Carnegie Mellon University
Heinz College

95-865 Australia Lecture 3: Clustering Part I

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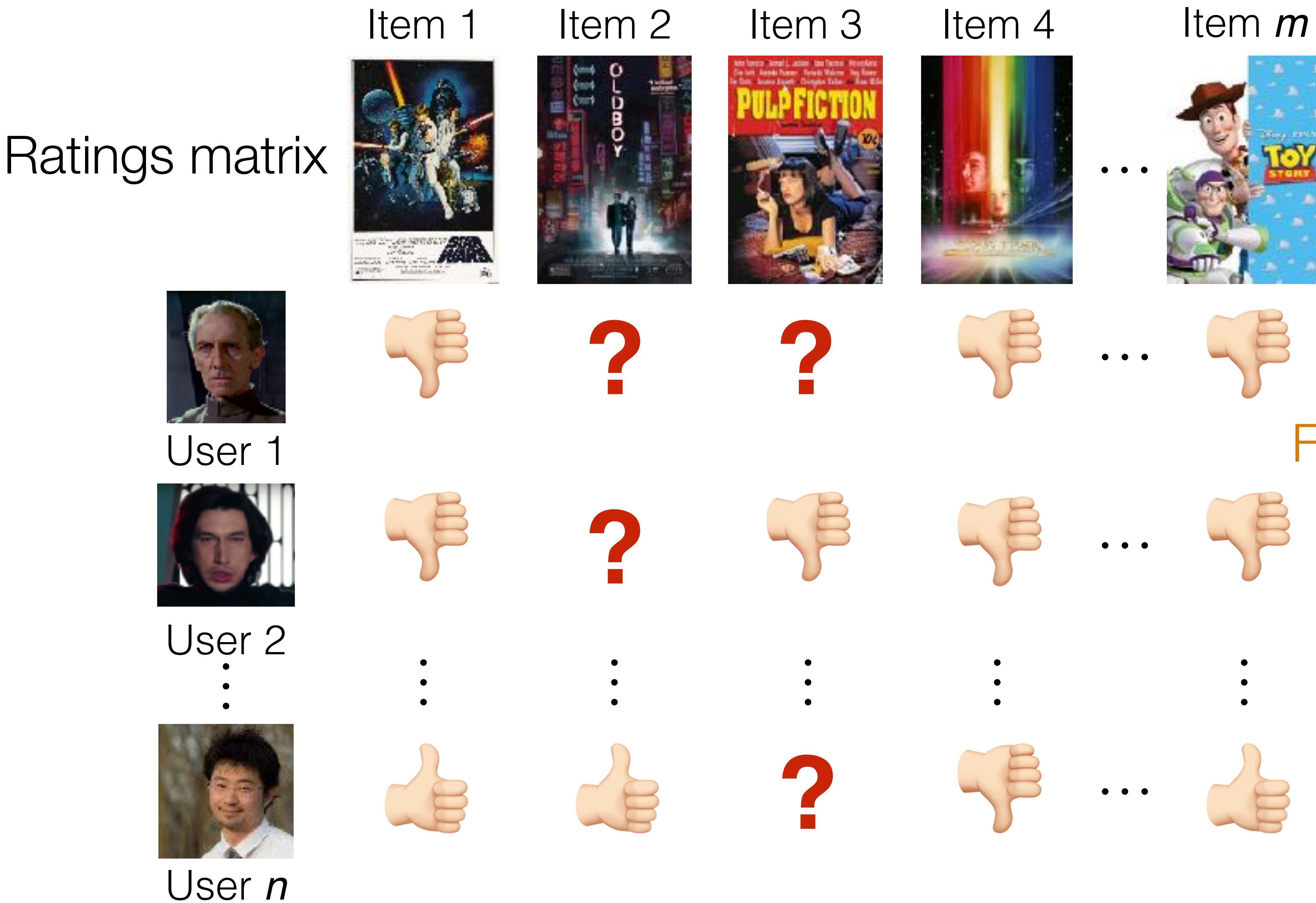
Suppose Netflix asks you how to go about understanding what kind of TV show it should produce next. How would you go about doing it?

Image source: http://static3.businessinsider.com/image/58f900e37522cacd008b4ee9/scott-galloway-netflix-could-be-the-next-300-billion-company.jpg

We want to understand user tastes

Movie Recommendation Data



For simplicity: consider single snapshot in time

We can also scrape IMDb for a lot of semantic information (actresses, actors, genres, reviews, etc) about movies/TV shows

When looking for structure,
it's helpful to hypothesize
what structure there might be

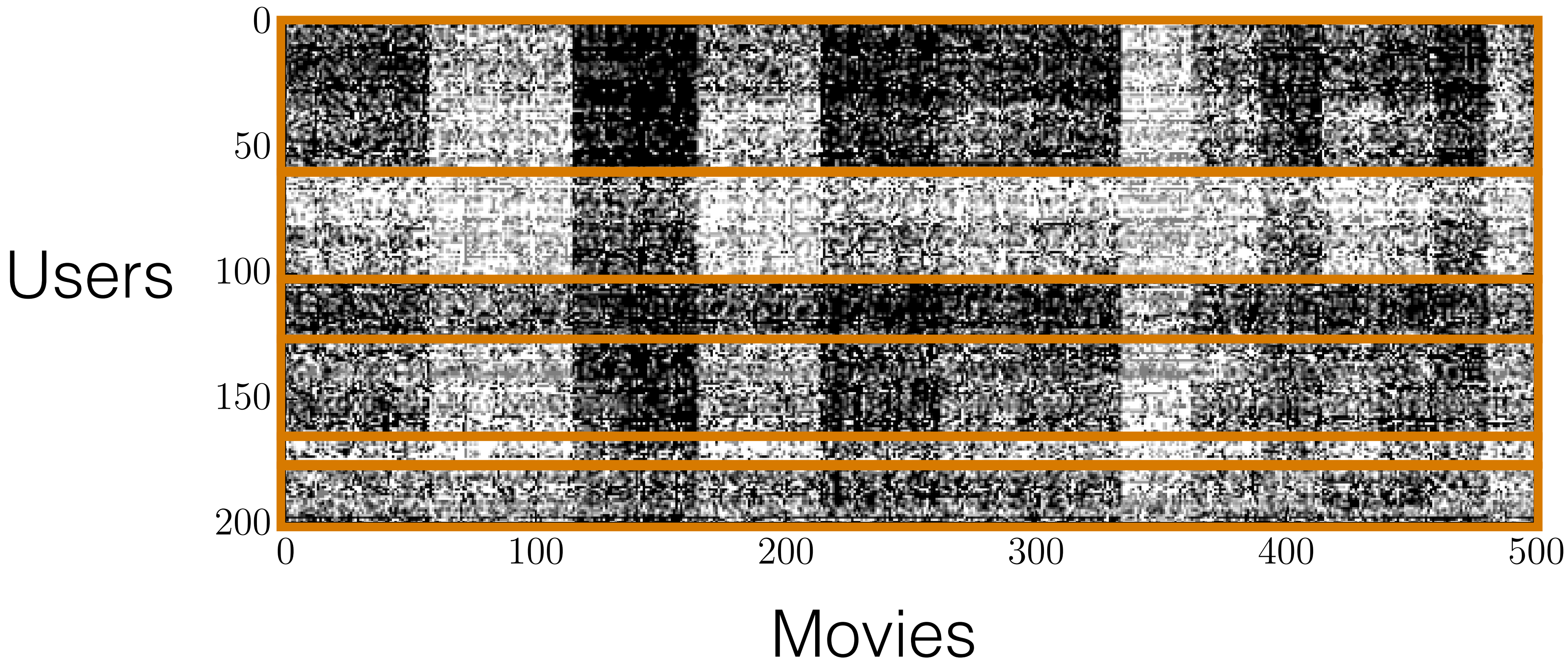
Movie Recommendation Data

Simple hypothesis: There are clusters of users with similar taste

Is the Hypothesis on Users True?

black = user dislikes movie

white = user likes movie



There are blocks of similar users!

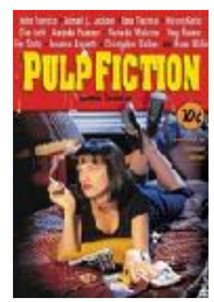
In fact there are blocks of similar items as well!

Dense part of Netflix Prize data

The Art of Defining Similarity

- There usually is no “best” way to define similarity

Example: cosine similarity between users



User u  Y_u | $+1$ | -1

User v  Y_v | $+1$ | $+1$

$$\frac{\langle Y_u, Y_v \rangle}{\|Y_u\| \|Y_v\|} = 0$$

The Art of Defining Similarity

- There usually is no “best” way to define similarity

Example: cosine similarity $\dfrac{\langle Y_u, Y_v \rangle}{\|Y_u\| \|Y_v\|}$

- Also popular: define a distance first and then turn it into a similarity

Example: Euclidean distance $\|Y_u - Y_v\|$

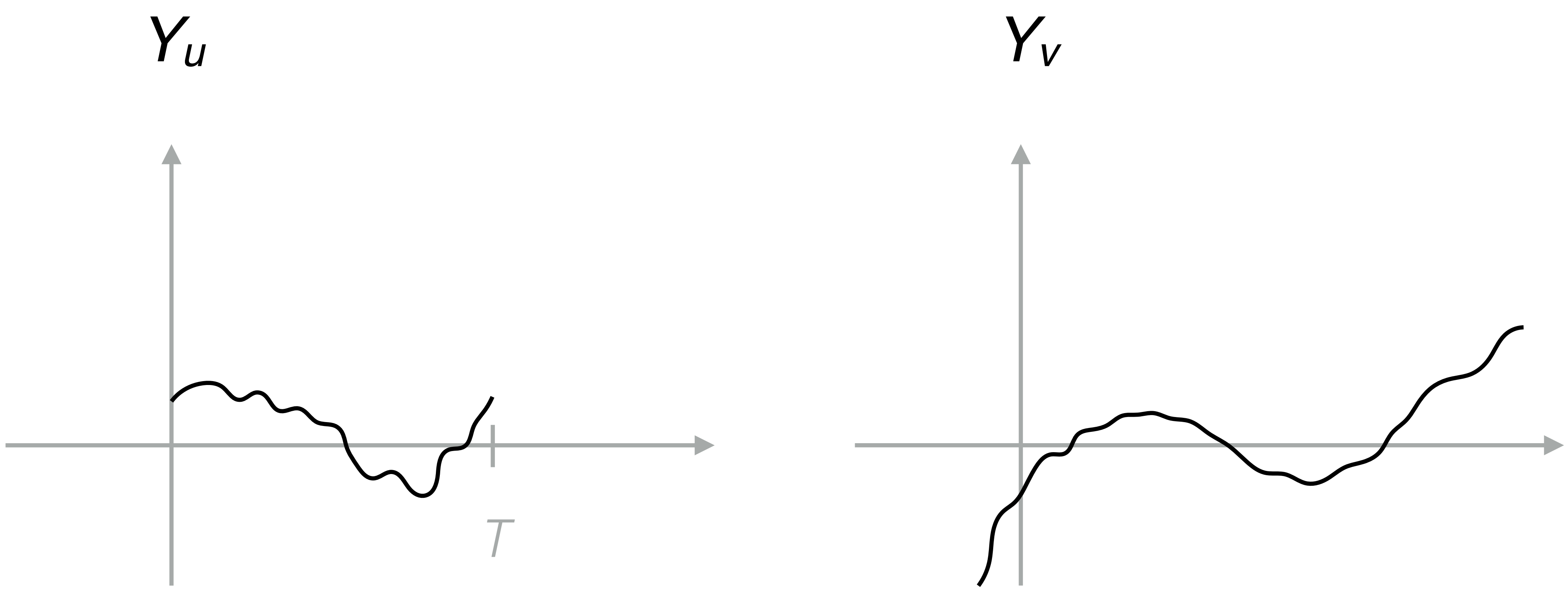
Turn into similarity with decaying exponential $\downarrow$

$$\exp(-\gamma \|Y_u - Y_v\|)$$

where $\gamma > 0$

Example: Time Series

How would you compute a distance between these?



Only observe time steps between 0 and T

Example: Time Series

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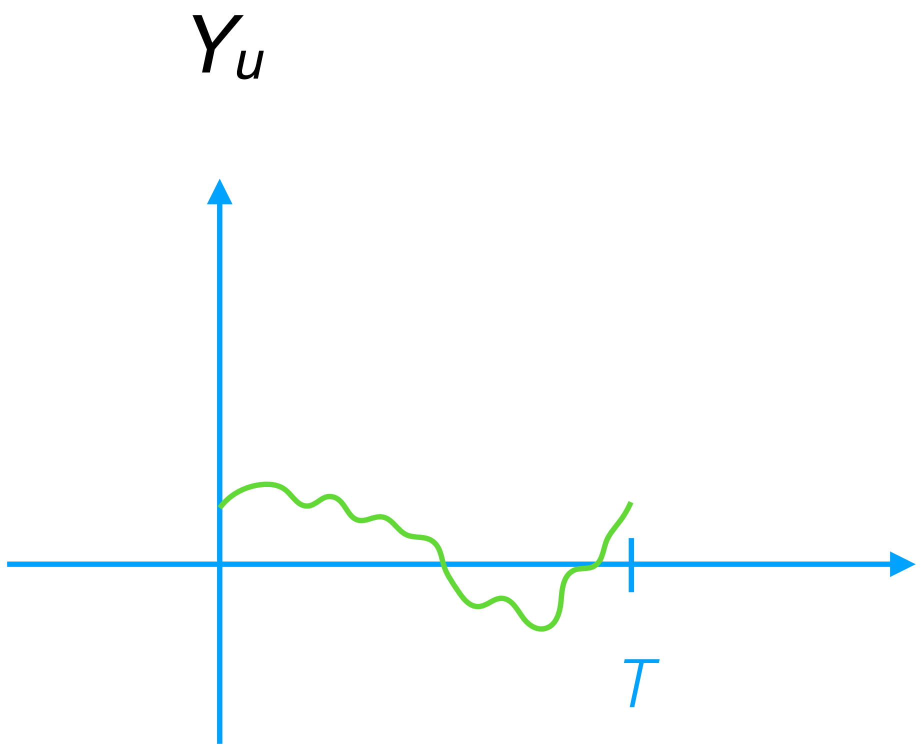

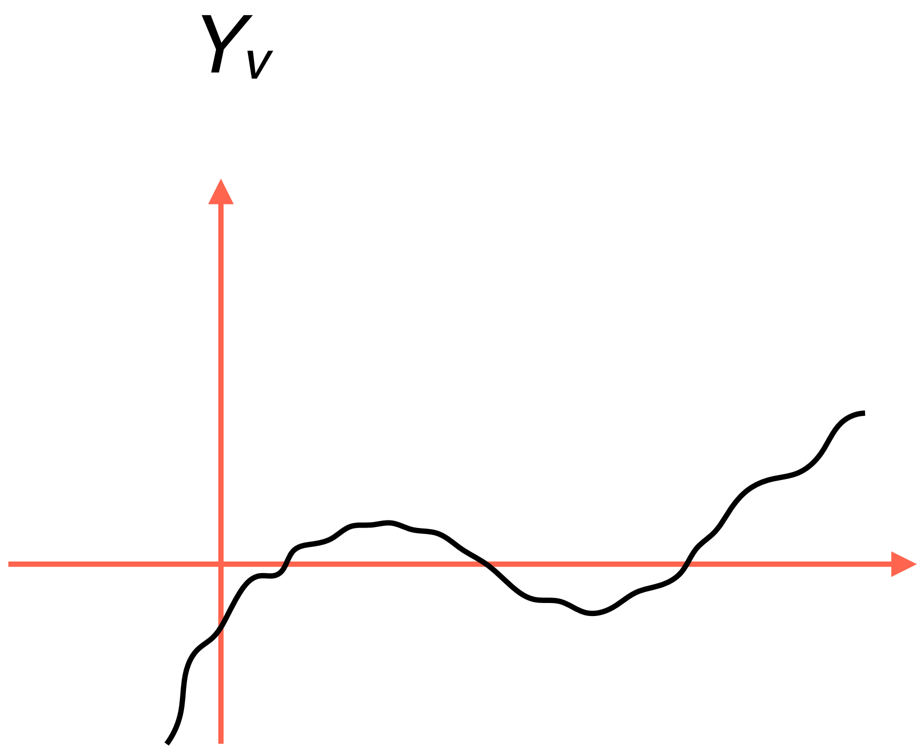

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Example: Time Series

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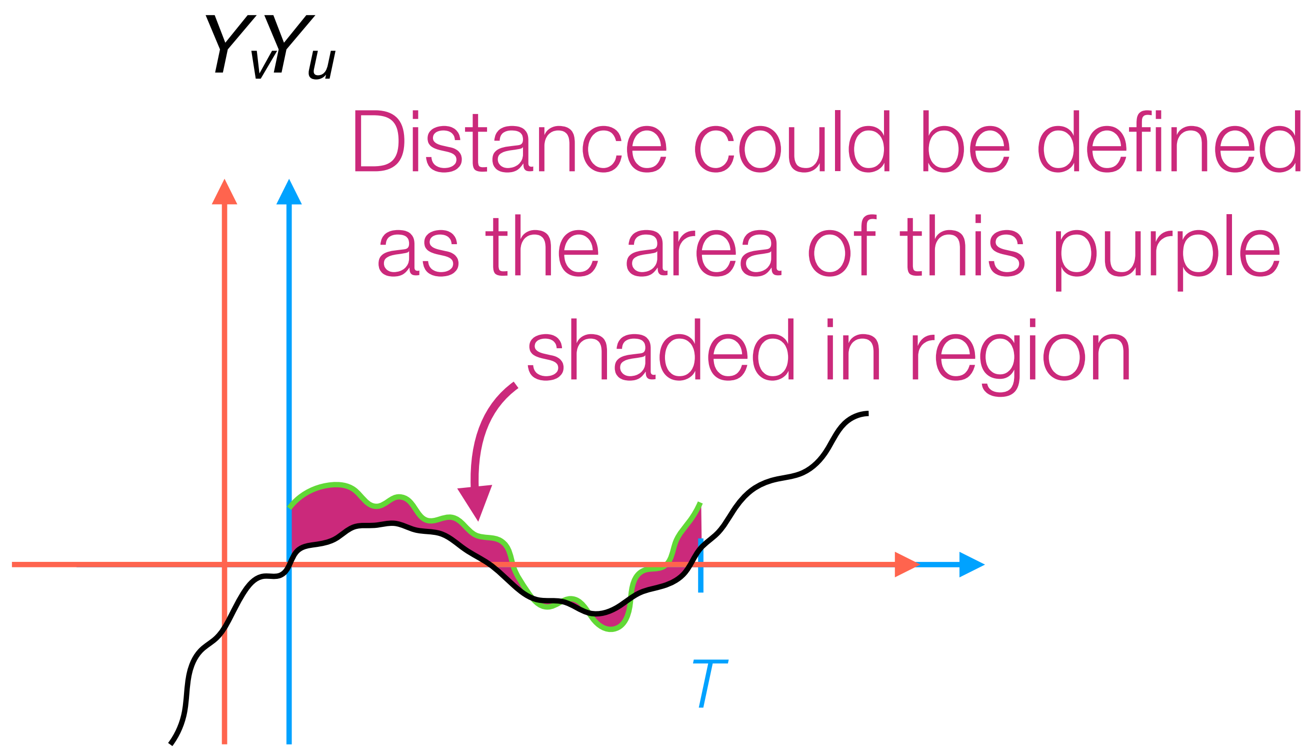


One solution: Align them first

In practice: for time series, very popular to use "dynamic time warping" to first align (it works kind of like how spell check does for words)

Similarity Diagnostics

- As you try different similarity functions, easy thing to check:
  - Pick any data point
  - Compute its similarity to all the other data points, and rank them in decreasing order from most similar to least similar
  - Inspect the top most similar data points — do they seem reasonable?

If the most similar points are not interpretable, it's quite likely that your similarity function isn't very good =(

Going from Similarities to Clusters

There's a whole zoo of clustering methods

Two main categories we'll talk about:

Generative models

1. Pretend data generated by specific model with parameters

2. Learn the parameters ("fit model to data")

3. Use fitted model to determine cluster assignments

We start here

Hierarchical clustering

Top-down: Start with everything in 1 cluster and decide on how to recursively split

Bottom-up: Start with everything in its own cluster and decide on how to iteratively merge clusters

We're going to start with perhaps the most famous of clustering methods

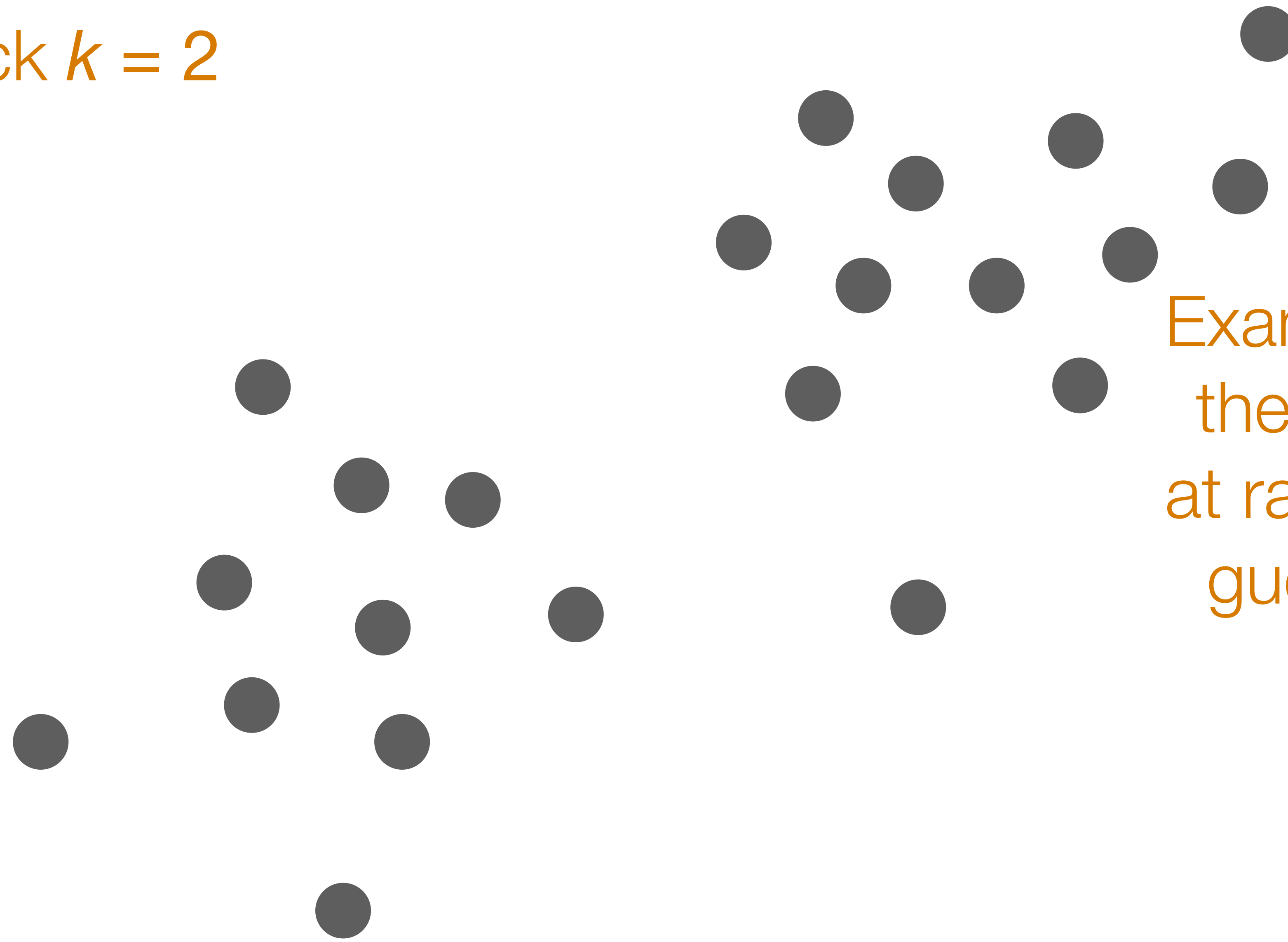
It won't yet be apparent what this method has to do with generative models

k-means

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

Step 0: Pick *k*

We'll pick $k = 2$



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

k-means

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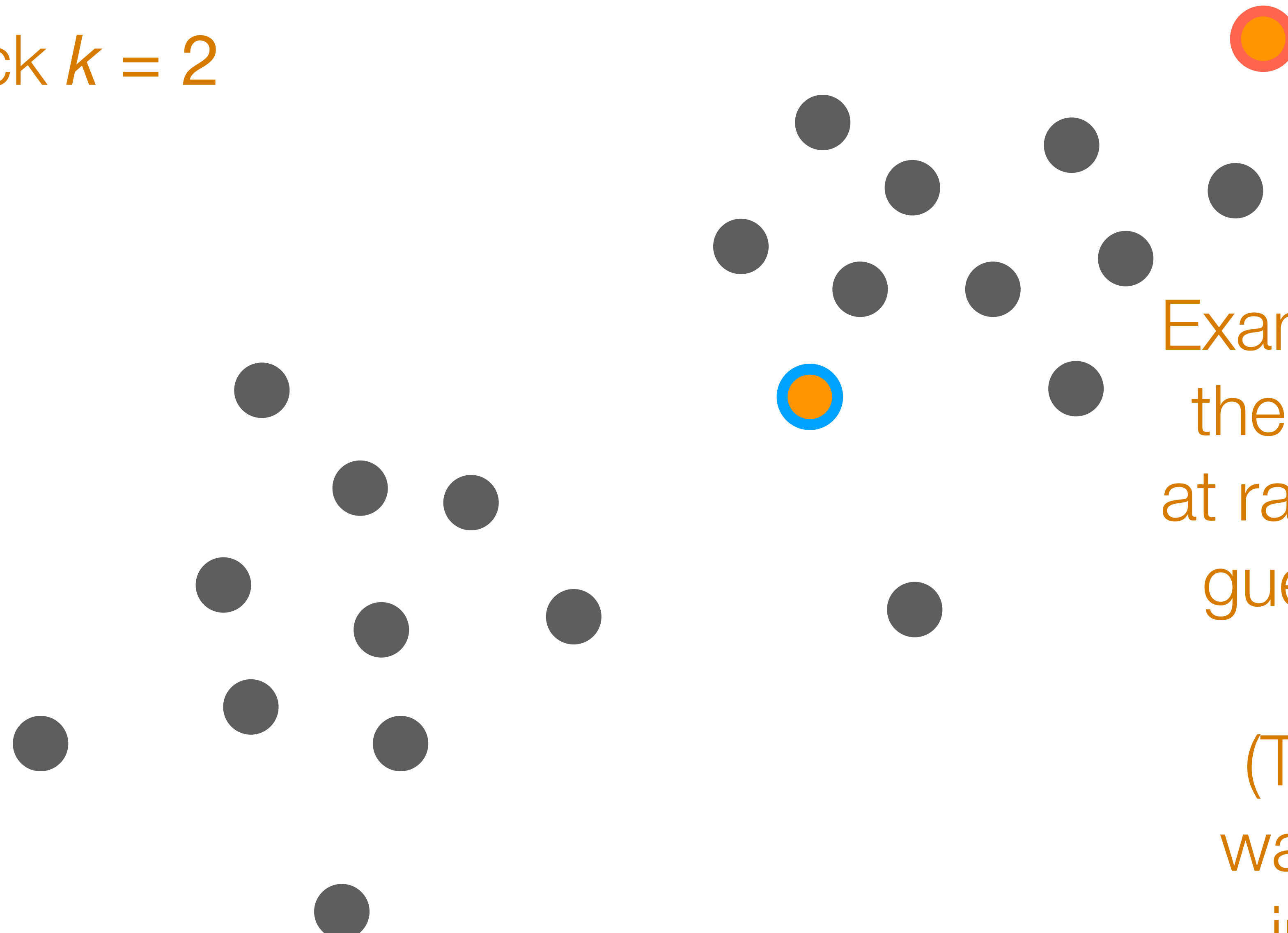

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(There are many ways to make the initial guesses)

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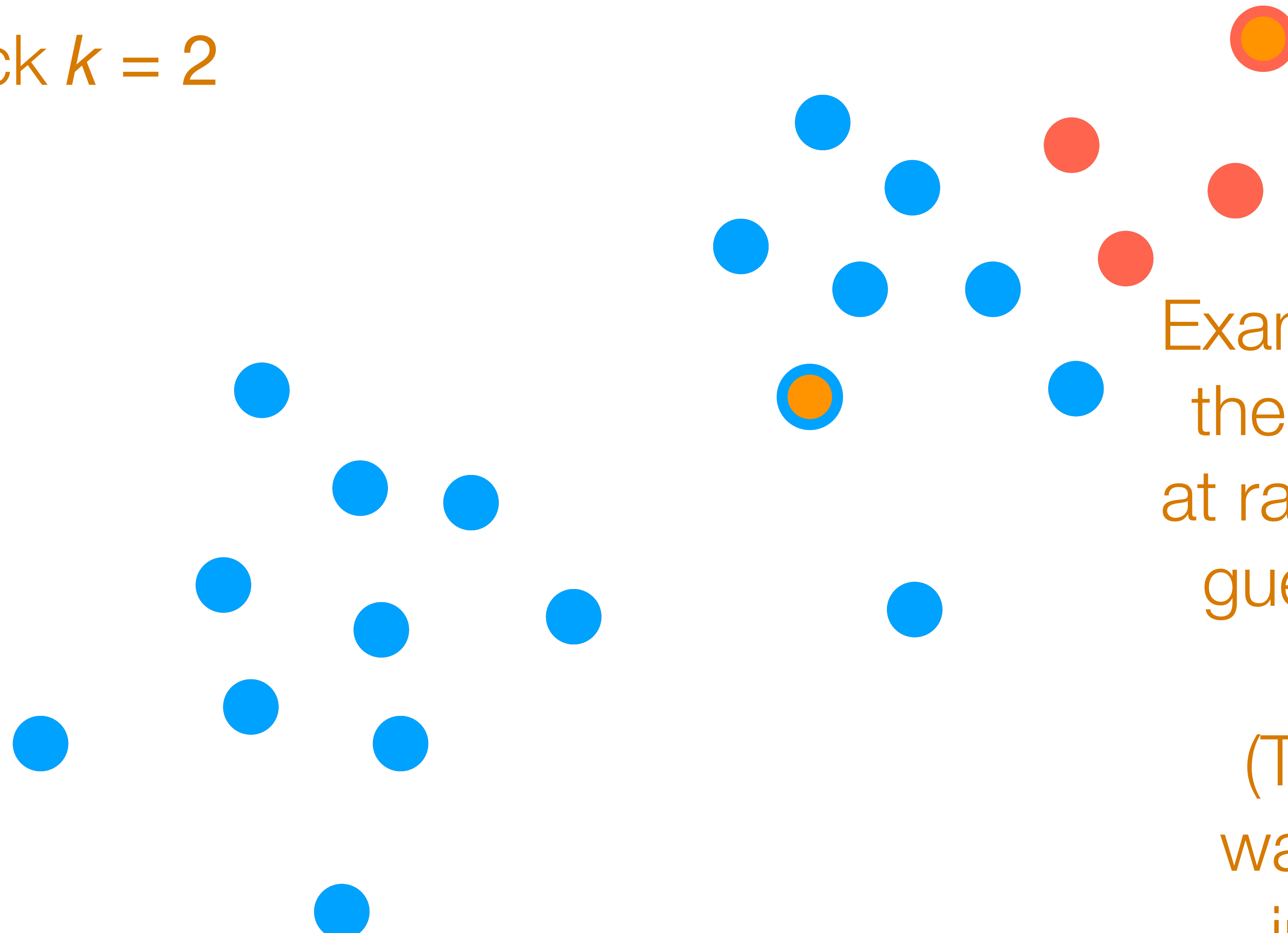

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Step 2: Assign each point to belong to the closest cluster

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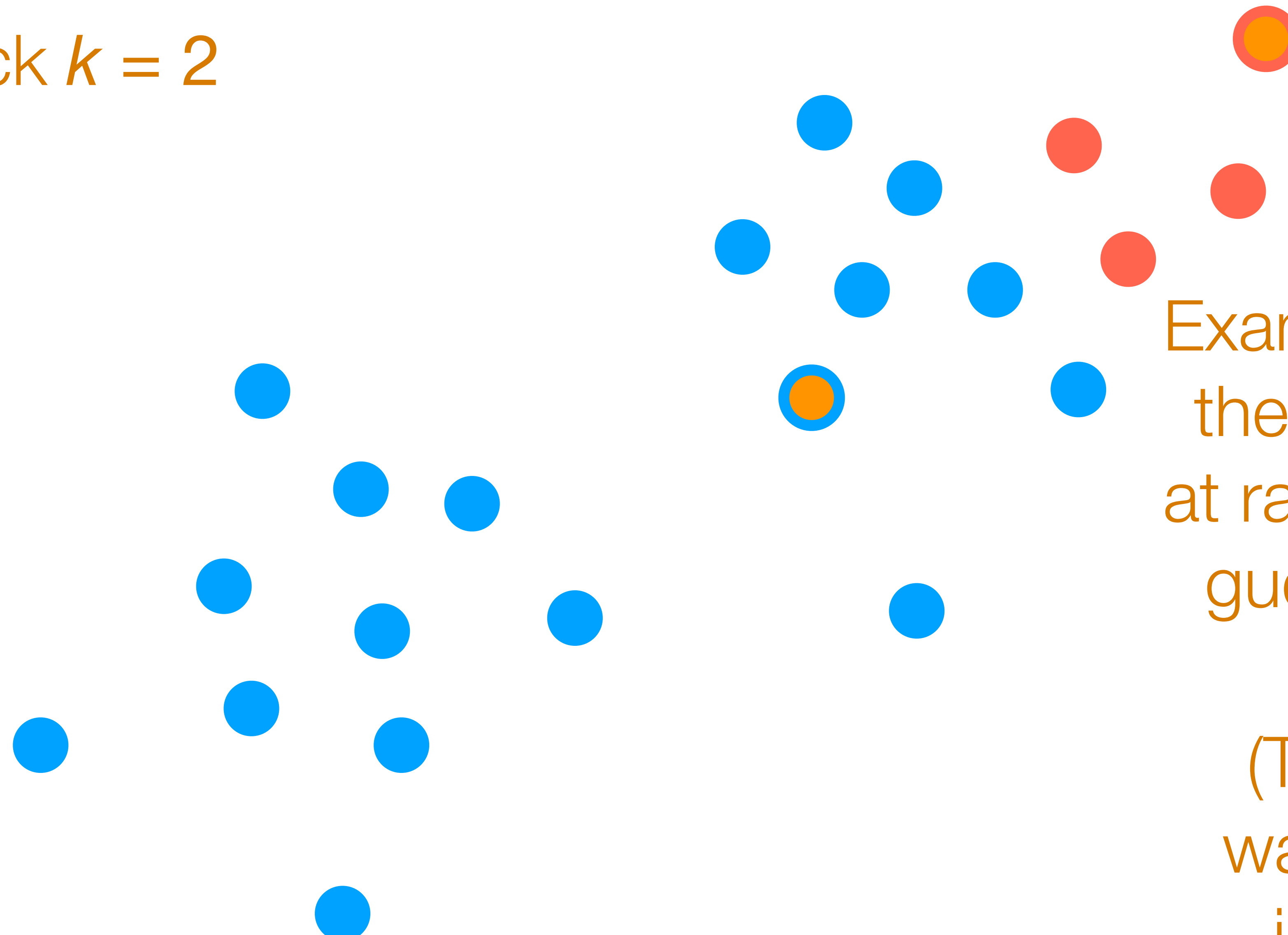

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Step 2: Assign each point to belong to the closest cluster

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

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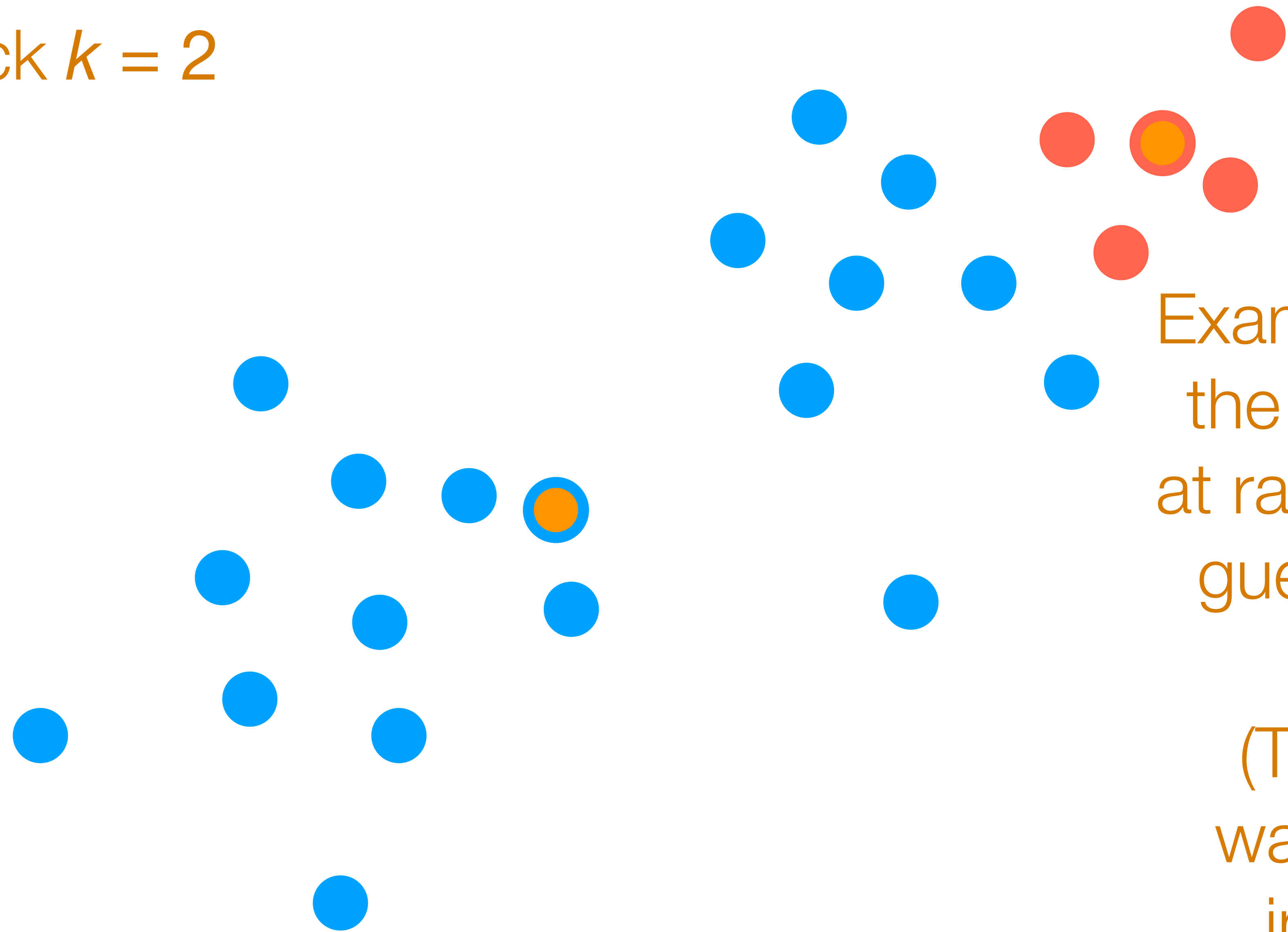

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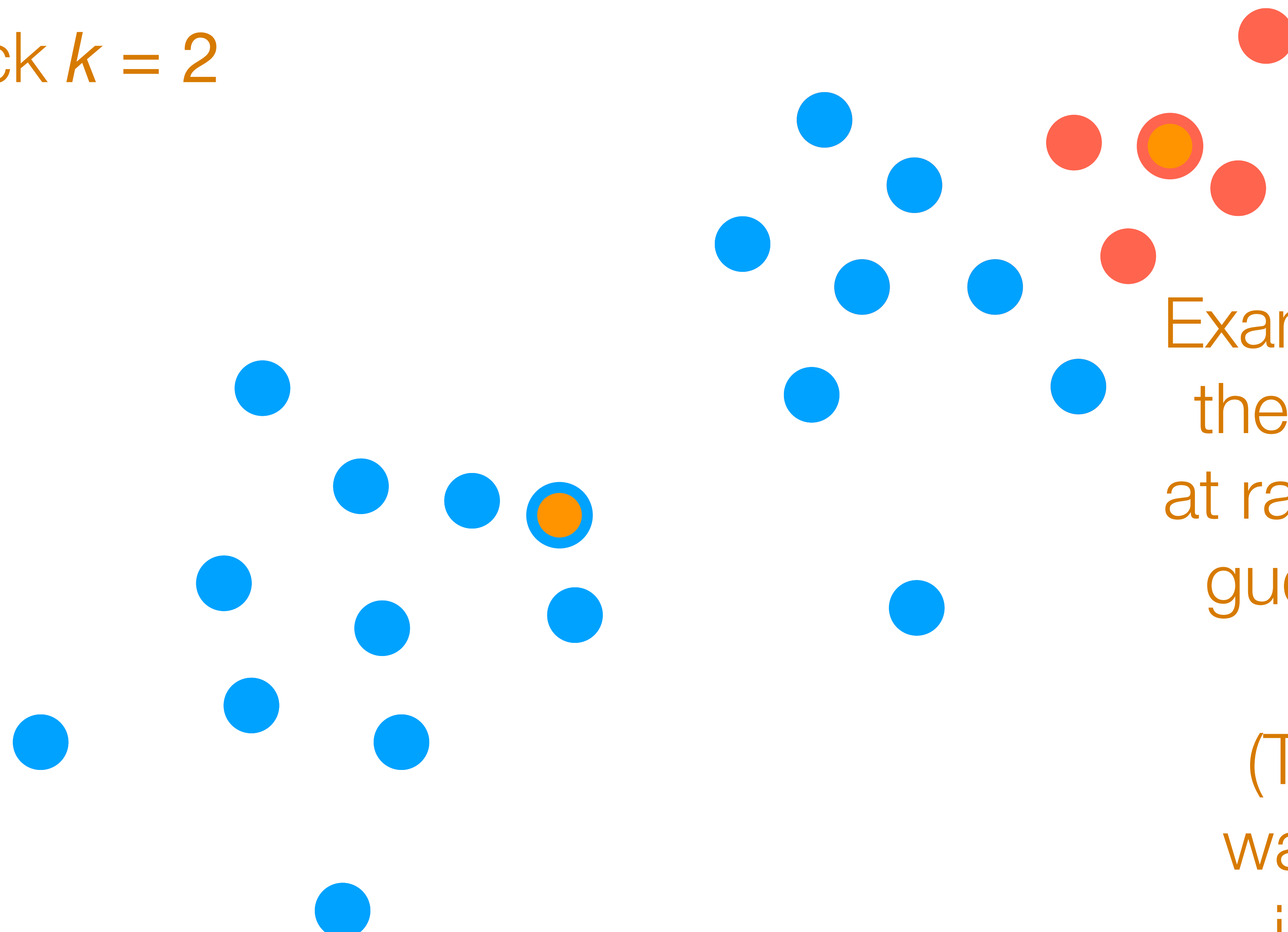

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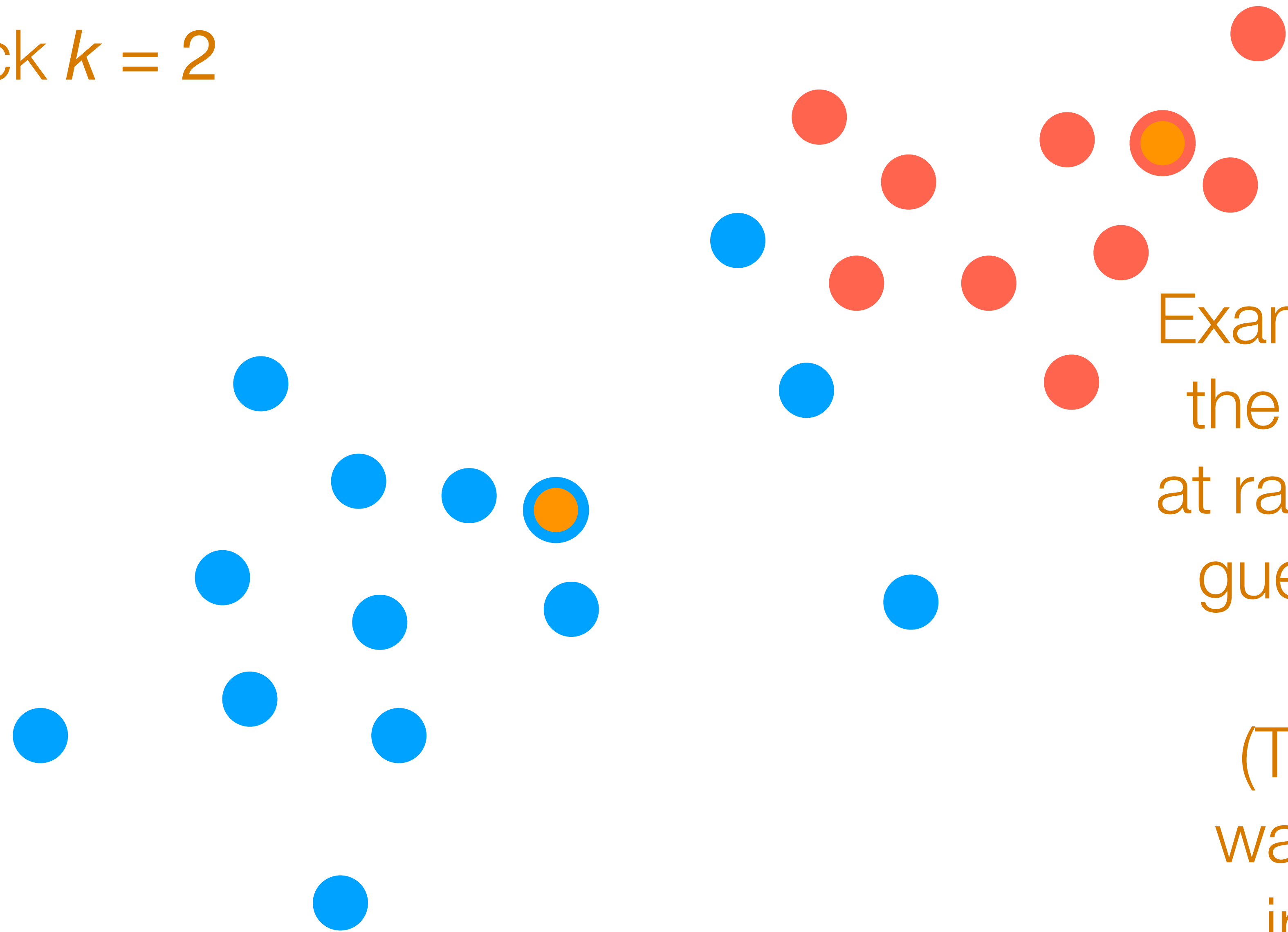

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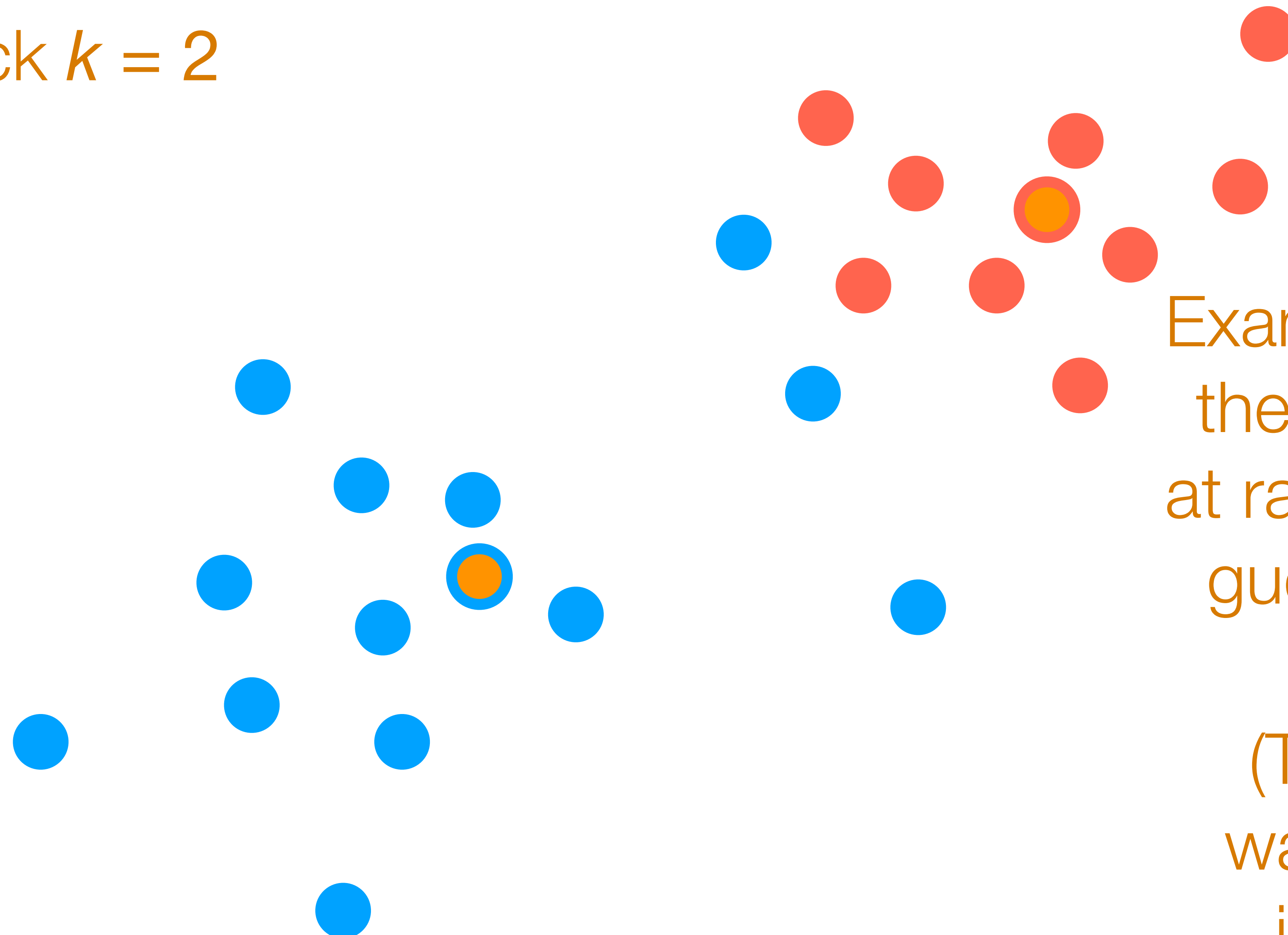

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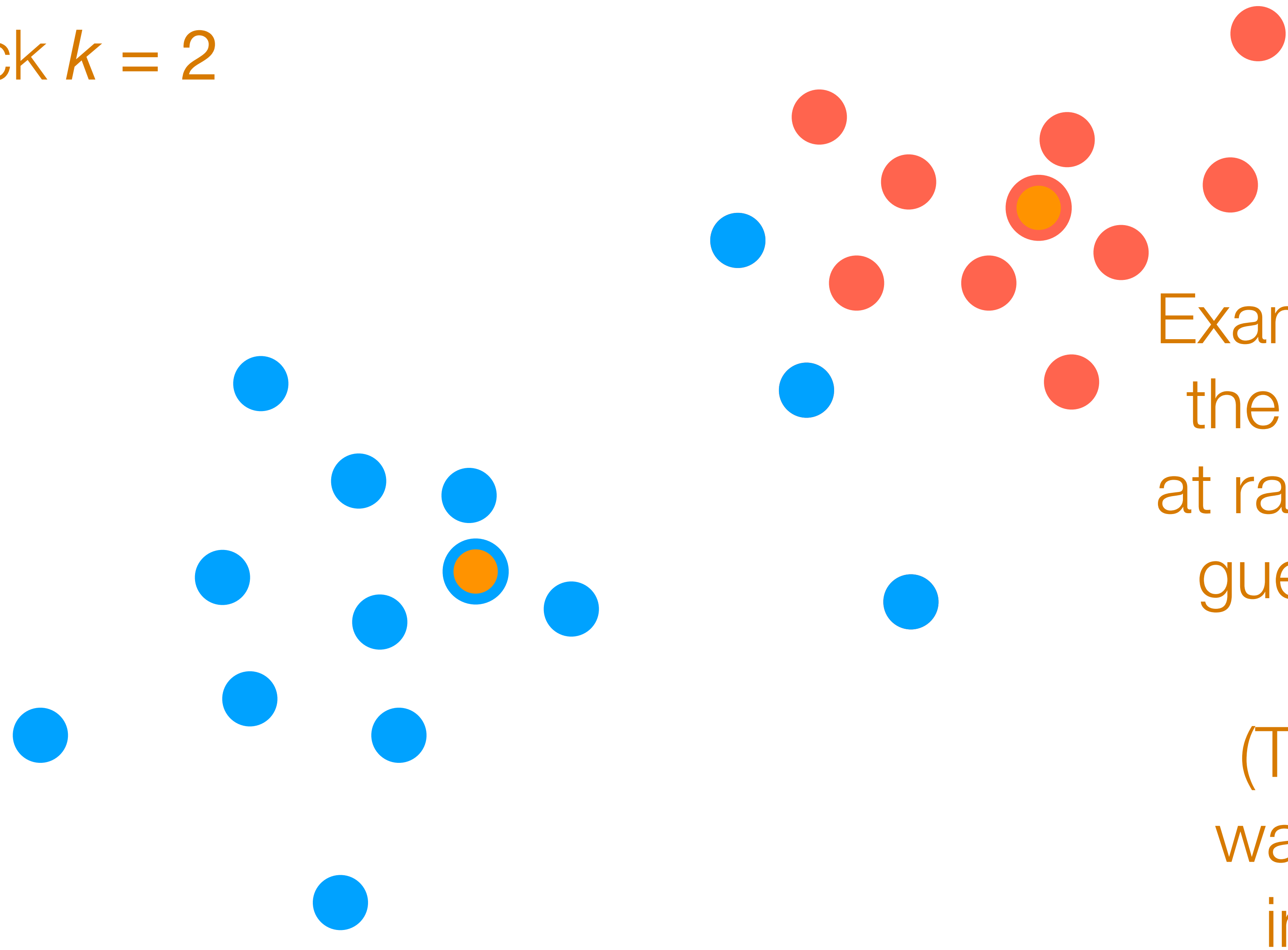

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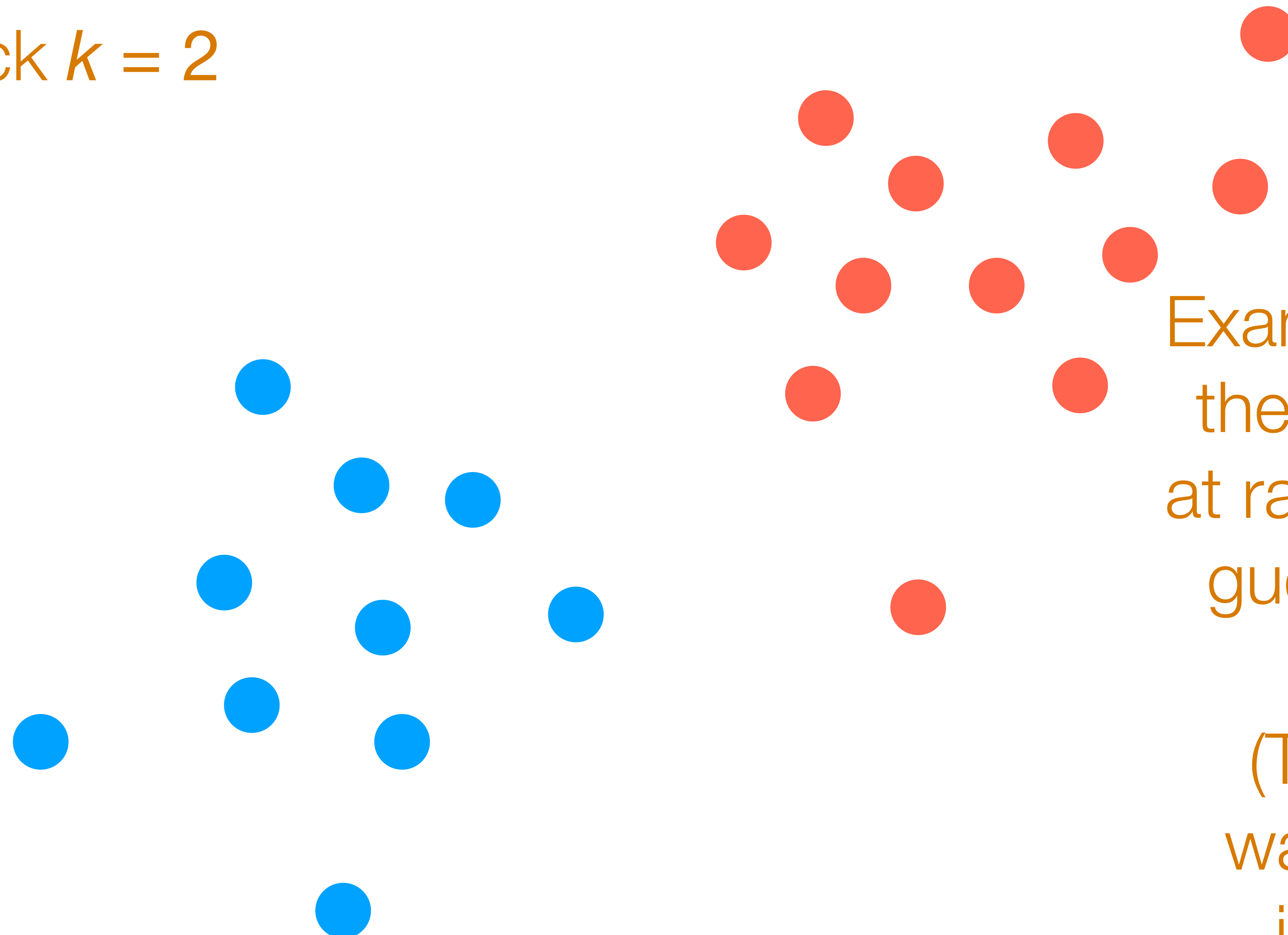

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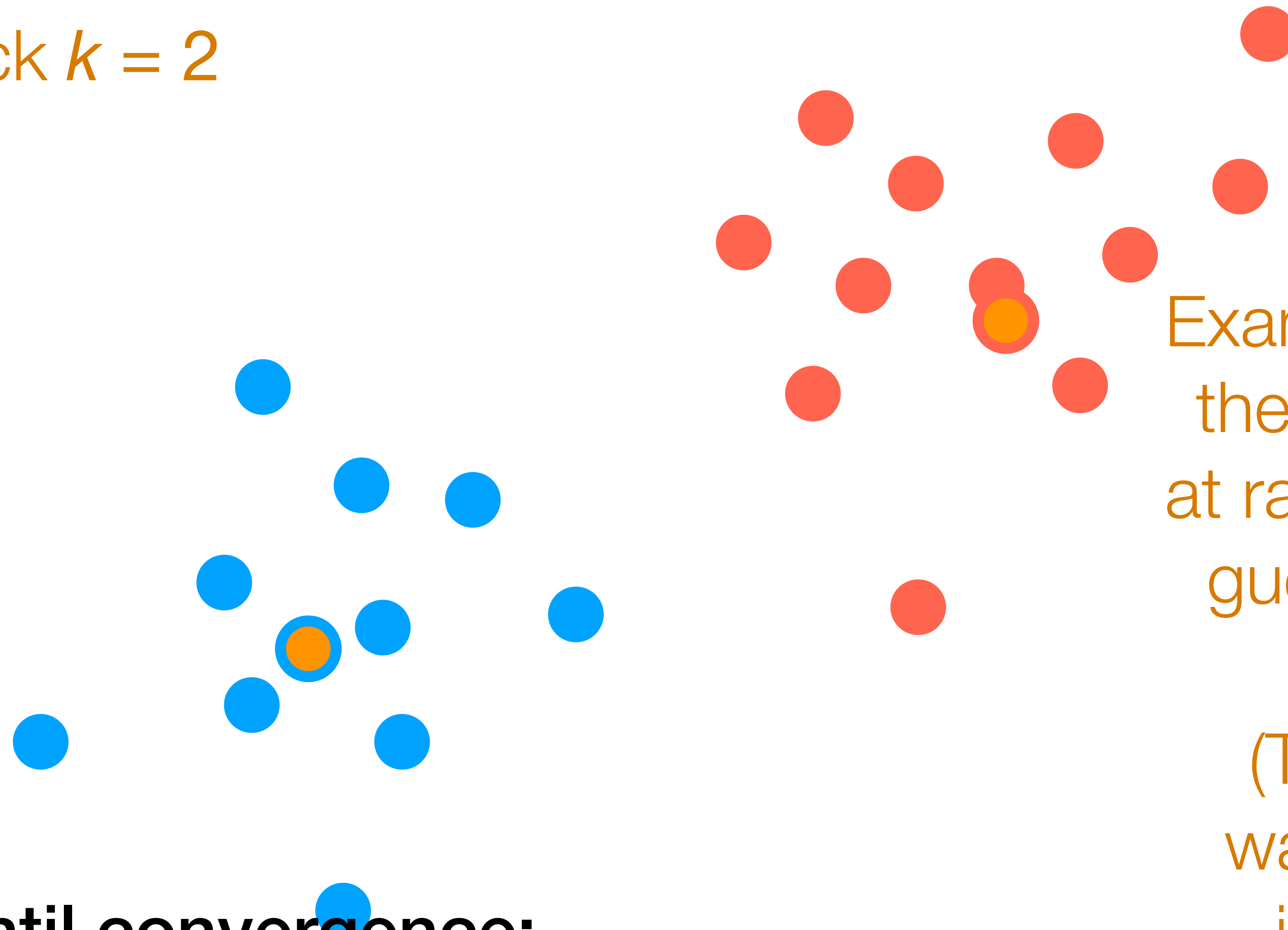

Example: choose *k* of the points uniformly at random to be initial guesses for cluster centers

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Repeat until convergence:

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

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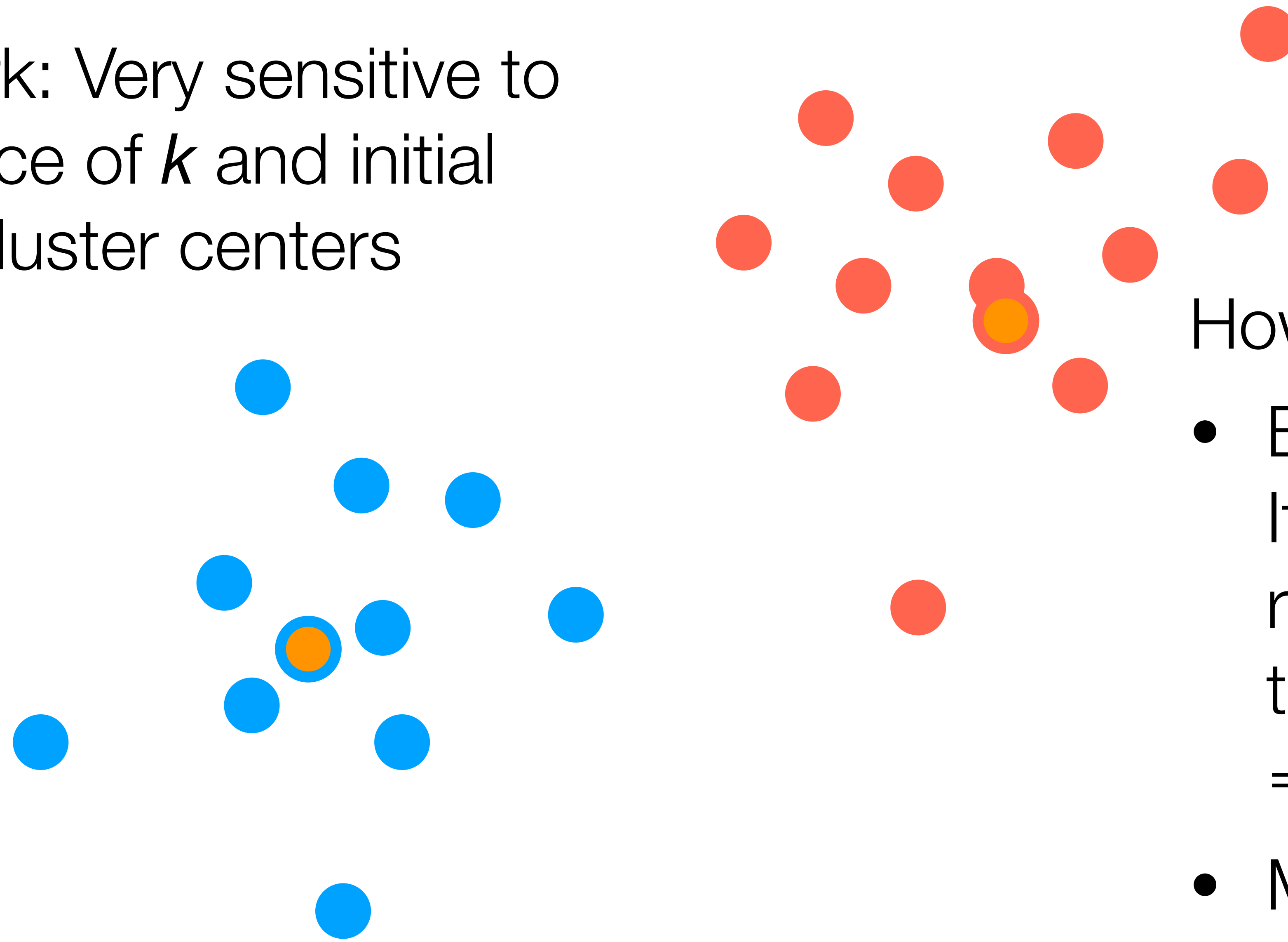
k-means

Final output: cluster centers, cluster assignment for every point

Remark: Very sensitive to choice of *k* and initial cluster centers



How to pick *k*?

- Basic check: If you have really, really tiny clusters $\Rightarrow$ decrease *k*
- More details later

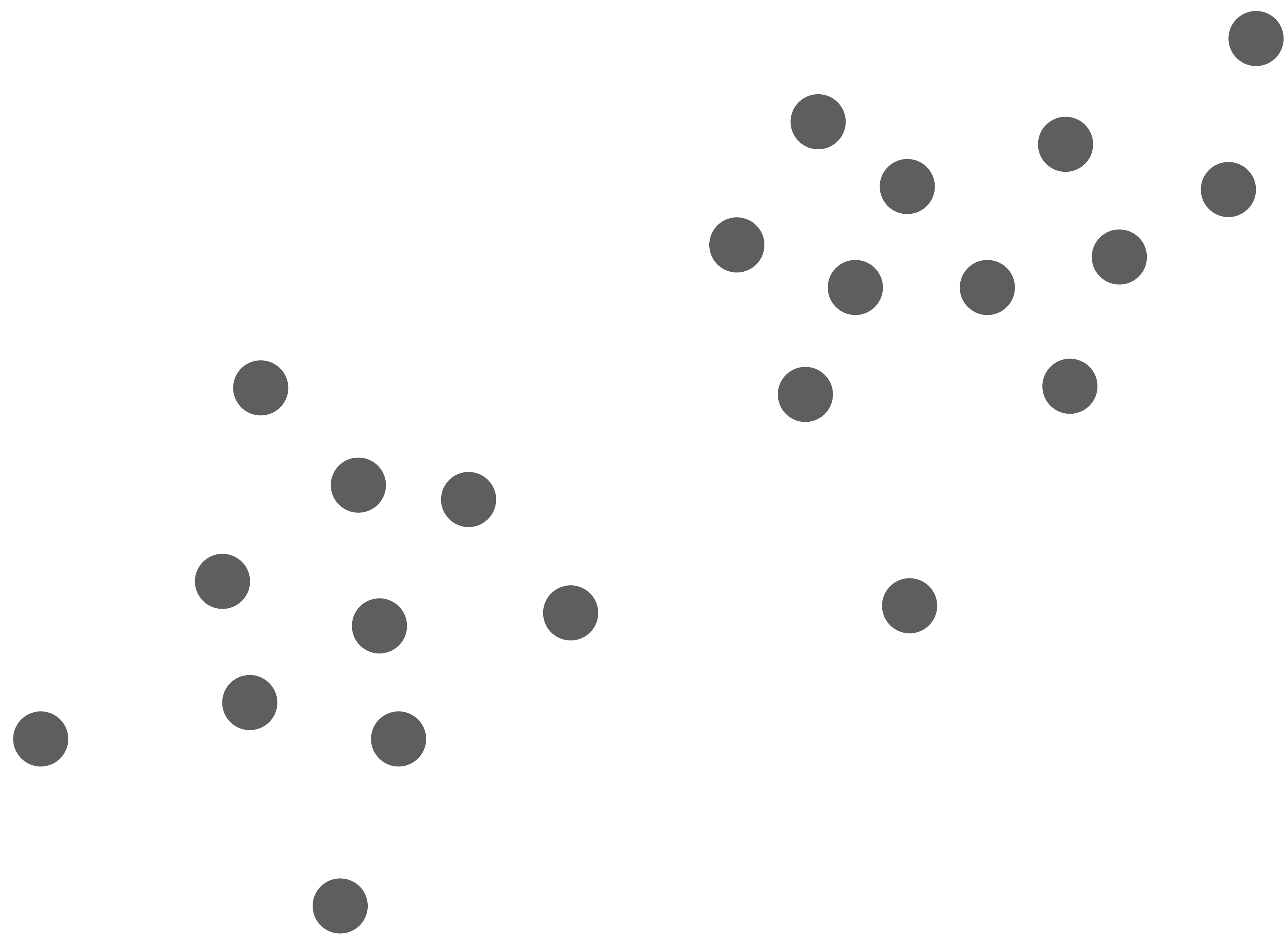
Suggested way to pick initial cluster centers: "*k*-means++" method

(rough intuition: incrementally add centers; favor adding center far away from centers chosen so far)

When does *k*-means work well?

k-means is related to a more general model, which will help us understand *k*-means

Gaussian Mixture Model (GMM)



What random process could have generated these points?

Generative Process

Think of flipping a coin

each outcome: heads or tails

Each flip doesn't depend on any of the previous flips

Generative Process

Think of flipping a coin

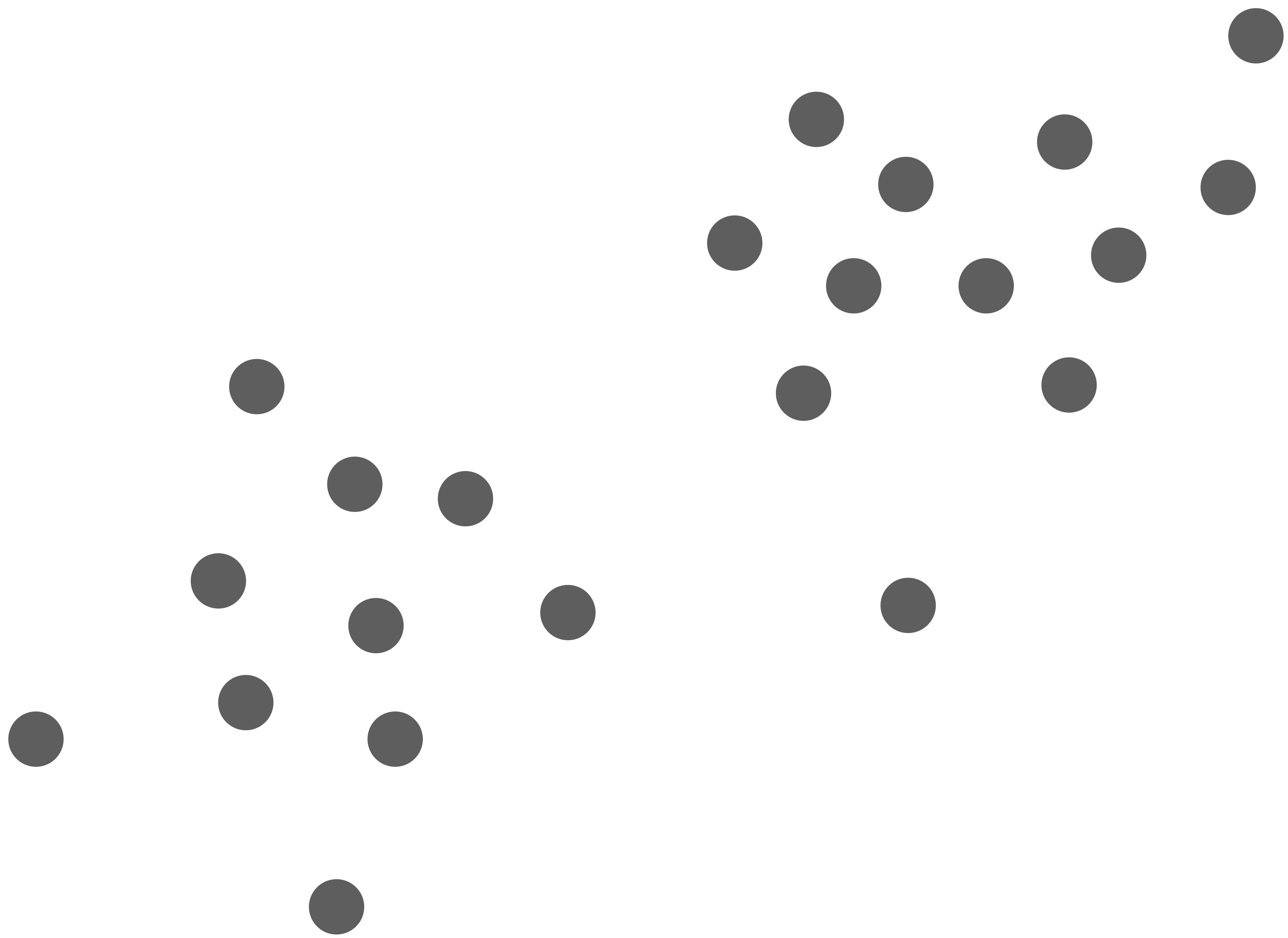
each outcome: 2D point

Each flip doesn't depend on any of the previous flips

Okay, maybe it's bizarre to think of it as a coin…

If it helps, just think of it as you pushing a button and a random 2D point appears…

Gaussian Mixture Model (GMM)



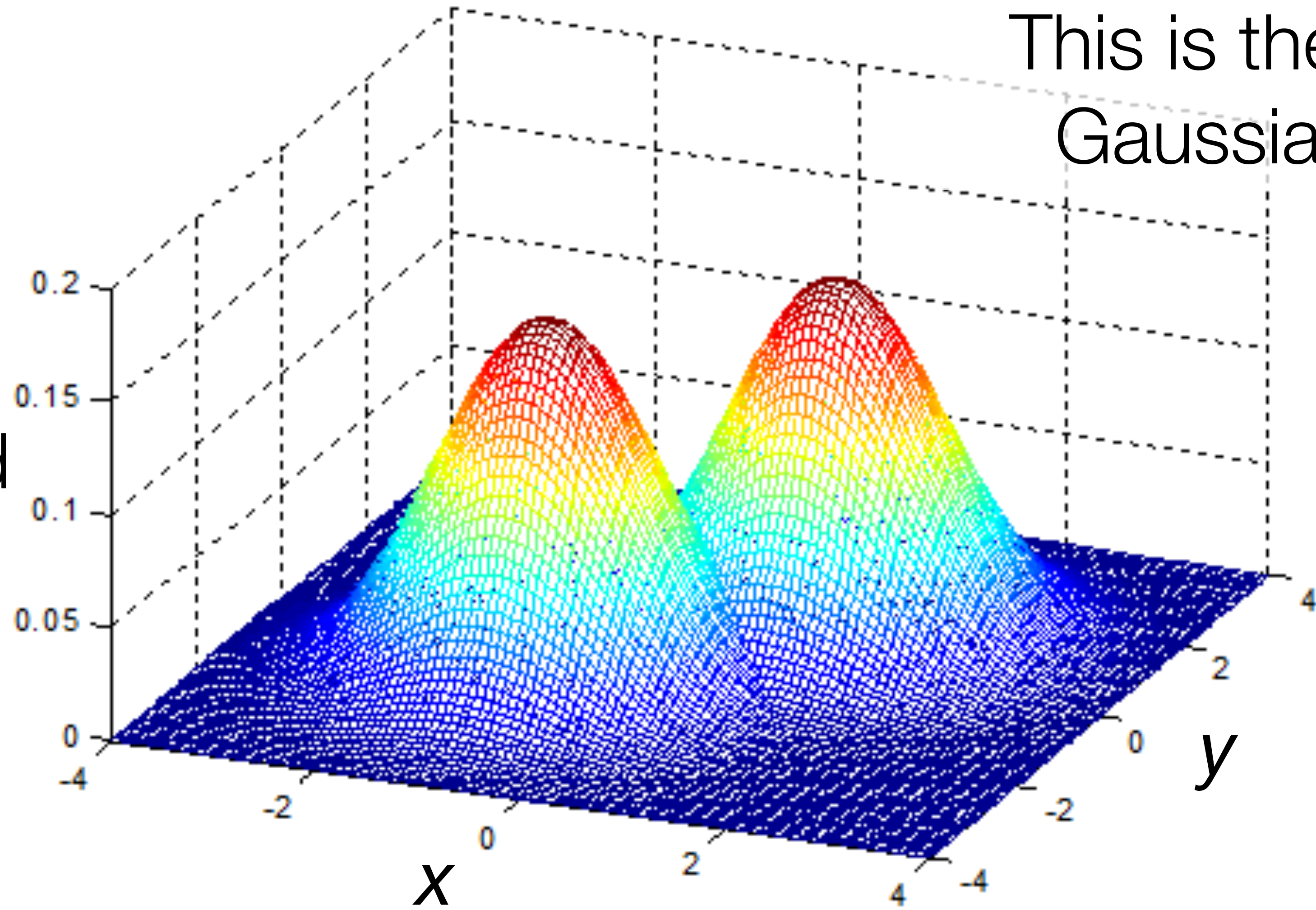
We now discuss a way to generate points in this manner

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



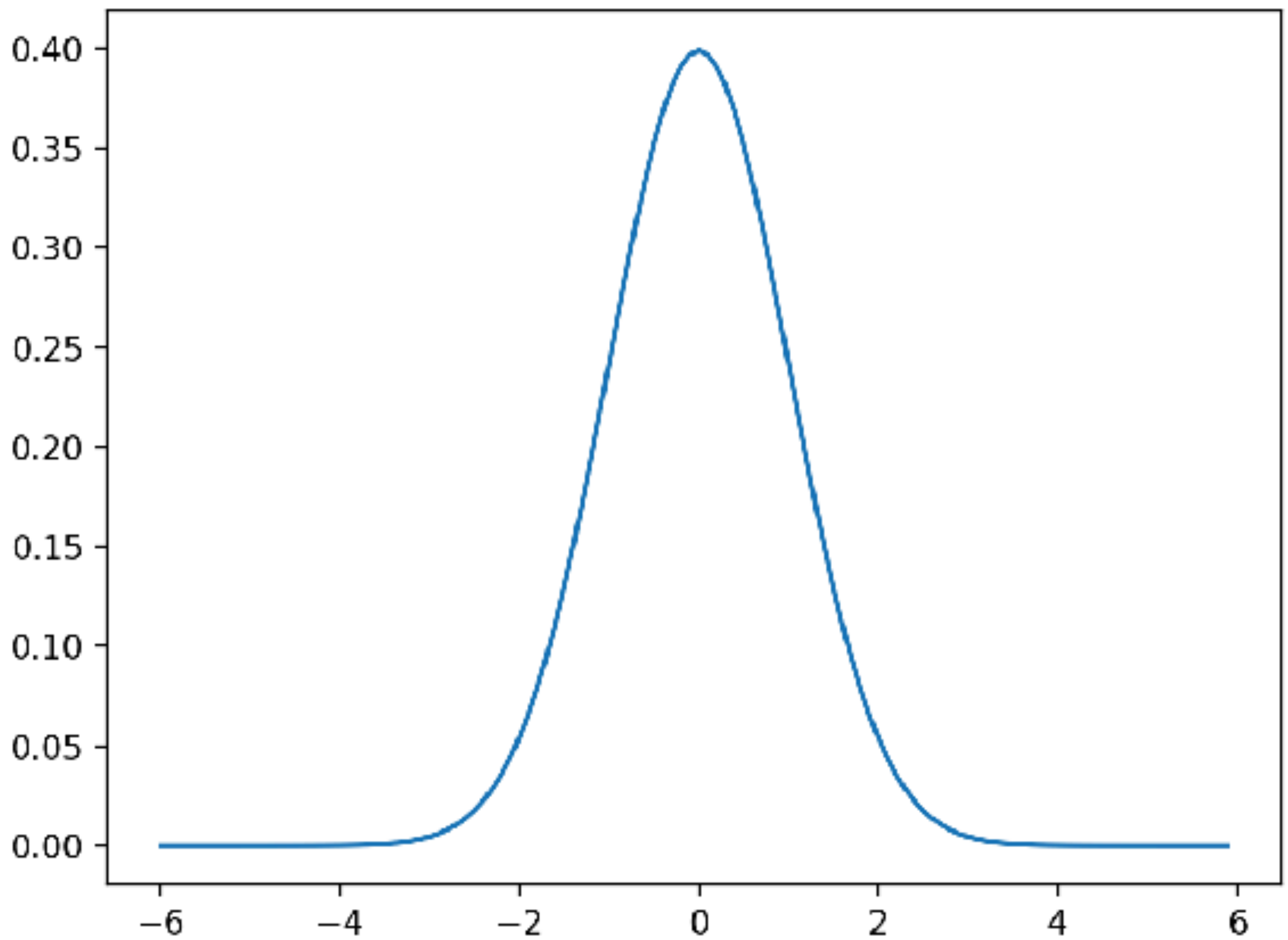
Red = more likely

Blue = less likely

Example of a 2D probability distribution

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

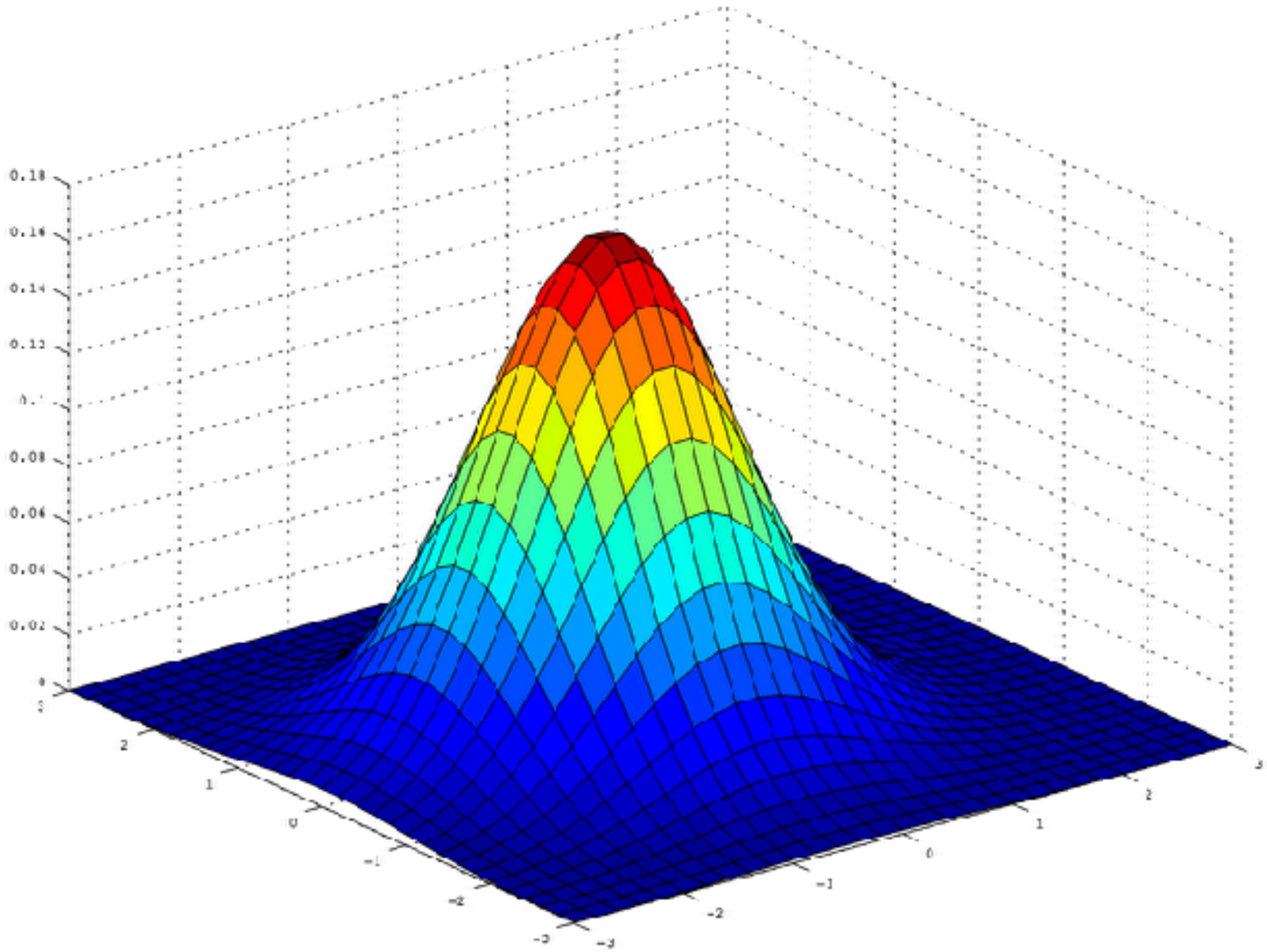
Quick Reminder: 1D Gaussian



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/OlWce.png

Gaussian Mixture Model (GMM)

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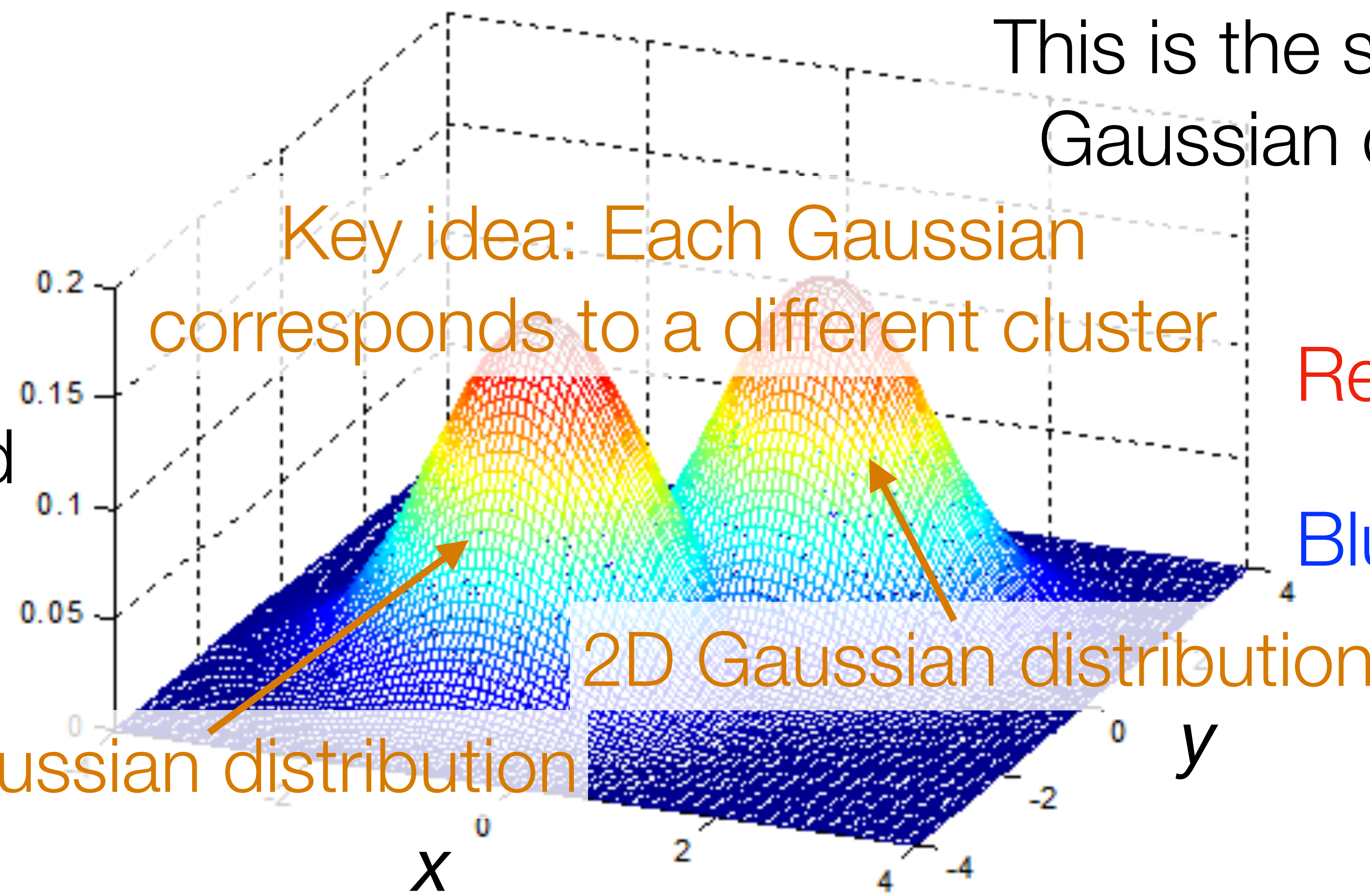

Red = more likely

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Example of a 2D probability distribution

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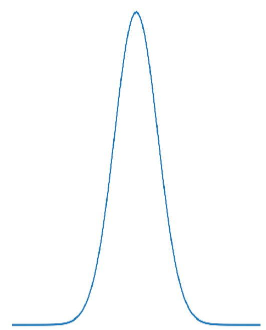
Gaussian Mixture Model (GMM)

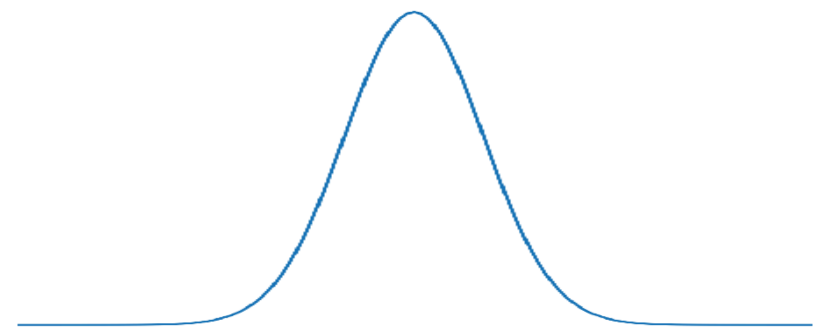
- For a fixed value *k* and dimension *d*, a GMM is the sum of *k* *d*-dimensional Gaussian distributions so that the overall probability distribution looks like *k* mountains (We've been looking at *d* = 2)
  - Each mountain corresponds to a different cluster
  - Different mountains can have different peak heights
  - One missing thing we haven't discussed yet: different mountains can have different shapes

2D Gaussian Shape

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



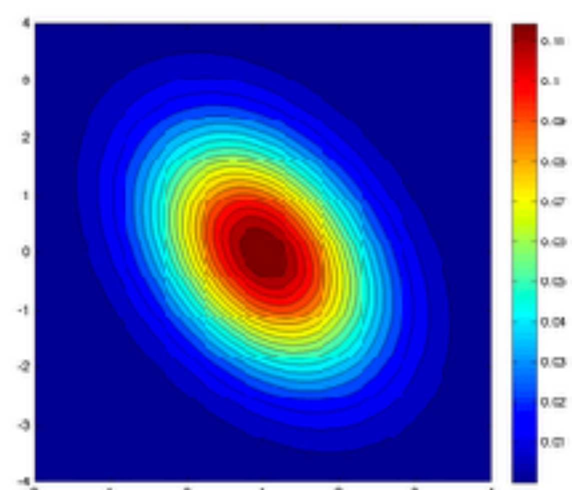
Less uncertainty



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

Gaussian Mixture Model (GMM)

- For a fixed value k and dimension d, a GMM is the sum of k d-dimensional Gaussian distributions so that the overall probability distribution looks like k mountains (We've been looking at $d = 2$)
  - Each mountain corresponds to a different cluster
  - Different mountains can have different peak heights
  - Different mountains can have different ellipse shapes (captures "covariance" information)

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 this looks like?

Example: 1D GMM with 2 Clusters

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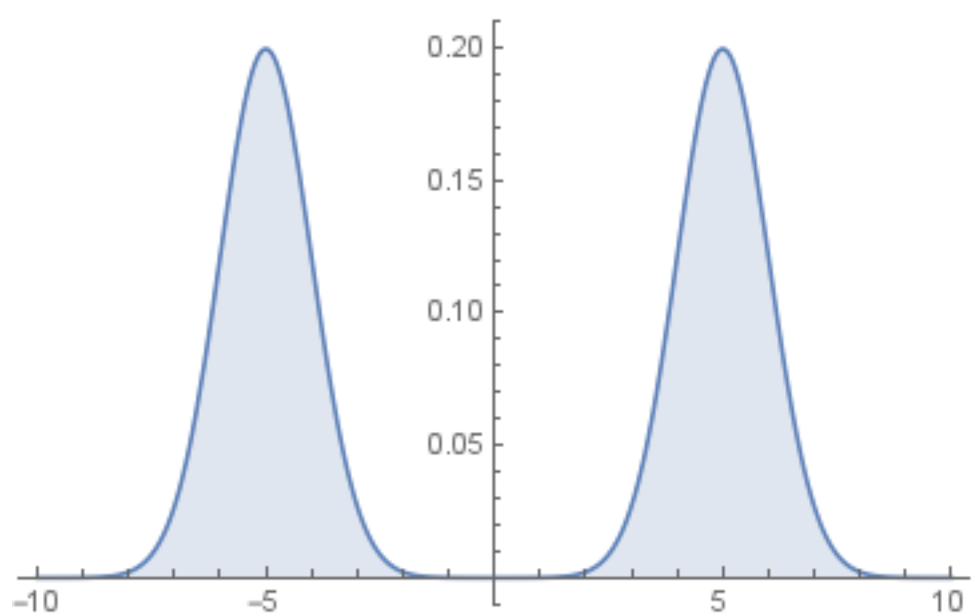

Example: 1D GMM with 2 Clusters

<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 this looks like?

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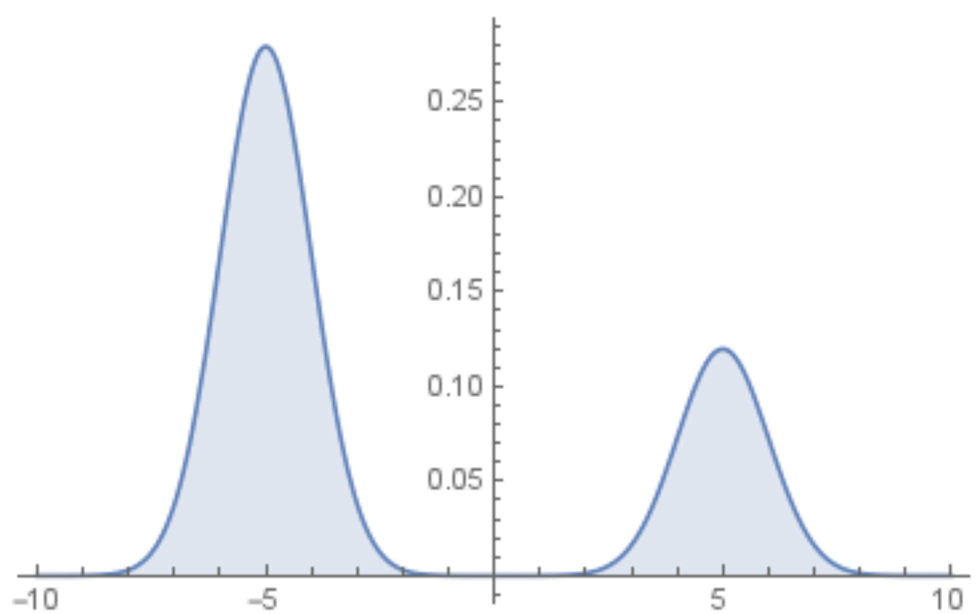

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<u>Cluster 2</u>

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 = π_1

Gaussian mean = μ_1

Gaussian std dev = σ_1

<u>Cluster 2</u>

Probability of generating a point from cluster 2 = π_2

Gaussian mean = μ_2

Gaussian std dev = σ_2

How to generate 1D points from this GMM:

1. Flip biased coin (with probability of heads π_1)
2. If heads: sample 1 point from Gaussian mean μ_1, std dev σ_1

   If tails: sample 1 point from Gaussian mean μ_2, std dev σ_2

Example: 1D GMM with *k* Clusters

Cluster 1		Cluster k
Probability of generating a point from cluster 1 = π_1	…	Probability of generating a point from cluster k = π_k
Gaussian mean = μ_1		Gaussian mean = μ_k
Gaussian std dev = σ_1		Gaussian std dev = σ_k

How to generate 1D points from this GMM:

1. Flip biased k-sided coin (the sides have probabilities $\pi_1, \ldots, \pi_k$)
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, std dev σ_Z

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:

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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, std dev σ_Z

Example: 2D GMM with k Clusters

Cluster 1

Probability of generating a point from cluster 1 = π_1

Gaussian mean = μ_1 2D point

Gaussian **covariance** = Σ_1

2x2 matrix

…

Cluster k

Probability of generating a point from cluster k = π_k

Gaussian mean = μ_k 2D point

Gaussian **covariance** = Σ_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, …, k)
3. Sample 1 point from Gaussian mean μ_Z, **covariance** Σ_Z

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

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

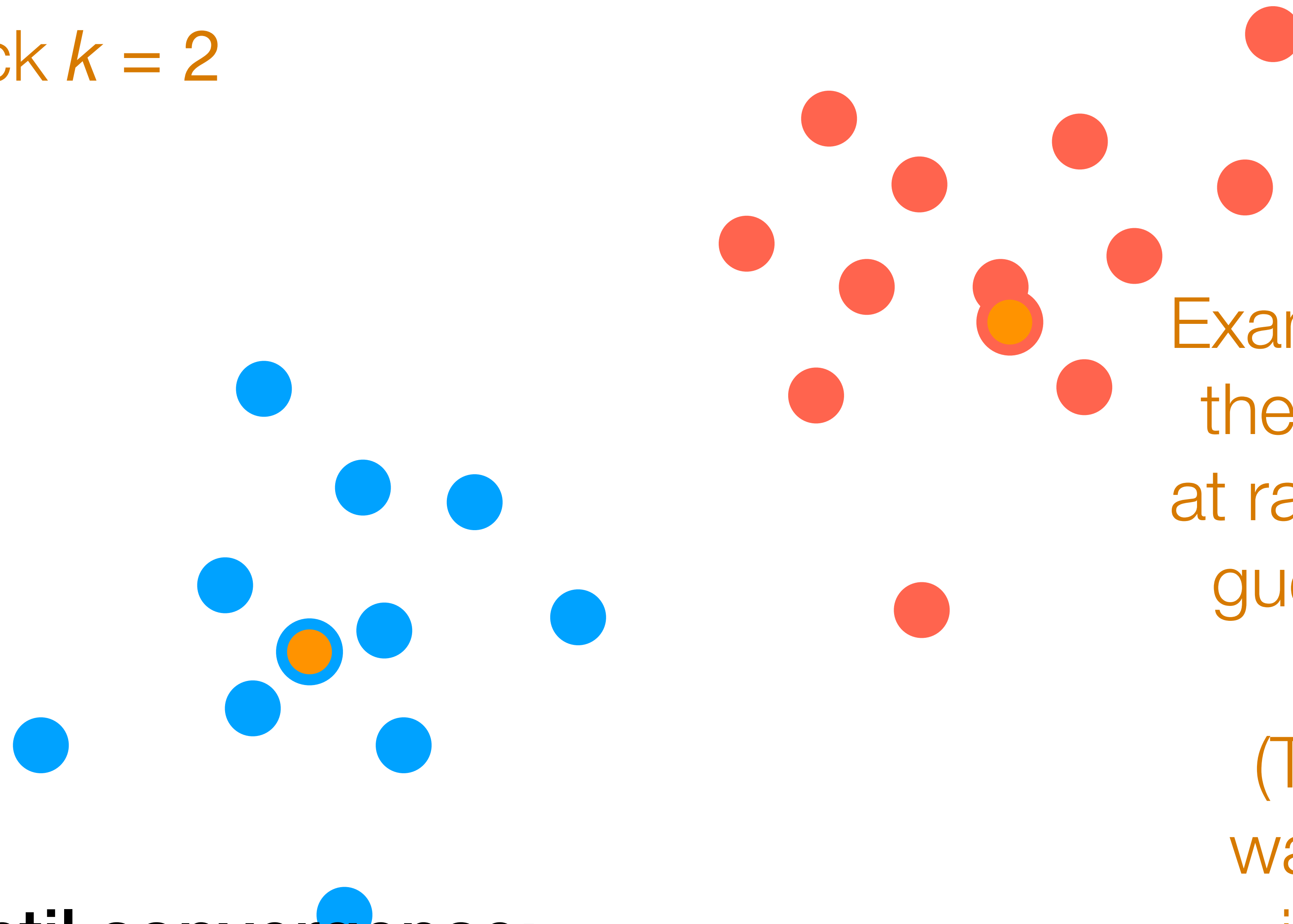
How do you turn this into a cluster assignment?

k-means

Step 0: Pick *k*

We'll pick $k = 2$

Step 1: Pick <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

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where cluster centers are

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(Rough Intuition) Learning a GMM

Step 0: Pick k

Step 1: Pick <u>guesses</u> for **cluster means and covariances**

Repeat until convergence:

Step 2: Compute probability of each point 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

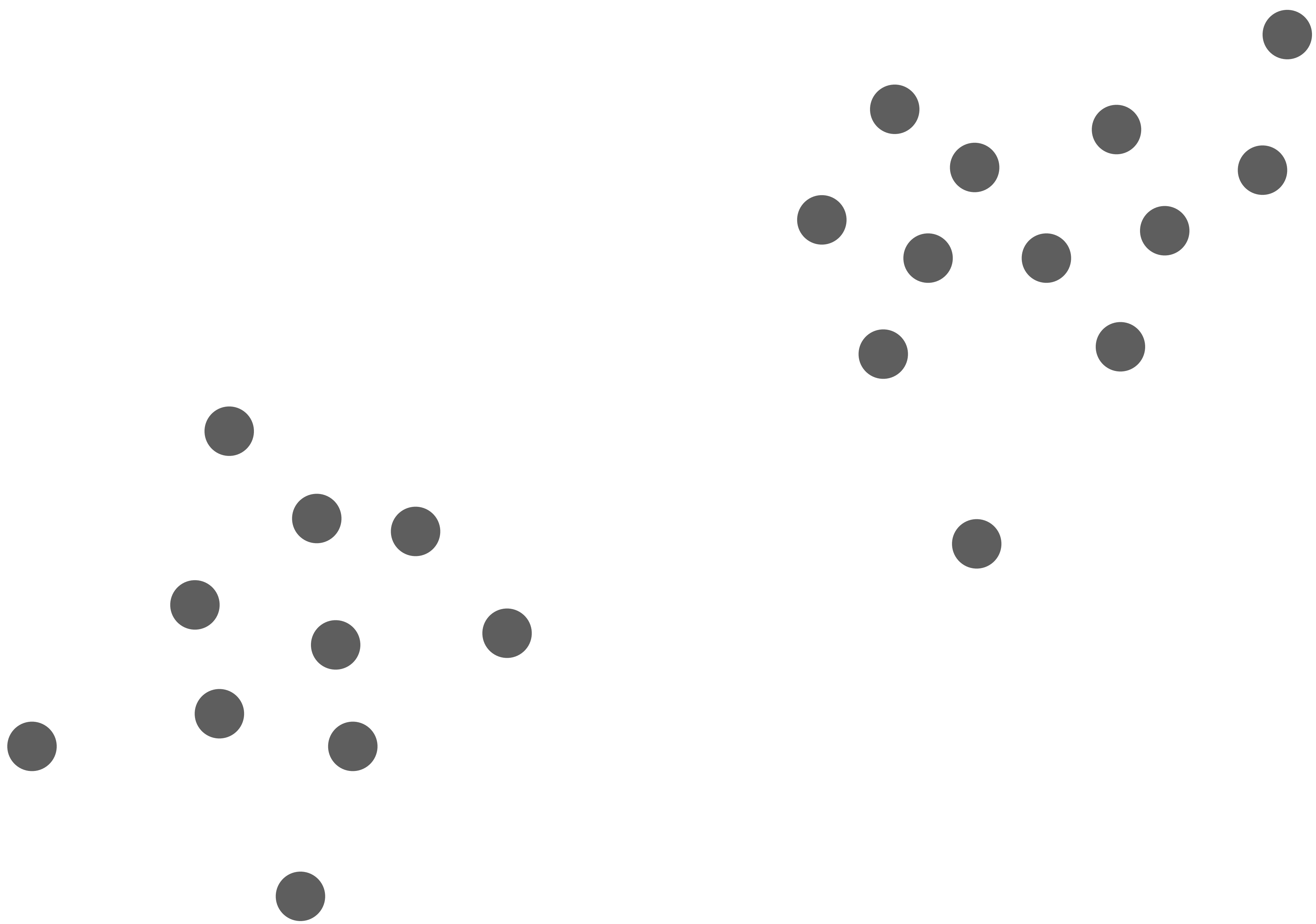
If the ellipses are all circles and have the same "skinniness" (e.g., in the 1D case it means they all have same std dev):

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

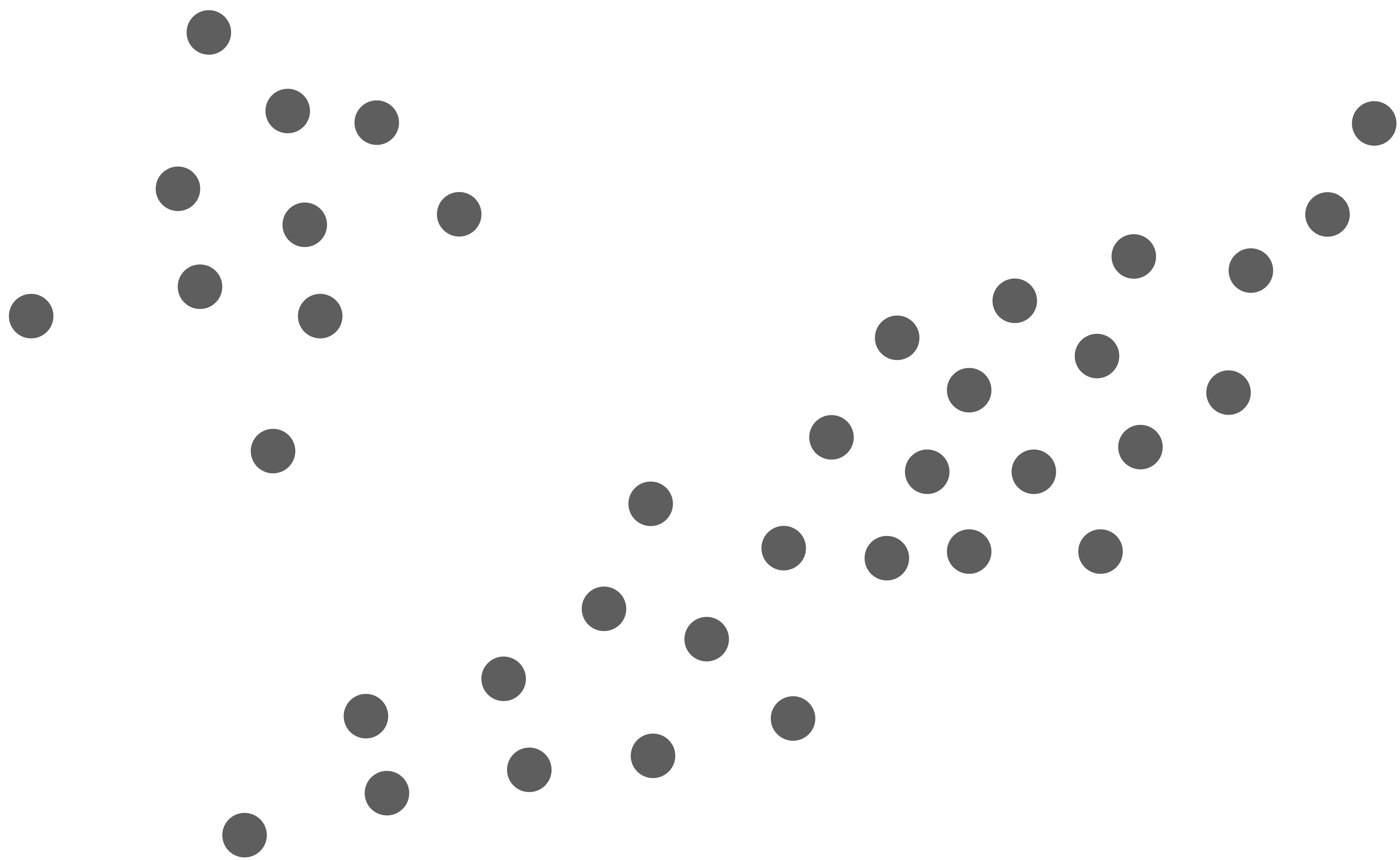
- Notice that *k*-means does a "hard" assignment of each point to a cluster, whereas the EM algorithm does a "soft" (probabilistic) assignment of each point to a cluster

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



Learning a GMM

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

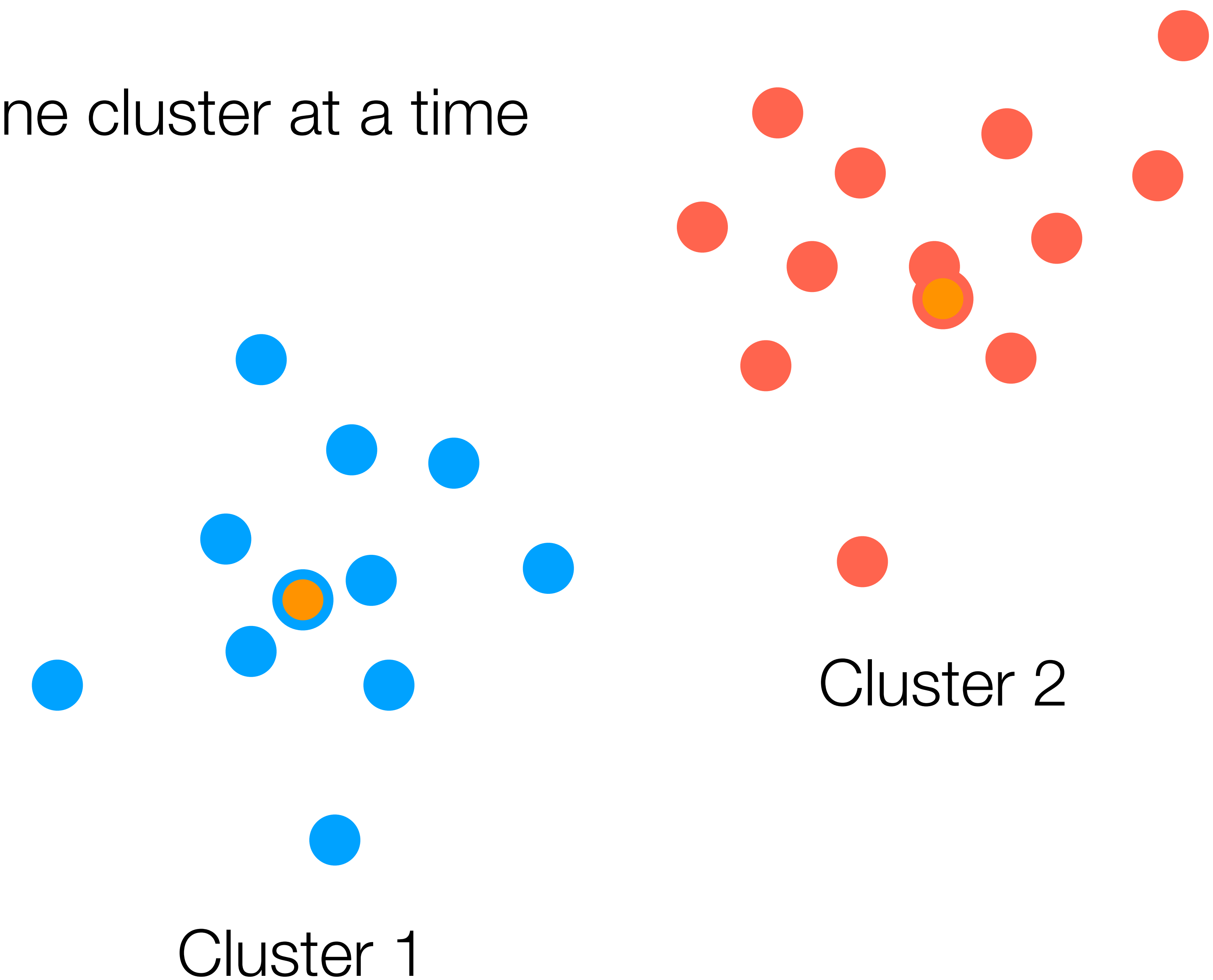
No single way of choosing k is the "best" way

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

But hey it’s worth a shot

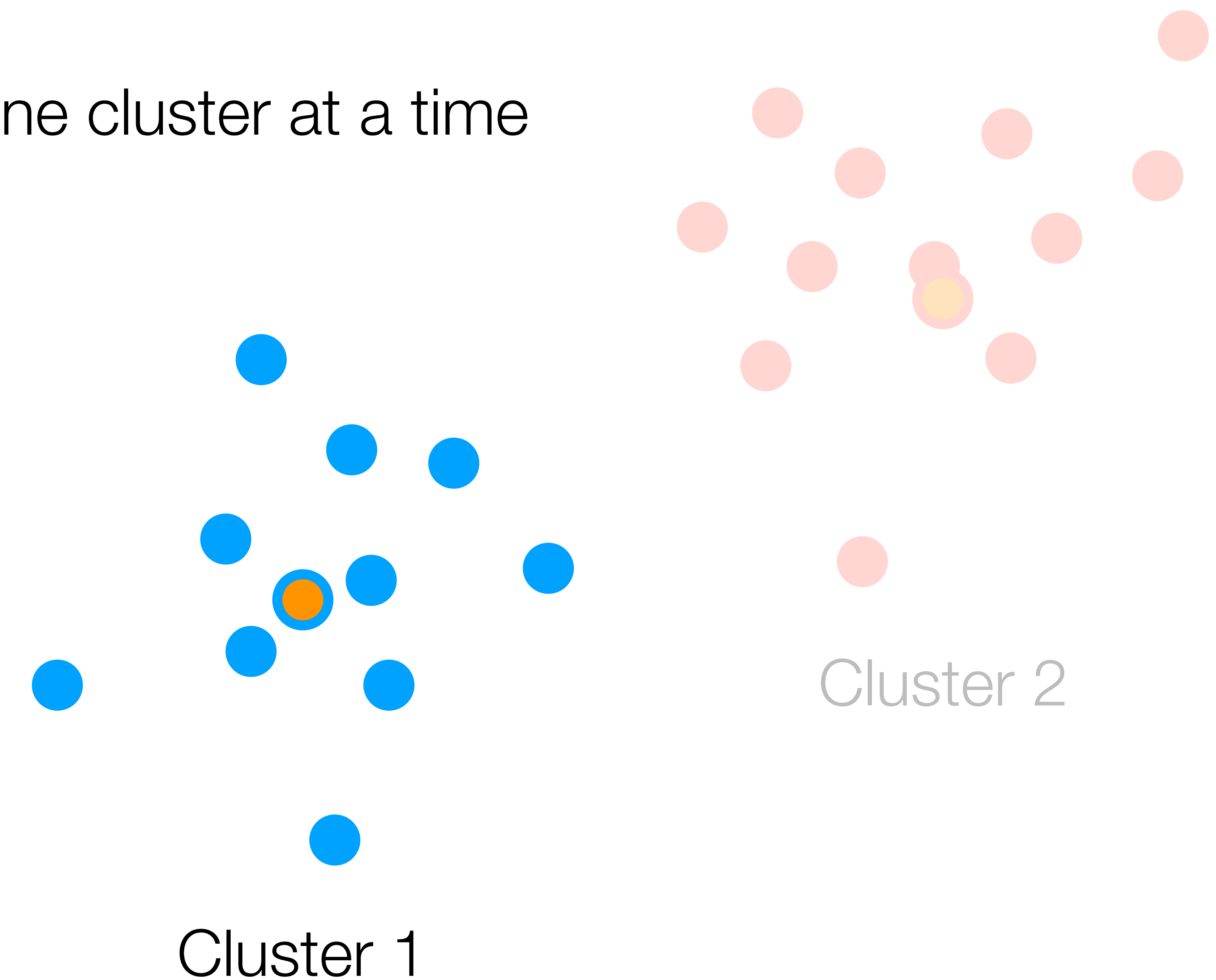
Residual Sum of Squares

Look at one cluster at a time



Residual Sum of Squares

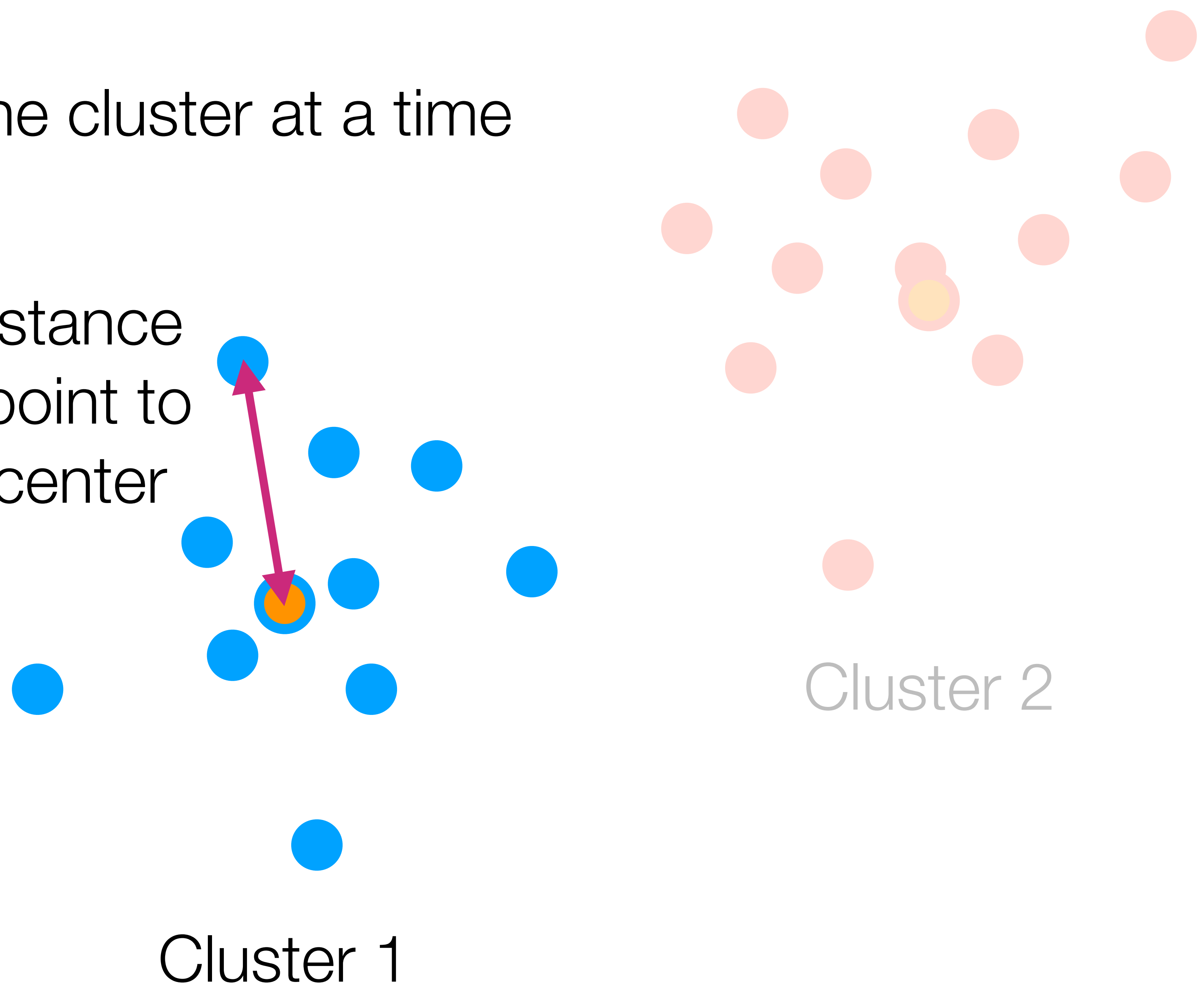
Look at one cluster at a time



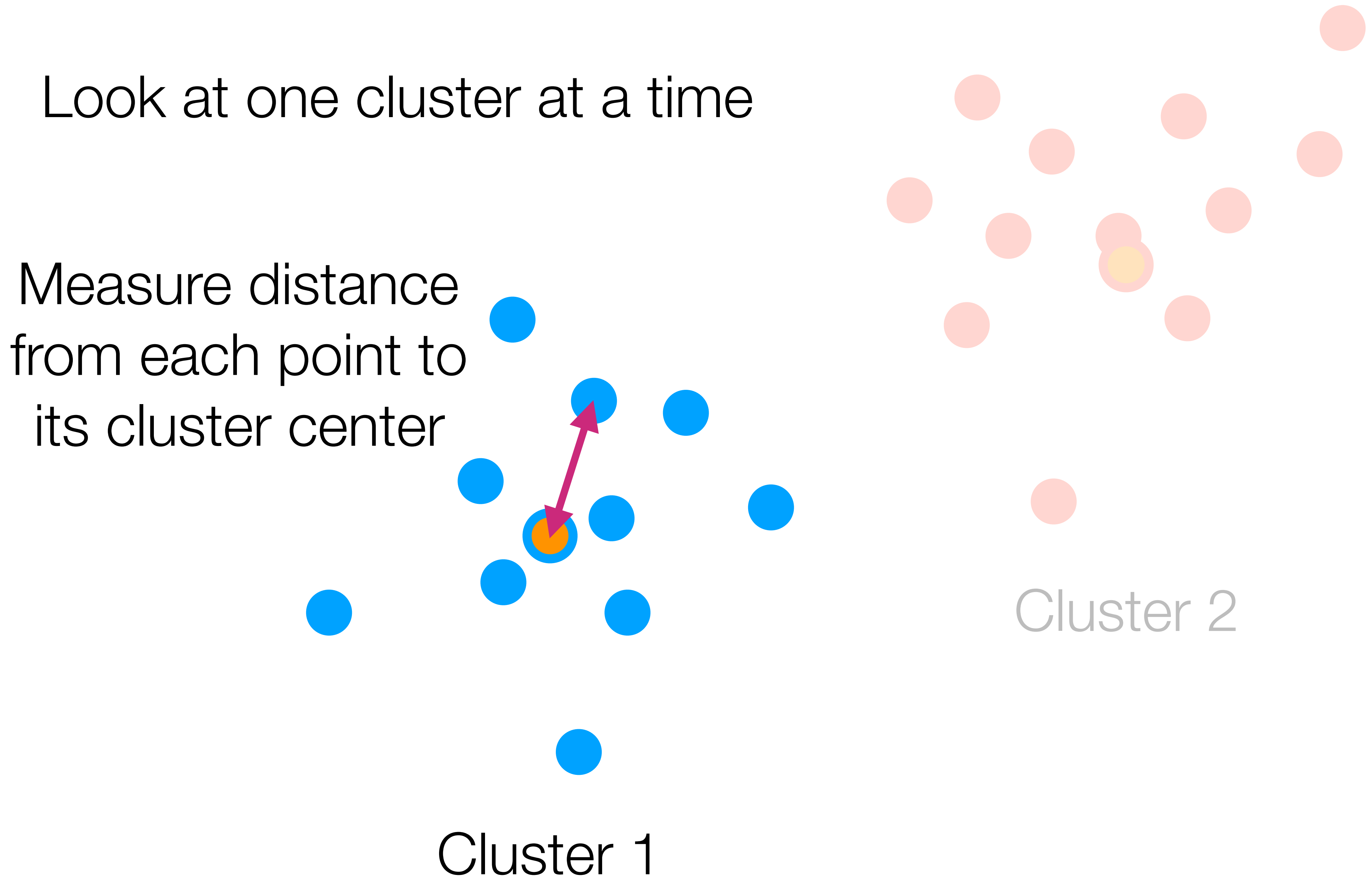
Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



Residual Sum of Squares



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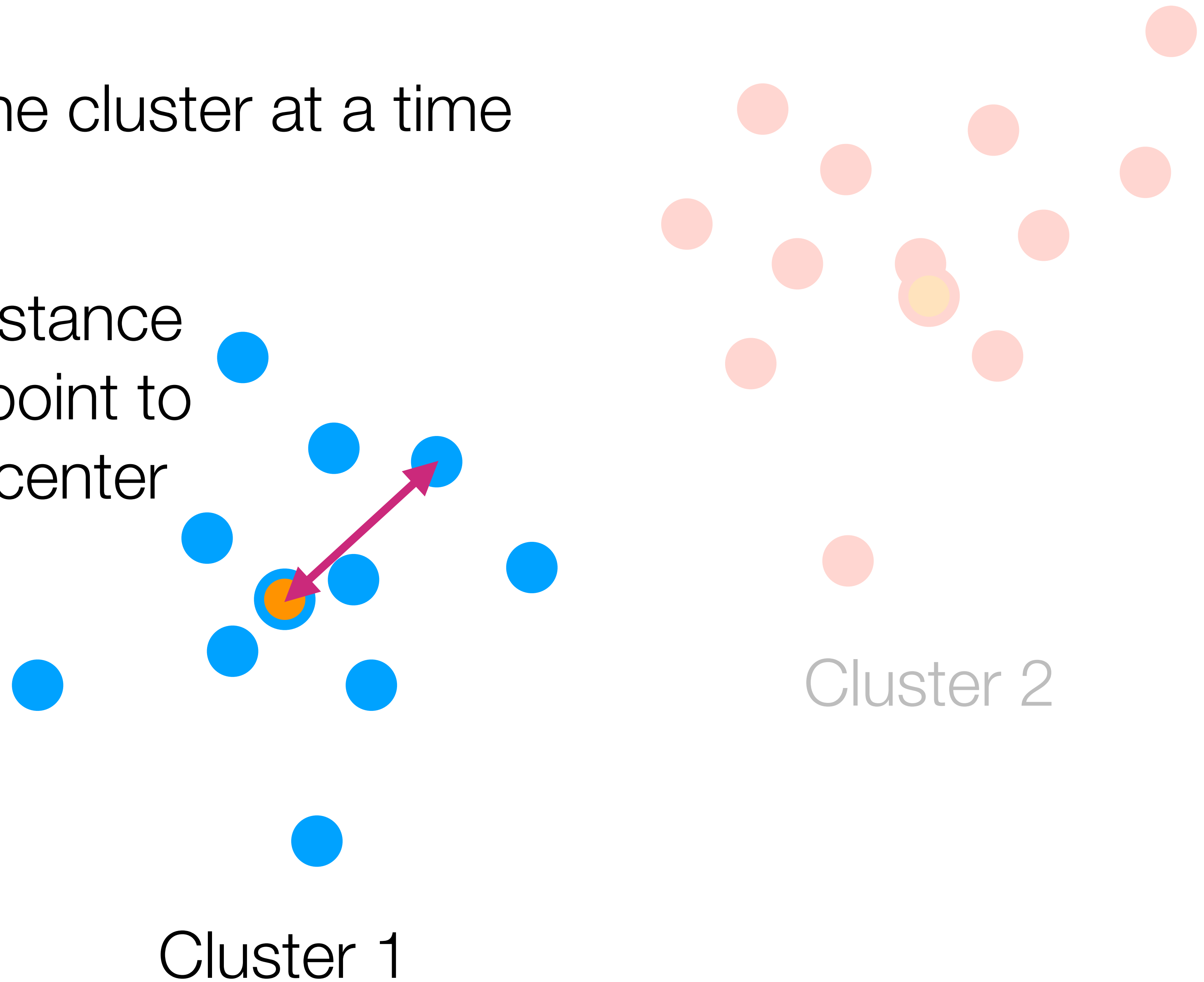

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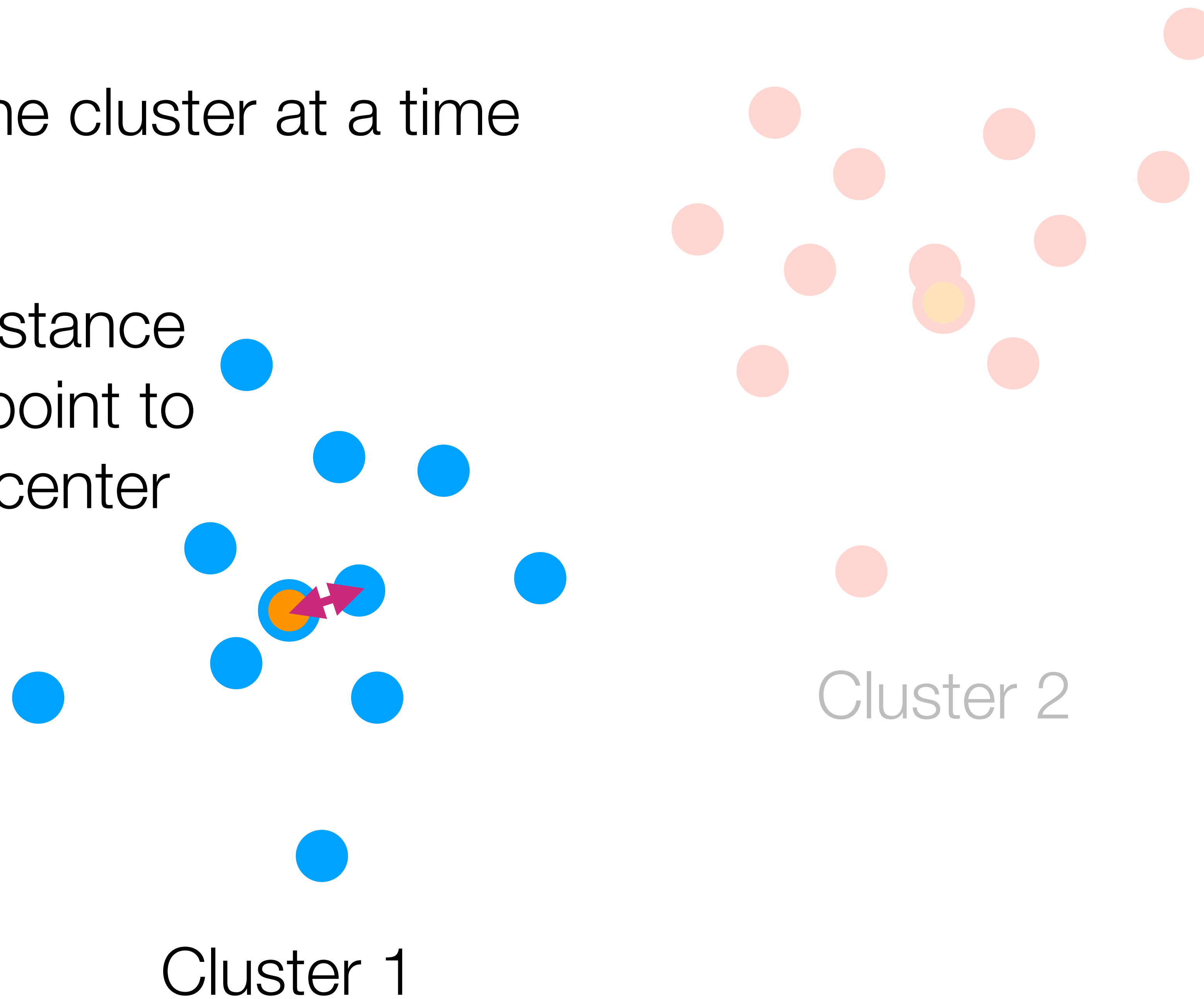

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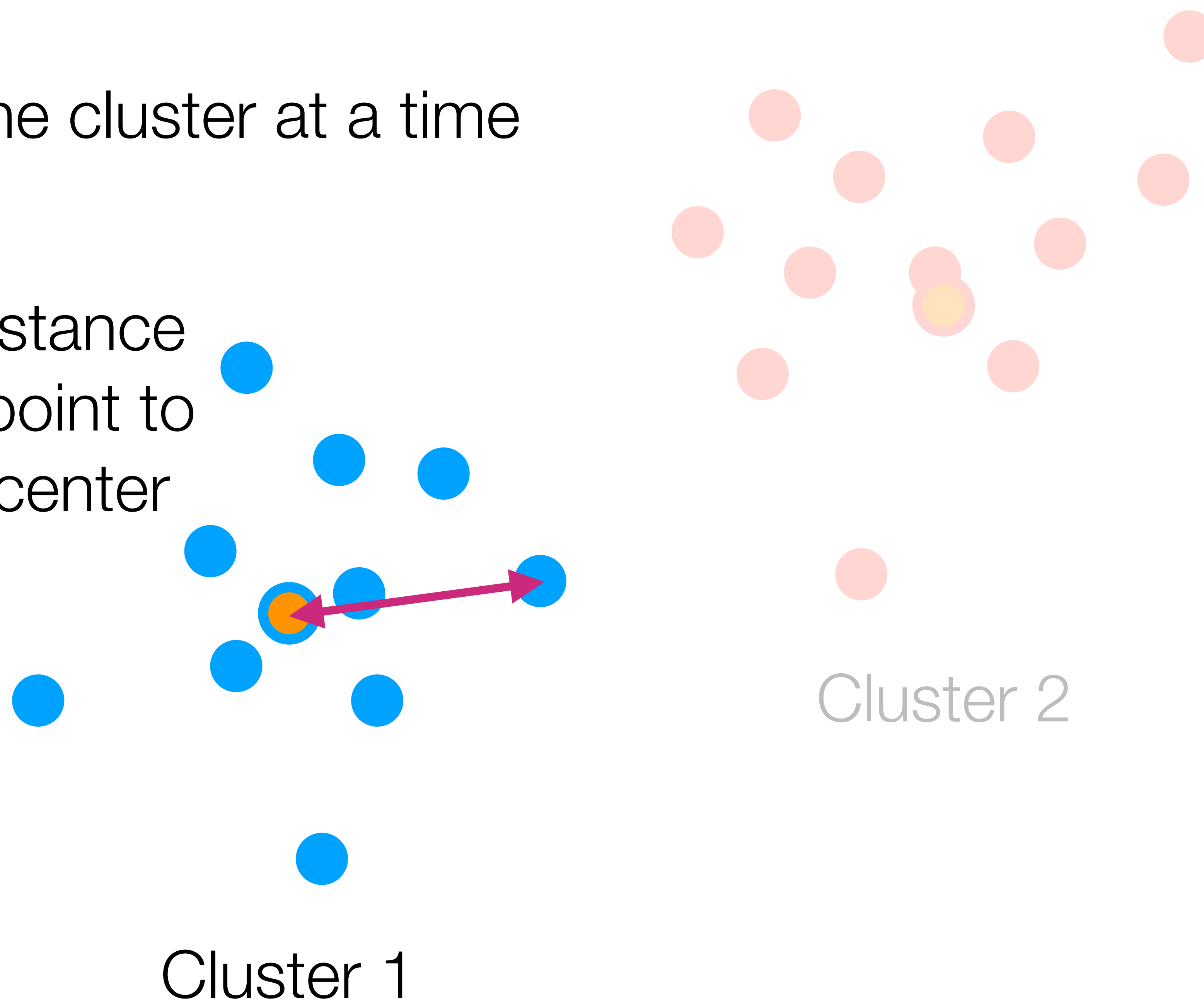

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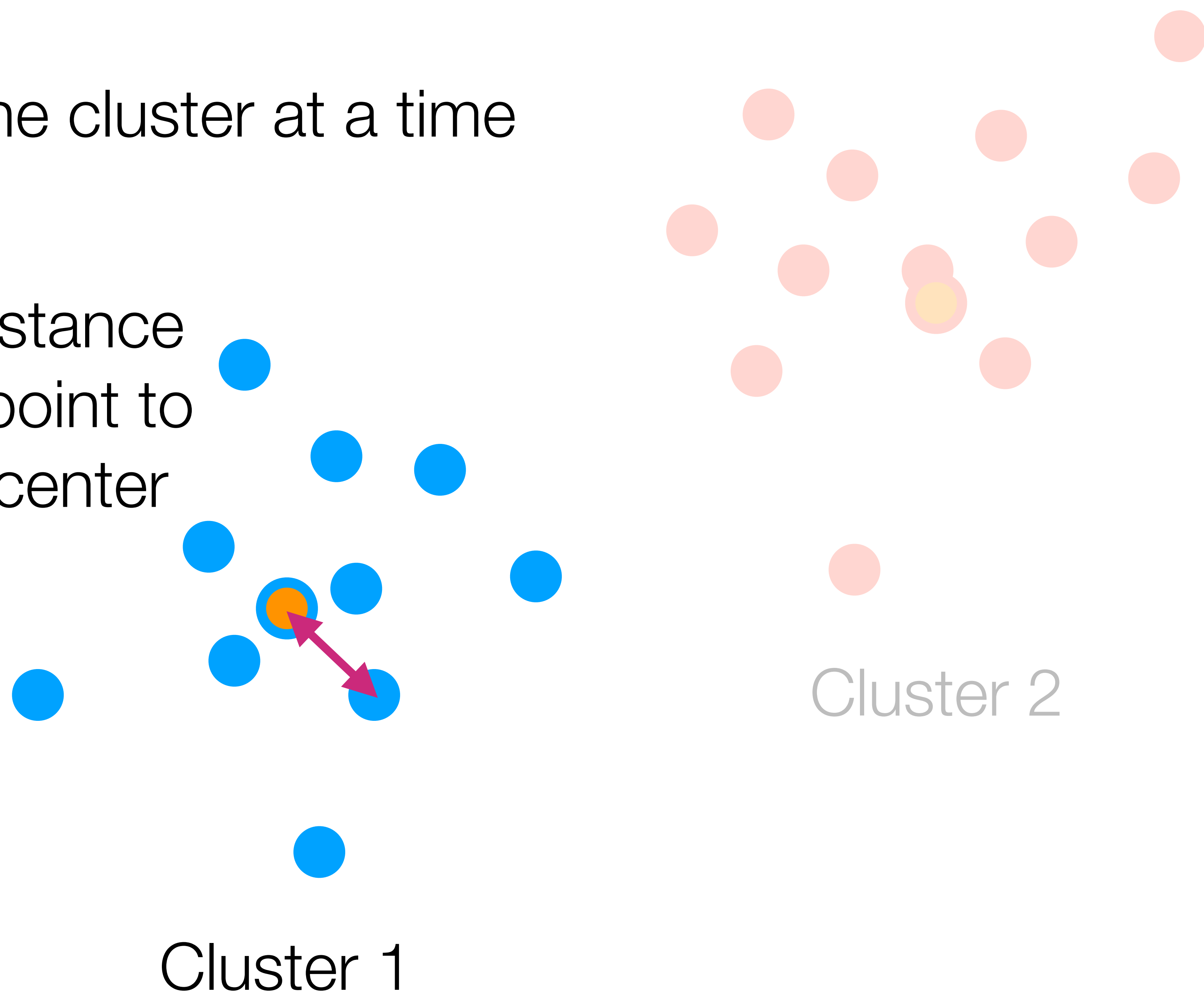

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Measure distance
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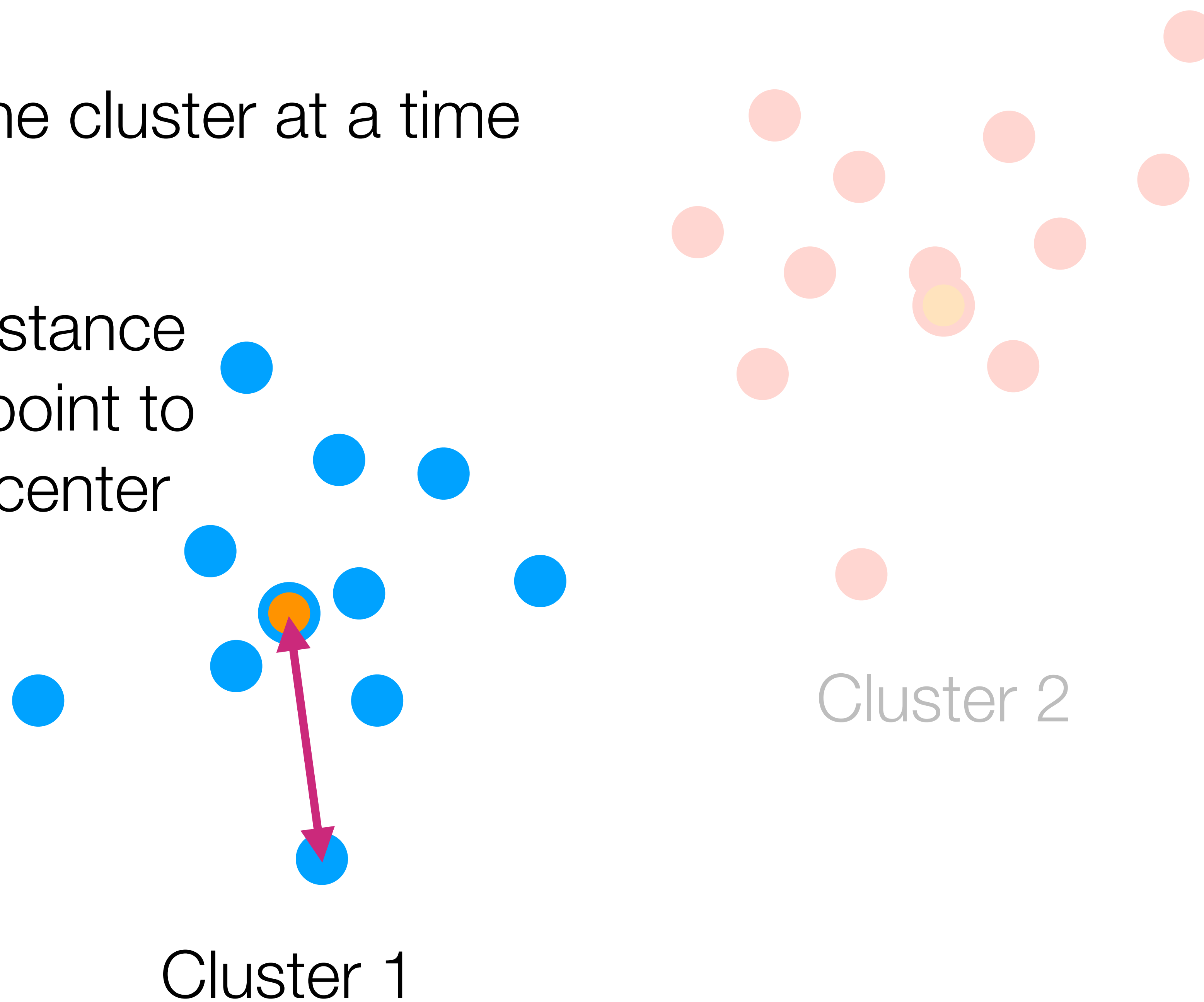

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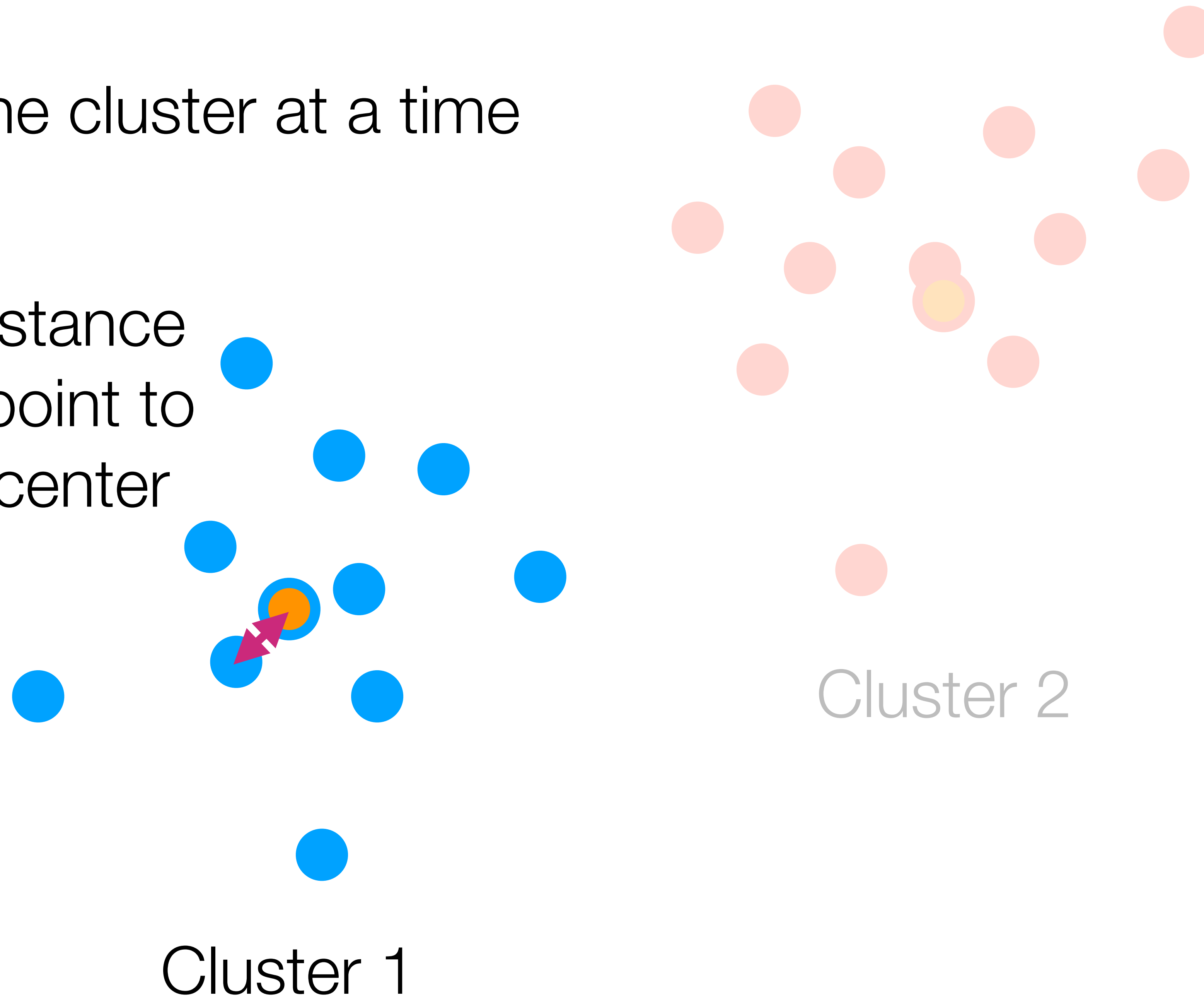

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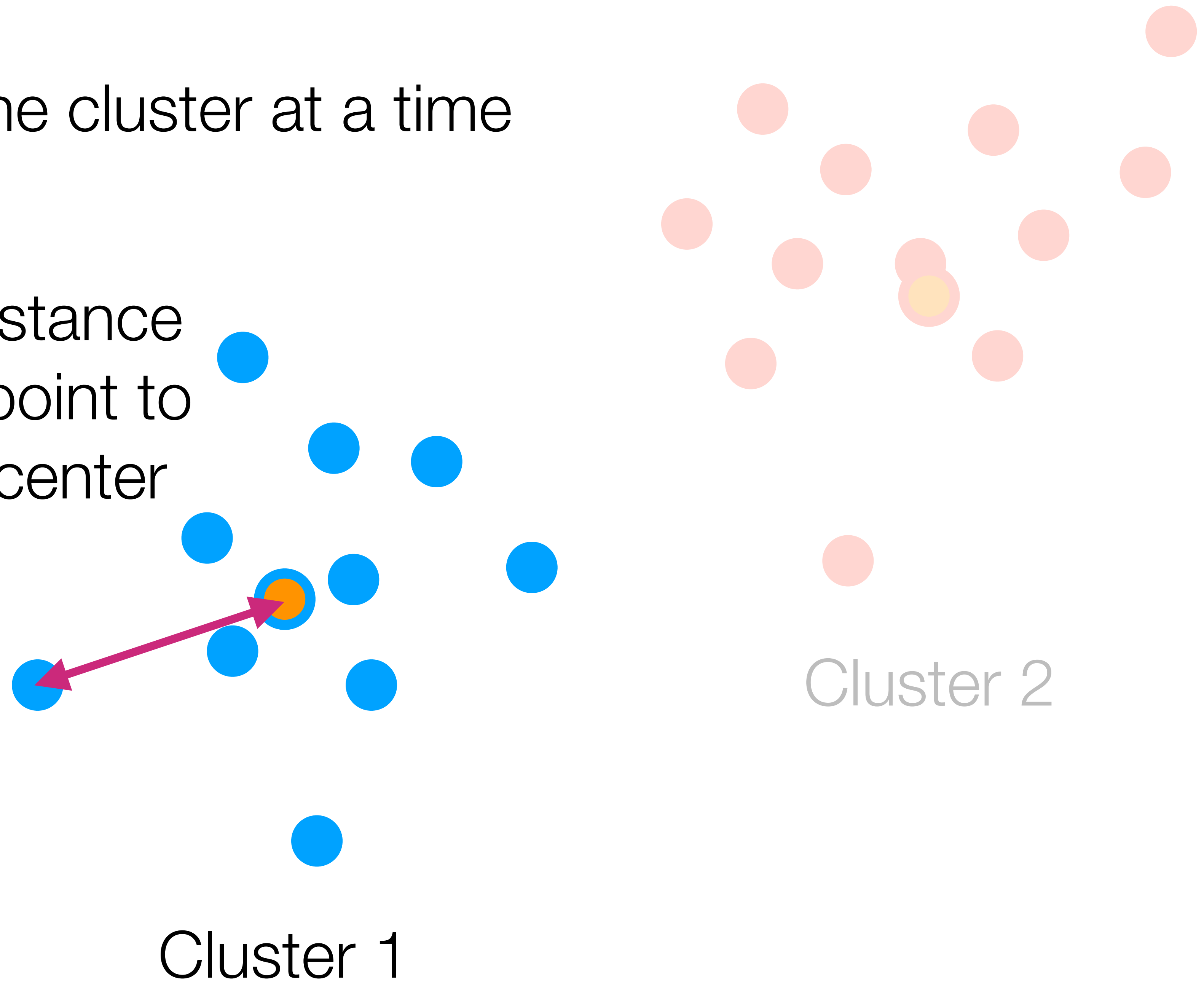

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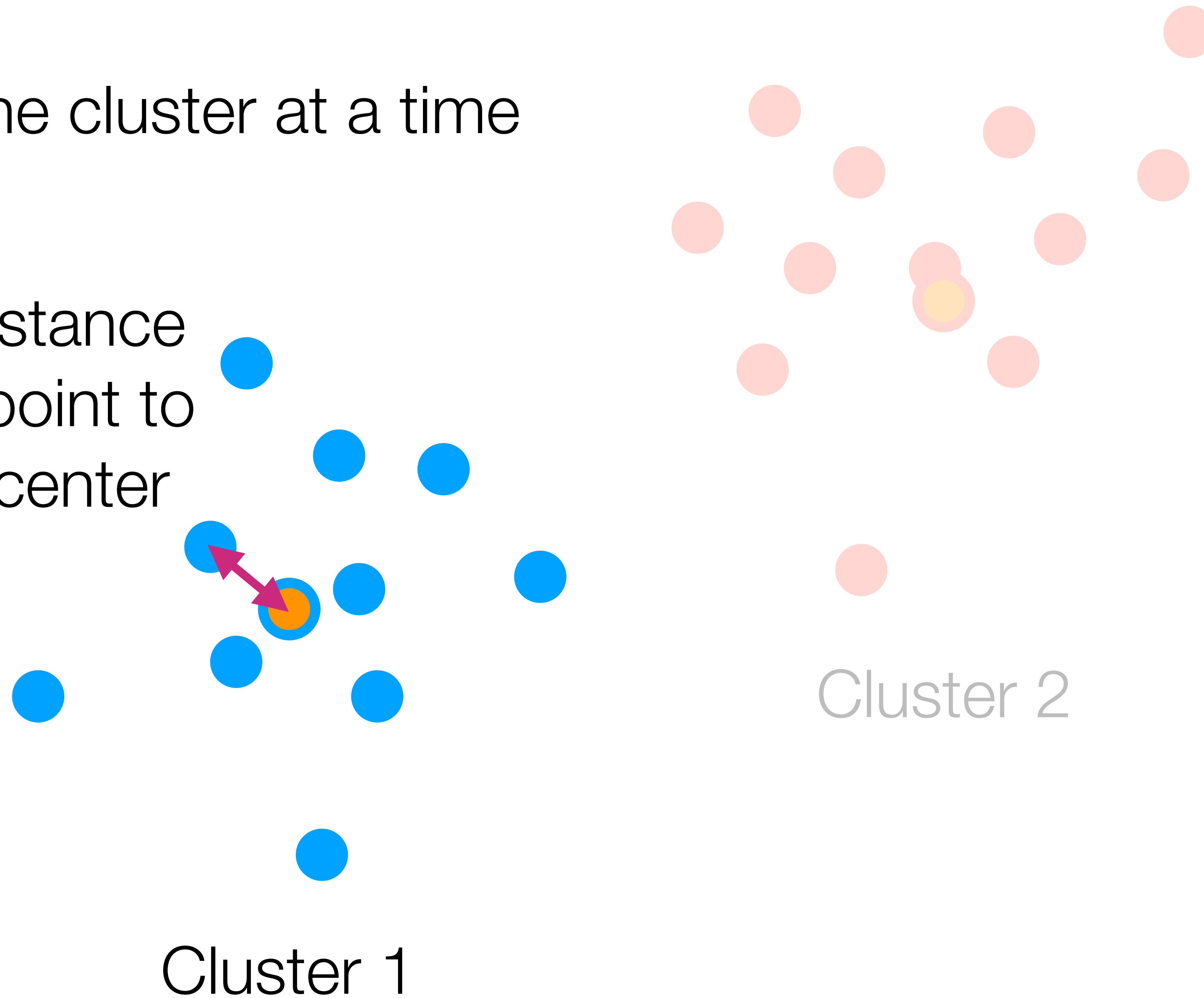
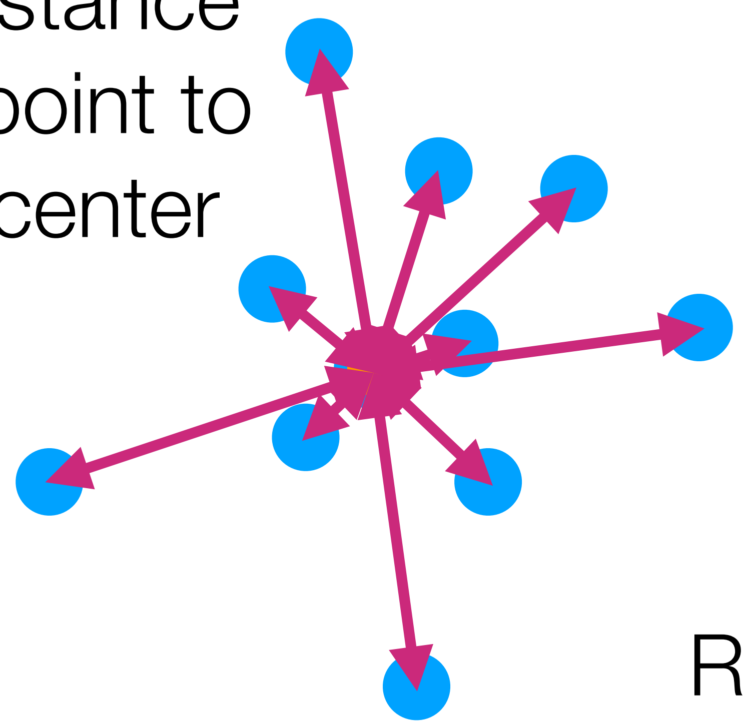
Measure distance from each point to its cluster center



Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center

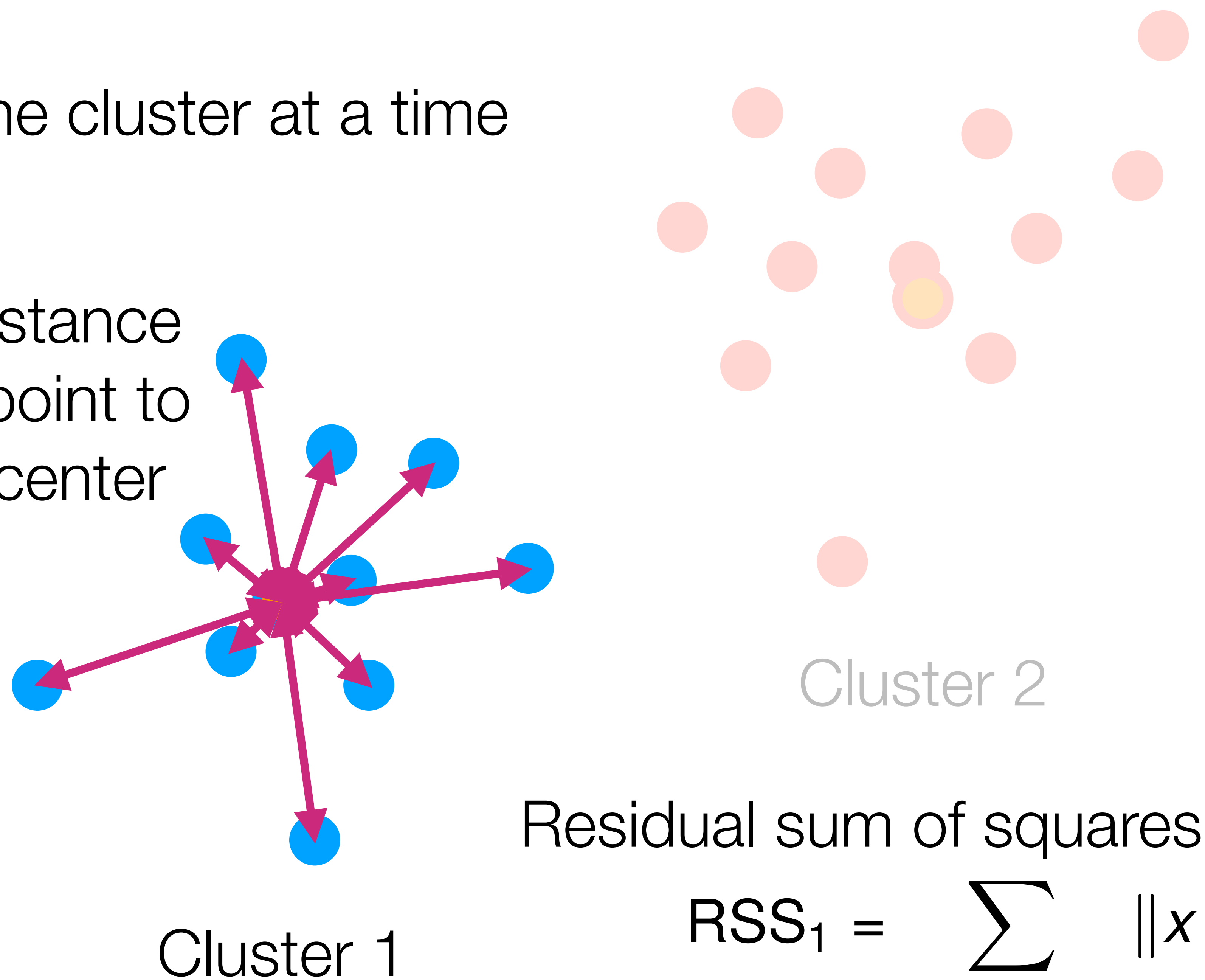


Residual sum of squares for cluster 1:
sum of *squared* purple lengths

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:

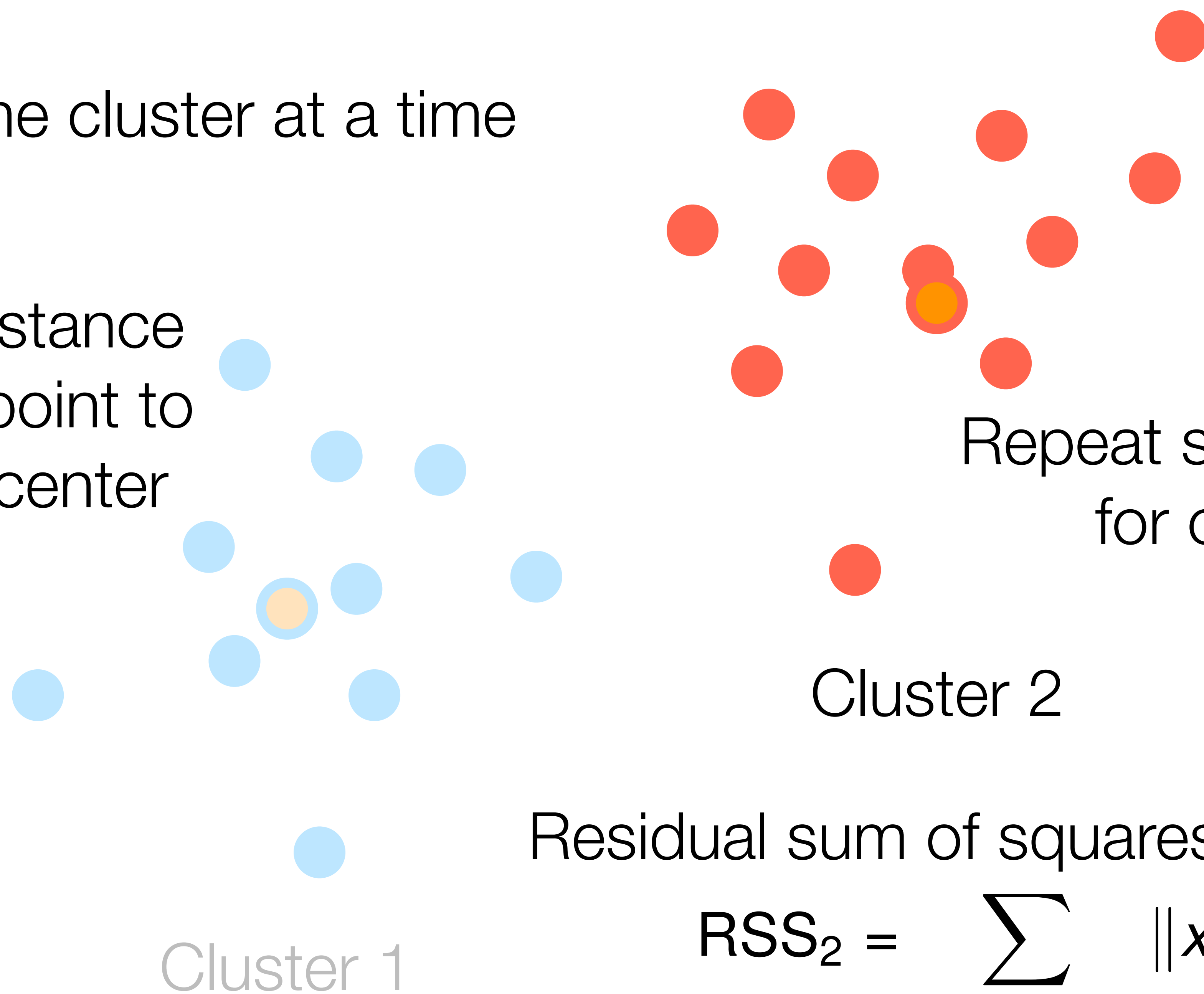
$$\mathrm{RSS}_1 = \sum_{x \in \text{cluster } 1} \|x - \mu_1\|^2$$

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