Carnegie Mellon University
Heinz College

# 94-775 Lecture 7: Interpreting Clusters, Gaussian Mixture Models, Automatically Choosing *k*

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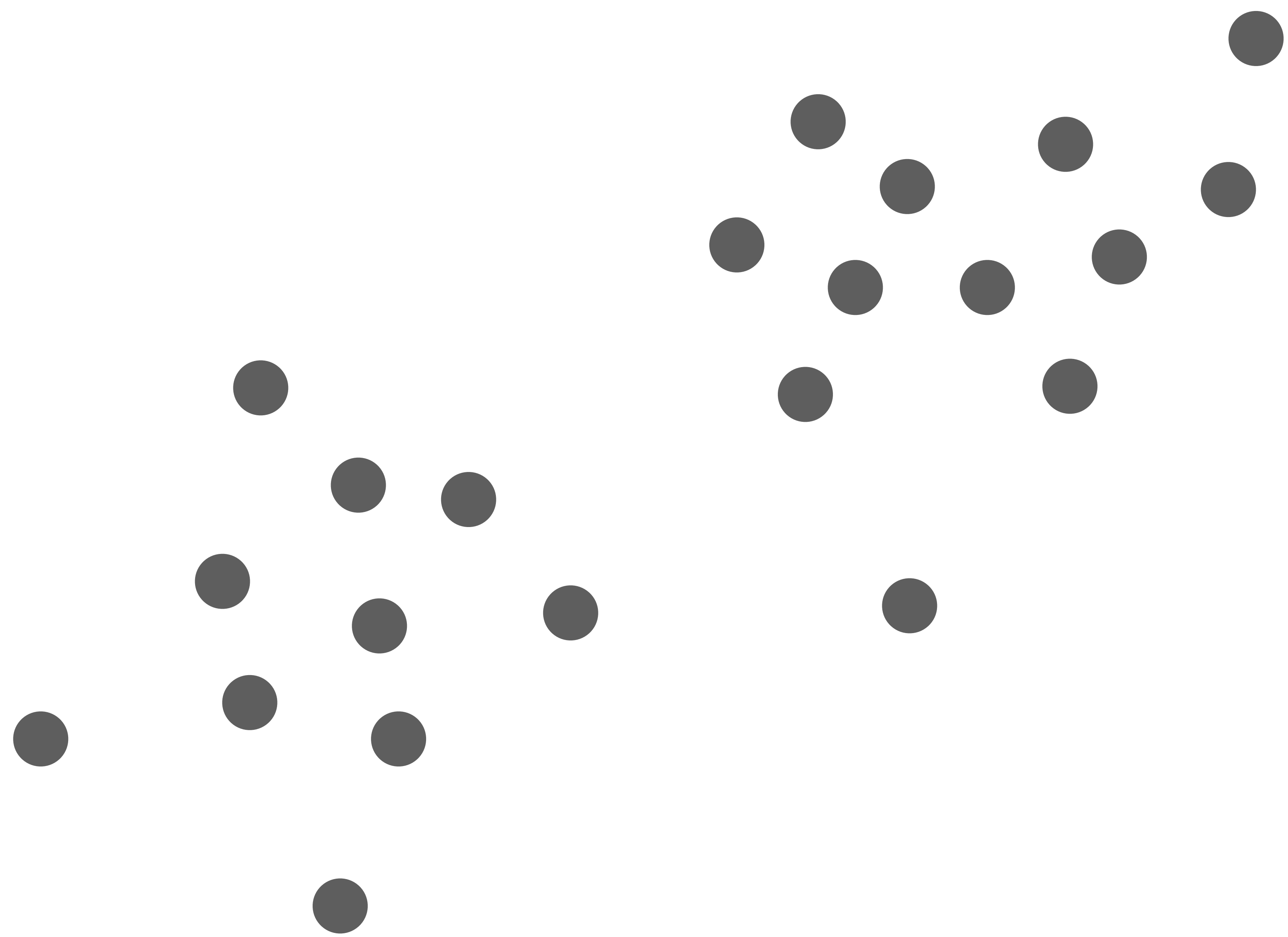
# A Sketch of How to Interpret Clusters

Demo

# Gaussian Mixture Model (GMM)



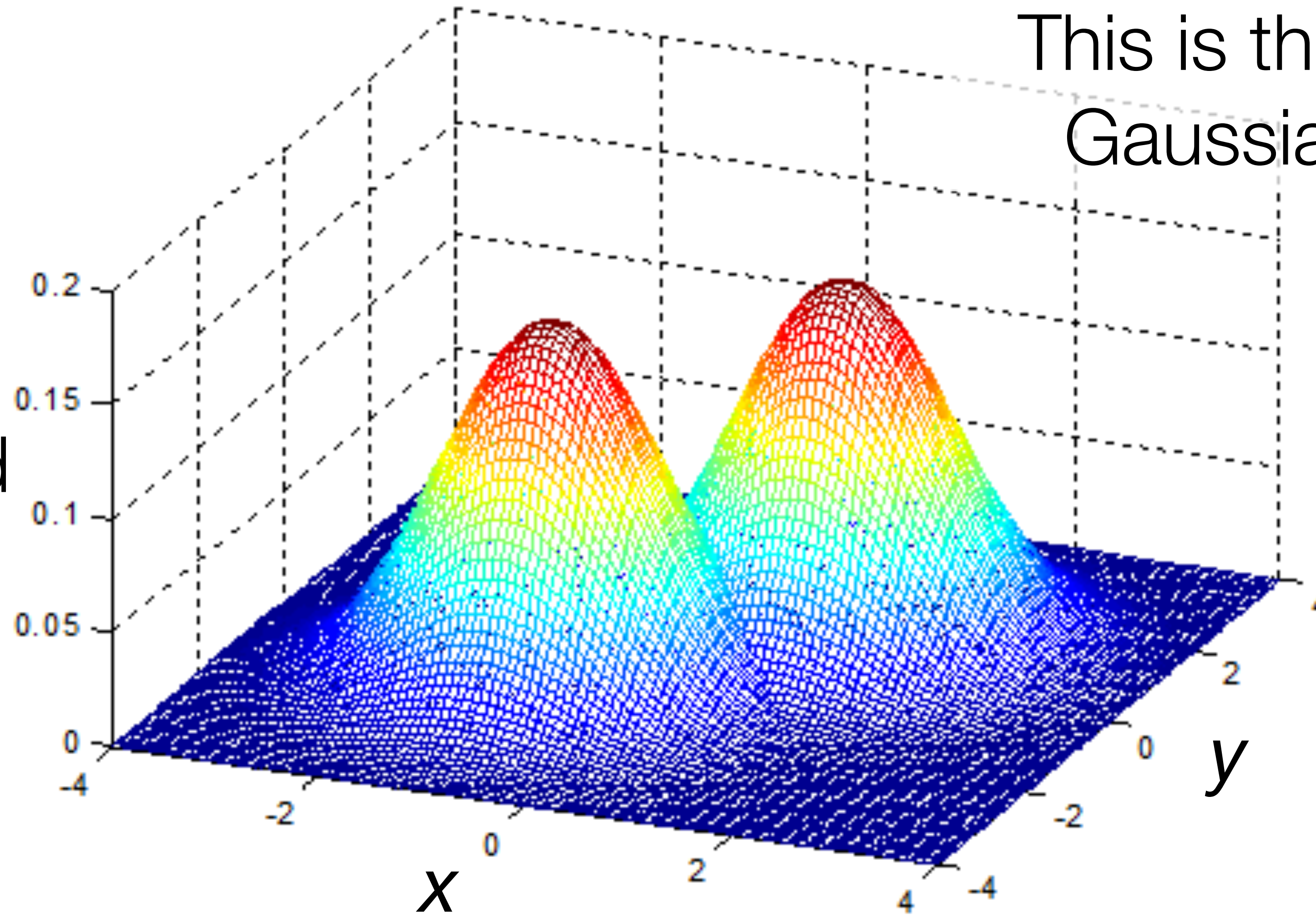
GMM: assume these points generated in a particular way

# Gaussian Mixture Model (GMM)

Assume: points sampled independently from a probability distribution

This is the sum of two 2D Gaussian distributions!

how probable point generated at ($x$, $y$) is



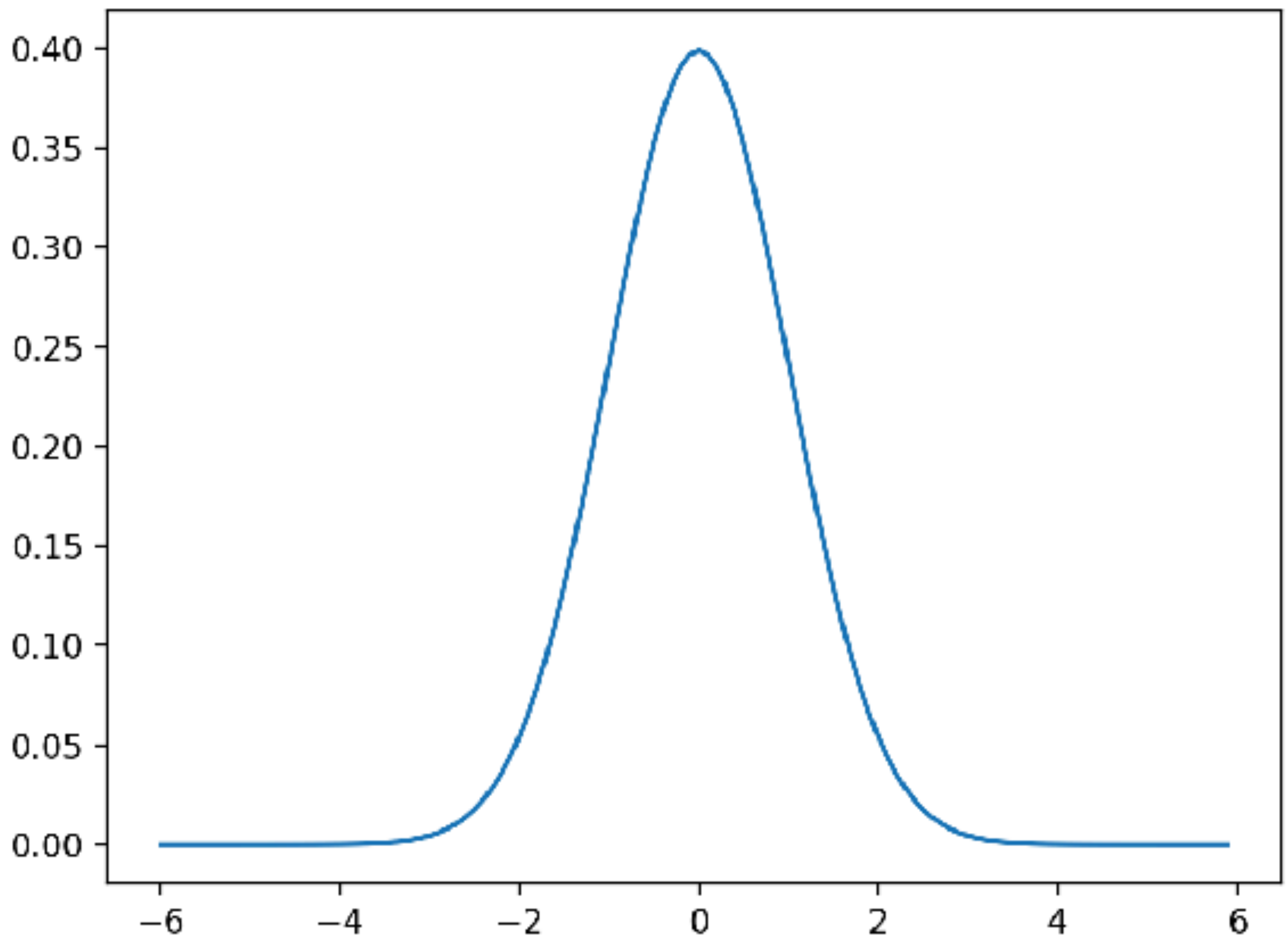

Red = more likely

Blue = less likely

Example of a 2D probability distribution

Image source: https://www.intechopen.com/source/html/17742/media/image25.png

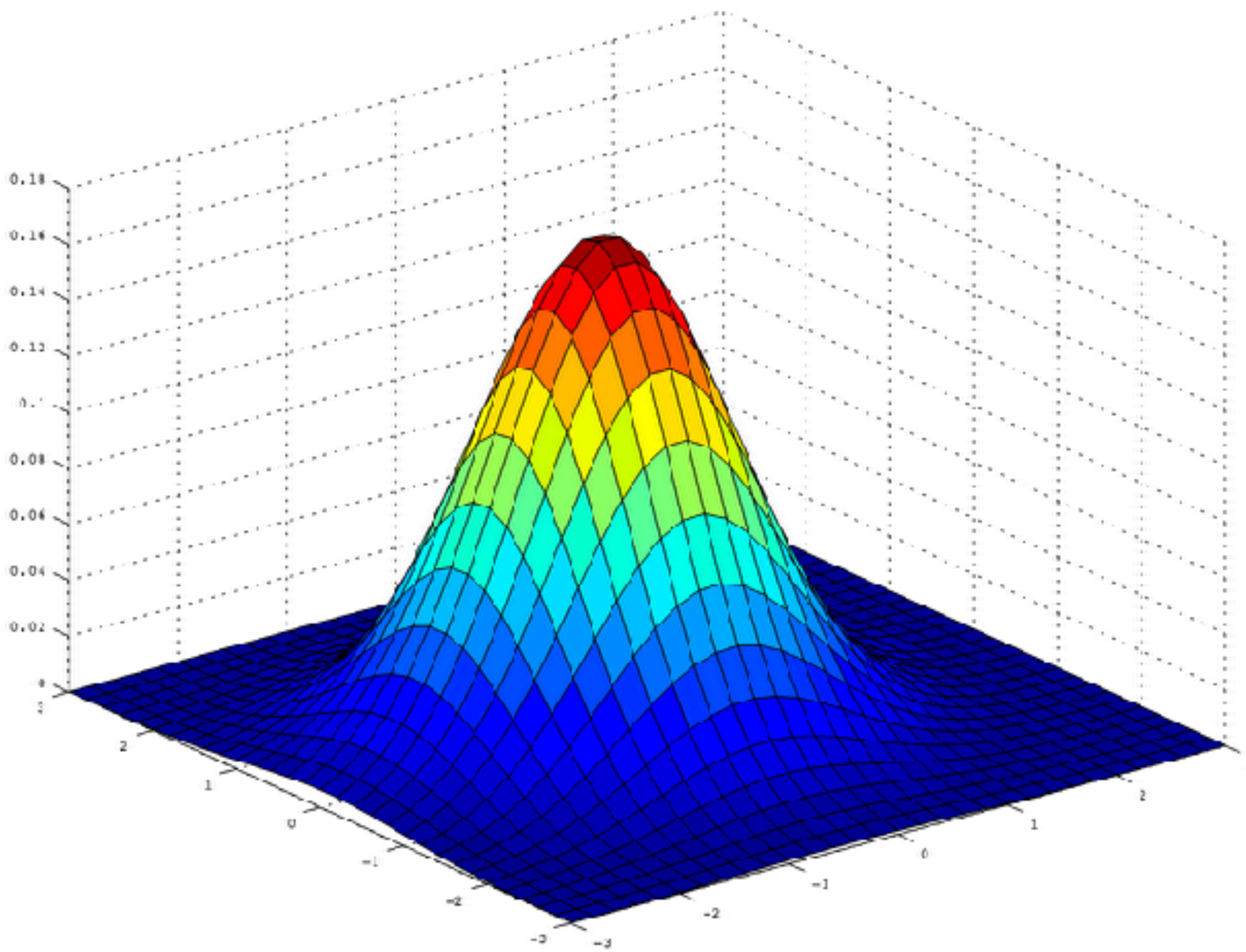
# Quick Reminder: 1D Gaussian




This is a 1D Gaussian distribution

Image source: https://matthew-brett.github.io/teaching//smoothing_intro-3.hires.png

# 2D Gaussian




This is a 2D Gaussian distribution

Image source: https://i.stack.imgur.com/OIWce.png

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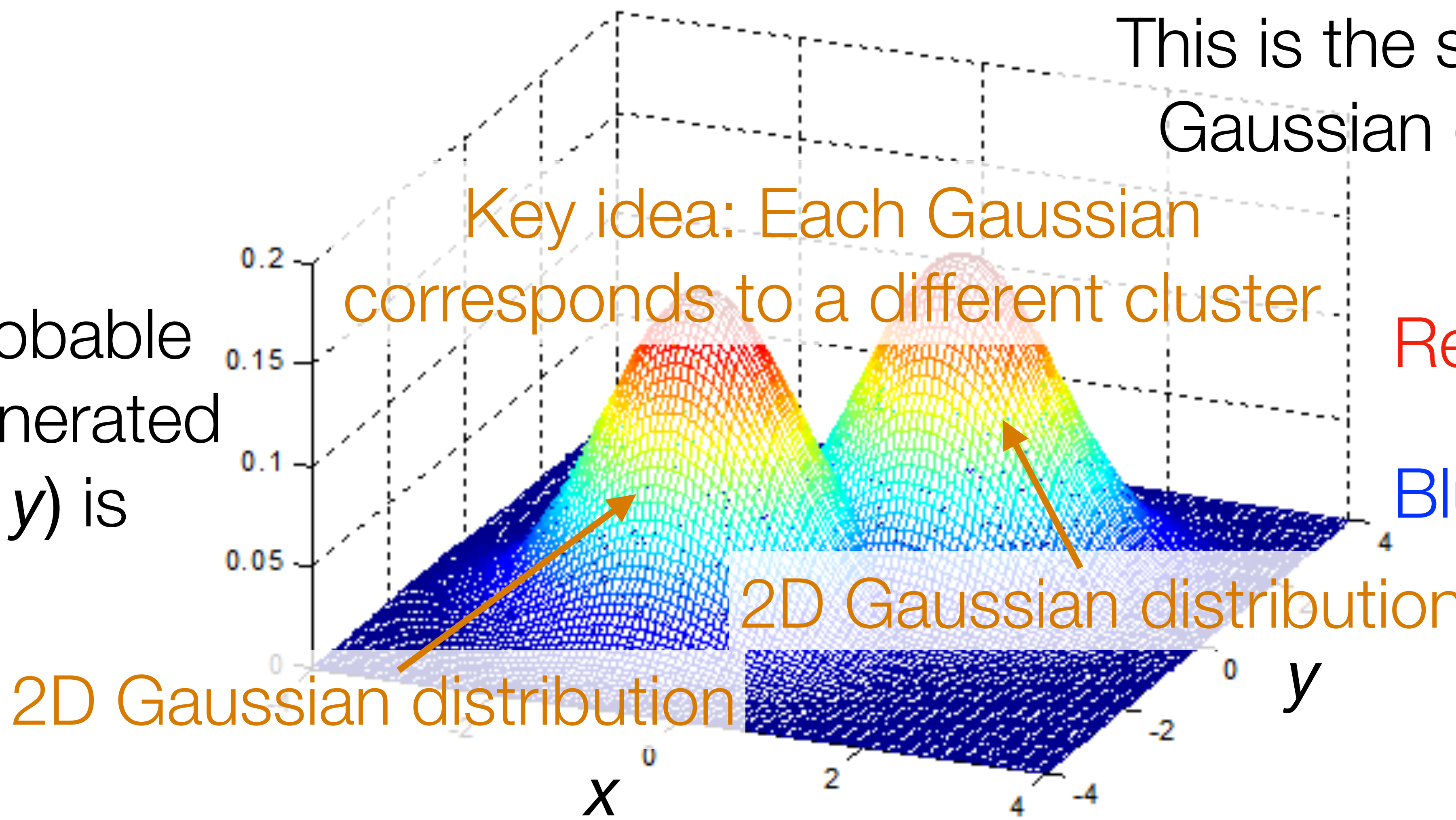


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# Example: 1D GMM with 2 Clusters

<u>Cluster 1</u>

Probability of generating a point from cluster 1 = 0.5

Gaussian mean = –5

Gaussian std dev = 1

<u>Cluster 2</u>

Probability of generating a point from cluster 2 = 0.5

Gaussian mean = 5

Gaussian std dev = 1

What do you think the probability distribution looks like?

# Example: 1D GMM with 2 Clusters

<u>Cluster 1</u>

Probability of generating a point from cluster 1 = 0.5

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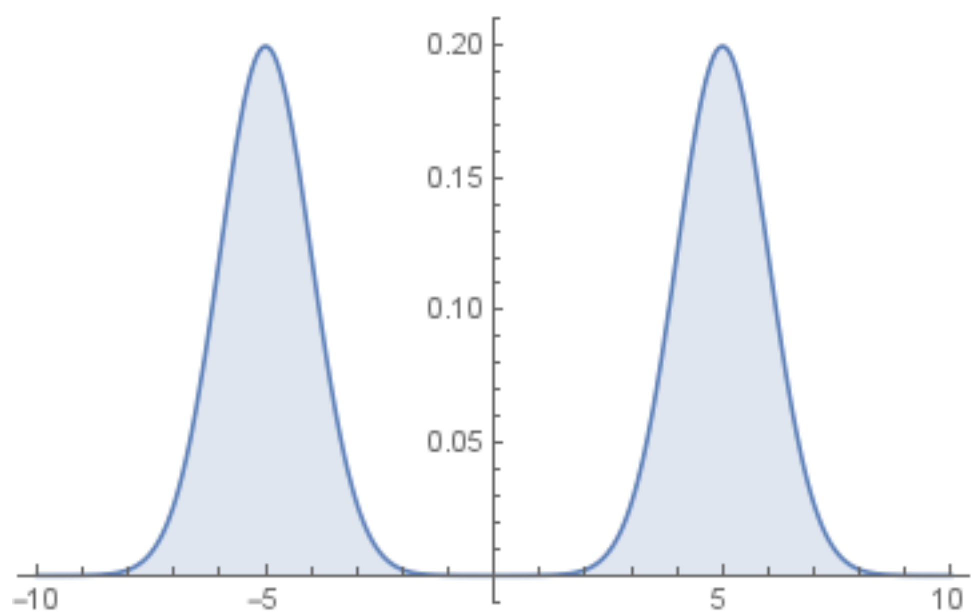


# Example: 1D GMM with 2 Clusters

<u>Cluster 1</u>

Probability of generating a point from cluster 1 = **0.7**

Gaussian mean = –5

Gaussian std dev = 1

<u>Cluster 2</u>

Probability of generating a point from cluster 2 = **0.3**

Gaussian mean = 5

Gaussian std dev = 1

What do you think the probability distribution looks like?

# Example: 1D GMM with 2 Clusters

<u>Cluster 1</u>

Probability of generating a point from cluster 1 = 0.7

Gaussian mean = –5

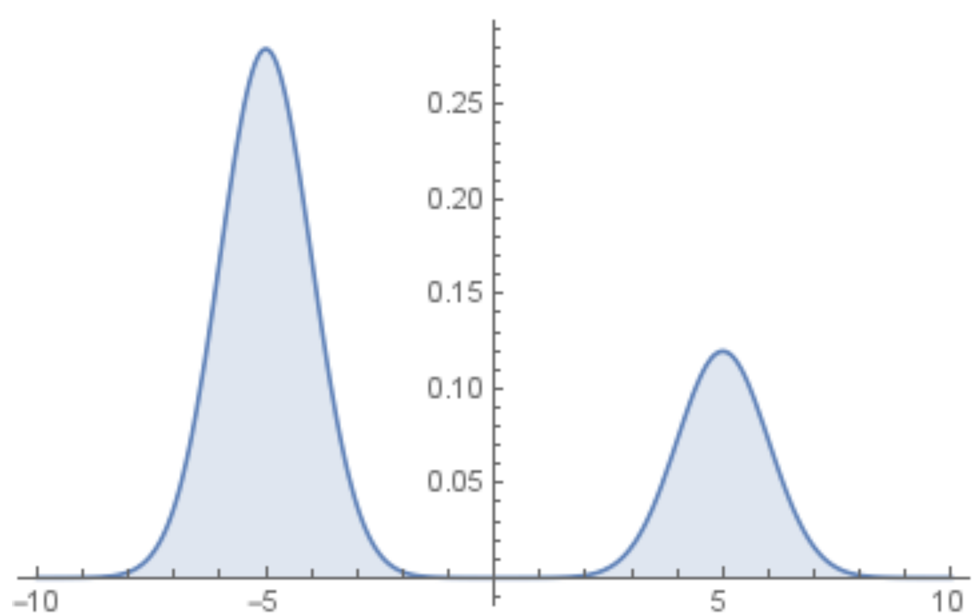
Gaussian std dev = 1

<u>Cluster 2</u>

Probability of generating a point from cluster 2 = 0.3

Gaussian mean = 5

Gaussian std dev = 1



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Gaussian mean = –5

Gaussian std dev = 1

<u>Cluster 2</u>

Probability of generating a point from cluster 2 = 0.3

Gaussian mean = 5

Gaussian std dev = 1

How to generate 1D points from this GMM:

1. Flip biased coin (with probability of heads 0.7)
2. If heads: sample 1 point from Gaussian mean -5, std dev 1

   If tails: sample 1 point from Gaussian mean 5, std dev 1

# Example: 1D GMM with 2 Clusters

<u>Cluster 1</u>

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

Gaussian mean = $\mu_1$

Gaussian std dev = $\sigma_1$

<u>Cluster 2</u>

Probability of generating a point from cluster 2 = $\pi_2$

Gaussian mean = $\mu_2$

Gaussian std dev = $\sigma_2$

How to generate 1D points from this GMM:

1. Flip biased coin (with probability of heads $\pi_1$)
2. If heads: sample 1 point from Gaussian mean $\mu_1$, std dev $\sigma_1$

   If tails: sample 1 point from Gaussian mean $\mu_2$, std dev $\sigma_2$

# Example: 1D GMM with *k* Clusters

Cluster 1

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

Gaussian mean = $\mu_1$

Gaussian std dev = $\sigma_1$

…

Cluster *k*

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

Gaussian mean = $\mu_k$

Gaussian std dev = $\sigma_k$

How to generate 1D 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 Gaussian mean $\mu_Z$, std dev $\sigma_Z$

# Example: 2D GMM with $k$ Clusters

Cluster 1

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

Gaussian mean = $\mu_1$ 2D point

Gaussian **covariance** = $\Sigma_1$

2x2 matrix

…

Cluster $k$

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

Gaussian mean = $\mu_k$ 2D point

Gaussian **covariance** = $\Sigma_k$

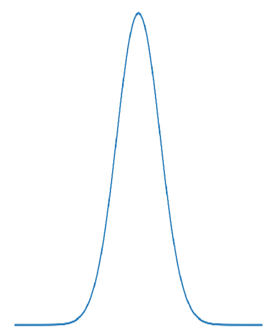
2x2 matrix

How to generate **2D** points from this GMM:

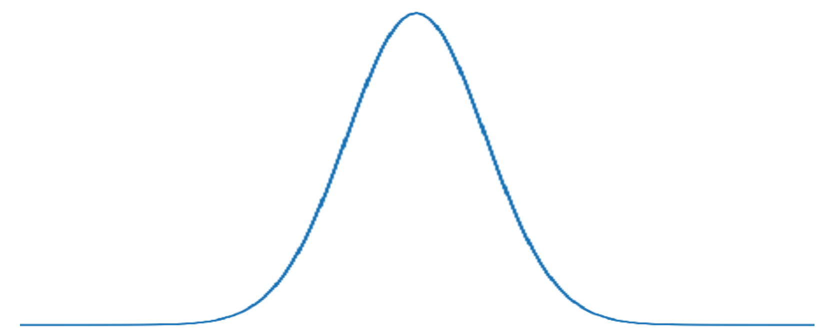
1. Flip biased $k$-sided coin (the sides have probabilities $\pi_1, \ldots, \pi_k$)
2. Let $Z$ be the side that we got (it is some value $1, \ldots, k$)
3. Sample 1 point from Gaussian mean $\mu_Z$, **covariance** $\Sigma_Z$

# 2D Gaussian Shape

In 1D, you can have a skinny Gaussian or a wide Gaussian



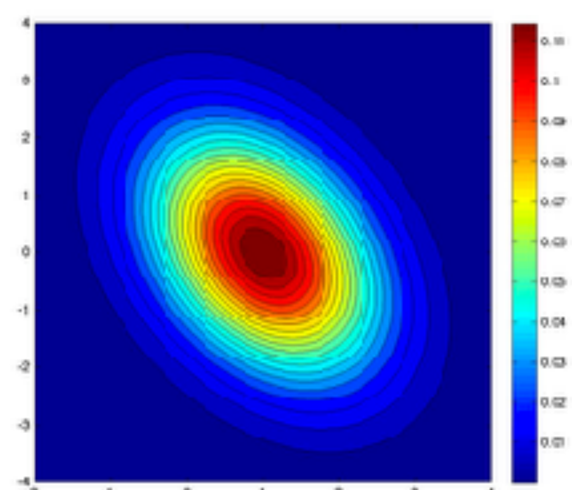
Less uncertainty



More uncertainty

In 2D, you can more generally have ellipse-shaped Gaussians

Ellipse enables encoding relationship between variables



Can't have arbitrary shapes

Top-down view of an example 2D Gaussian distribution

Image source: https://www.cs.colorado.edu/~mozer/Teaching/syllabi/ProbabilisticModels2013/homework/assign5/a52dgauss.jpg

# GMM with $k$ Clusters

Cluster 1

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

Gaussian mean = $\mu_1$ in $\mathbb{R}^d$

Gaussian covariance = $\Sigma_1$

$d$ x $d$ matrix

…

Cluster $k$

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

Gaussian mean = $\mu_k$ in $\mathbb{R}^d$

Gaussian covariance = $\Sigma_k$

$d$ x $d$ matrix

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 $\mu_Z$, covariance $\Sigma_Z$

# 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!

**"All models are wrong, but some are useful."**

*–George Edward Pelham 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

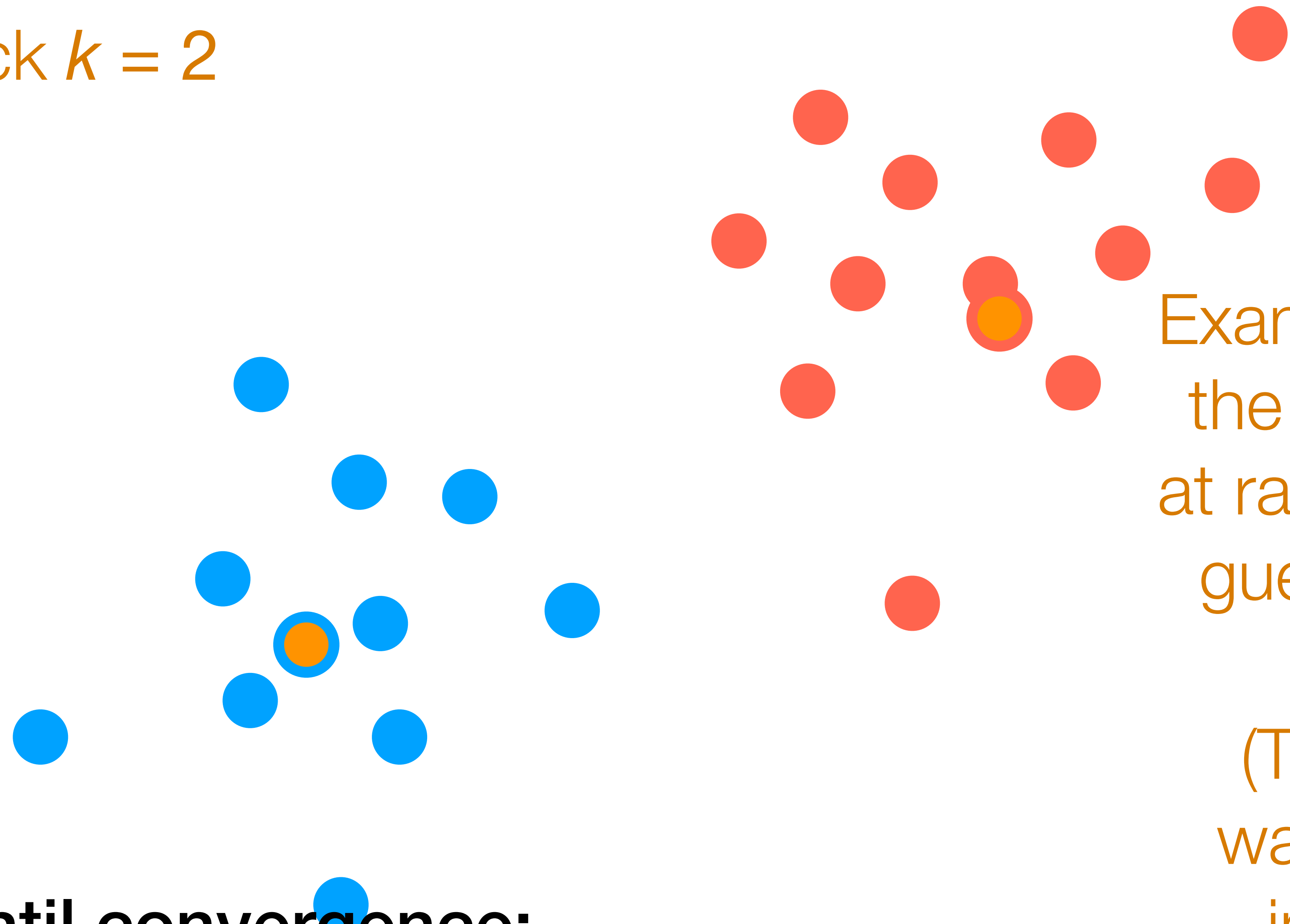
*How do you turn this into a cluster assignment?*

# *k*-means

Step 0: Pick *k*

We'll pick $k = 2$

Step 1: Pick guesses 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 guesses for
where cluster centers are

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# (Rough Intuition) Learning a GMM

Step 0: Pick *k*

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

**Repeat until convergence:**

Step 2: Assign each point a probability to belonging to each of the *k* clusters

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

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

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

# Relating *k*-means to GMM's

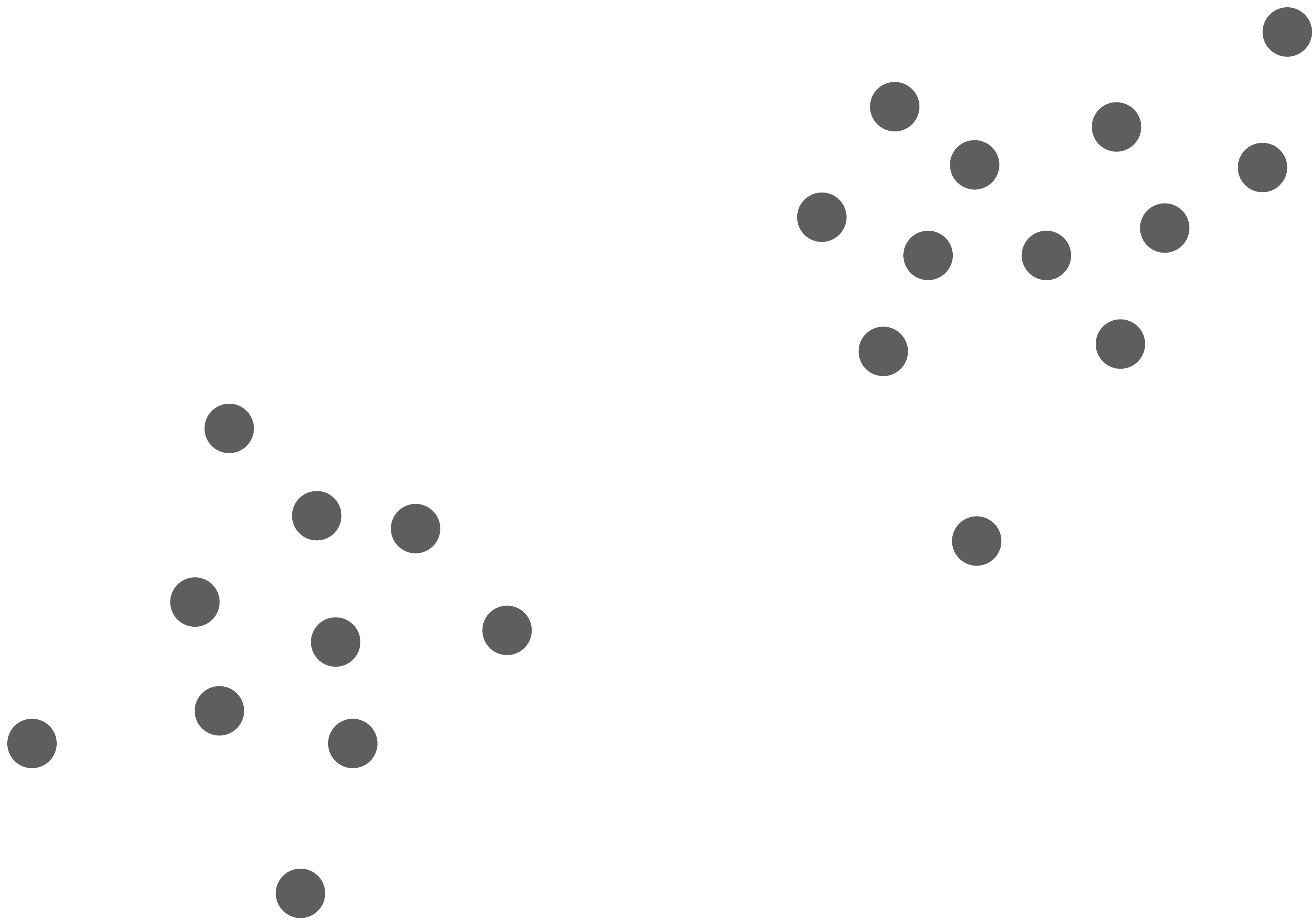
*k*-means approximates the EM algorithm for GMM's:

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

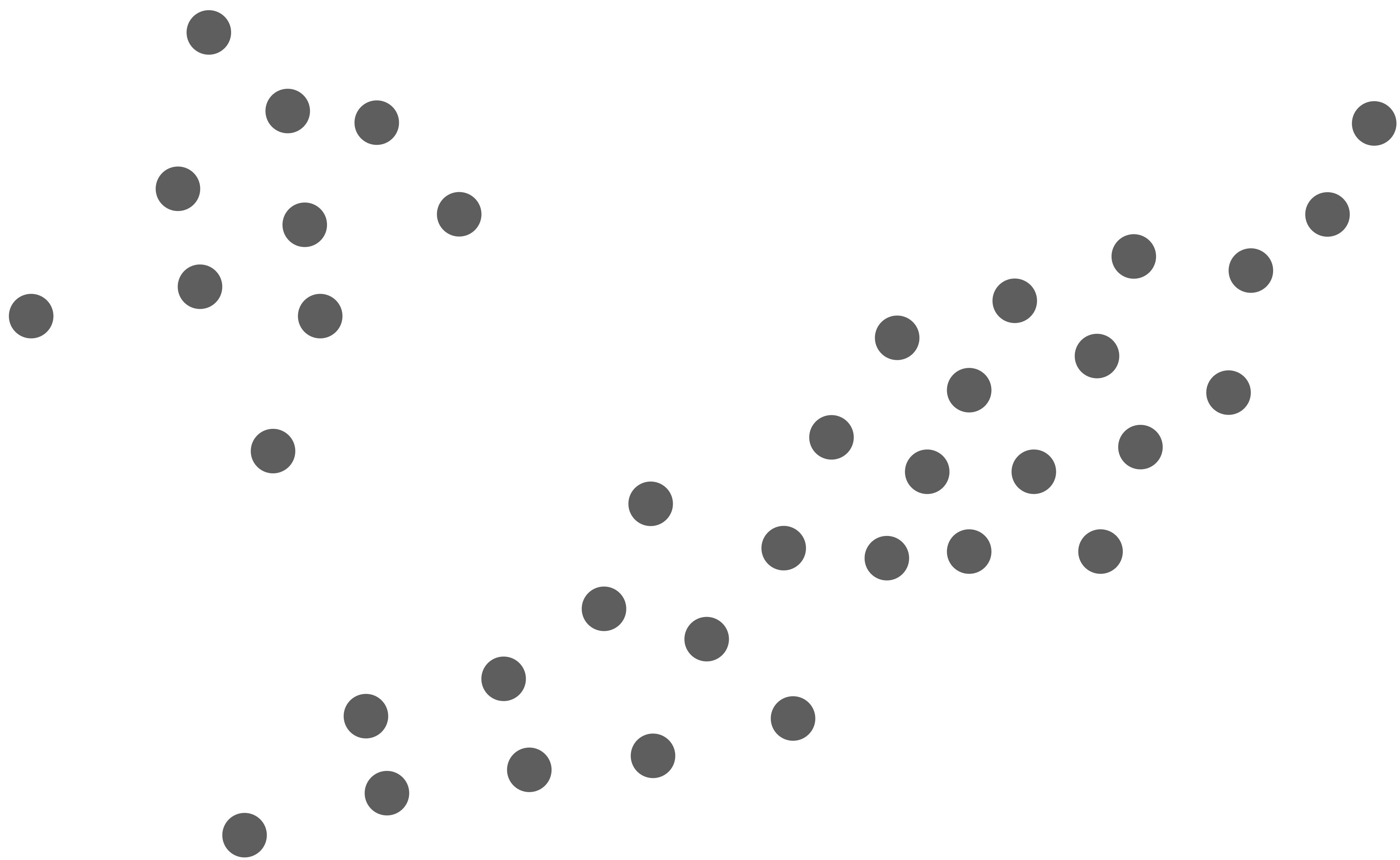
- *k*-means does not keep track of shape/correlation information between variables (so shape is circular)

**Interpretation:** We know when k-means should work! It should work when the data appear as if they're from a GMM with true clusters that "look like circles"

# *k*-means should do well on this



# But not on this



# 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

There are fancier ways for choosing $k$ (e.g., DP-GMMs)

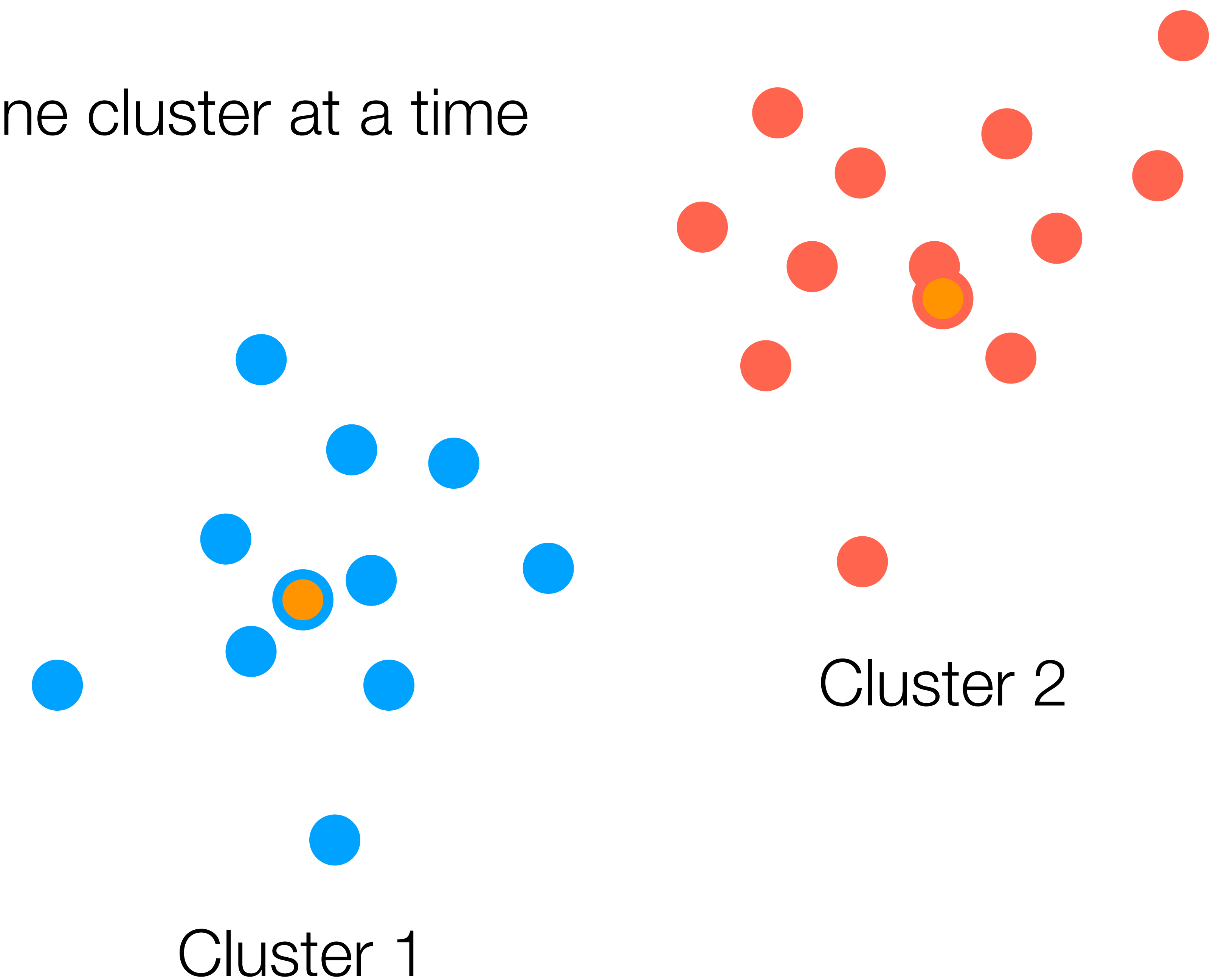
No single way of choosing $k$ is the “best” way

# 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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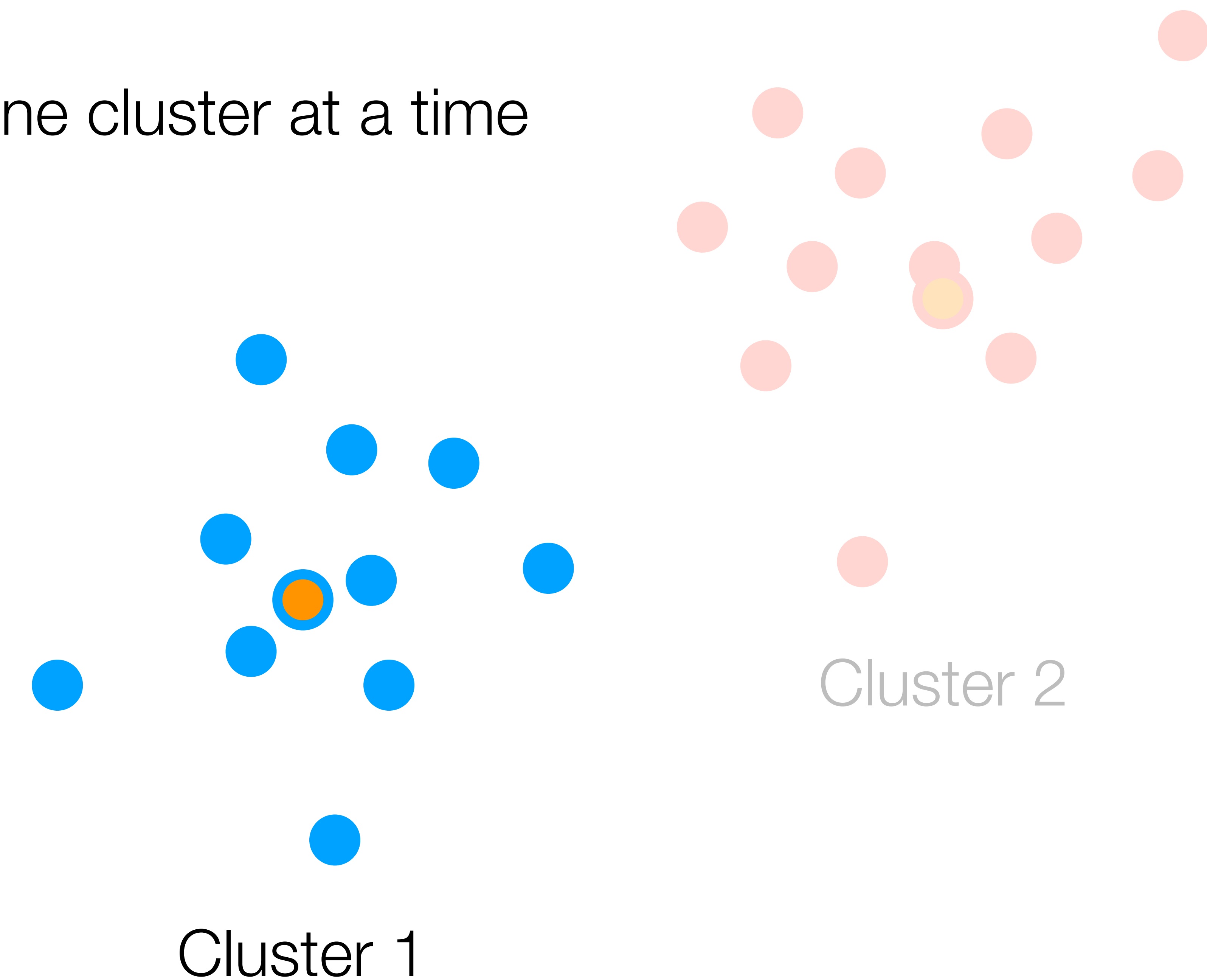
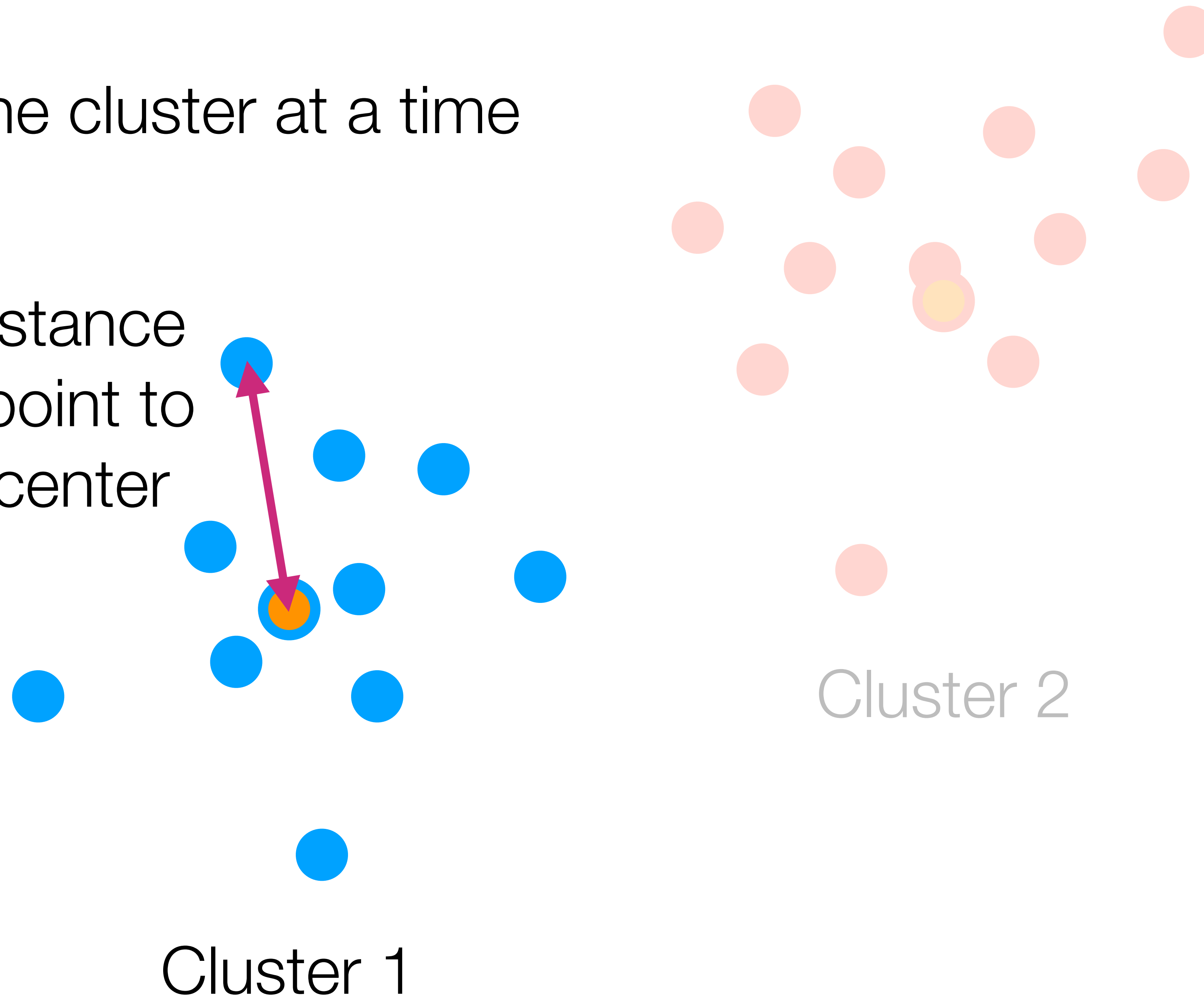


# Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



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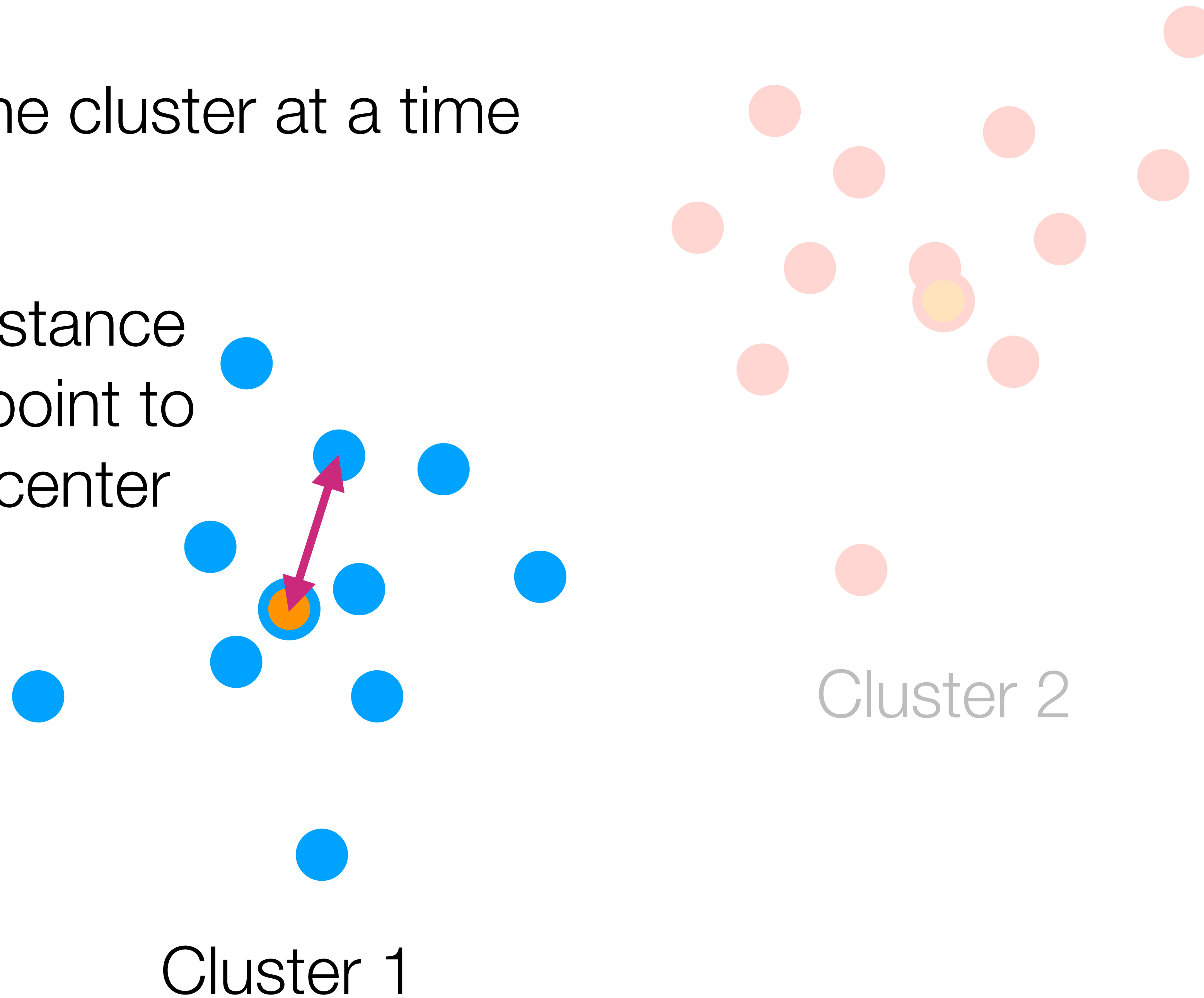

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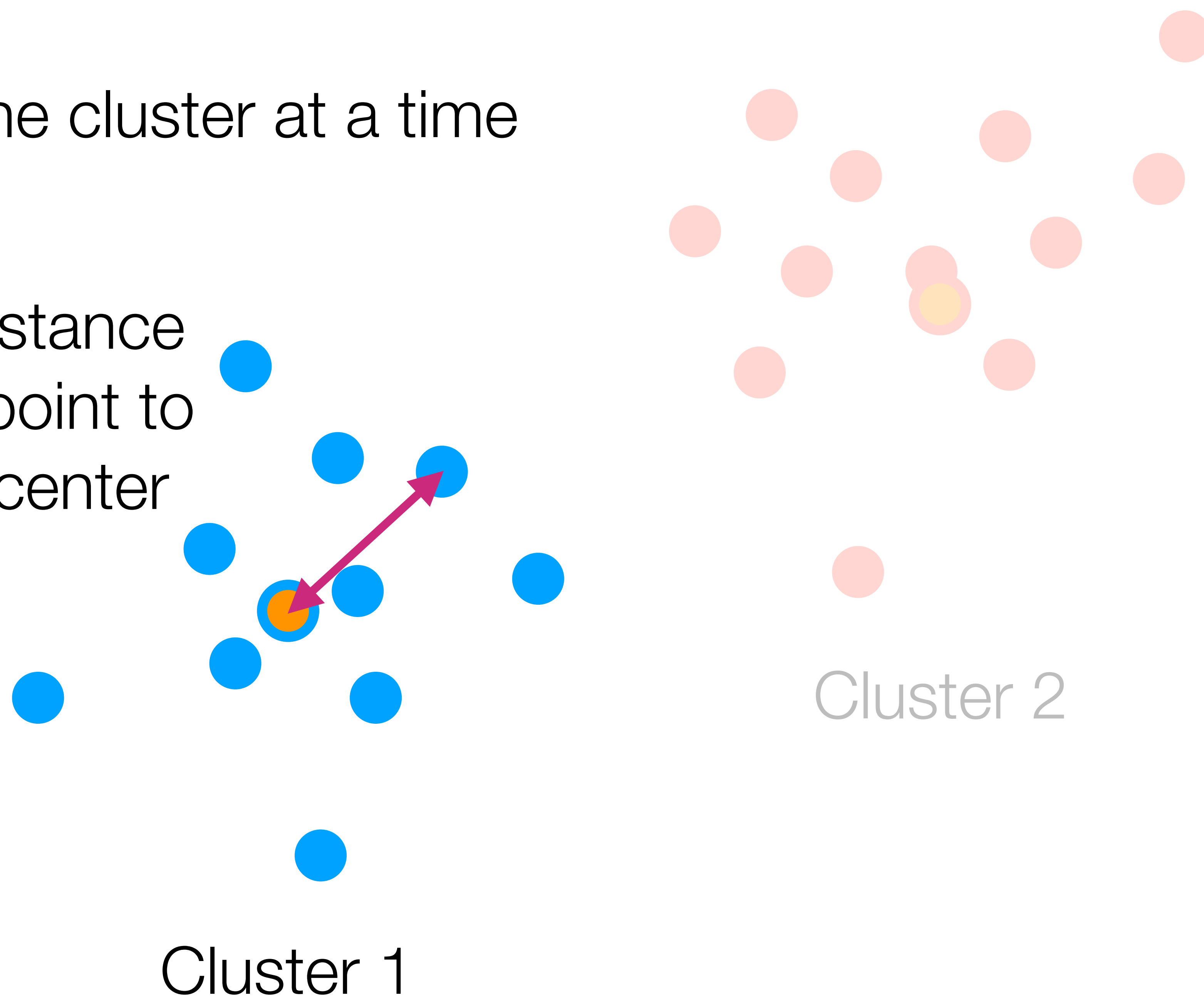

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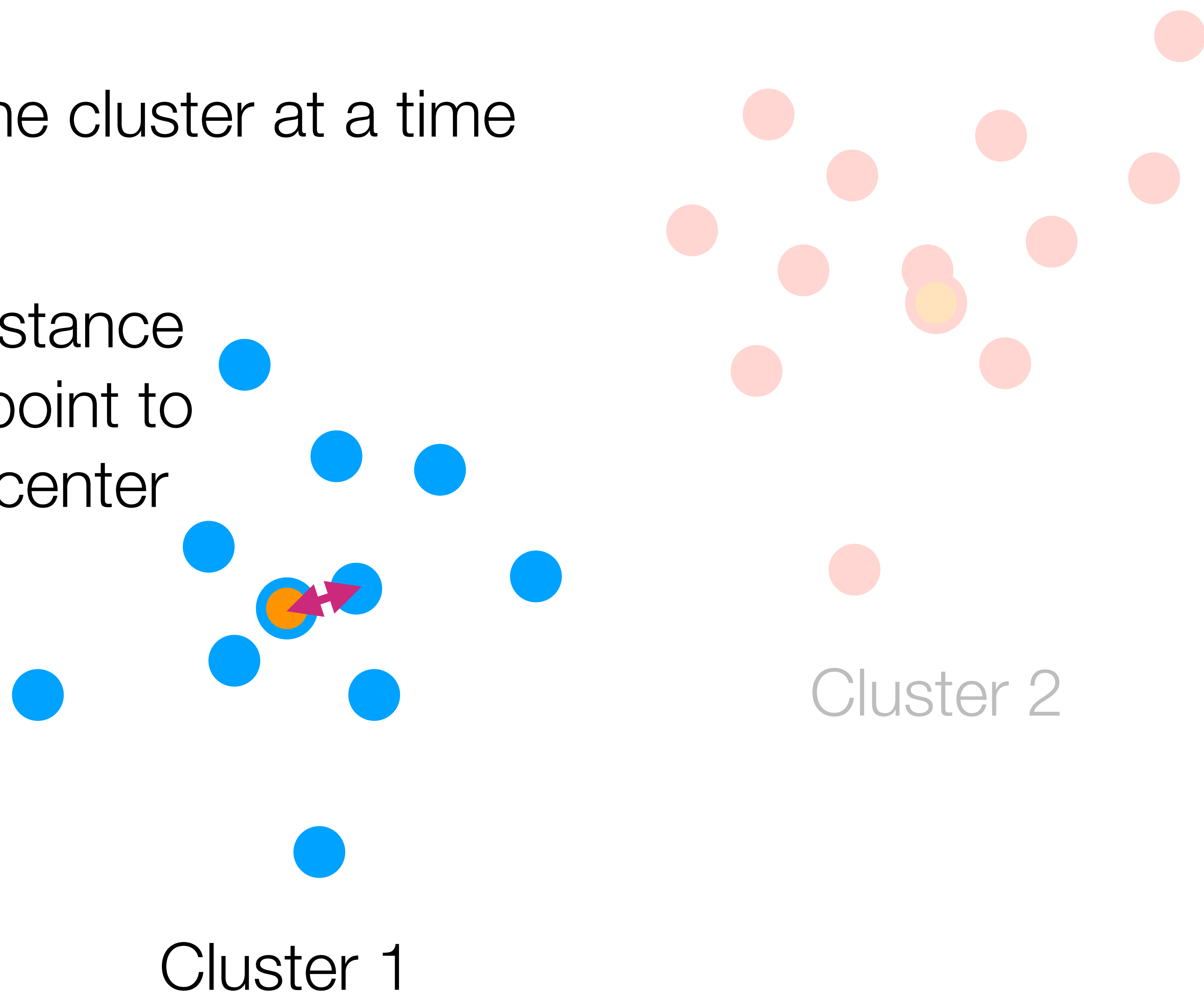

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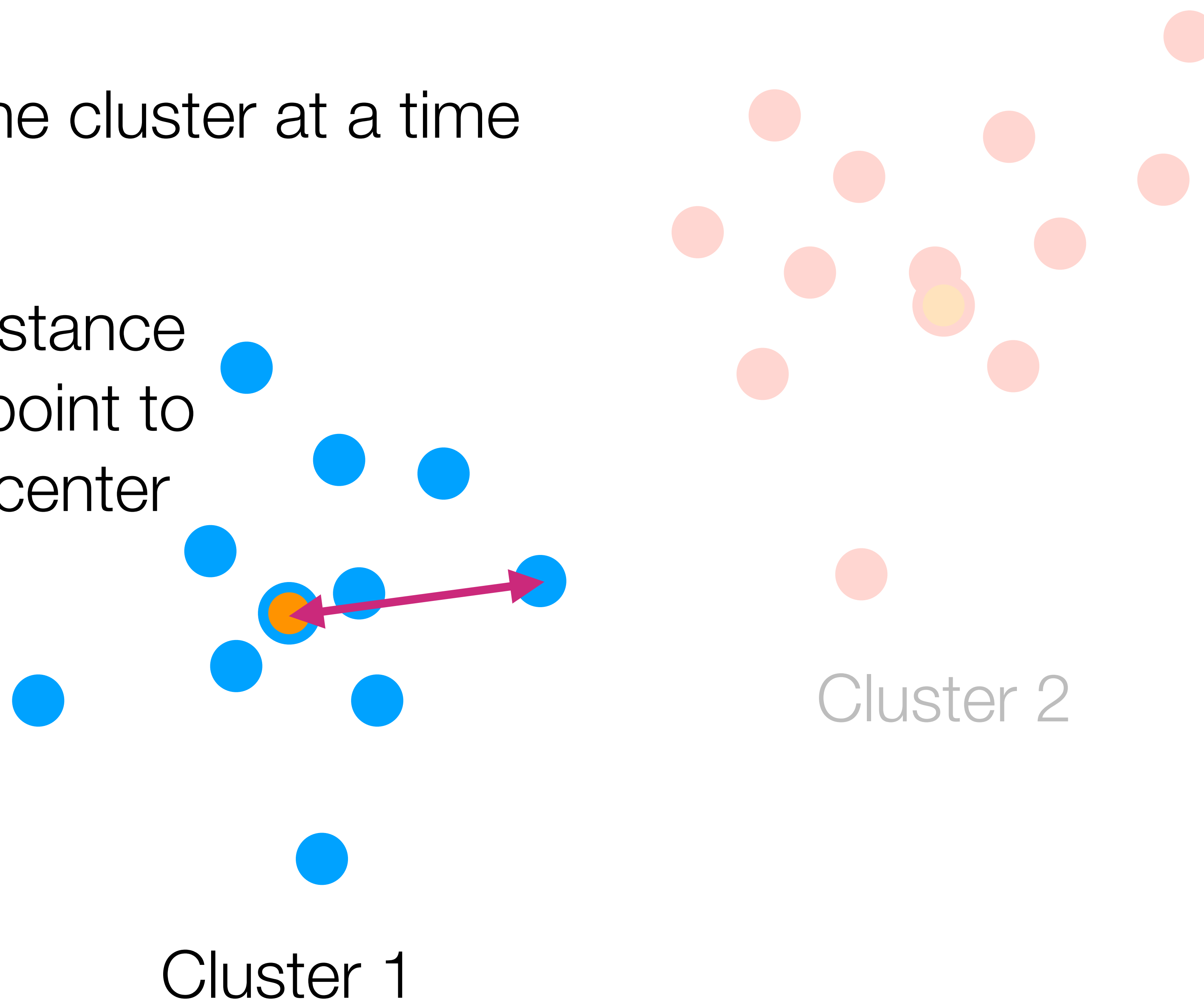

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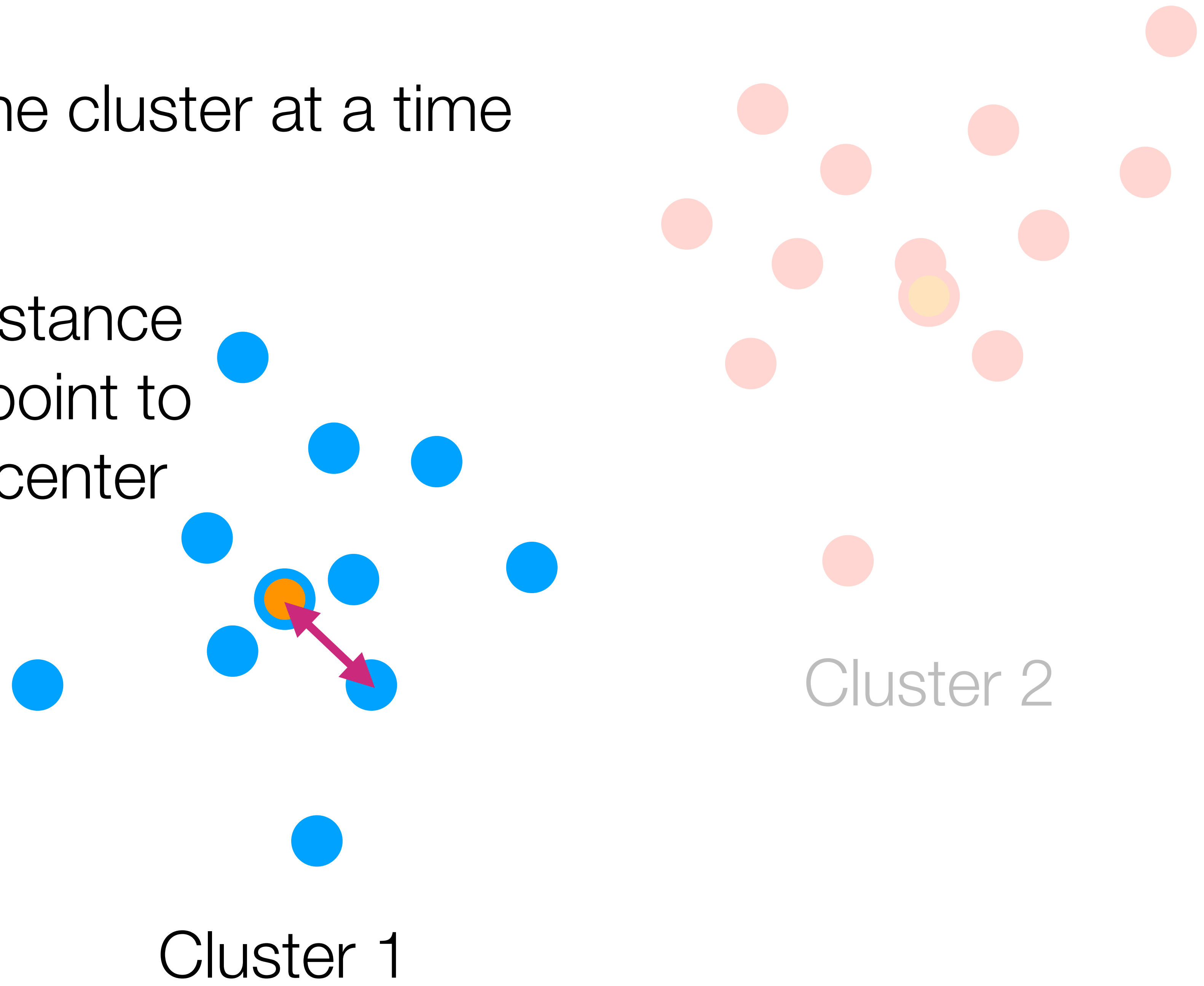

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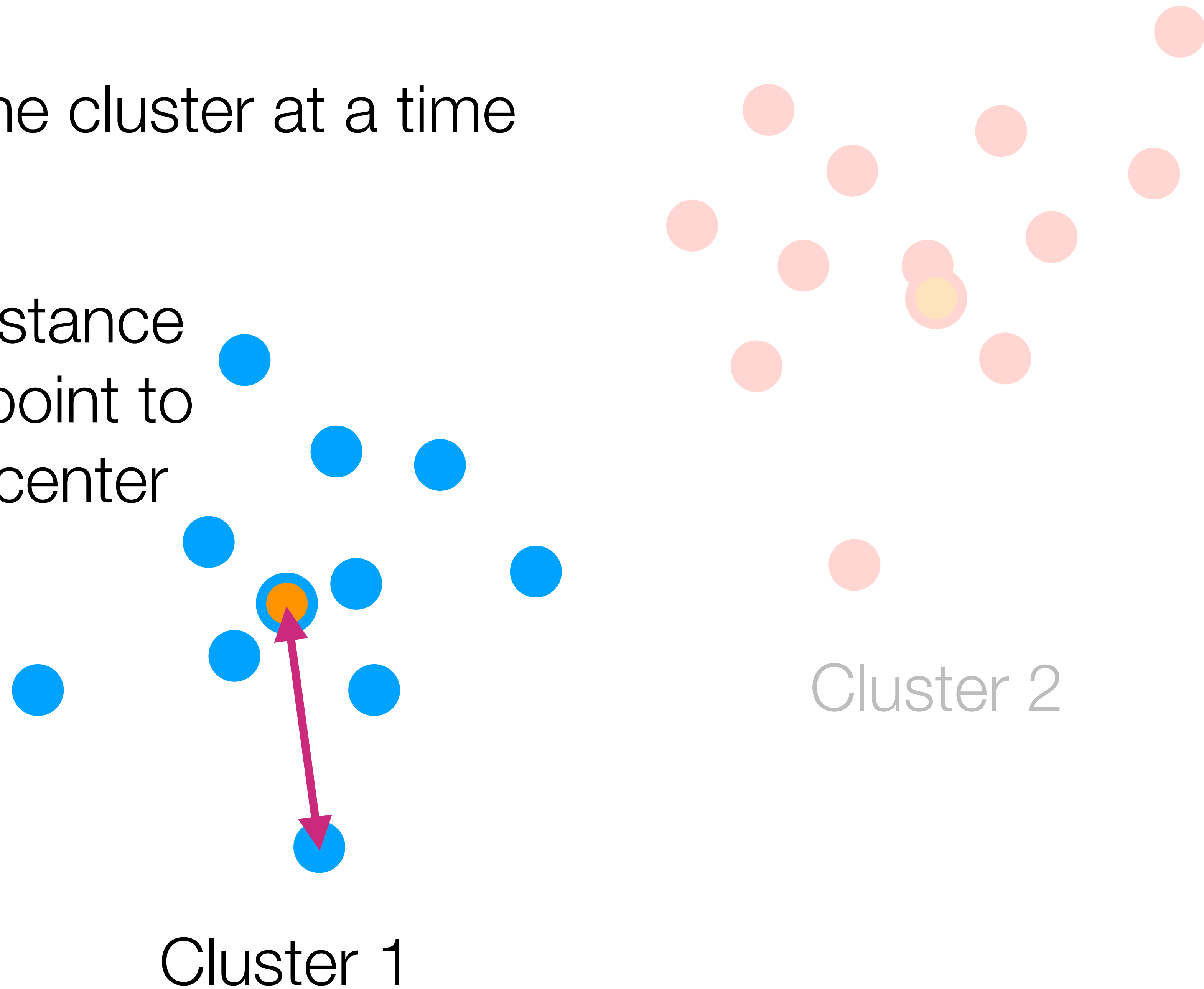

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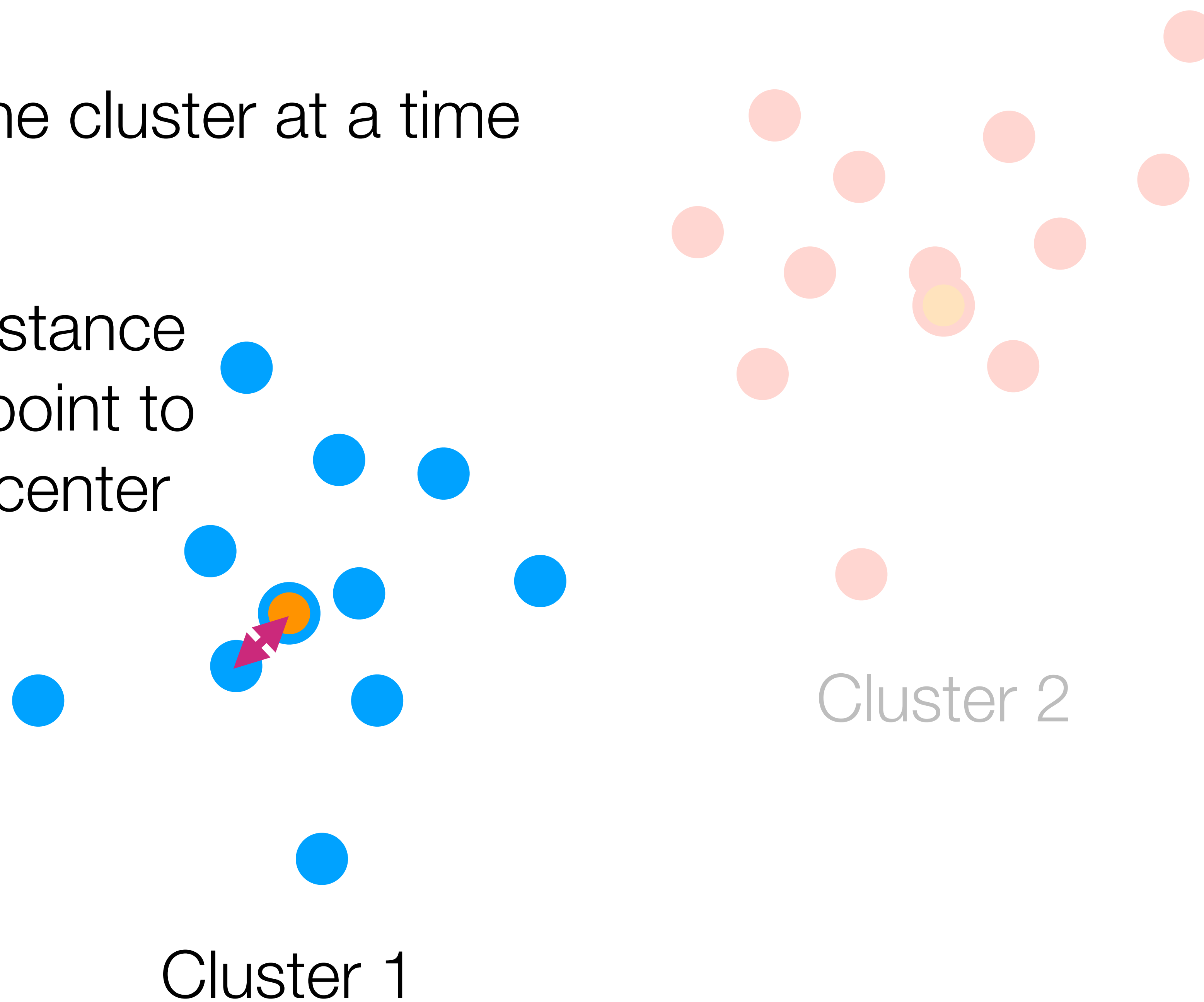

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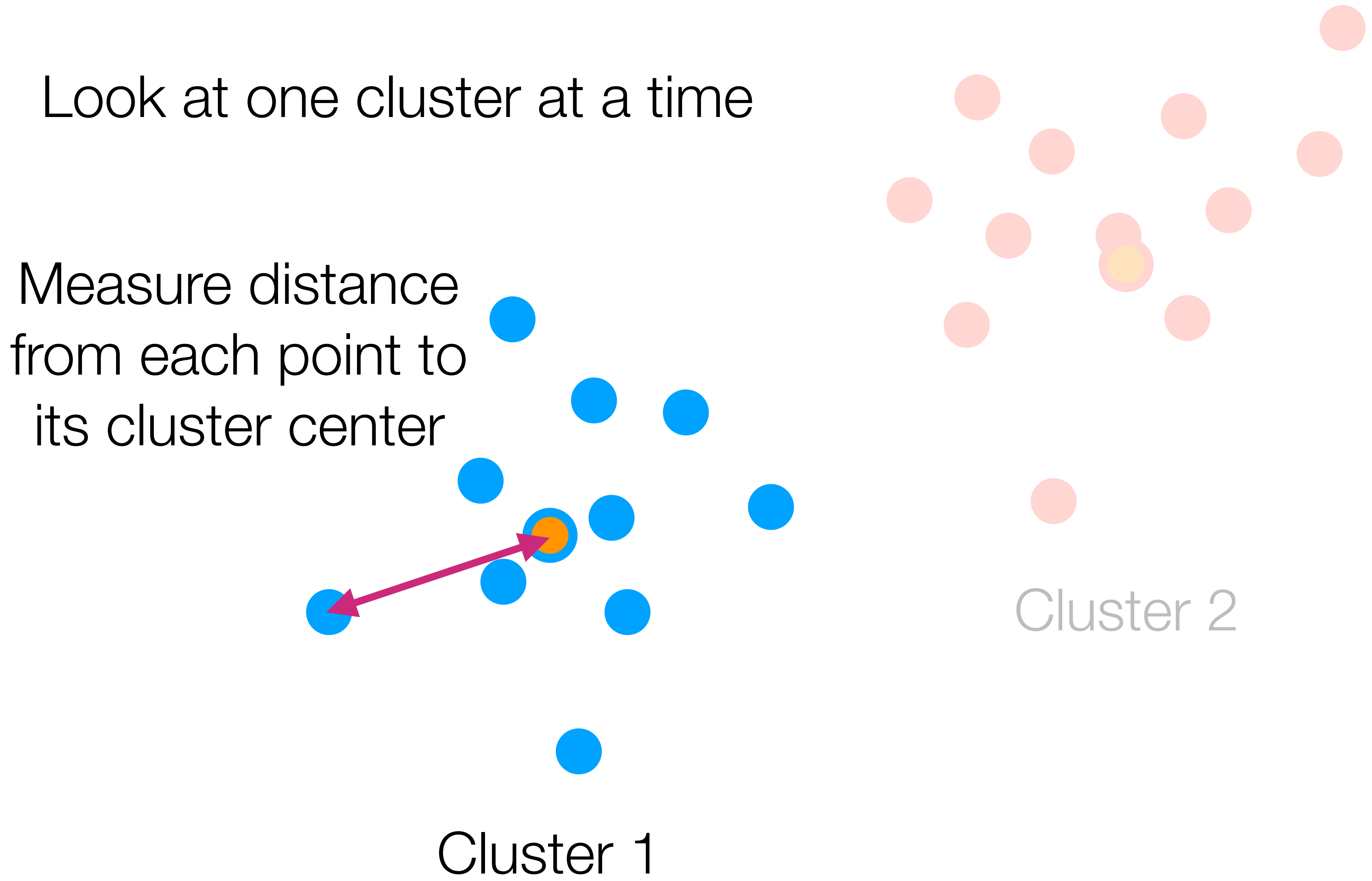

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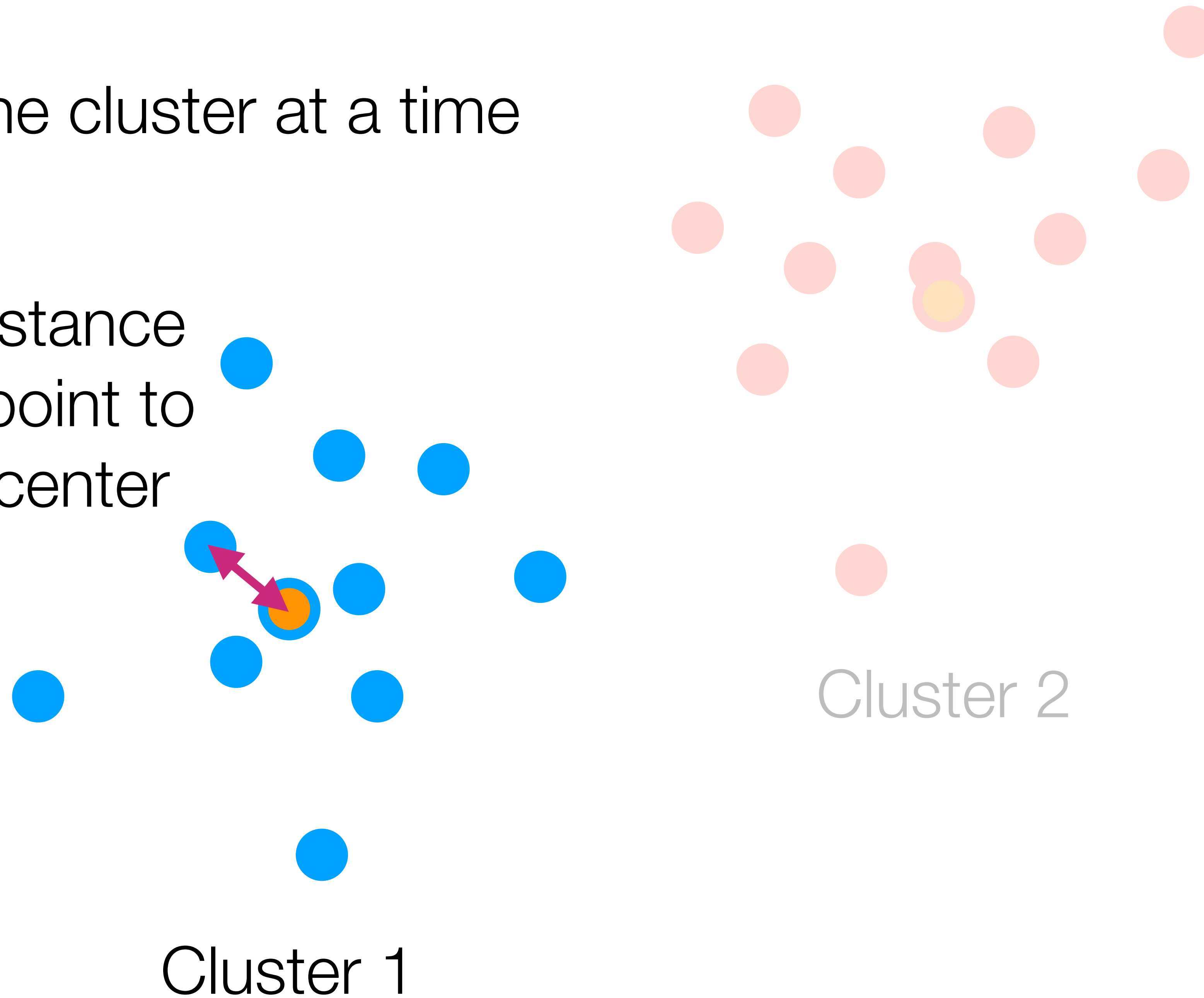

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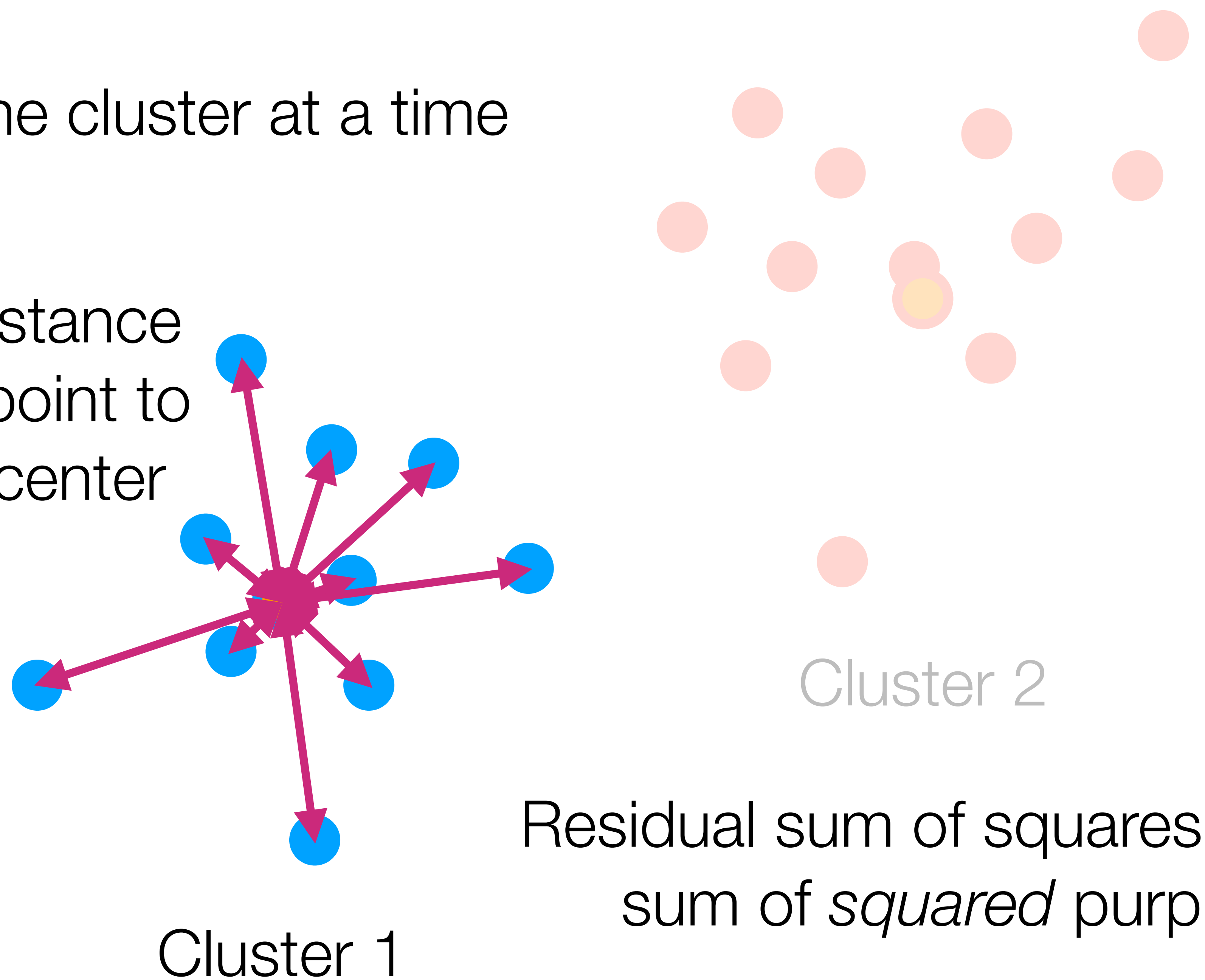
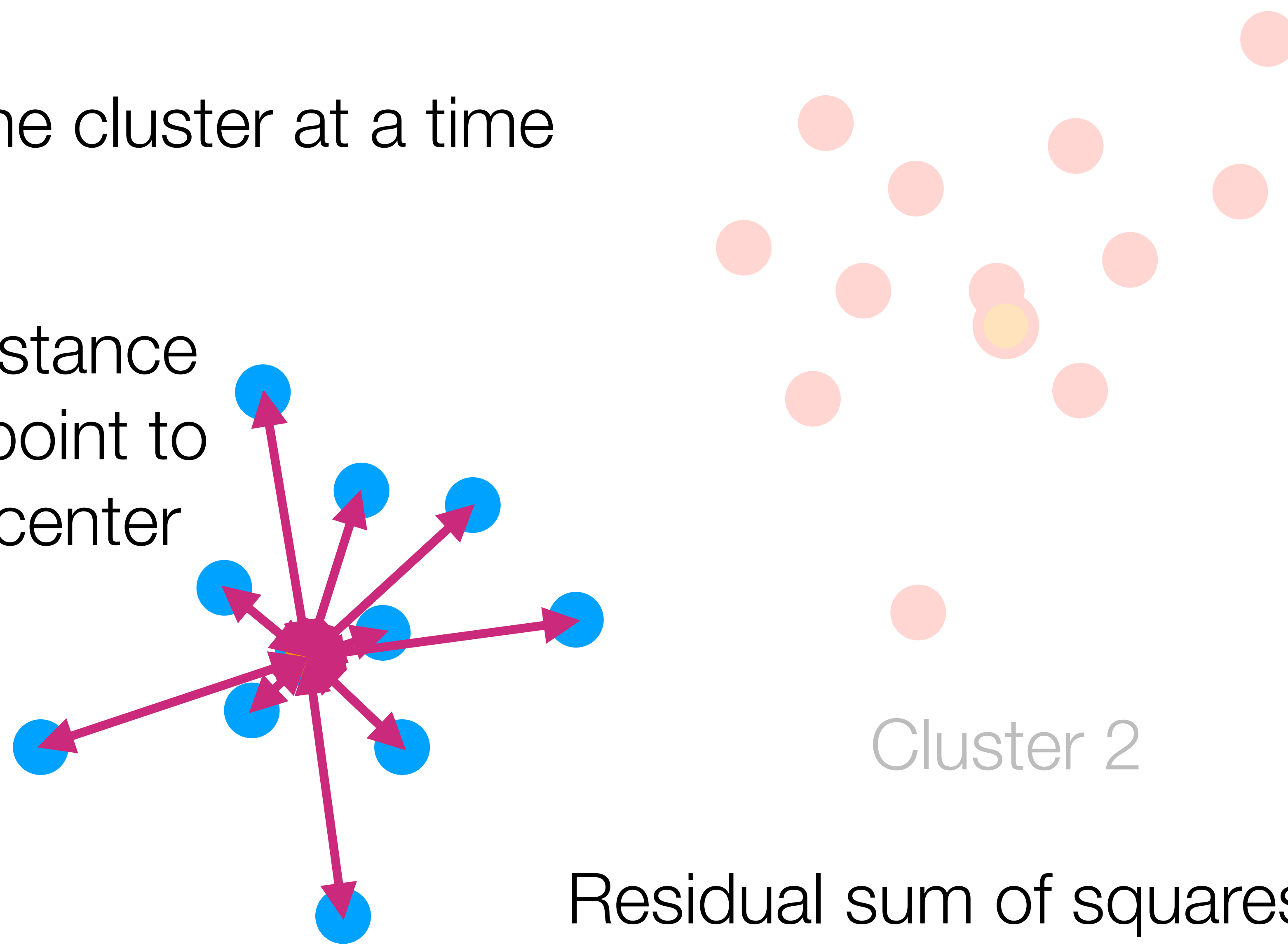



Residual sum of squares for cluster 1: sum of *squared* purple lengths

# Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



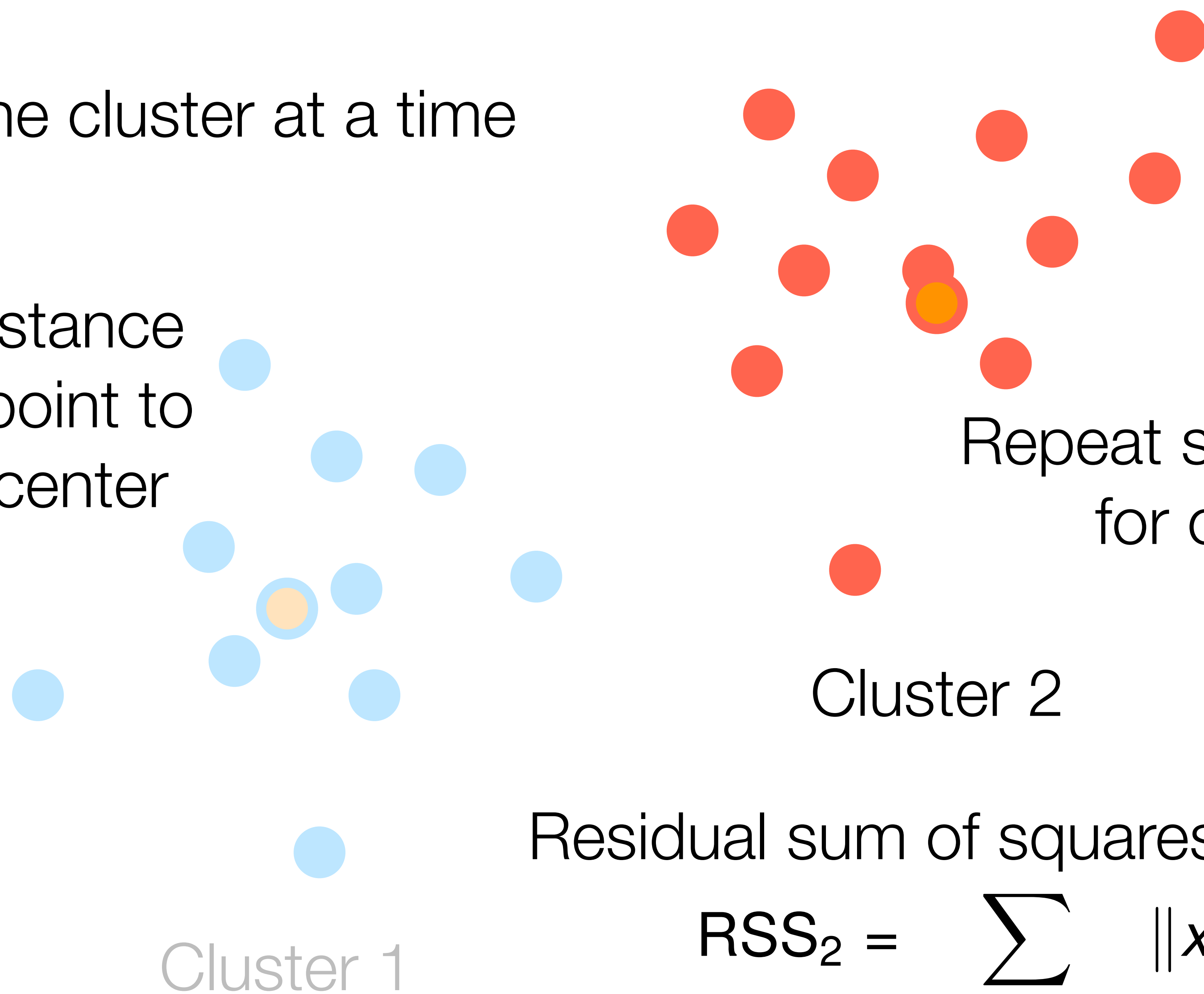

Residual sum of squares for cluster 1:

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

# 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:

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

# 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 *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