Carnegie Mellon University
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94-775/95-865 Lecture 6: Clustering Part II

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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, …, 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

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 covariance = Σ_1	…	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, …, 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 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

Repeat until convergence:

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

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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: 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)

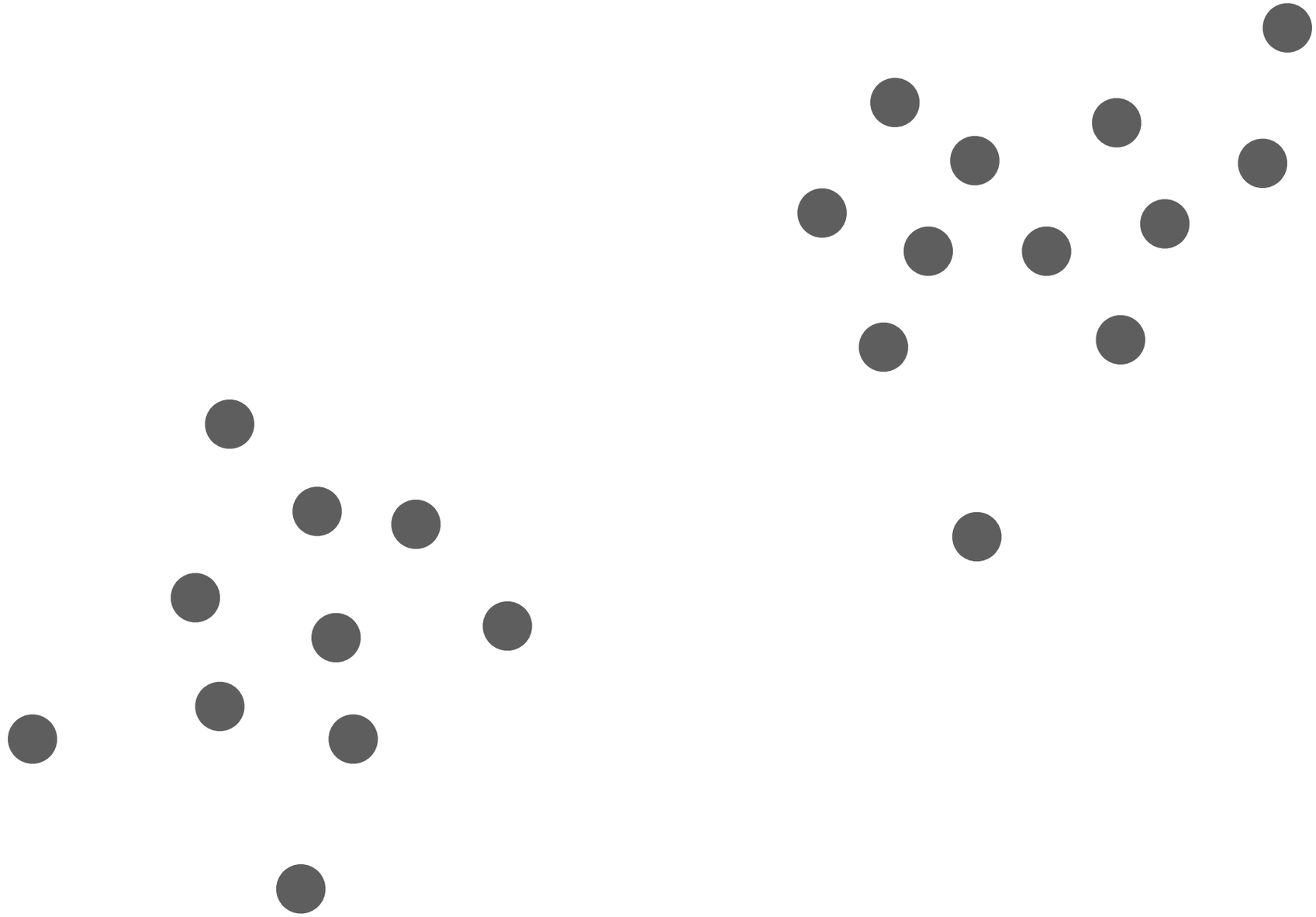
Relating *k*-means to GMM's

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):

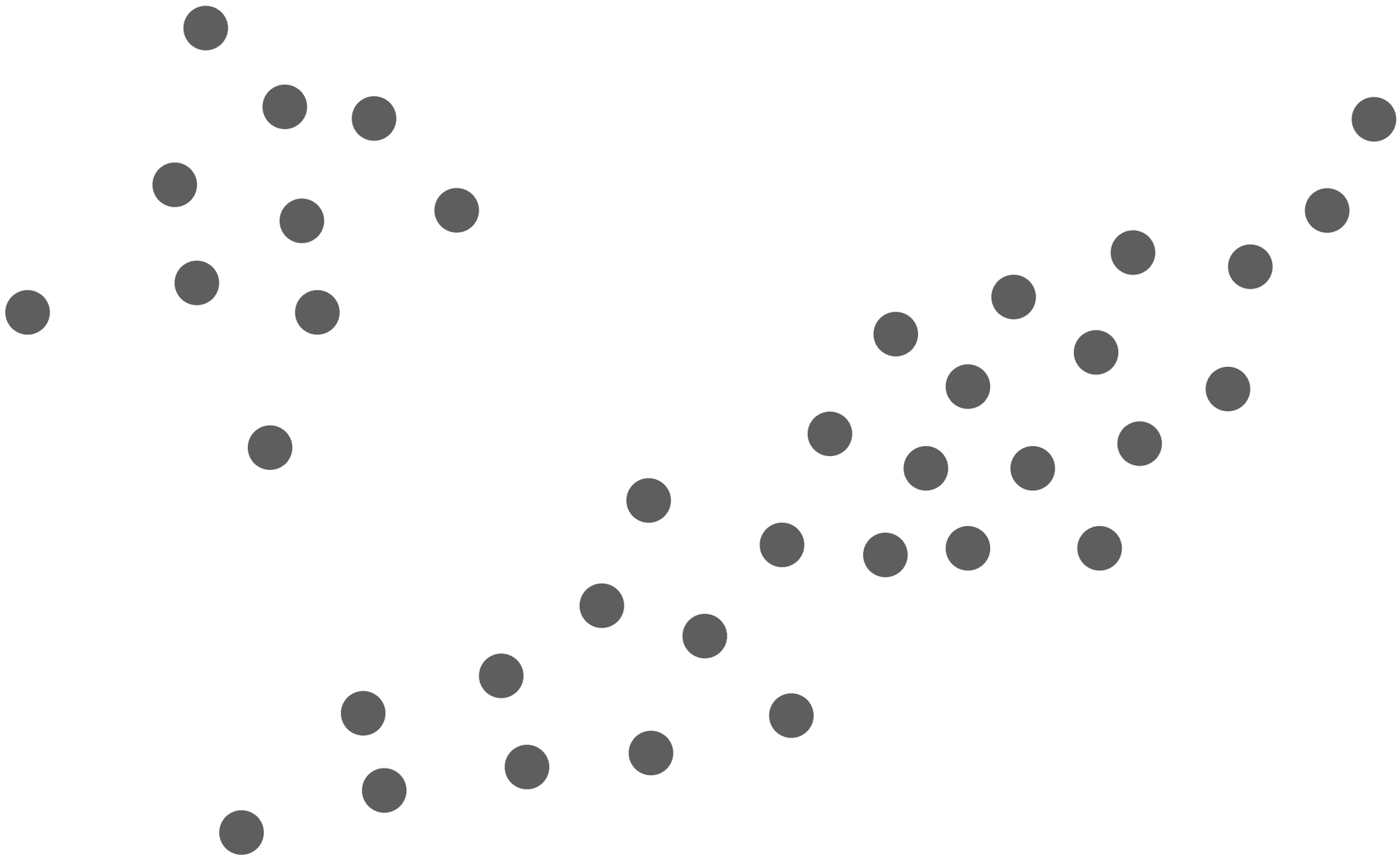
- *k*-means approximates the EM algorithm for GMM's
- Notice that ***k***-means does a "hard" assignment of each point to a cluster, whereas the EM algorithm does a "soft" (probabilistic) assignment of each point to a cluster

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 and Interpreting 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

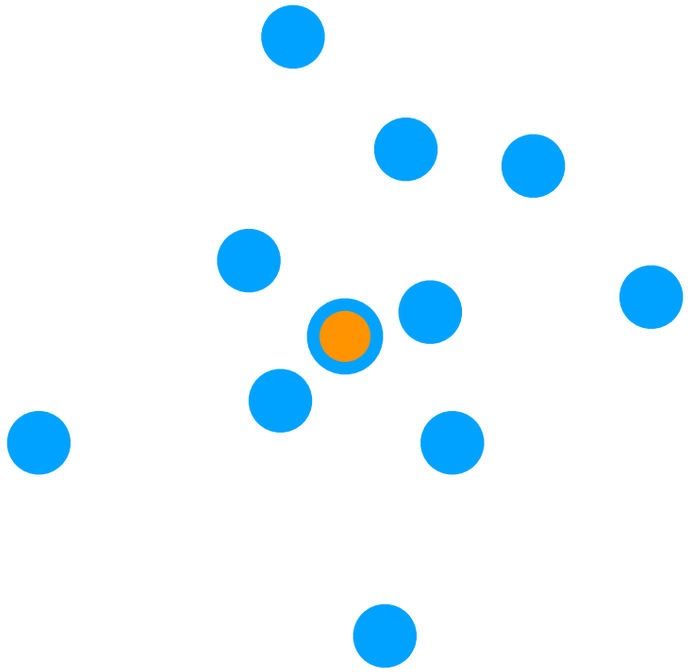
No single way of choosing *k* is the “best” way

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

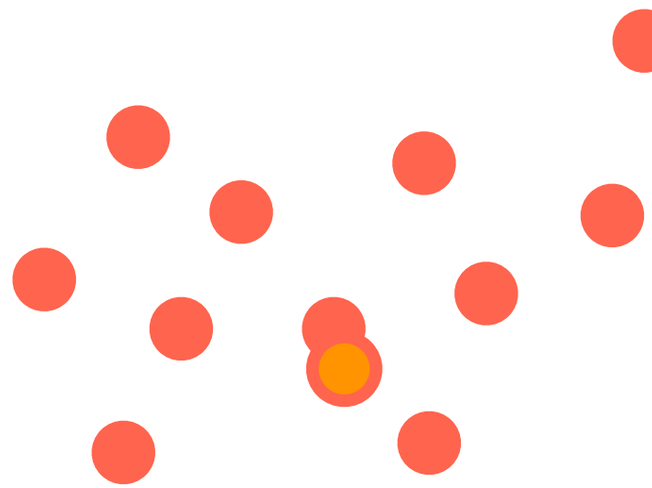
But hey it’s worth a shot

Residual Sum of Squares

Look at one cluster at a time



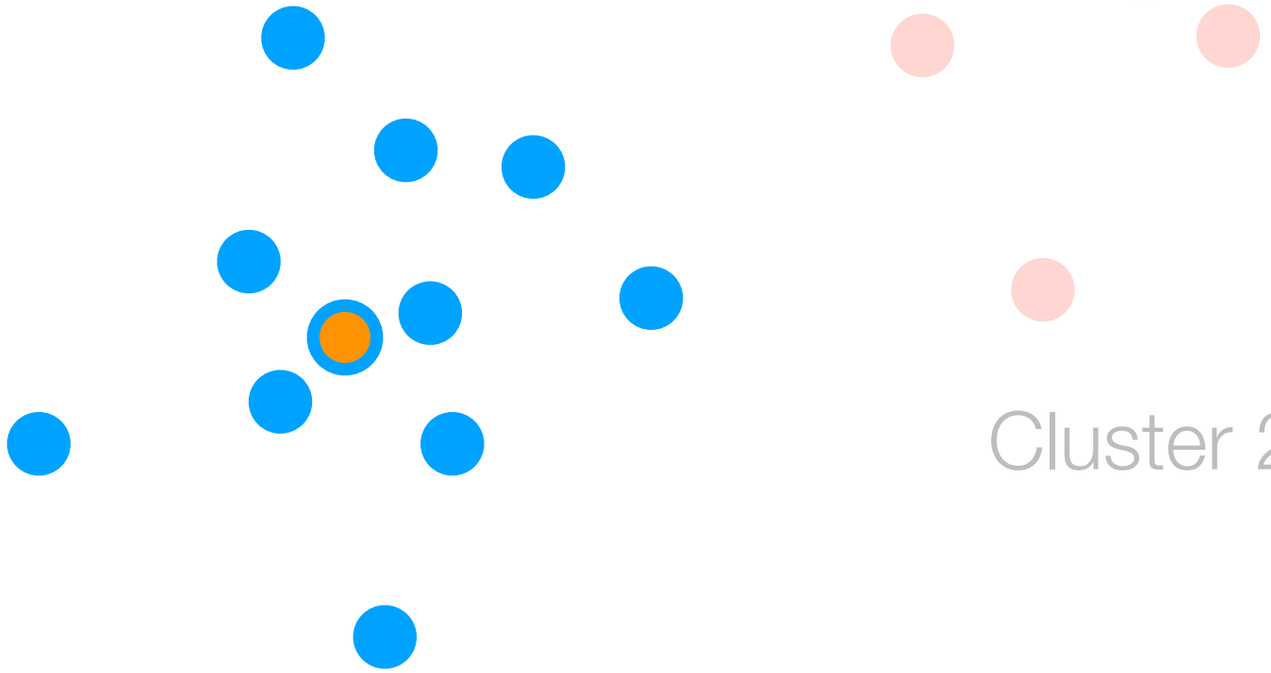
Cluster 1



Cluster 2

Residual Sum of Squares

Look at one cluster at a time



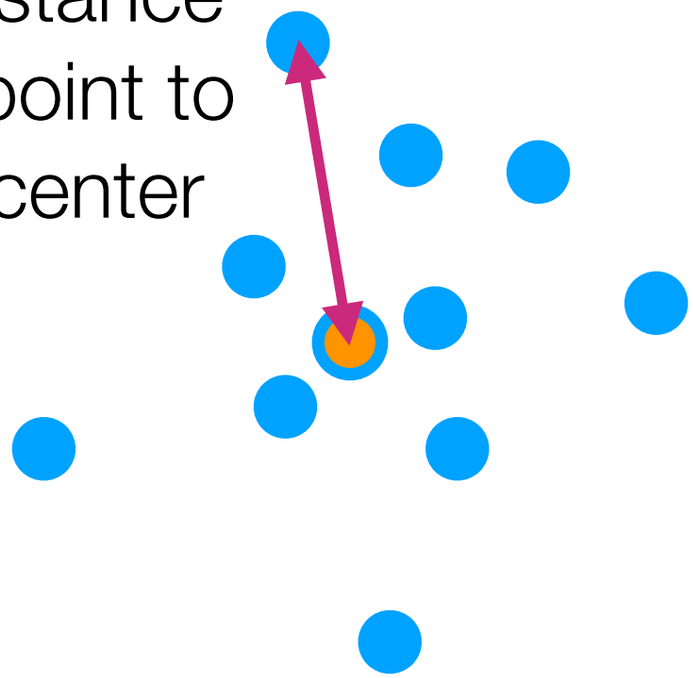
Cluster 1

Cluster 2

Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center



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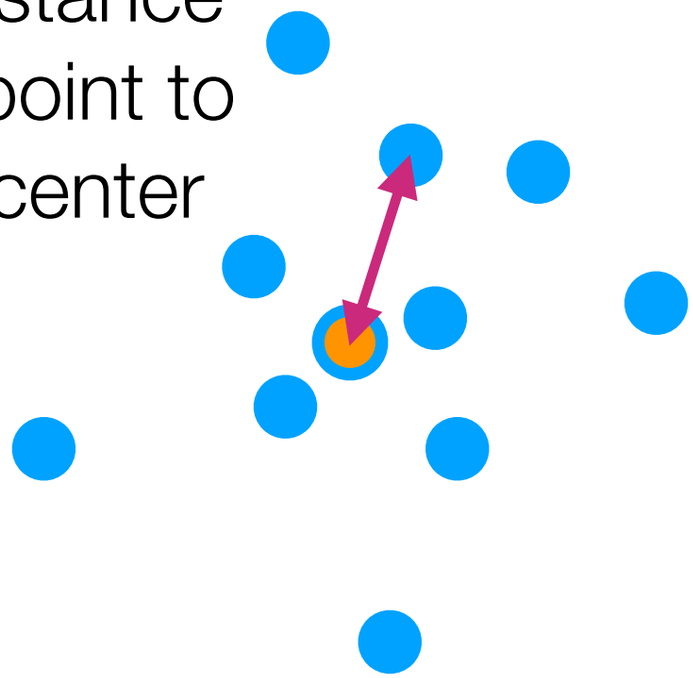

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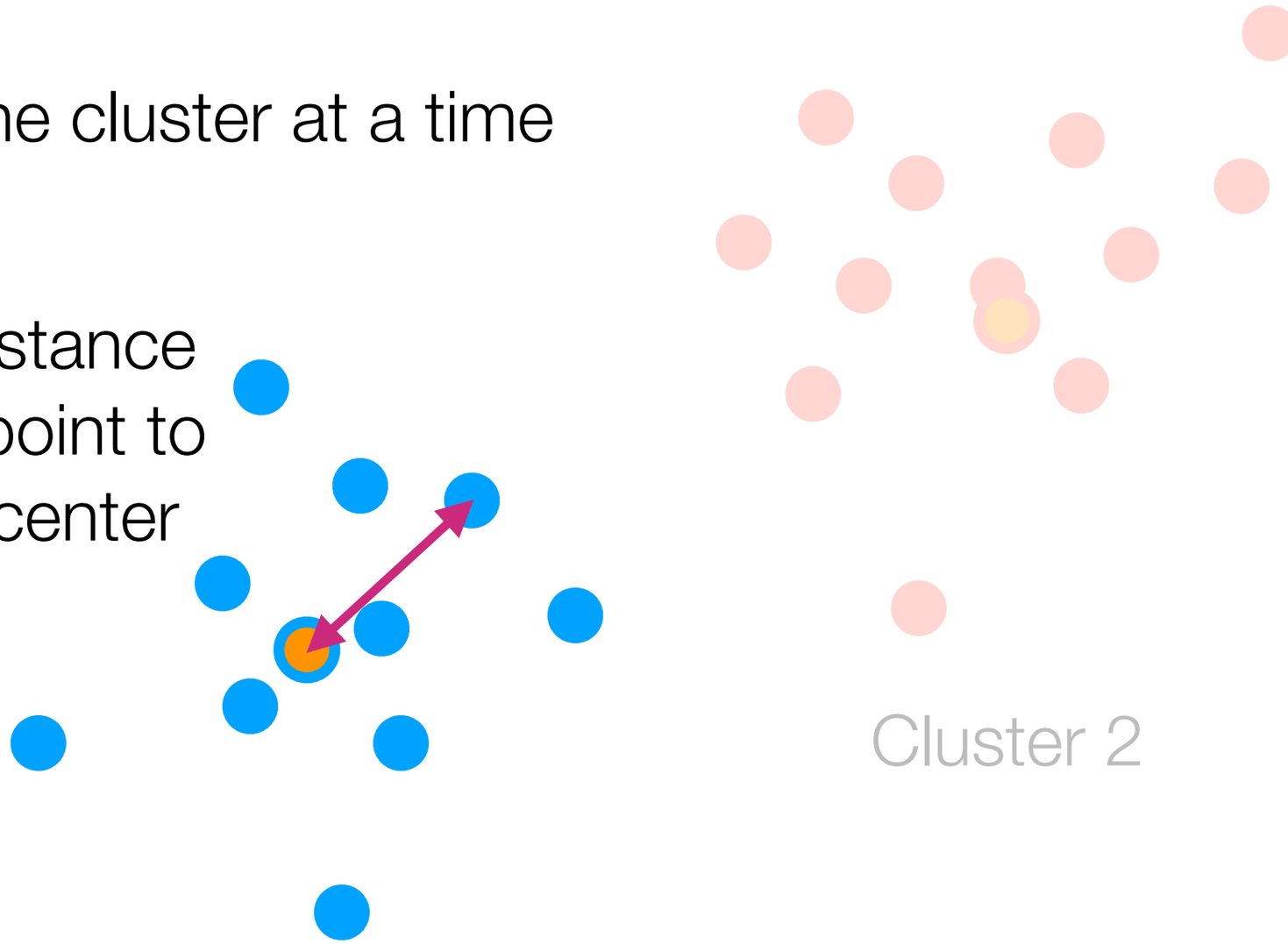

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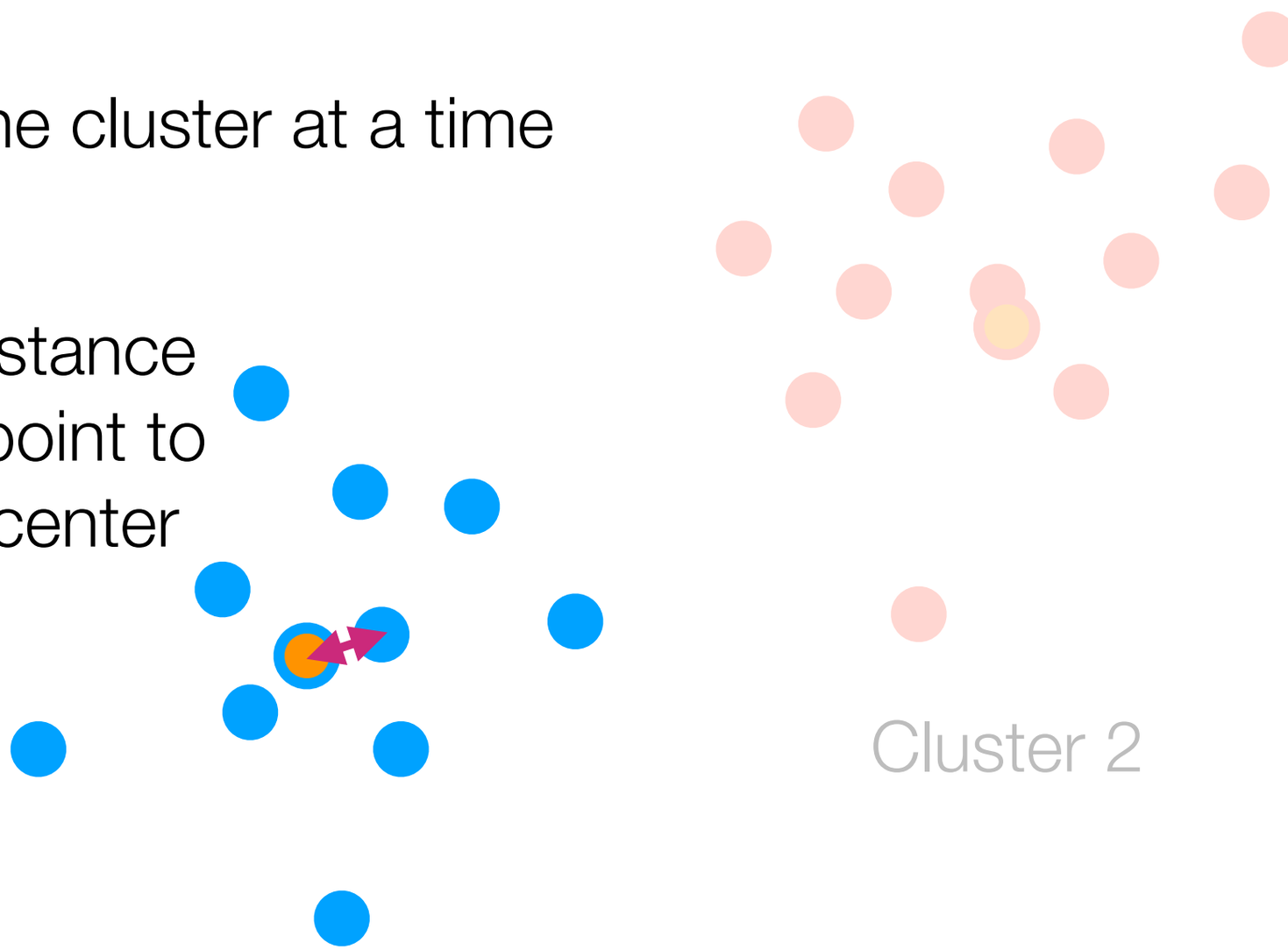

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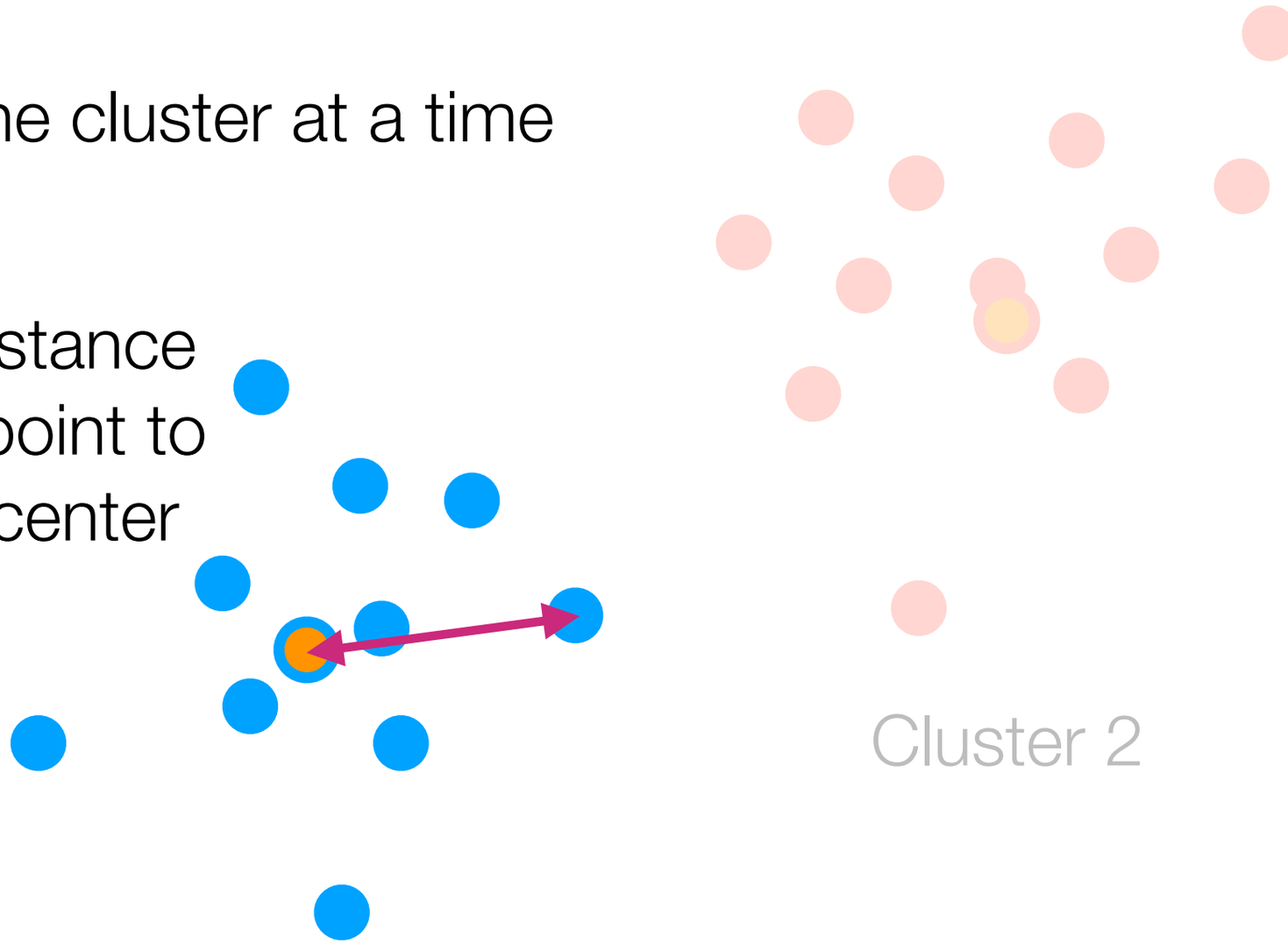

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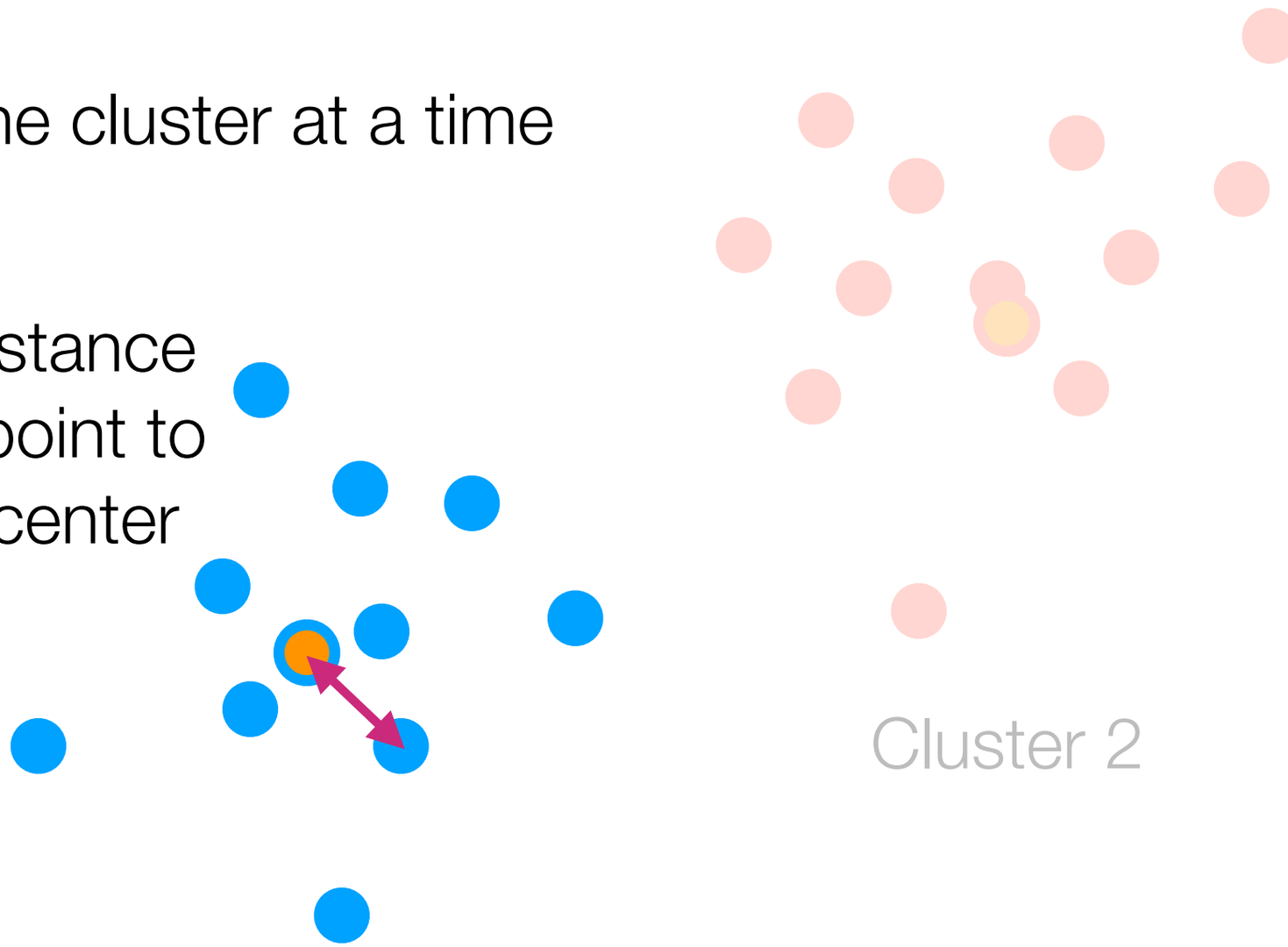

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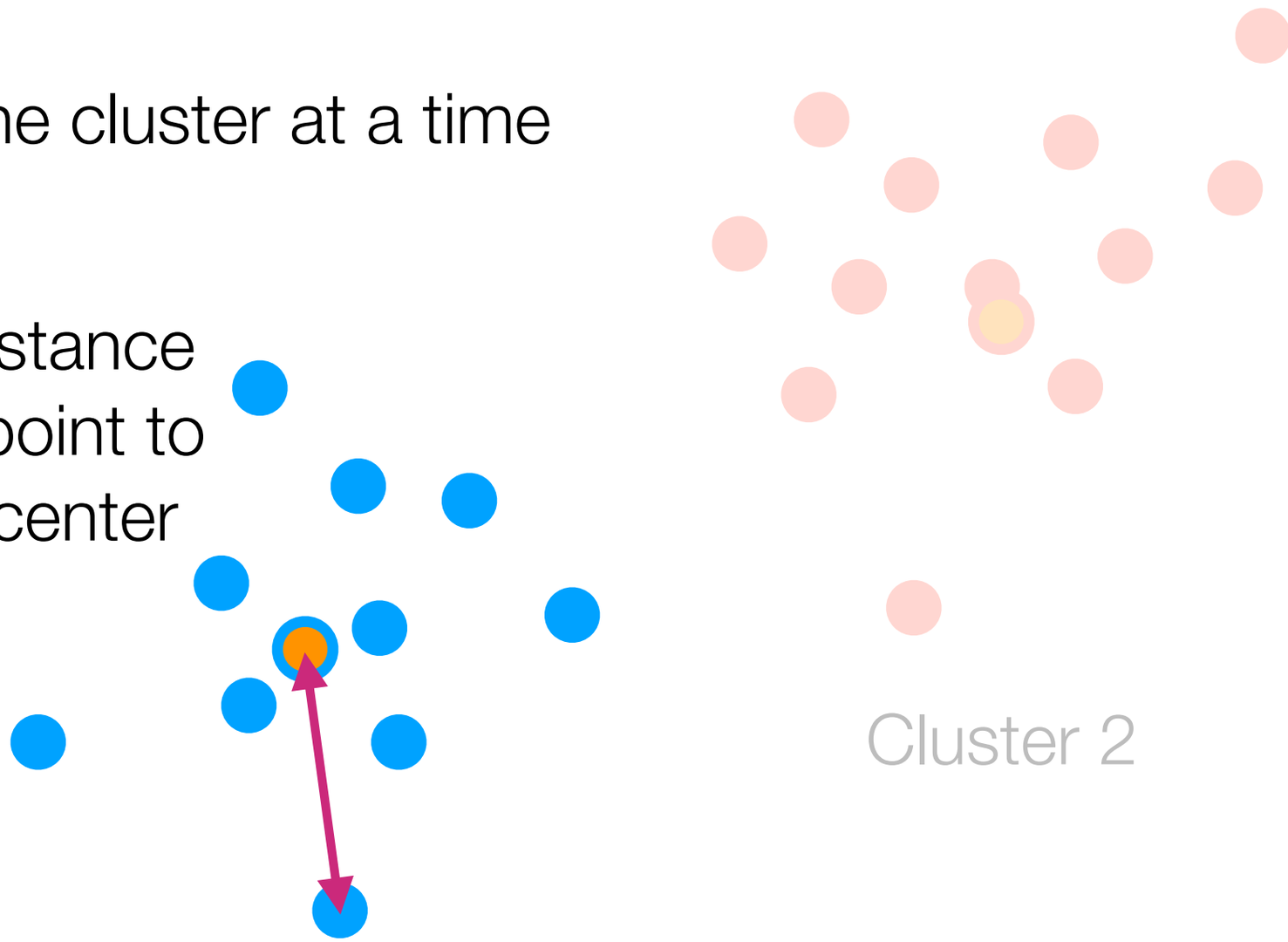

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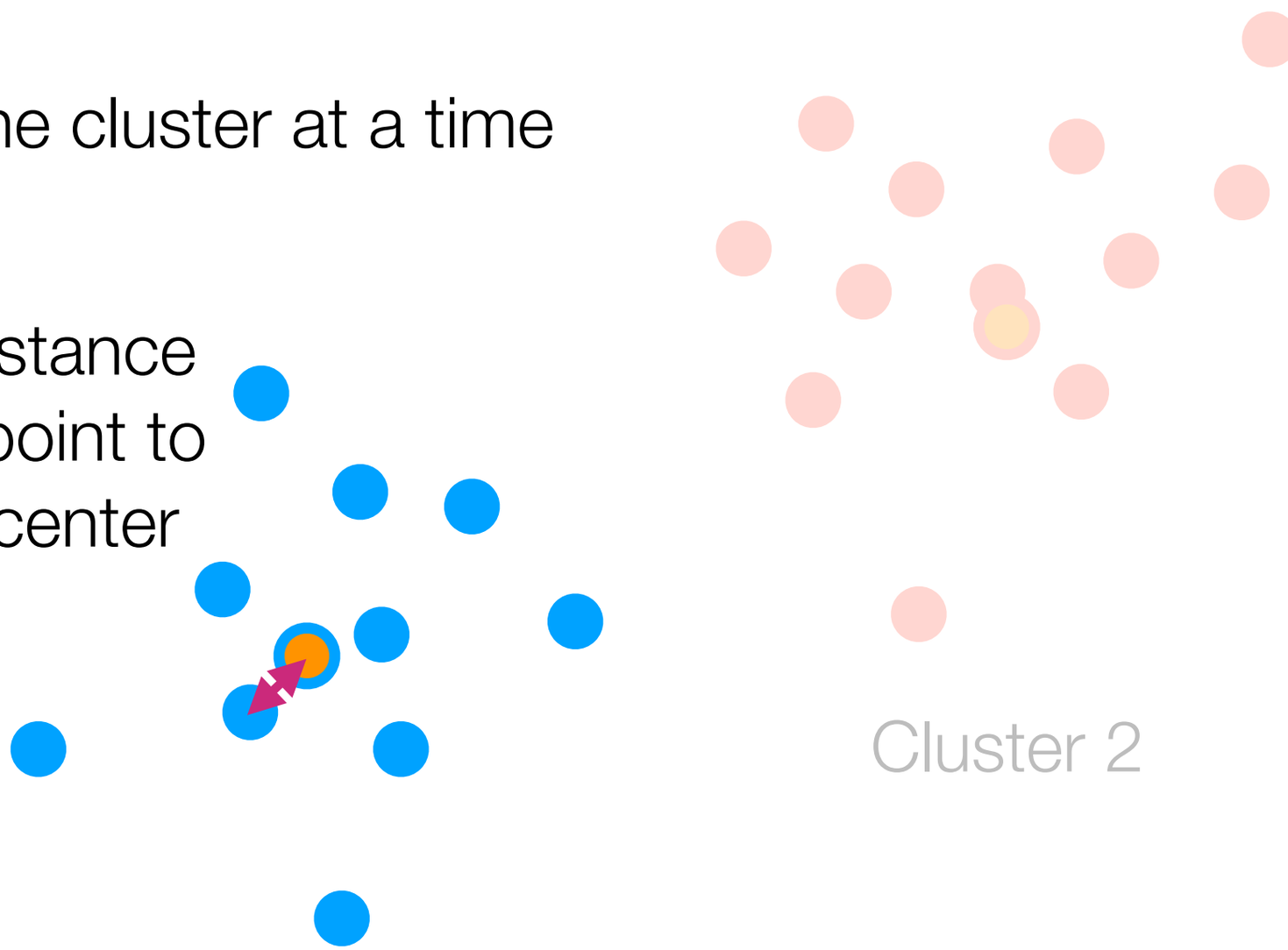

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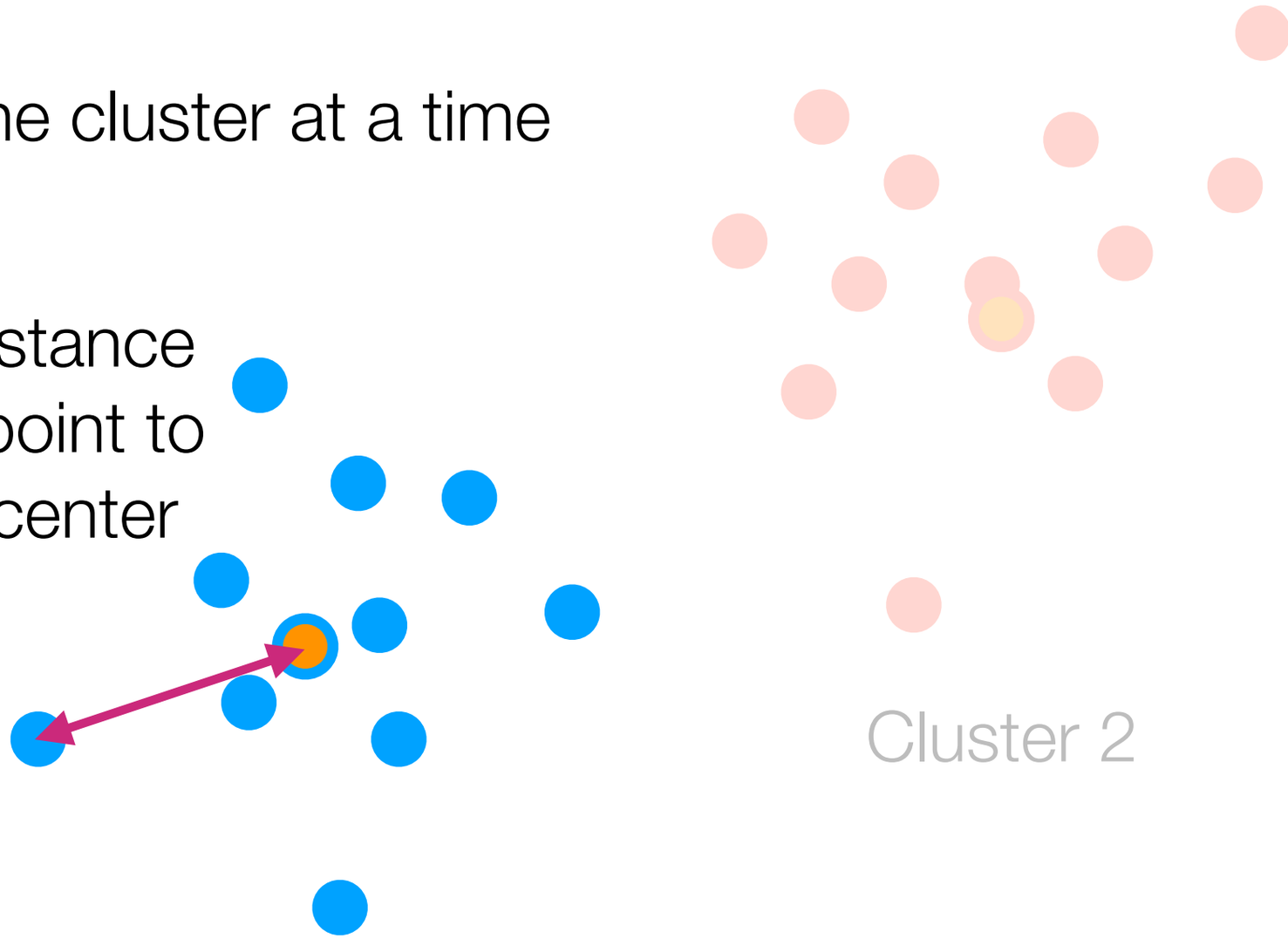


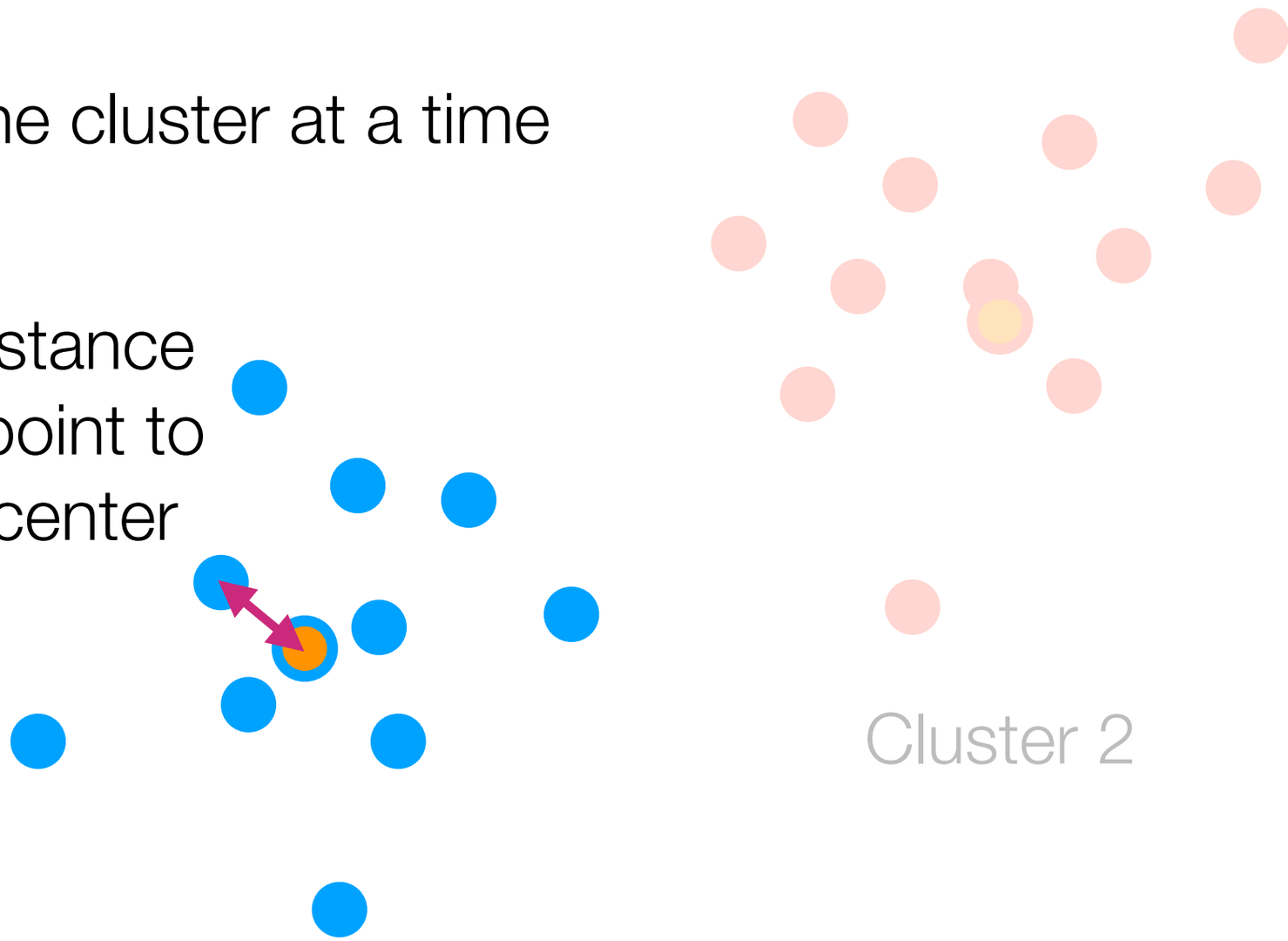
Cluster 1

Cluster 2

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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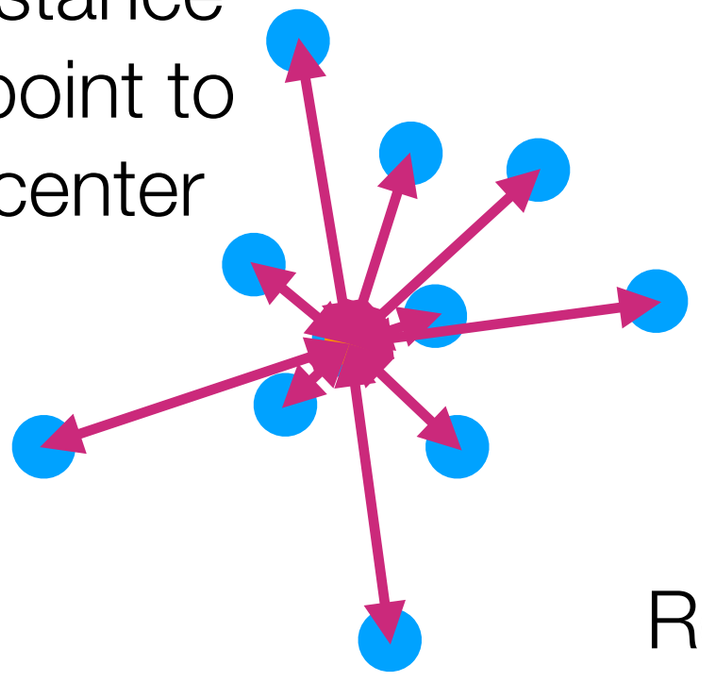


Cluster 1

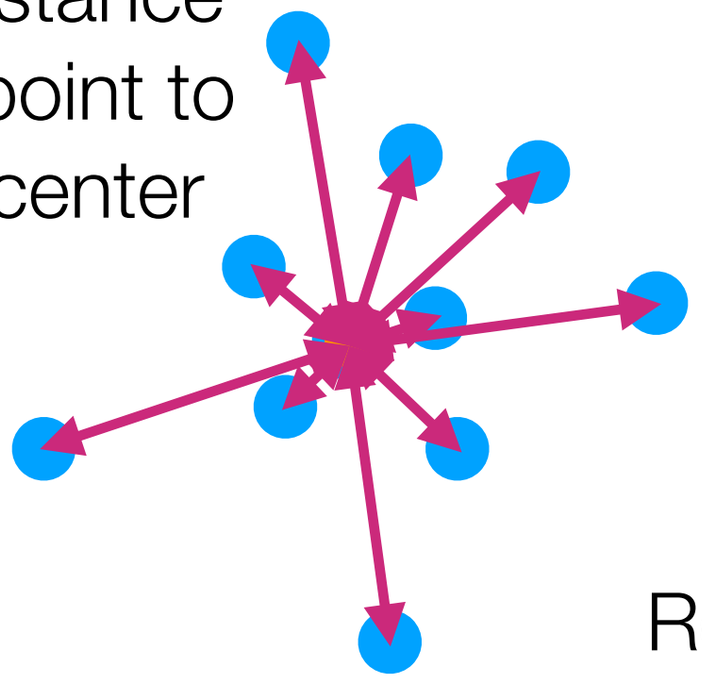
Cluster 2

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

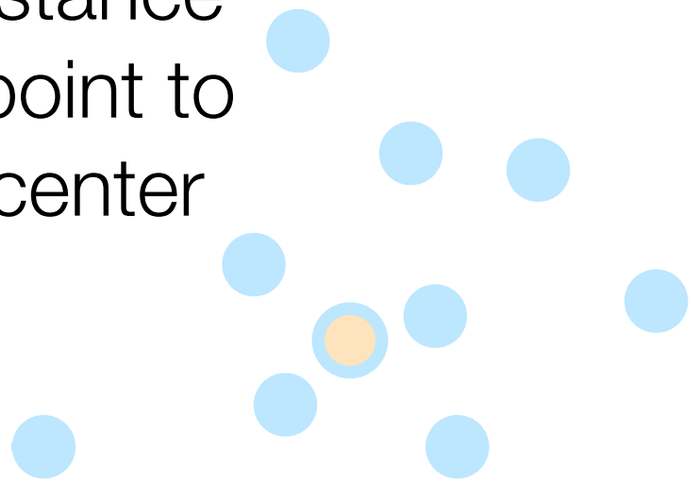
Residual sum of squares for cluster 1:

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

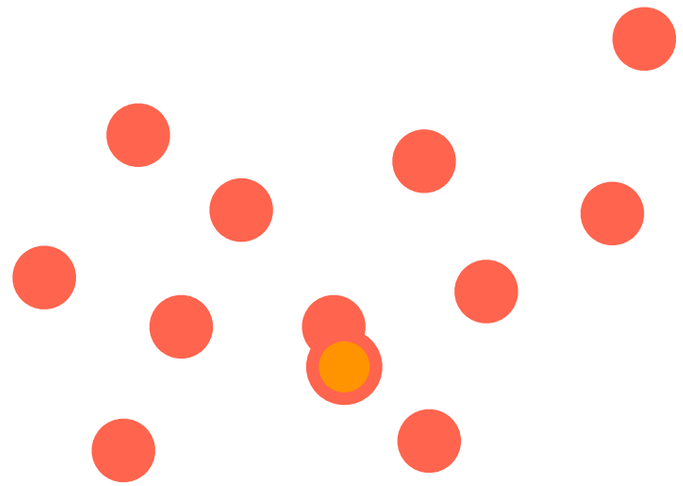
Residual Sum of Squares

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