Carnegie Mellon University
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Unstructured Data Analysis for Policy

Lecture 7: Clustering (cont'd)

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(Last time) Example: 1D GMM with *k* Clusters

Cluster 1

Probability of generating a point from cluster 1 = π_1

Gaussian mean = μ_1

Gaussian std dev = σ_1

…

Cluster ***k***

Probability of generating a point from cluster ***k*** = π_k

Gaussian mean = μ_k

Gaussian std dev = σ_k

How to generate 1D points from this GMM:

1. Flip biased ***k***-sided coin (the sides have probabilities $\pi_1, \dots, \pi_k$)
2. Let ***Z*** be the side that we got (it is some value 1, …, ***k***)
3. Sample 1 point from the Gaussian for cluster ***Z***

Example: 2D GMM with *k* Clusters

<u>Cluster 1</u> | <u>Cluster ***k***</u>

Probability of generating a point from cluster 1 $= \pi_1$

Gaussian mean $= \mu_1$

Gaussian covariance $= \Sigma_1$

$\cdots$

Probability of generating a point from cluster ***k*** $= \pi_k$

Gaussian mean $= \mu_k$ ← 2-dim.

Gaussian covariance $= \Sigma_k$ ← 2-by-2 matrices

How to generate 2D points from this GMM:

1. Flip biased ***k***-sided coin (the sides have probabilities $\pi_1, \dots, \pi_k$)
2. Let ***Z*** be the side that we got (it is some value 1, …, ***k***)
3. Sample 1 point from the Gaussian for cluster ***Z***

GMM with k Clusters

Cluster 1		Cluster **k**
Probability of generating a point from cluster 1 $= \pi_1$	…	Probability of generating a point from cluster **k** $= \pi_k$
Gaussian mean $= \mu_1$		Gaussian mean $= \mu_k$ ← d-dim.
Gaussian covariance $= \Sigma_1$		Gaussian covariance $= \Sigma_k$

↖ d-by-d matrices

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, …, **k**)
3. Sample 1 point from the Gaussian for cluster ***Z***

High-Level Idea of GMM

- Generative model that gives a *hypothesized* way in which data points are generated

<u>In reality, data are unlikely generated the same way!</u>

<u>In reality, data points might not even be independent!</u>

“All models are wrong, but some are useful.”

–George Box

High-Level Idea of GMM

- Generative model that gives a *hypothesized* way in which data points are generated

In reality, data are unlikely generated the same way!

In reality, data points might not even be independent!

- Learning ("fitting") the parameters of a GMM
  - Input: ***d***-dimensional data points, your guess for ***k***
  - Output: $\pi_1, \ldots, \pi_k, \mu_1, \ldots, \mu_k, \Sigma_1, \ldots, \Sigma_k$
- *After* learning a GMM:
  - For *any* ***d***-dimensional data point, can figure out probability of it belonging to each of the clusters

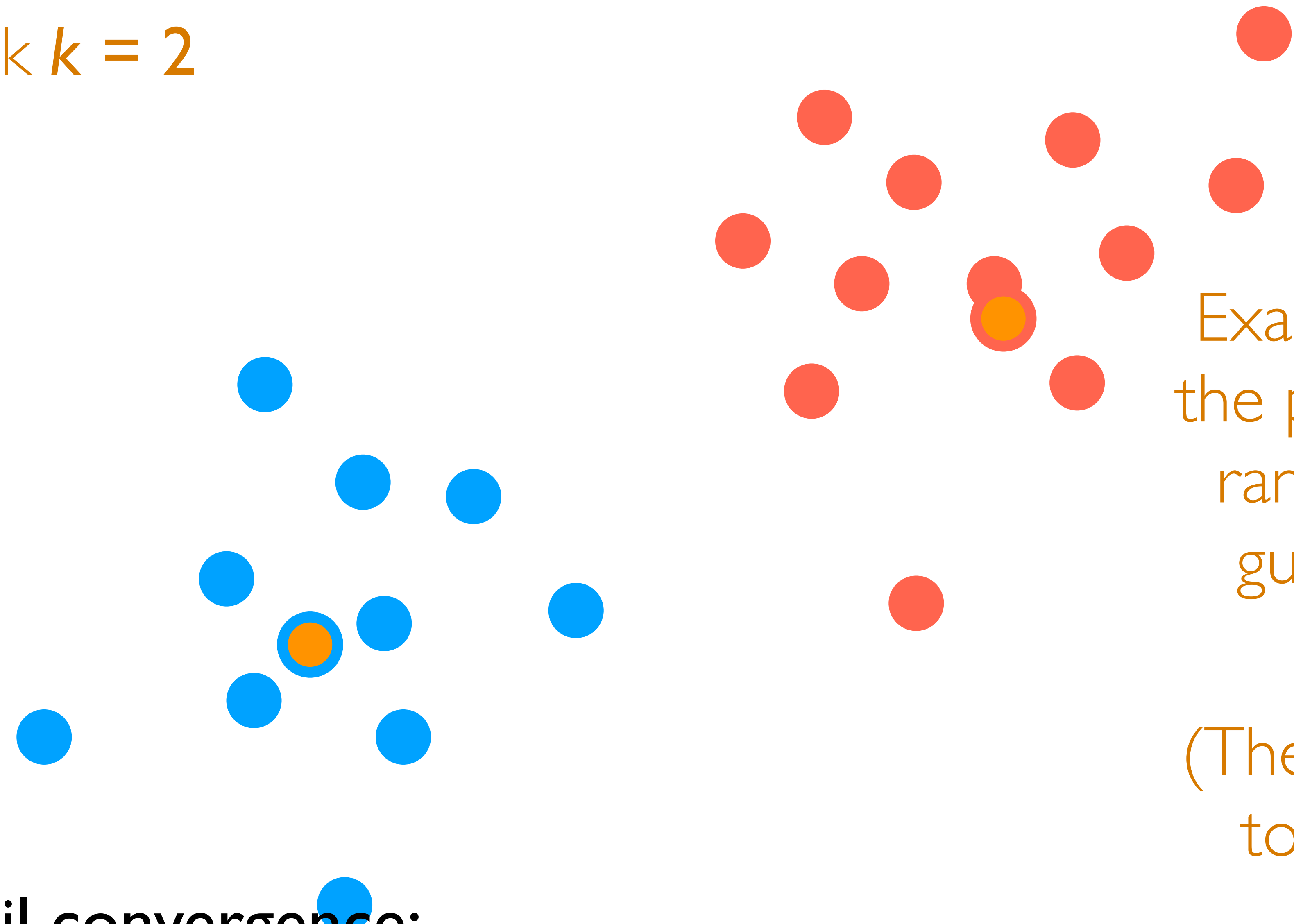
How do you turn this into a cluster assignment?

k-means

Step 0: Pick ***k***

We'll pick ***k* = 2**

Step 1: Pick <u>guesses</u> for where cluster centers are



Example: choose ***k*** of the points uniformly at random to be initial guesses for cluster centers

(There are many ways to make the initial guesses)

Repeat until convergence:

Step 2: Assign each point to belong to the closest cluster

Step 3: Update cluster means (to be the center of mass per cluster)

k-means

Step 0: Pick ***k***

Step 1: Pick <u>guesses</u> for where cluster centers are

Repeat until convergence:

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(Rough Intuition) Learning a GMM

Step 0: Pick ***k***

Step 1: Pick guesses for **cluster probabilities, means, and covariances**

(often done using ***k***-means)

Repeat until convergence:

Step 2: Compute probability of each point being in each of the ***k*** clusters

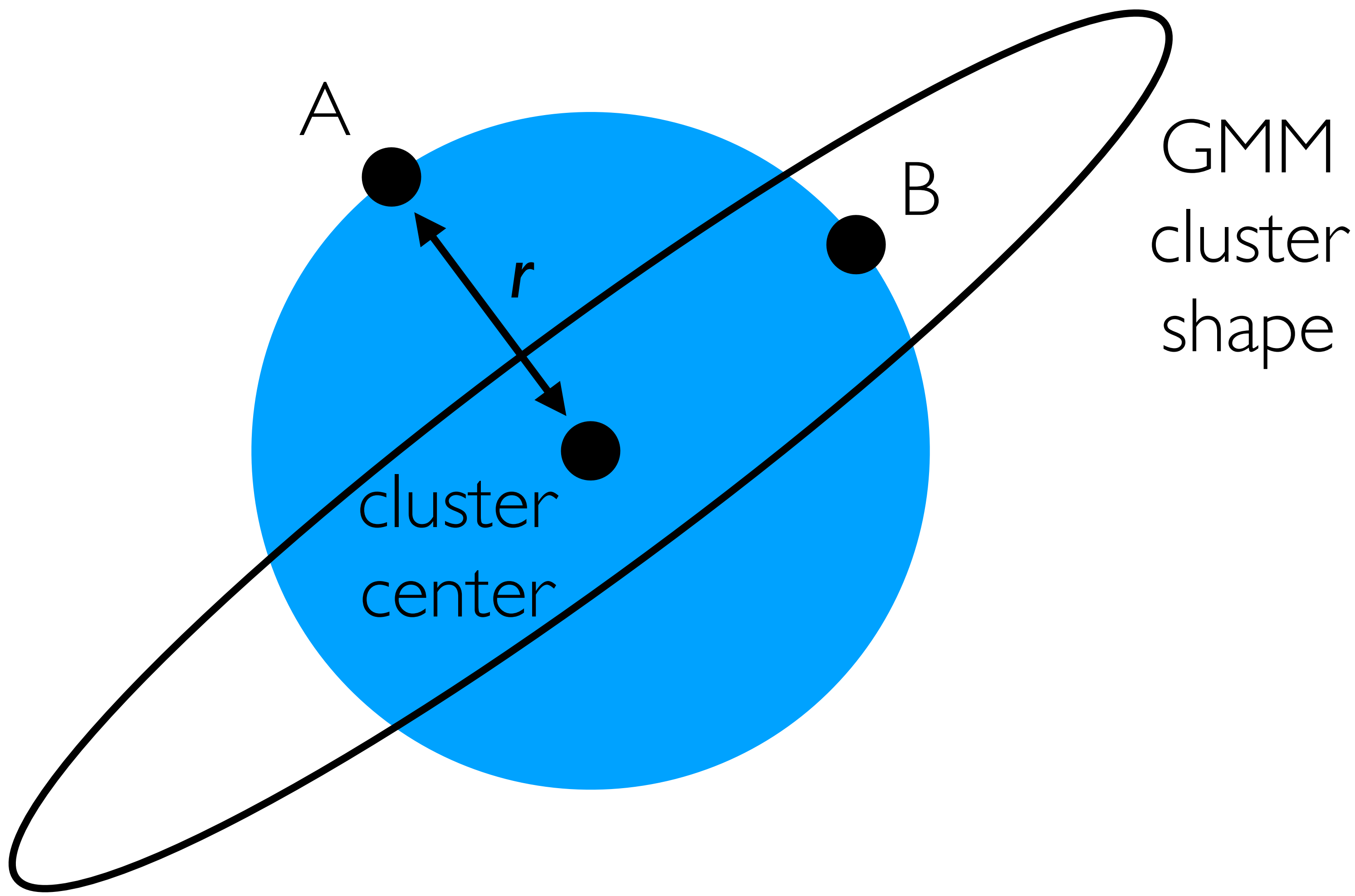
Step 3: Update **cluster probabilities, means, and covariances** accounting for probabilities of each point belonging to each of the clusters

This algorithm is called the **Expectation-Maximization (EM)** algorithm for GMM's (and approximately does maximum likelihood)

(Note: EM by itself is a general algorithm not just for GMM's)

(Rough Intuition) How Shape is Encoded by a GMM

For this ellipse-shaped Gaussian, point B is considered more similar to the cluster center than point A



k-means would think that point A and point B are equally similar to the cluster center (since both points are distance ***r*** away from the center)

Relating *k*-means to GMM's

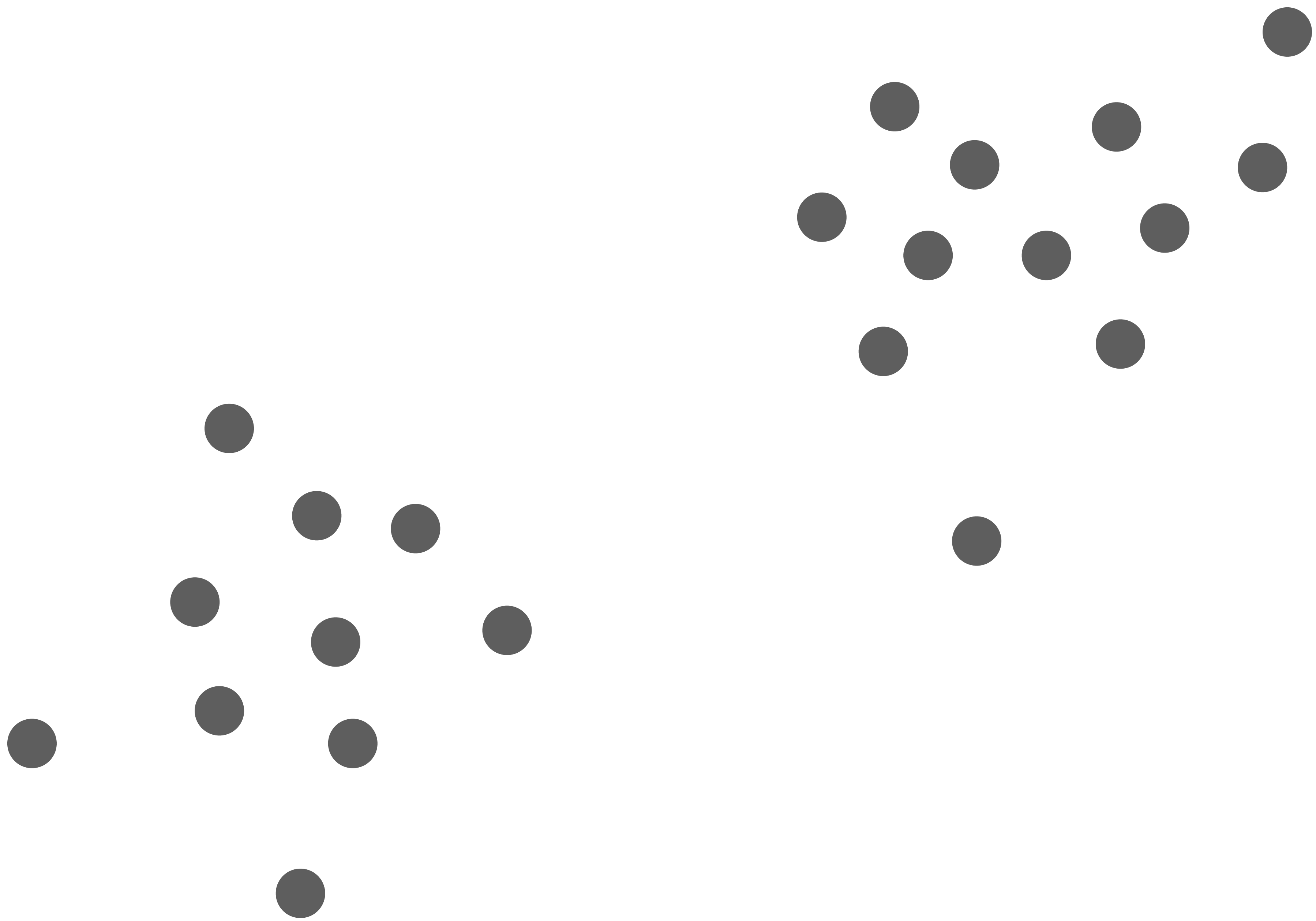
If the ellipses are all circles and have the same "skinniness" (e.g., in the 1D case it means they all have same std dev):

- ***k***-means approximates the EM algorithm for GMM's (as there is no need to keep track of cluster shape)

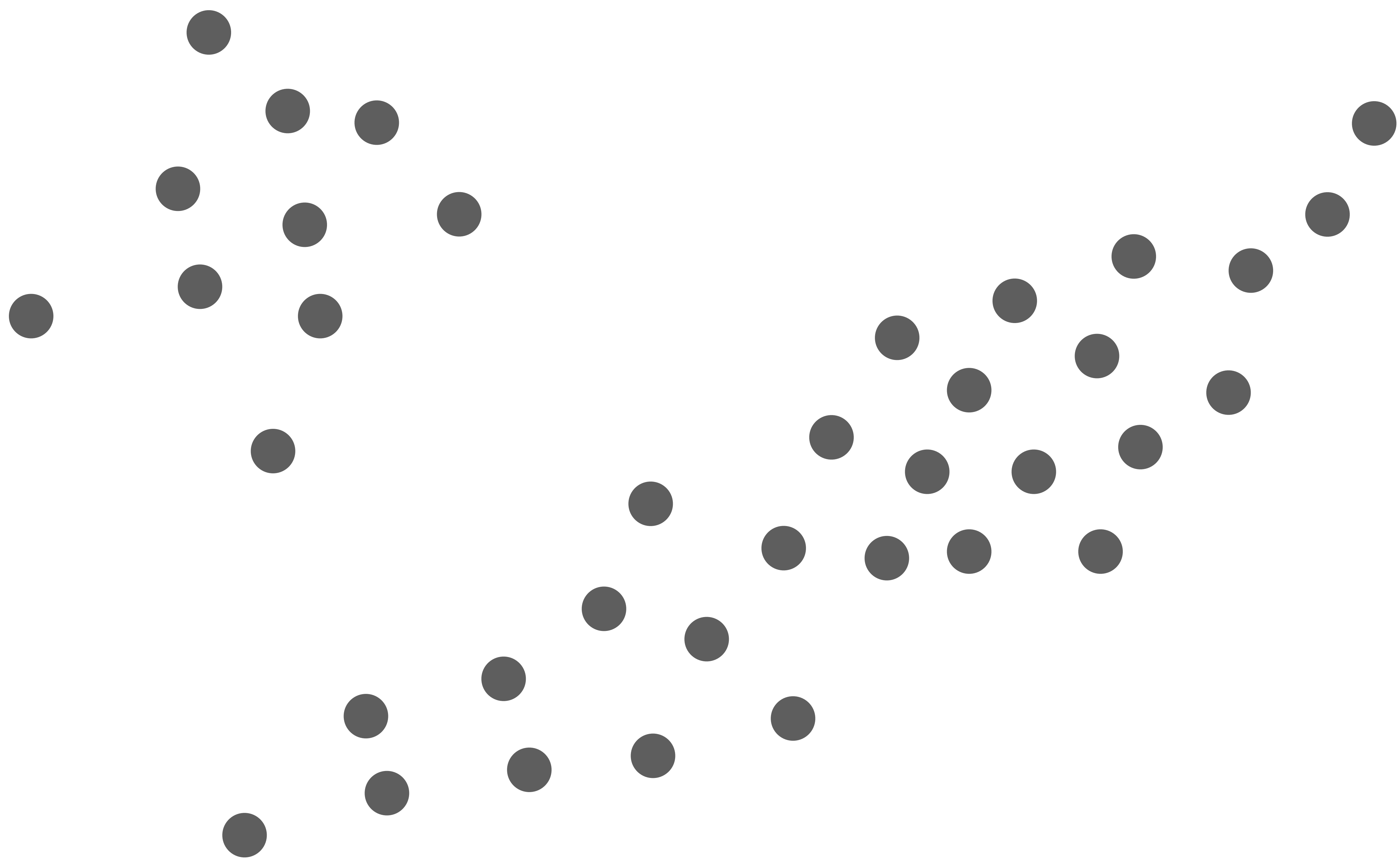
- ***k***-means does a "hard" assignment of each point to a cluster, whereas the EM algorithm does a "soft" (probabilistic) assignment

Interpretation: *When the data appear as if they're from a GMM with true clusters that "look like circles of equal size", then* ***k****-means should work well*

k-means should do well on this



But not on this



Relating *k*-means to GMM's

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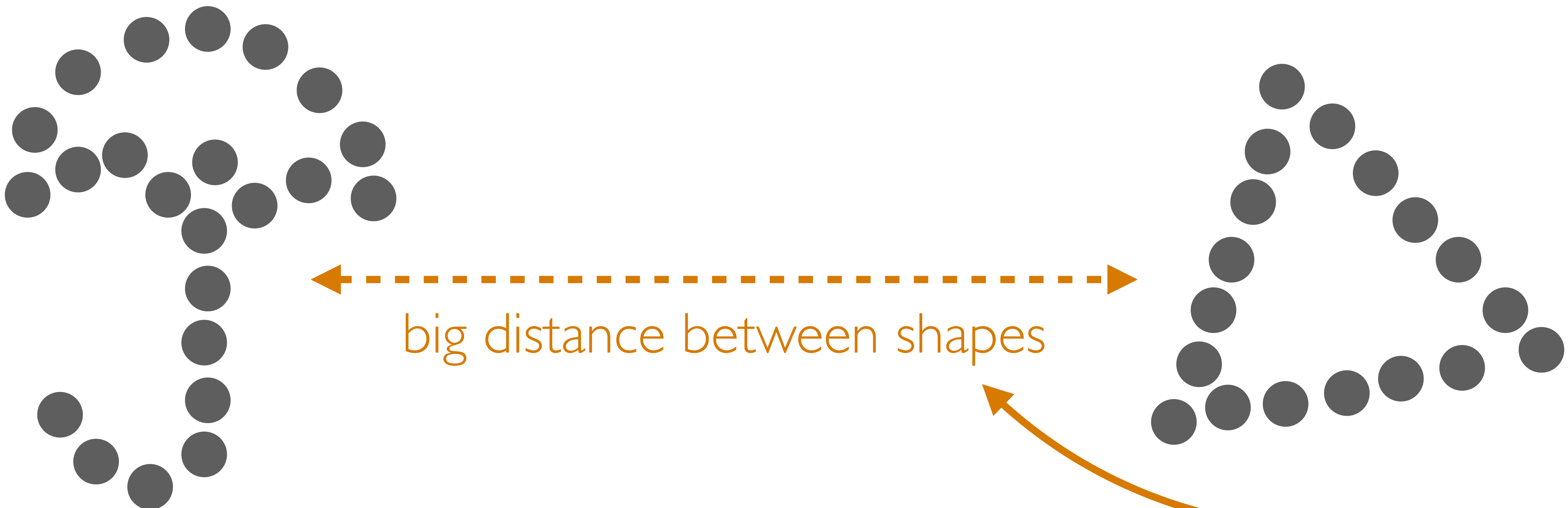
Interpretation: *When the data appear as if they're from a GMM with true clusters that "look like circles of equal size", then* ***k****-means should work well*

This is *not* the only scenario in which ***k***-means should work well

Even if data aren't generated from a GMM, *k*-means and GMM's can still cluster correctly

This dataset obviously doesn't look generated by a GMM



k-means with ***k*** = 2, and 2-component GMM will both work well in identifying the two shapes as separate clusters

Key idea: the clusters are very ***well-separated***
(so that *many* clustering algorithms will work well in this case!)

k-means & GMMs, Sketch of Interpretation

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

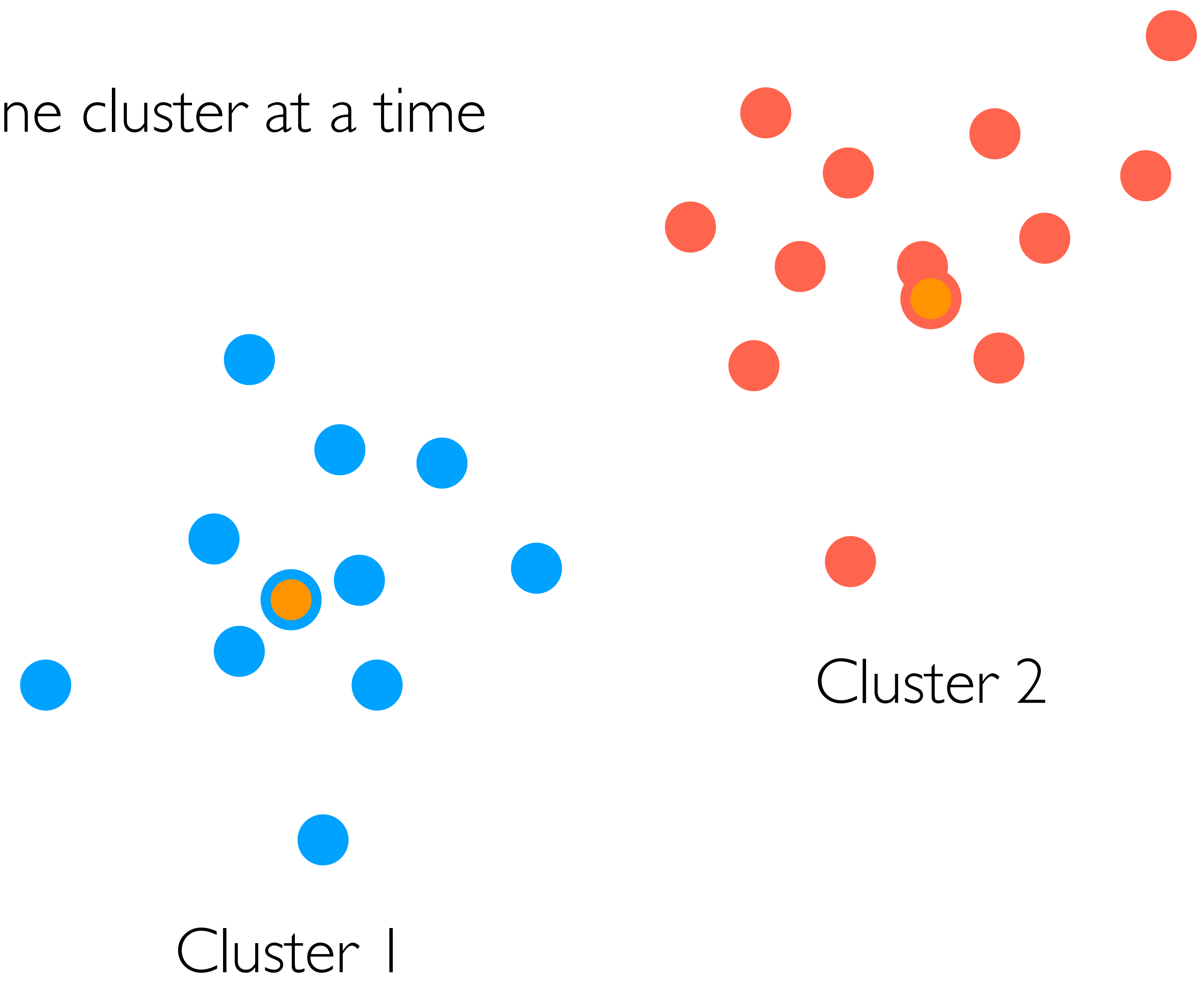
No single way of choosing ***k*** is the "best" way

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



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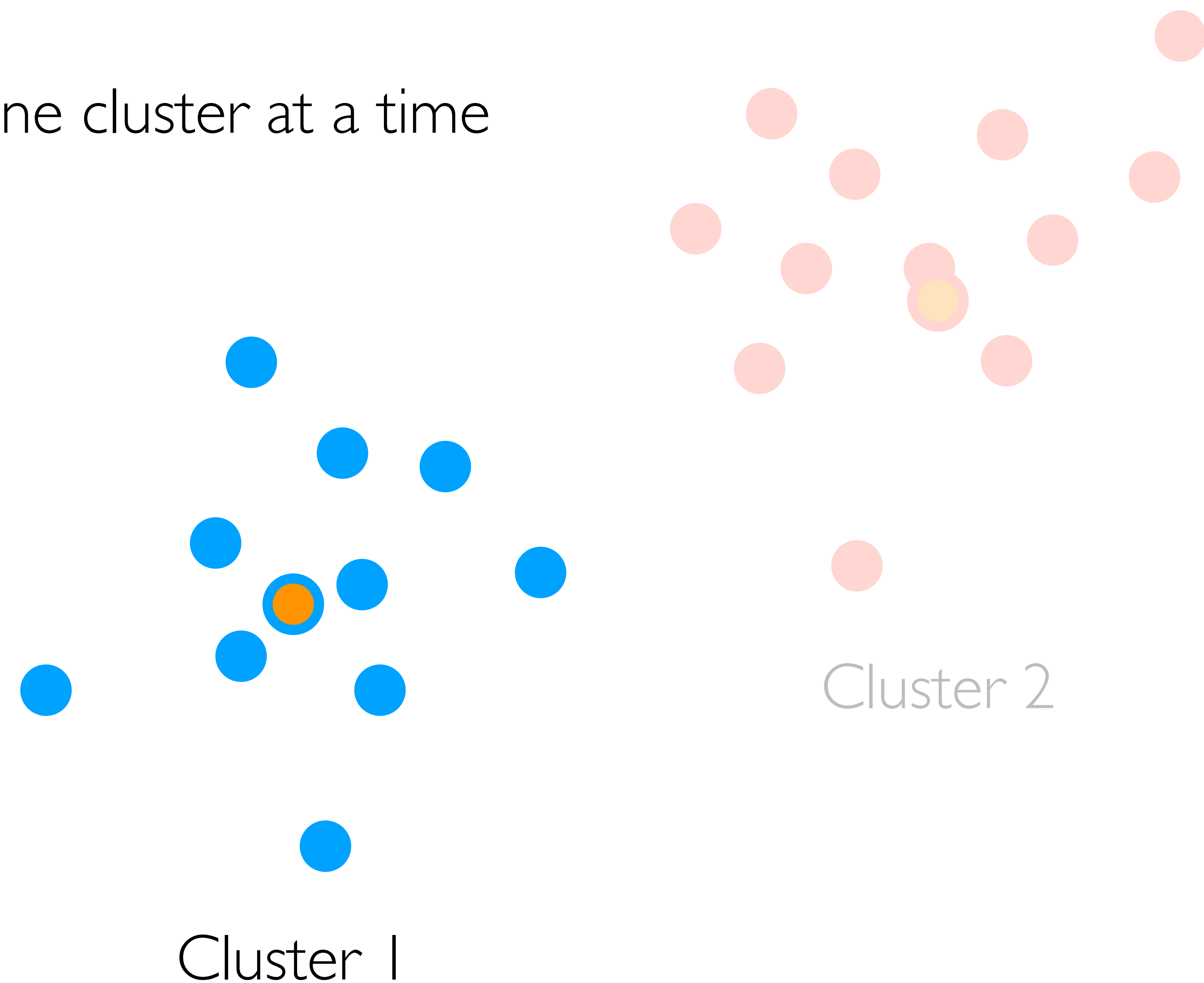

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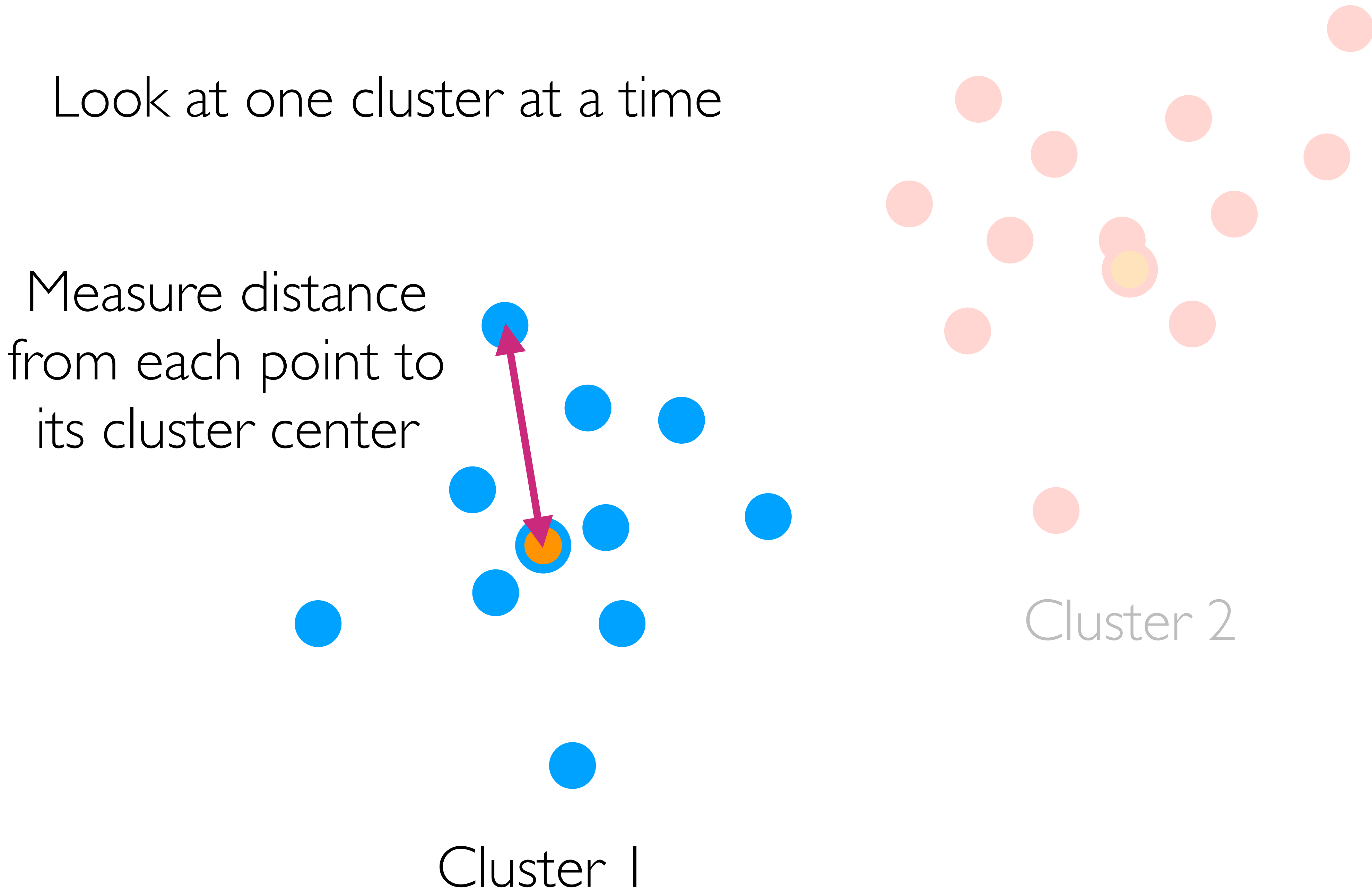
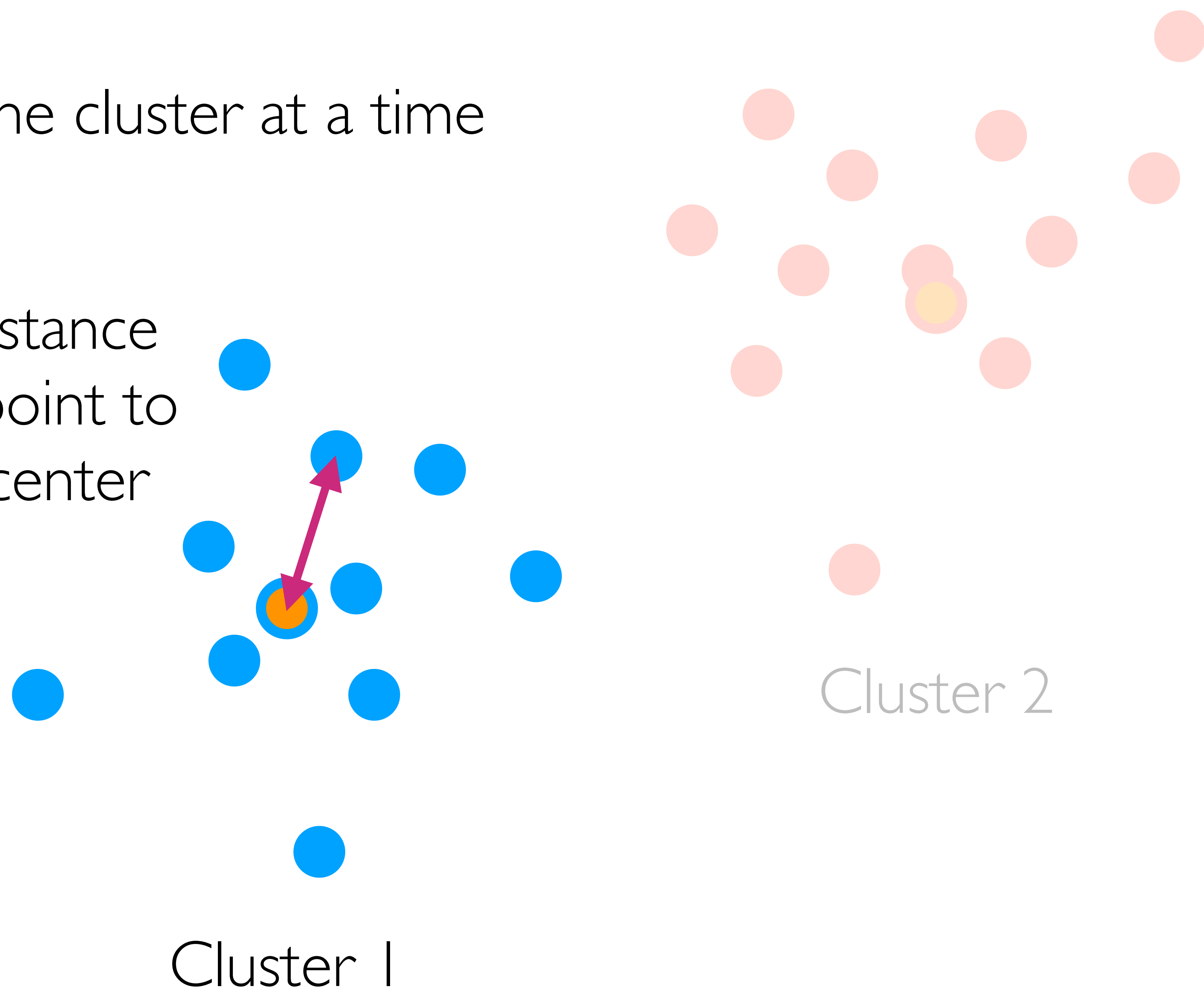


Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



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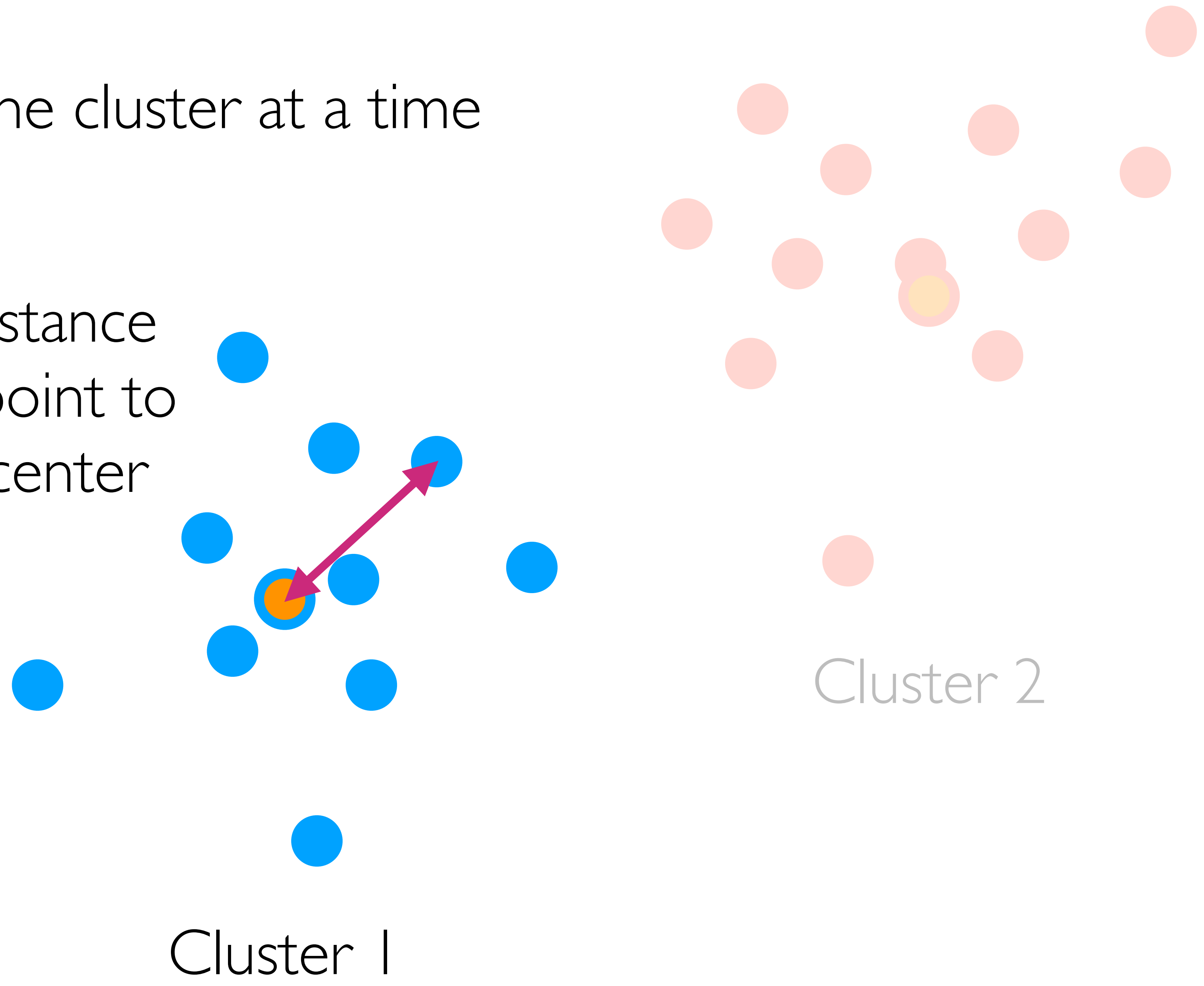

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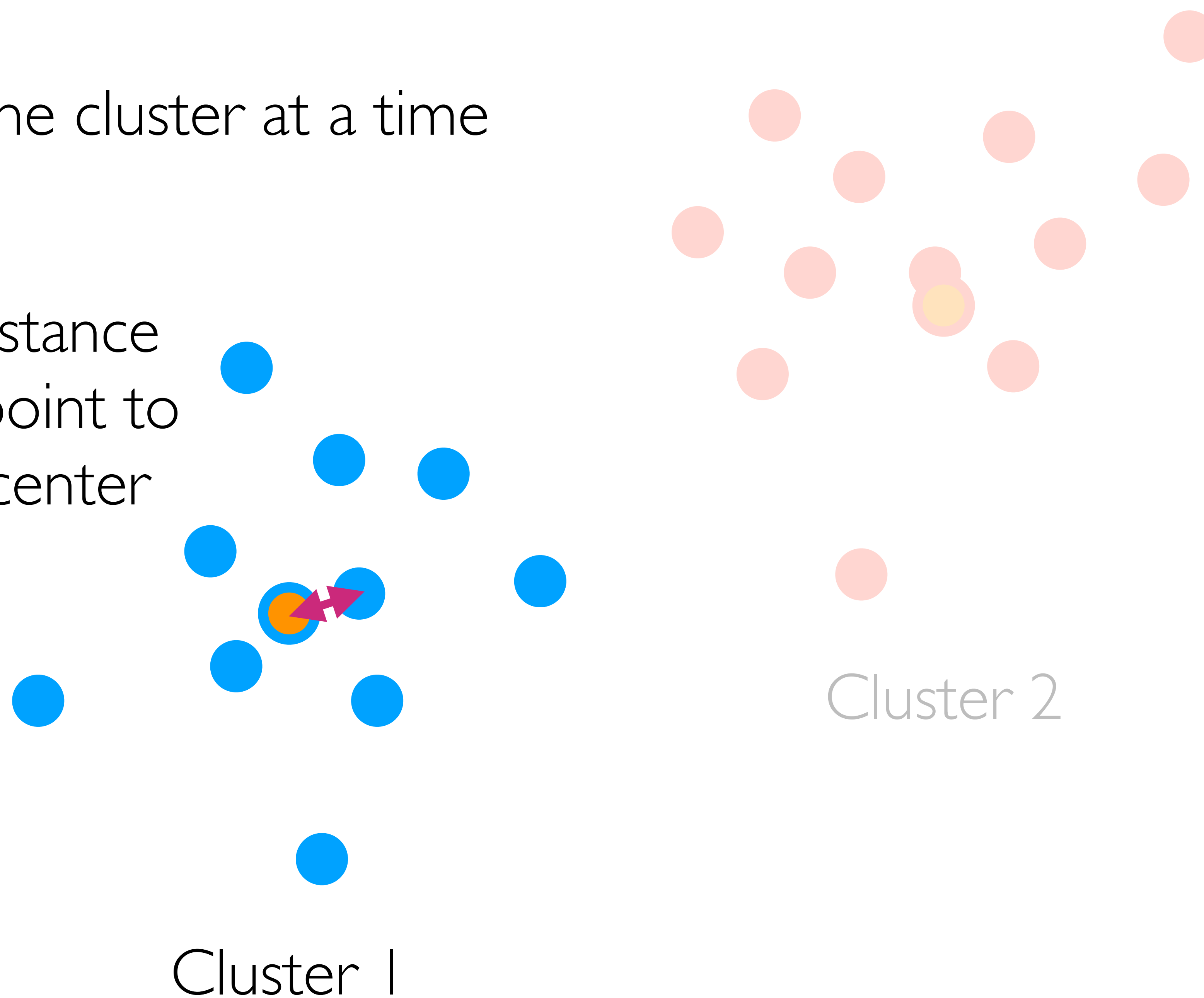

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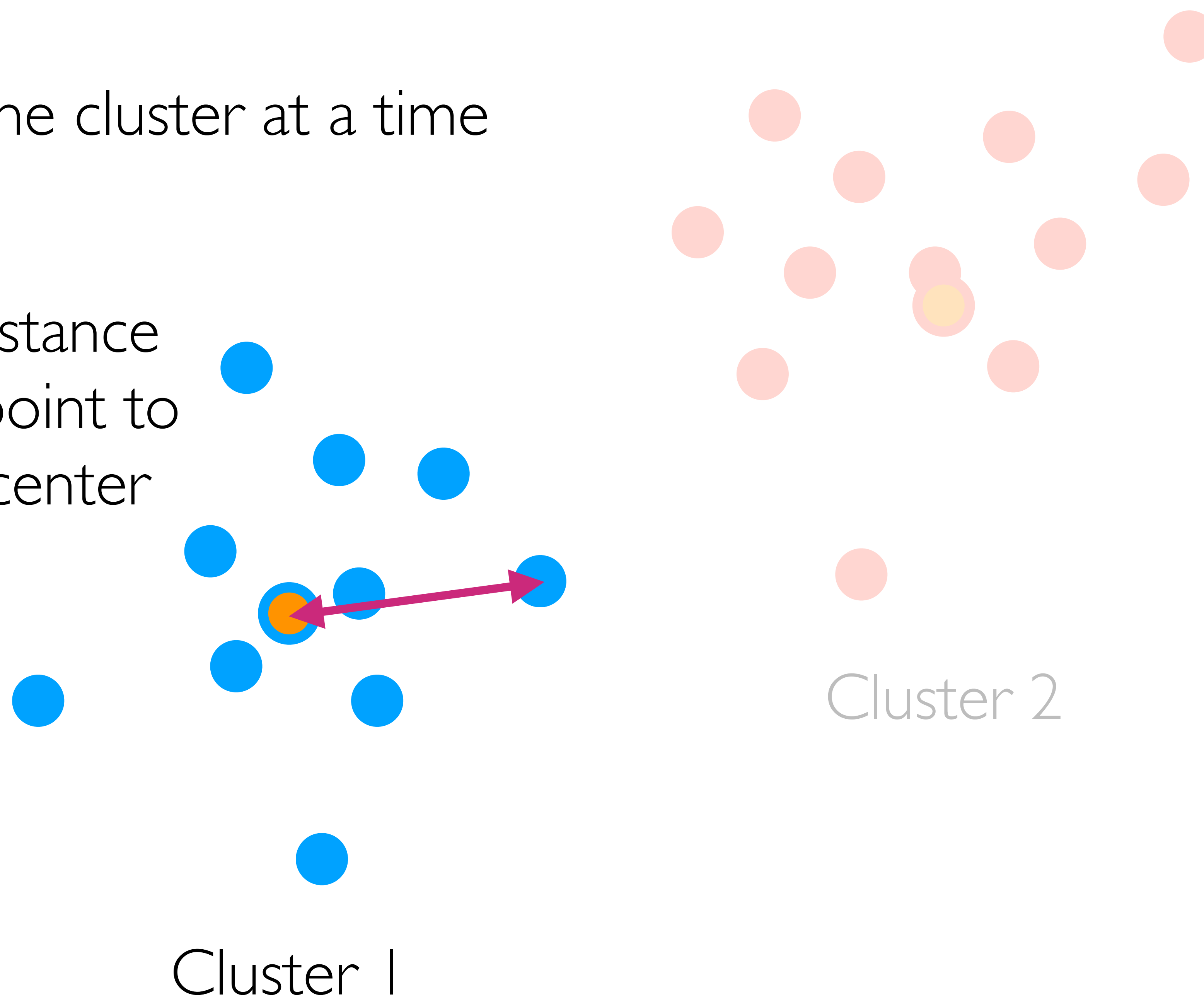

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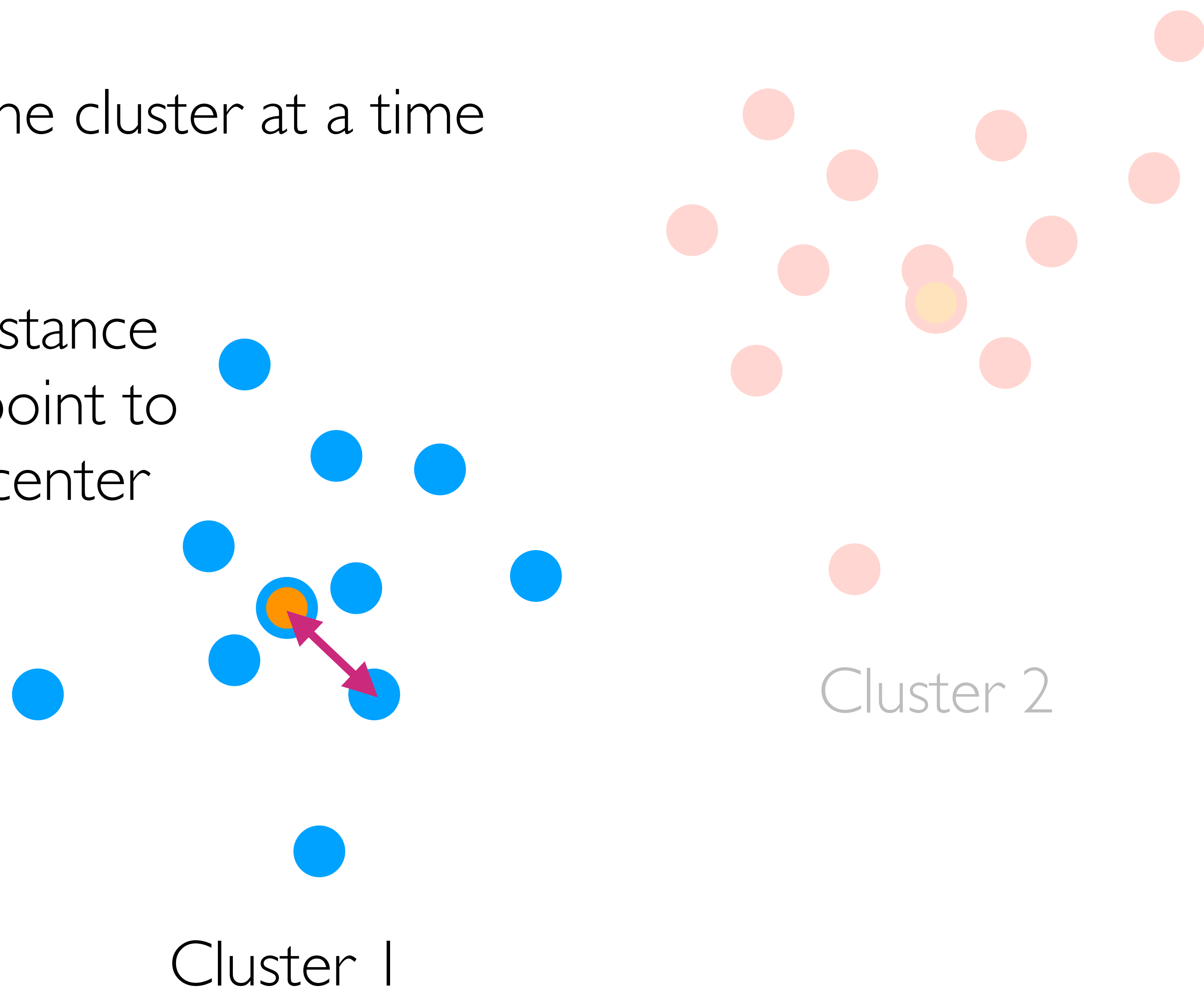

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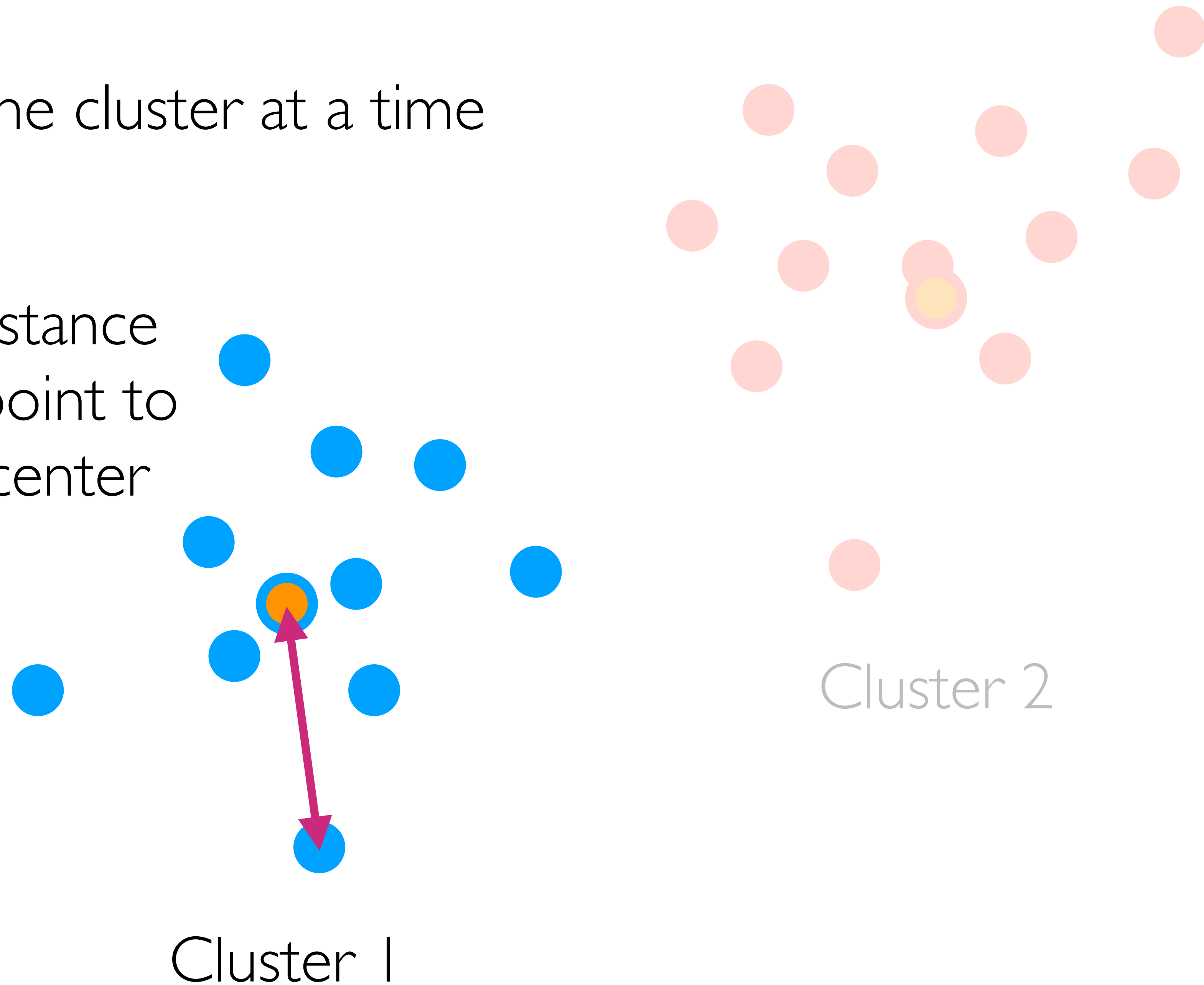

Residual Sum of Squares

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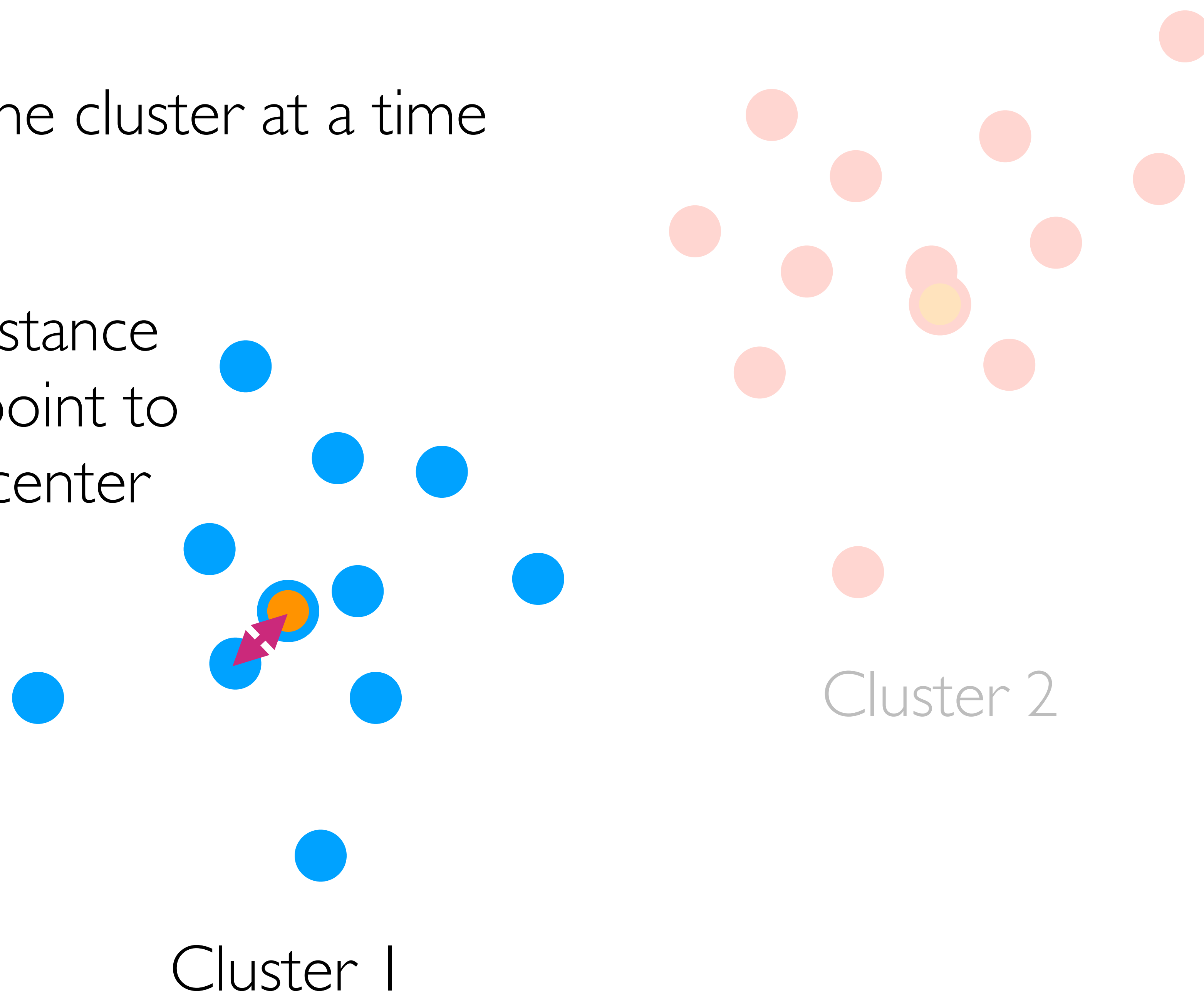

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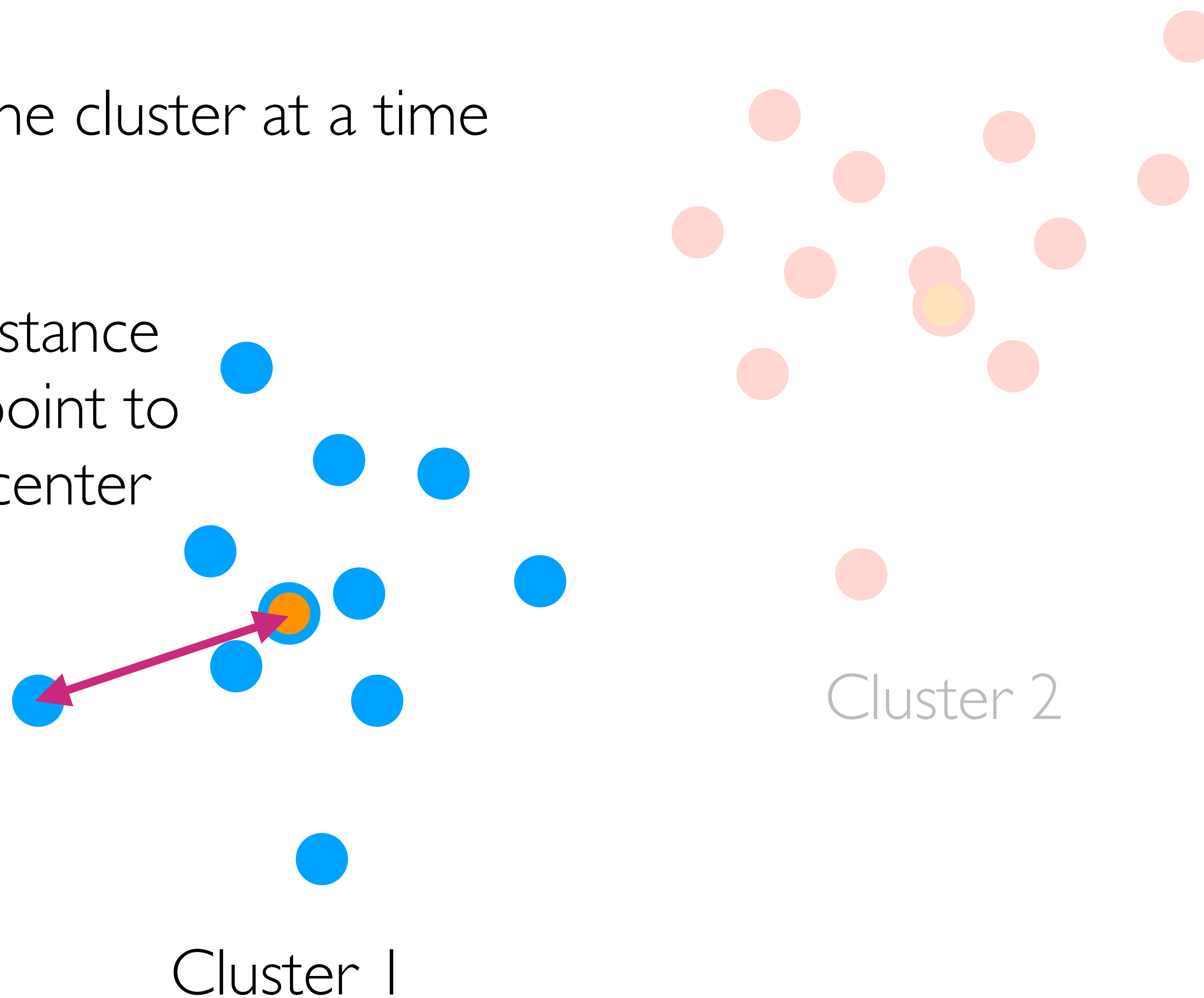

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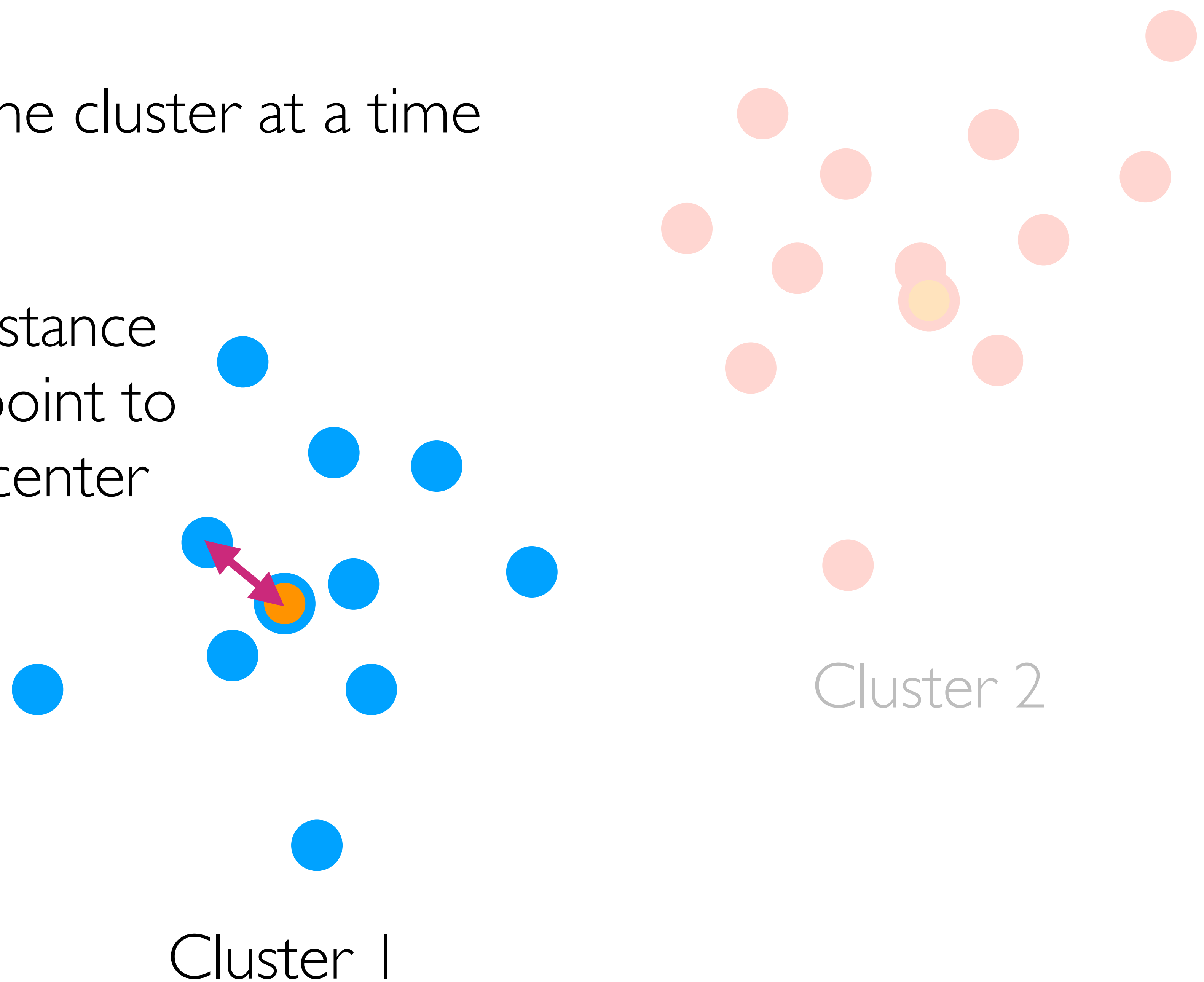

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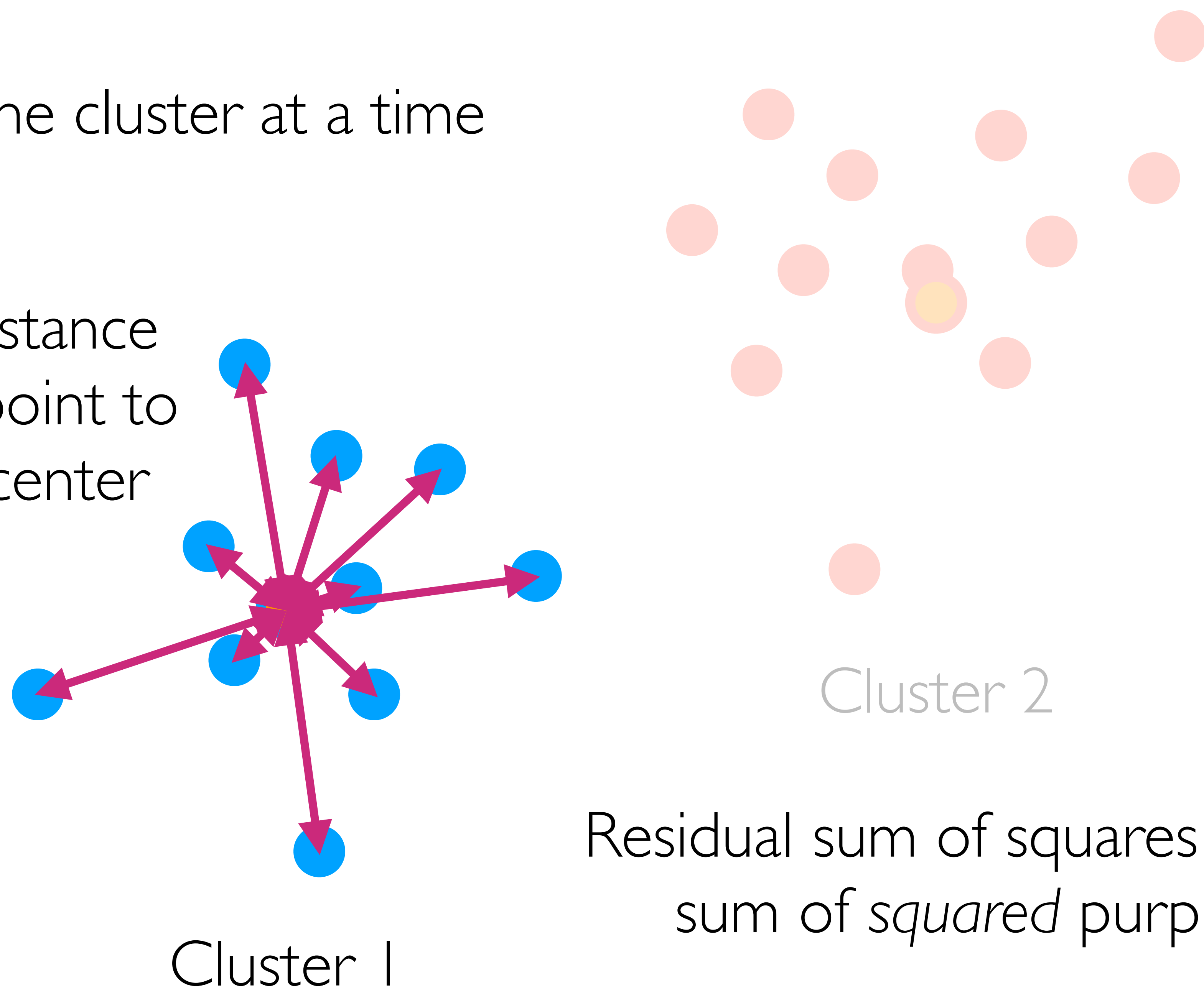
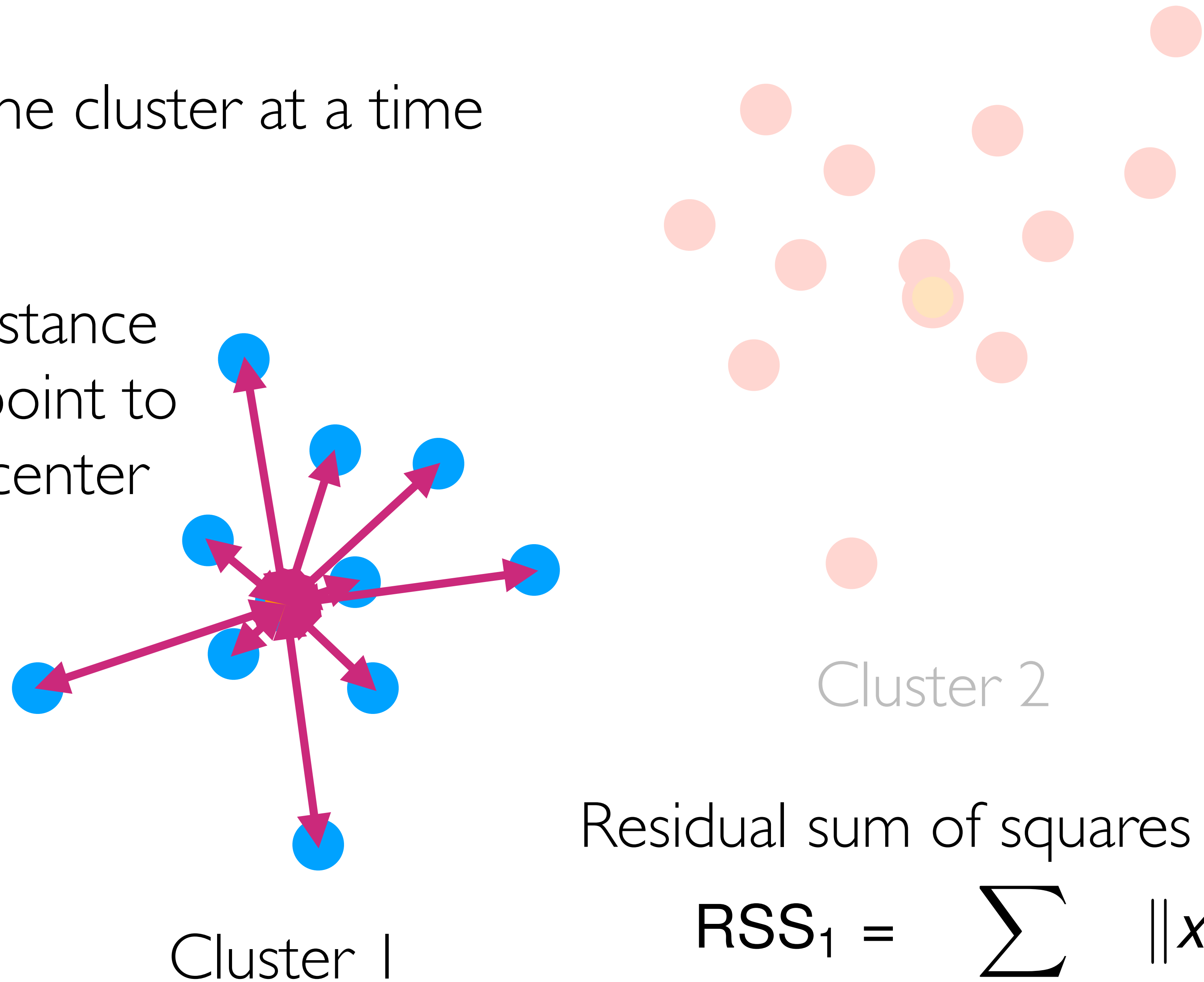


Residual sum of squares for cluster 1: sum of *squared* purple lengths

Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



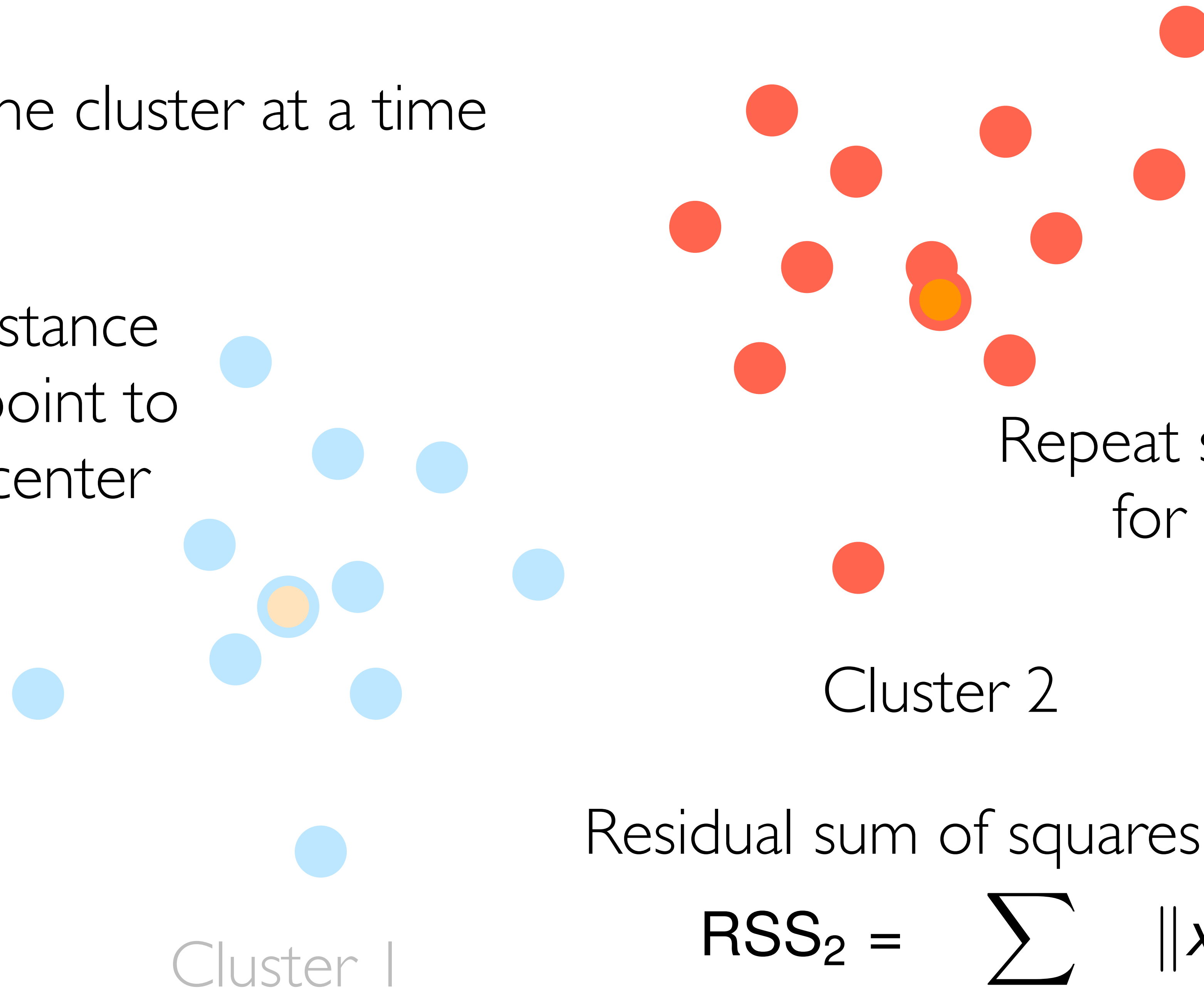
Residual sum of squares for cluster 1:

$$RSS_1 = \sum_{x \in \text{cluster } 1} \|x - \mu_1\|^2$$

Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



Repeat similar calculation for other cluster

Residual sum of squares for cluster 2:

$$RSS_2 = \sum_{x \in \text{cluster 2}} \|x - \mu_2\|^2$$

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*

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

mean of *all* points

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

A good score function to use for choosing $\boldsymbol{k}$:

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

$\boldsymbol{n}$ = total # points

Pick $\boldsymbol{k}$ with highest **CH(*k*)**

(Choose $\boldsymbol{k}$ among 2, 3, … up to pre-specified max)

Automatically Choosing *k*

Demo