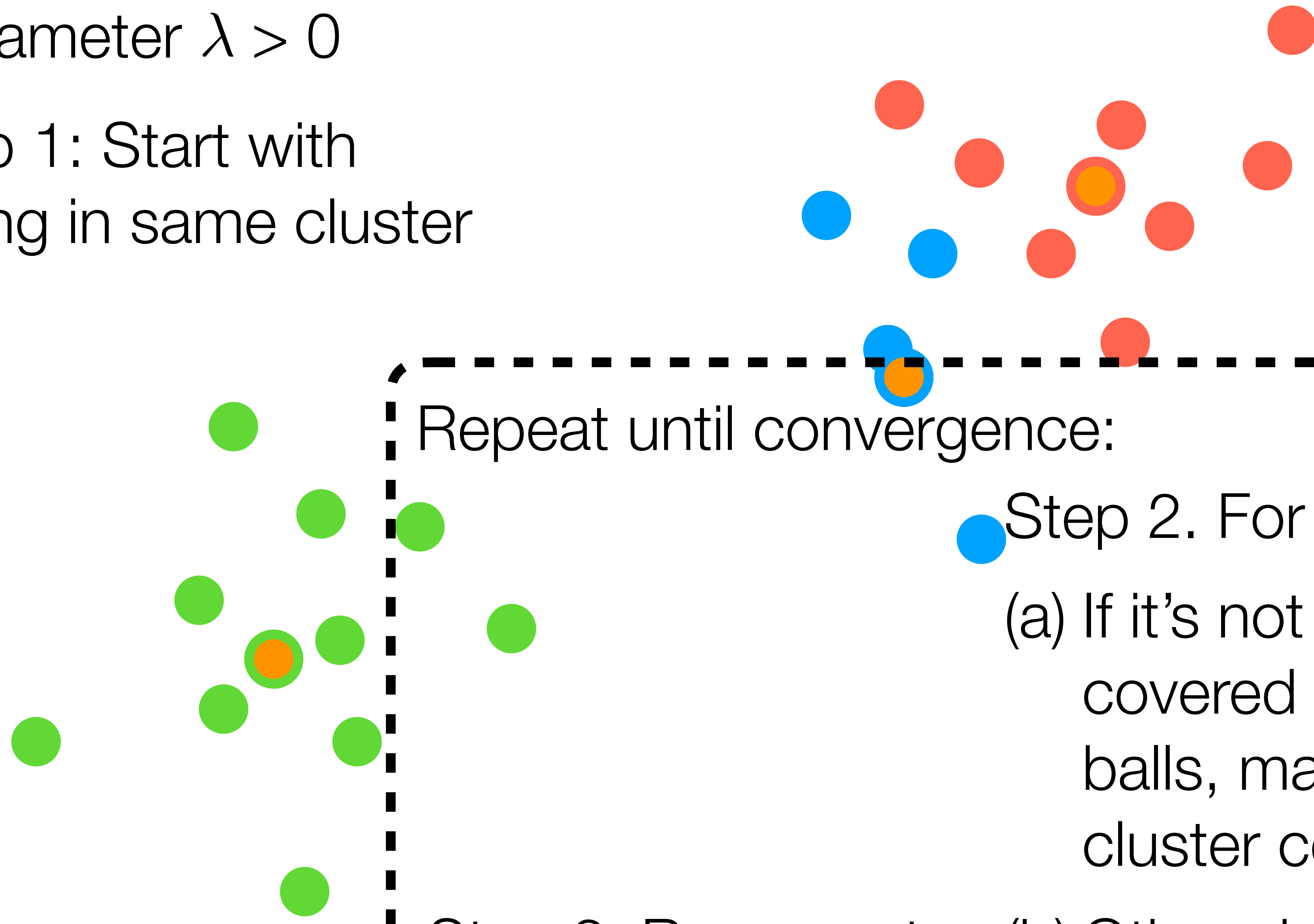


Repeat until convergence:

Step 2. For each point:

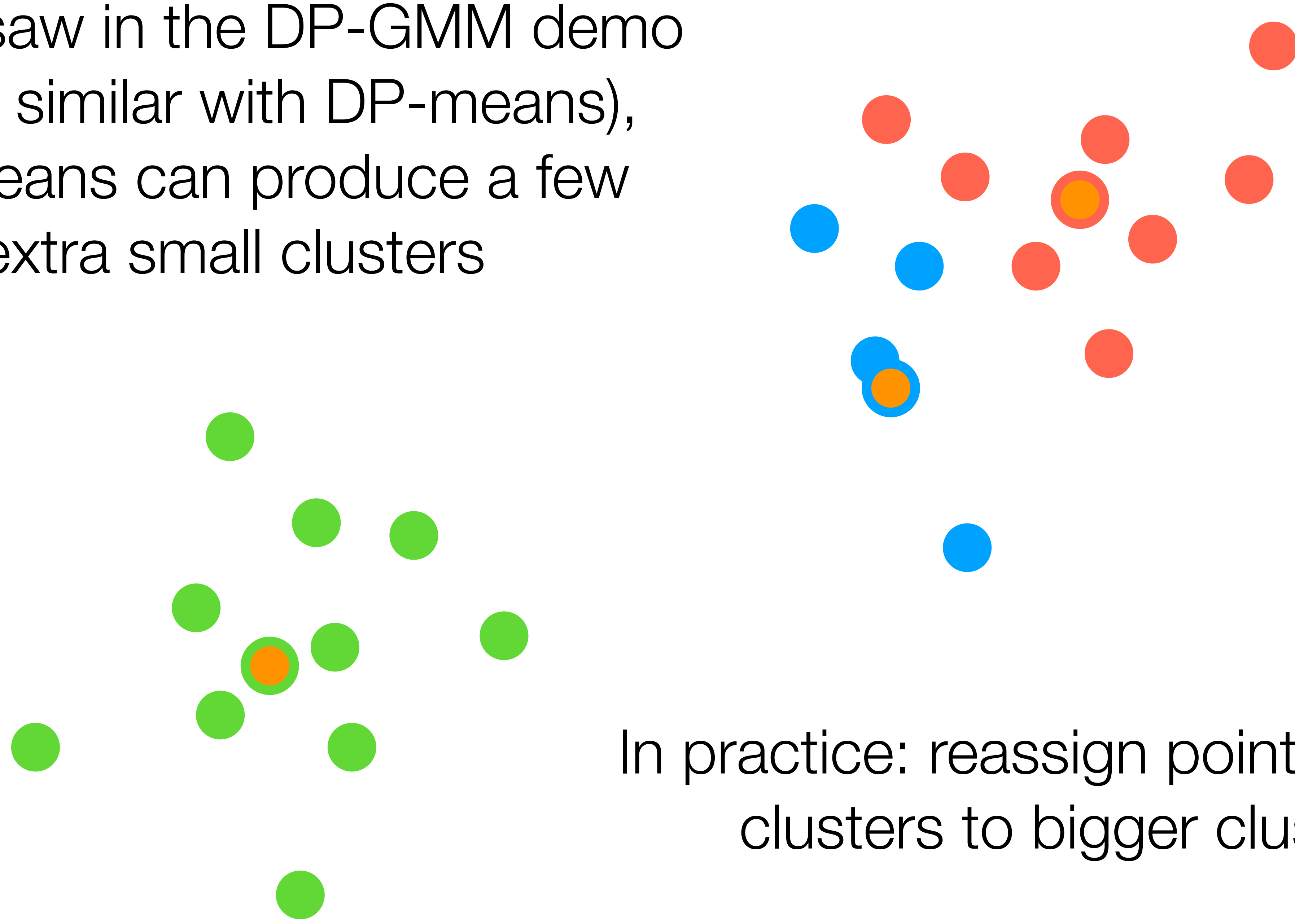
(a) If it's not currently covered by gray balls, make it a new cluster center

(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: reassign points in small
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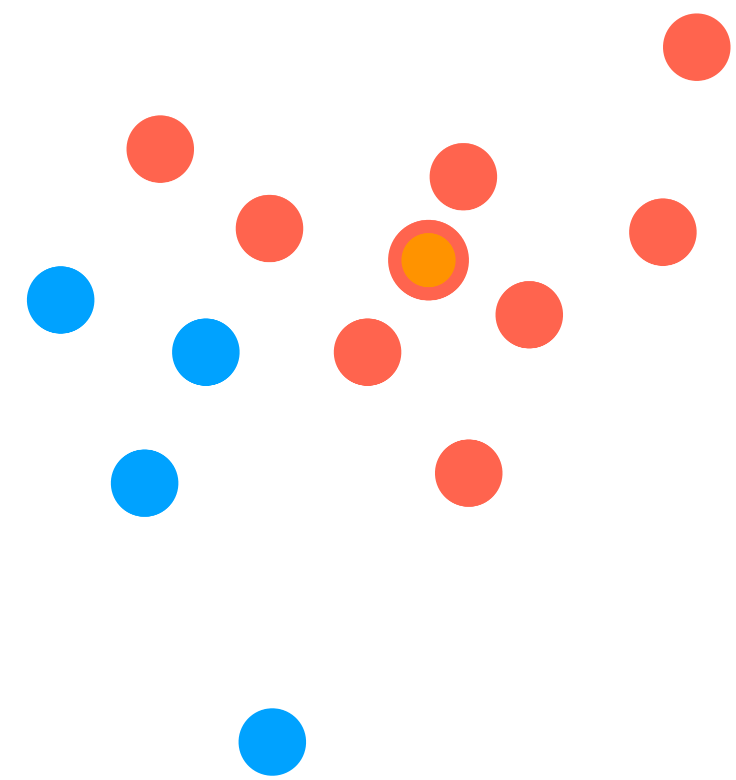

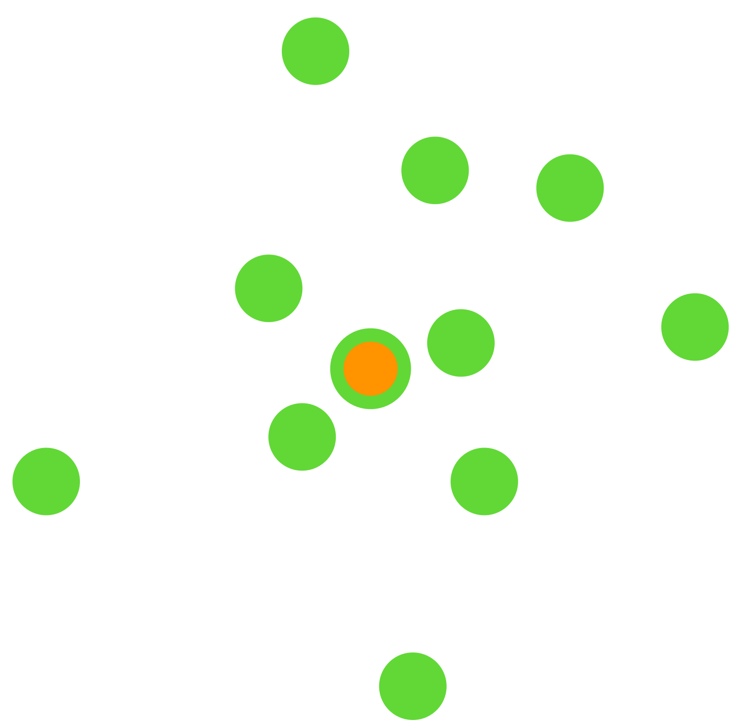

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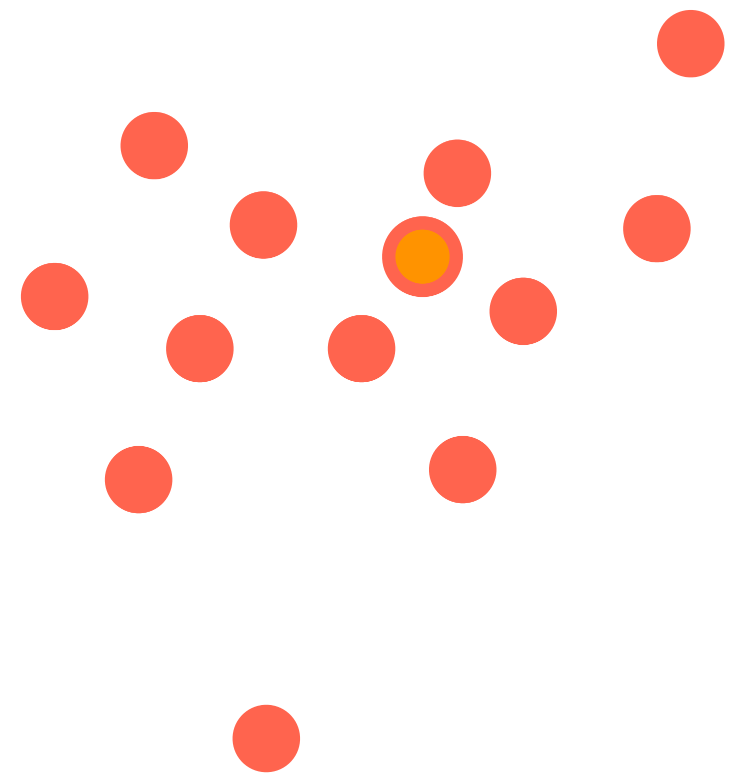

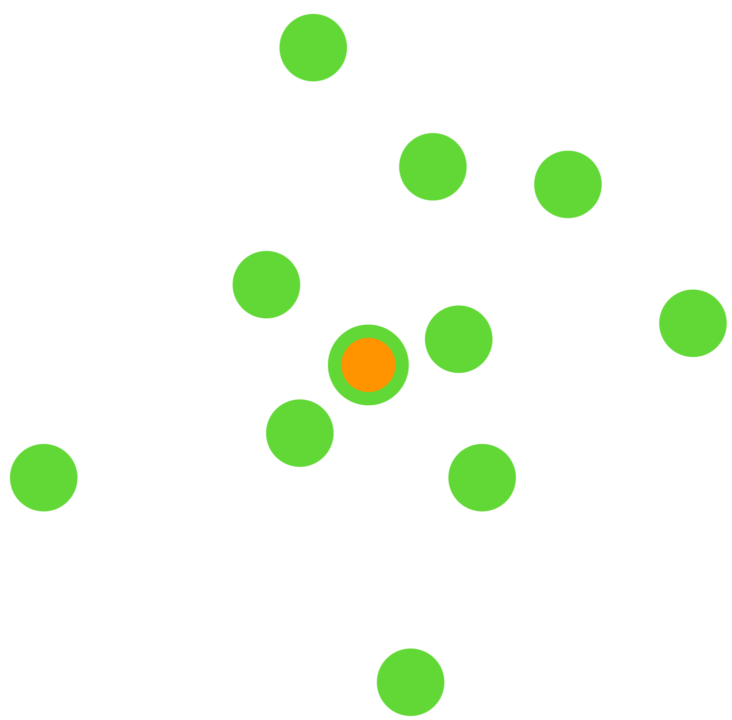

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Can recompute cluster centers

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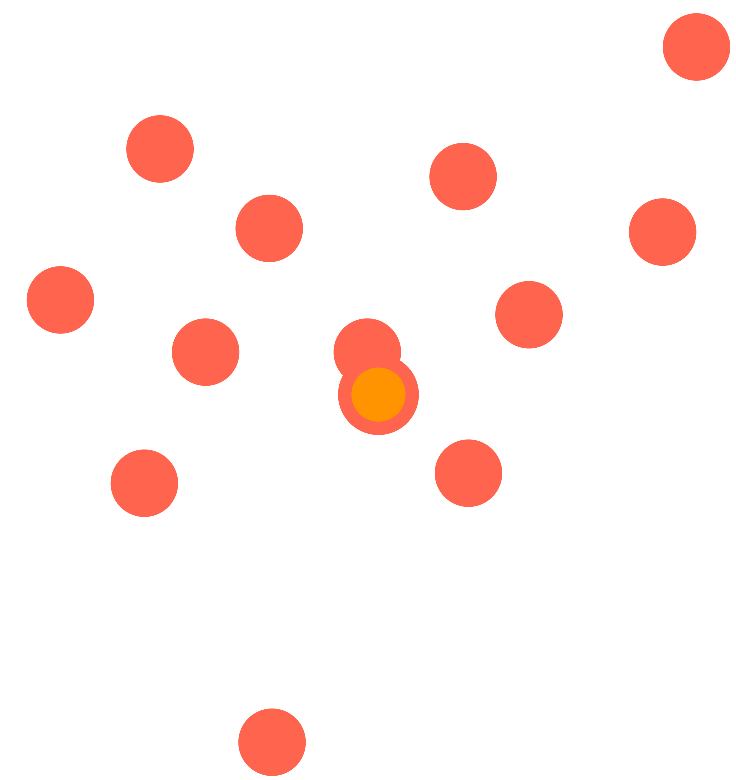
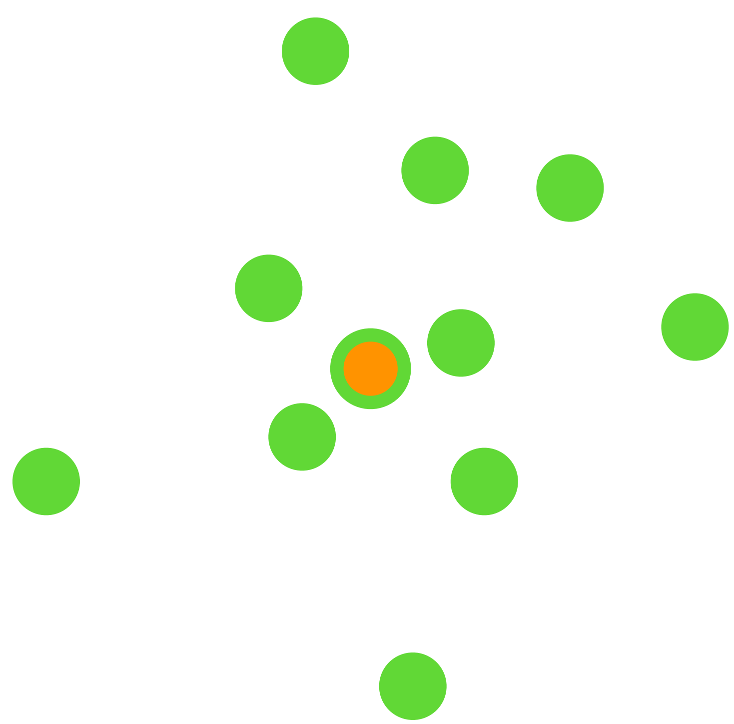




In practice: reassign points in small clusters to bigger clusters

Can recompute cluster centers

Big picture: DP-means & DP-GMM have a “concentration” 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 provides a decent solution!

Other Ways for Choosing *k*

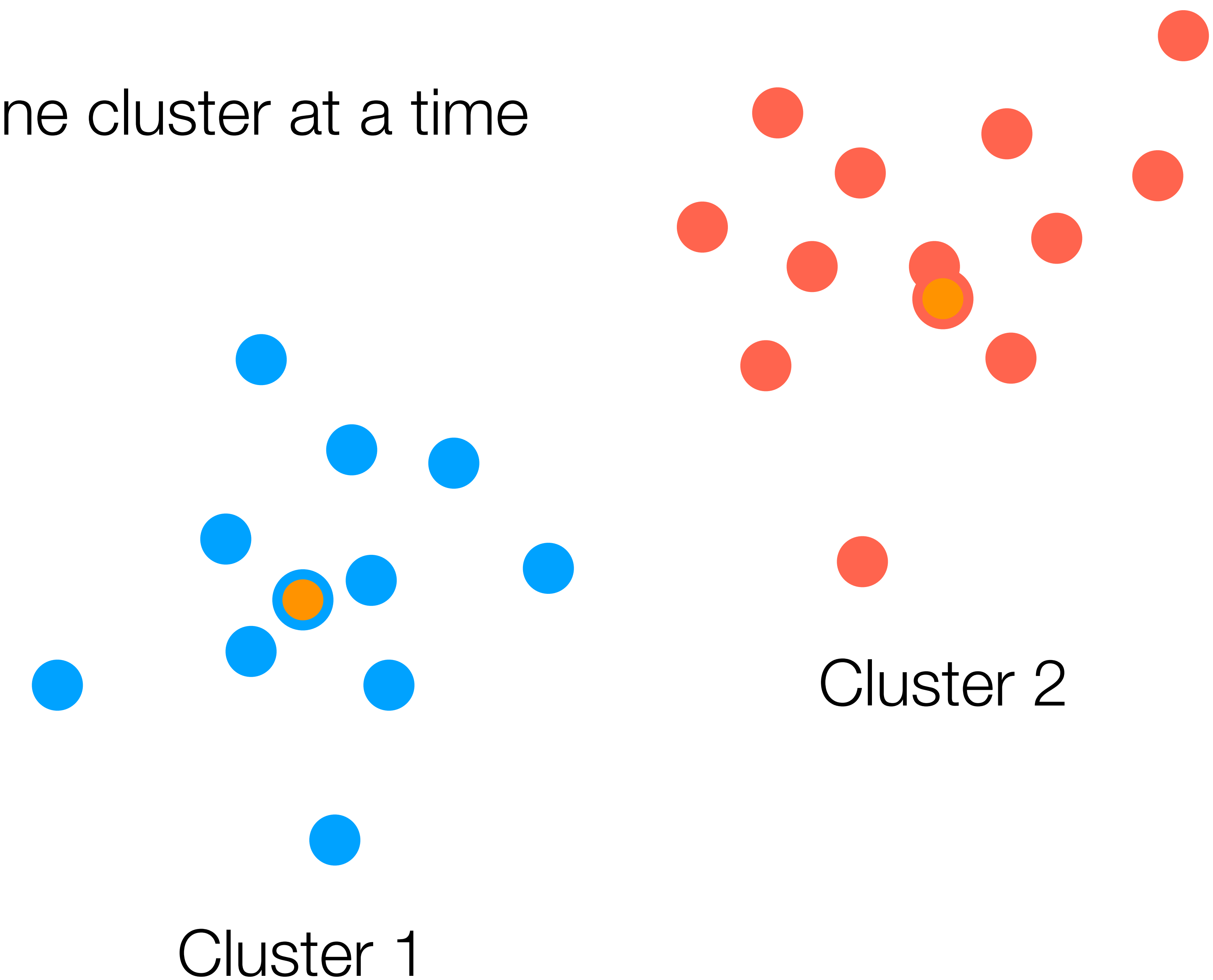
- Choose a cost function to compute for different *k*
  - In general, not easy! Need some intuition for what “good” clusters are
  - Ideally: cost function should relate to your application of interest
- Pick *k* achieving lowest cost

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

But hey it’s worth a shot

Residual Sum of Squares

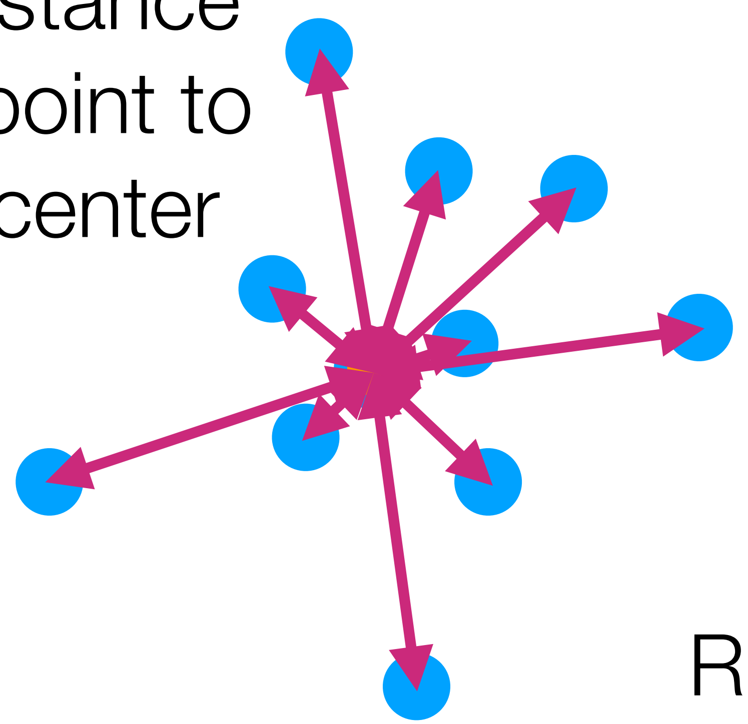
Look at one cluster at a time



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

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Measure distance
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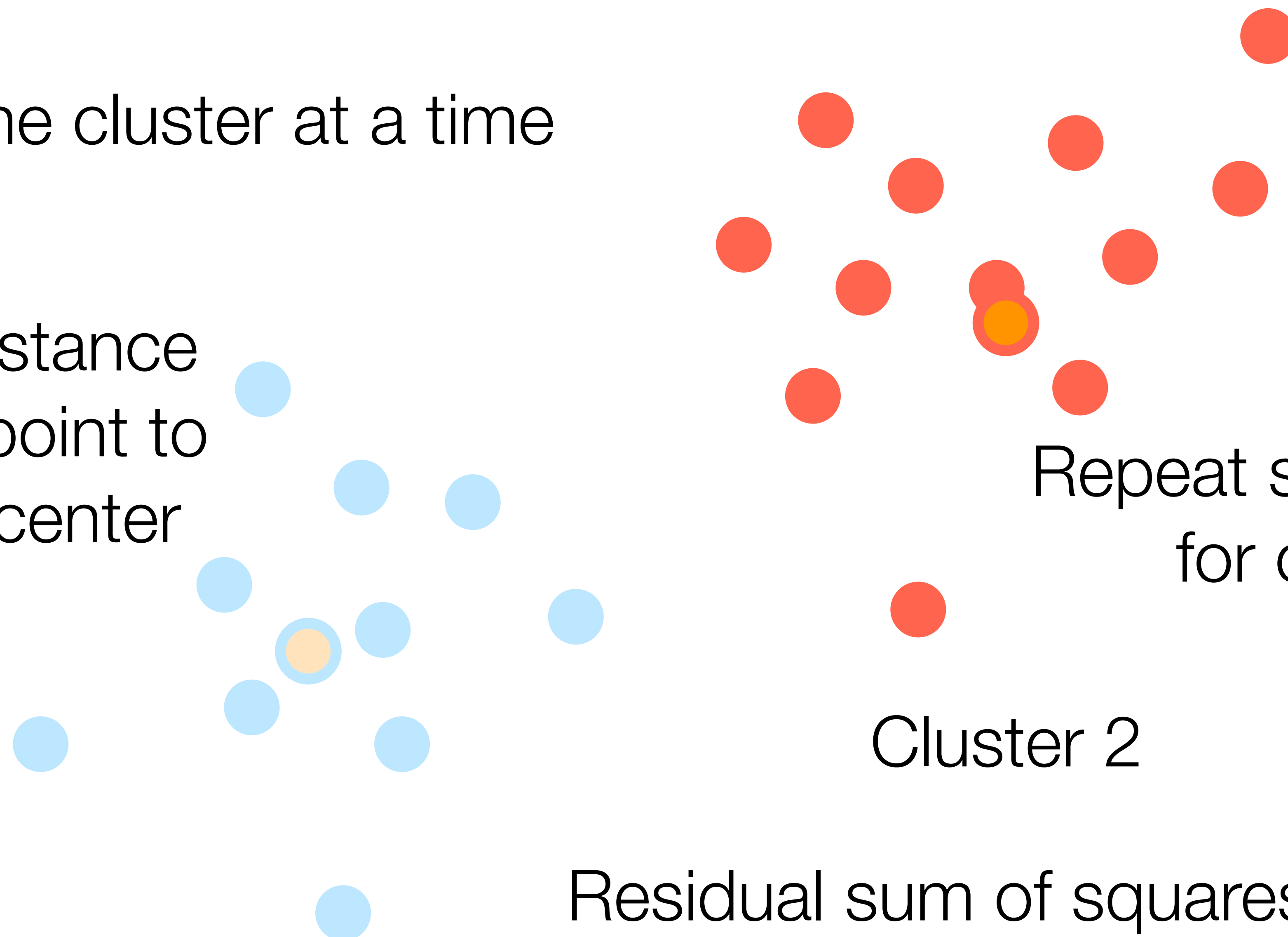

Repeat similar calculation
for other cluster

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

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

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 RSS not a good way to choose *k*?

What is RSS 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*

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

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)

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