GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 15: K-MEANS CLUSTERING

- DATA EXPLORATION
- SUPERVISED LEARNING: REGRESSION
- SUPERVISED LEARNING: CLASSIFICATION
- UNSUPERVISED LEARNING
- VARIOUS TOPICS

- LOGISTIC REGRESSION
- NAIVE BAYES
- RANDOM FORESTS
- SUPPORT VECTOR MACHINES
- COMPETITION (LAST CLASS)

Questions?

- DATA EXPLORATION
- SUPERVISED LEARNING: REGRESSION
- SUPERVISED LEARNING: CLASSIFICATION
- UNSUPERVISED LEARNING
  - CLUSTERING (TODAY)
  - DIMENSION REDUCTION
- VARIOUS TOPICS

DATA EXPLORATION

SUPERVISED LEARNING: REGRESSION

SUPERVISED LEARNING: CLASSIFICATION

UNSUPERVISED LEARNING

VARIOUS TOPICS

Data exploration presentations are held next lesson!

CLUSTERING (TODAY)

DIMENSION REDUCTION

I. CLUSTER ANALYSIS
II. K-MEANS CLUSTERING
III. CLUSTER VALIDATION
IV. IMPLEMENTING K-MEANS IN PYTHON (EXERCISE)

- DESCRIBE UNSUPERVISED LEARNING AND CLUSTERING
- DESCRIBE WHAT K-MEANS DOES
- APPLY K-MEANS IN SKLEARN
- BE ABLE TO IMPLEMENT K-MEANS IN PYTHON

I. CLUSTER ANALYSIS

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

supervised	*making predictions*
unsupervised	*discovering patterns*

Q: What is a cluster?

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A: A group of **similar** *data points.*

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The concept of similarity is central to the definition of a cluster, and therefore to cluster analysis.

Examples: distance between points, number of common words, etc.

Q: What is the purpose of cluster analysis?

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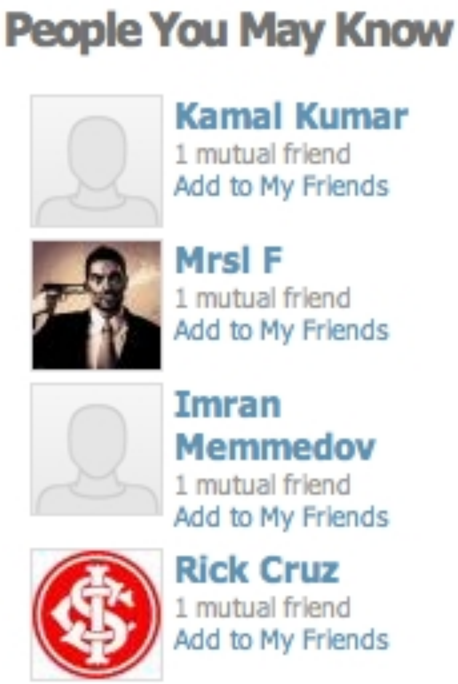
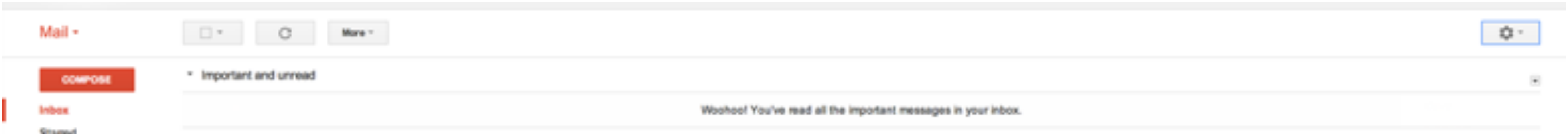
A: To enhance our understanding of a dataset by dividing the data into groups.


People You May Know
Kamal Kumar
1 mutual friend
Add to My Friends
Mrsl F
1 mutual friend
Add to My Friends
Imran Memmedov
1 mutual friend
Add to My Friends
Rick Cruz
1 mutual friend
Add to My Friends



Priority Inbox: Unsupervised Learning

Group mails into groups and decide which group represents important mails

Q: How do you solve a clustering problem?

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A: Think of a cluster as a "potential class"; then the solution to a clustering problem is to programmatically determine these classes.

II. K-MEANS CLUSTERING

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

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greedy – *captures local structure (depends on initial conditions)*

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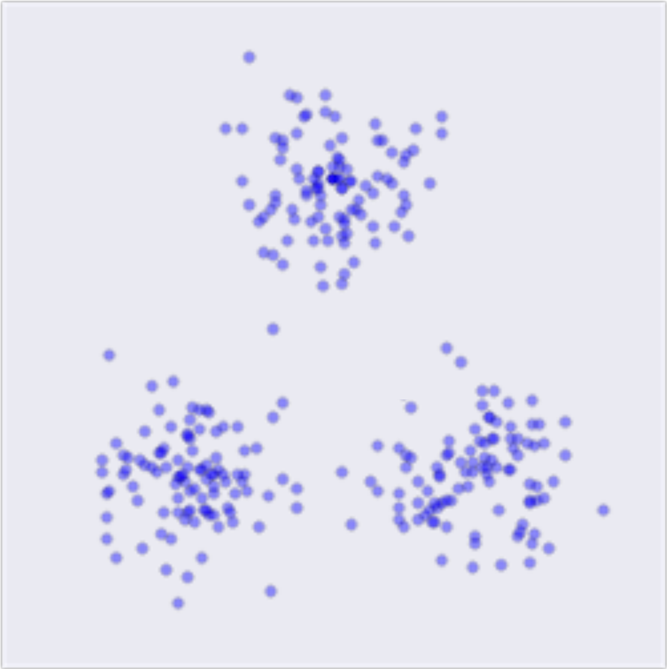
A: A **greedy** *learner that* **partitions** *a data set into k clusters.*

greedy – *captures local structure (depends on initial conditions)*

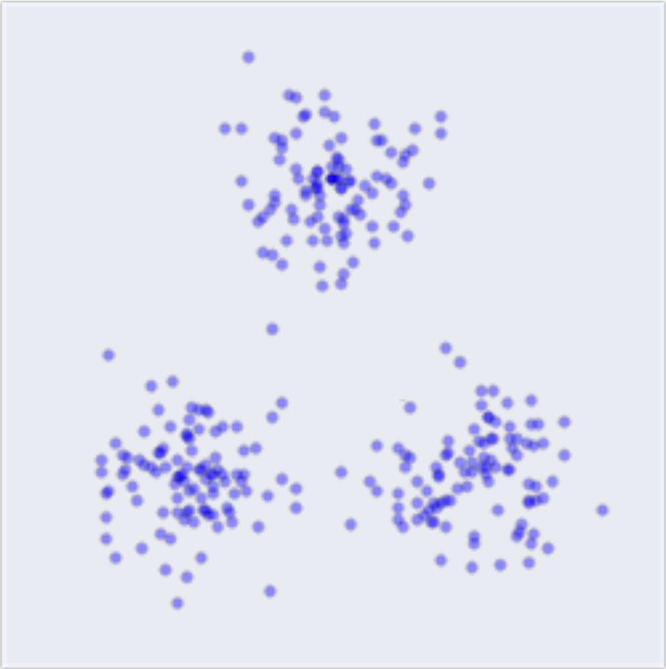
partition – *each point belongs to exactly one cluster*

K-means is algorithmically pretty efficient

(time & space complexity is linear in number of records)

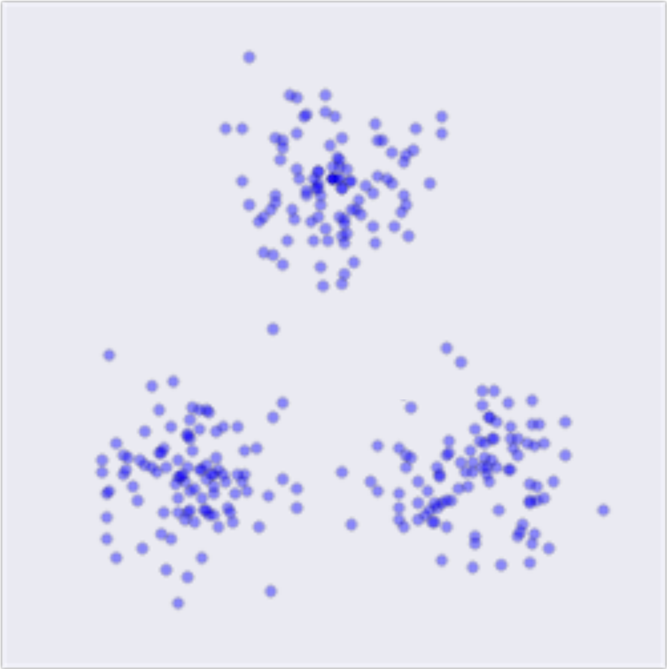


Suppose we are given some unsupervised data (i.e., no class labels)

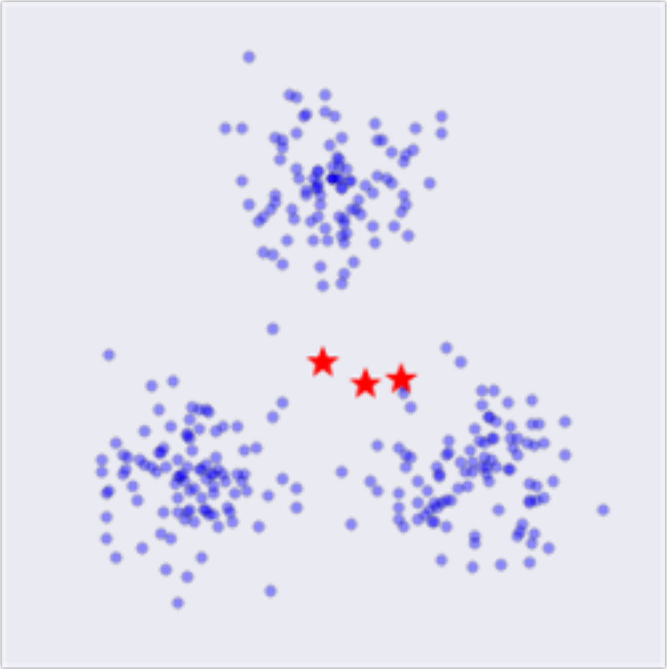


Suppose we are given some unsupervised data (i.e., no class labels)

We could like to infer class labels from the data, i.e., cluster the data into similar groups

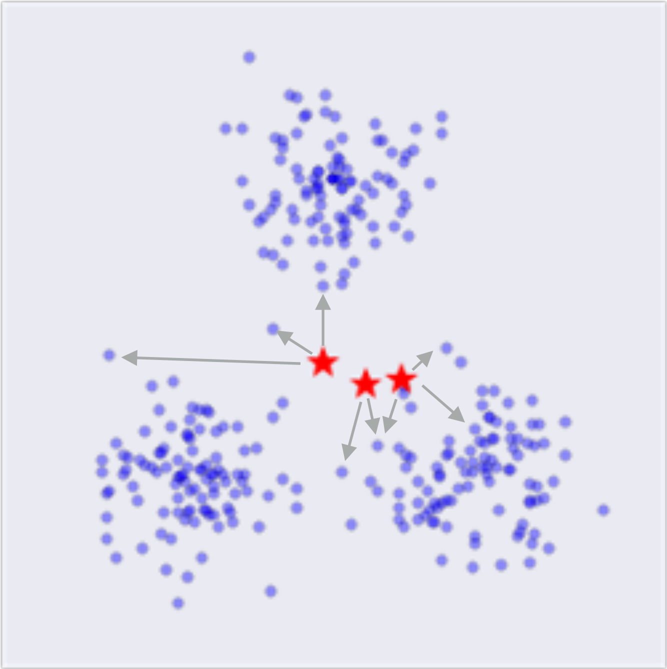


Steps of k-means algorithm



Steps of k-means algorithm

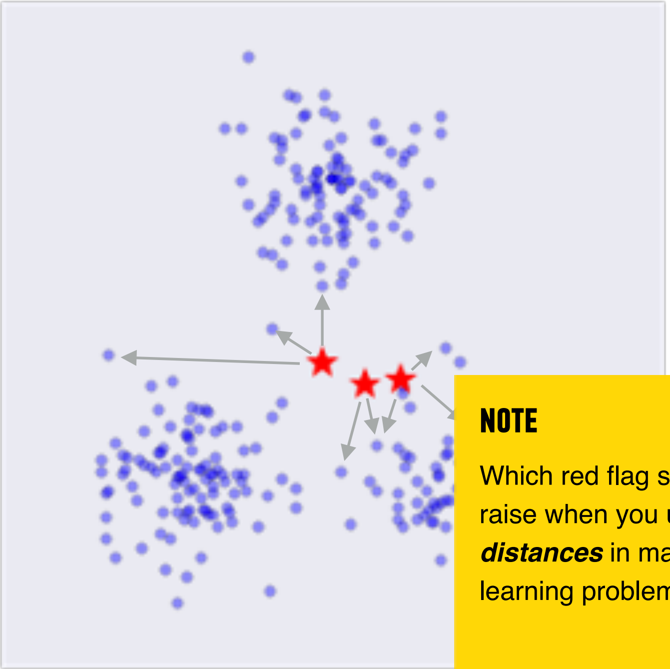
Start with k cluster centers chosen at random



Steps of k-means algorithm

Start with k cluster centers chosen at random

1. *Compute distances from each point to centers*



NOTE

Which red flag should raise when you use ***distances*** in machine learning problems?

Steps of k-means algorithm

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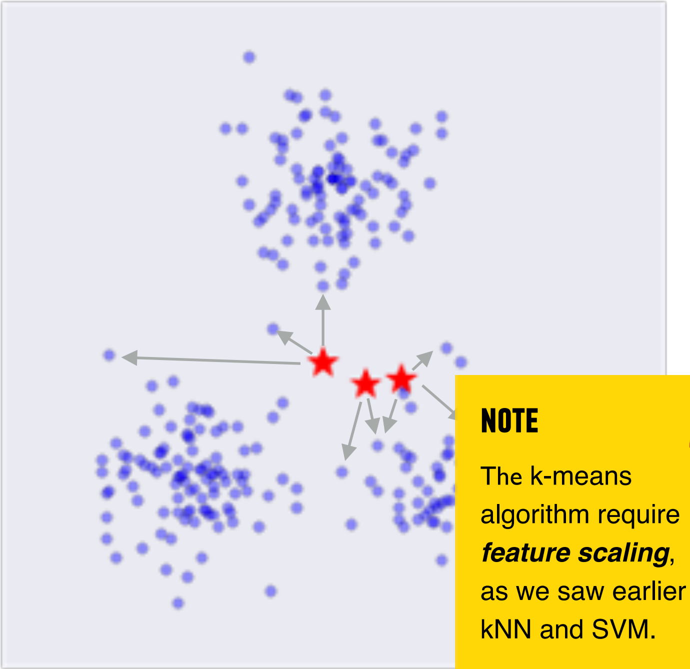

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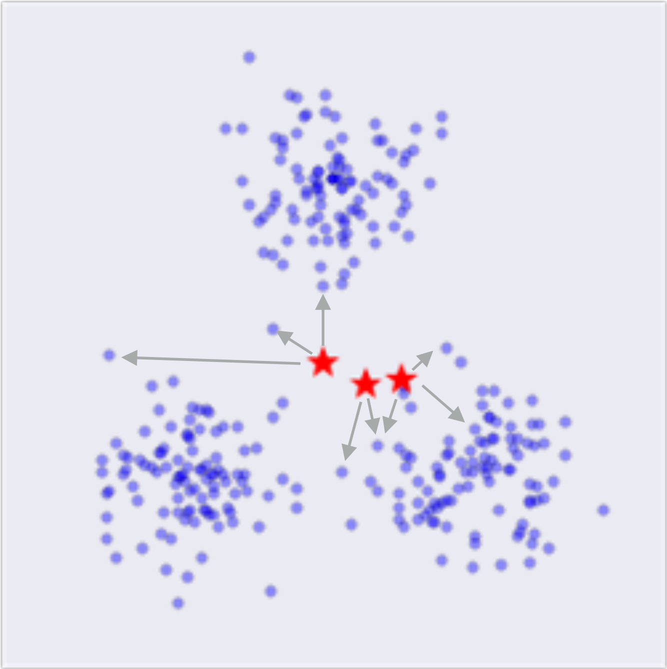
NOTE

The k-means algorithm require ***feature scaling***, as we saw earlier with kNN and SVM.



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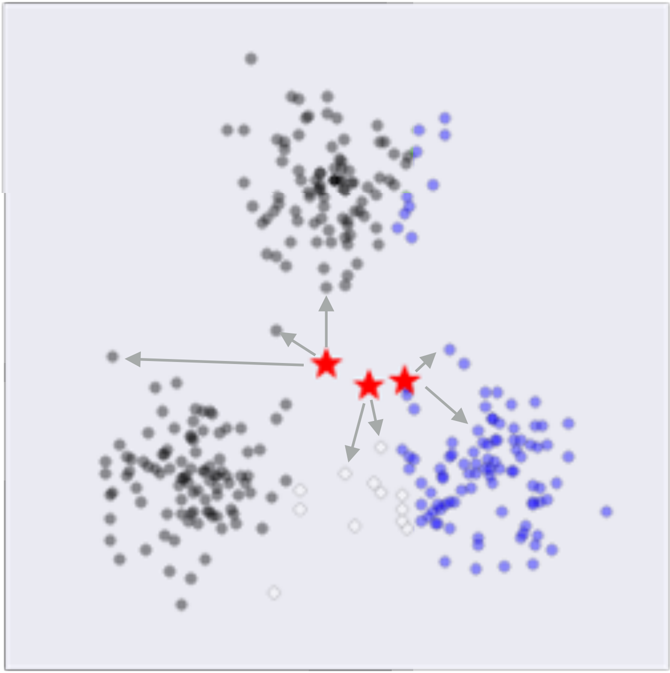
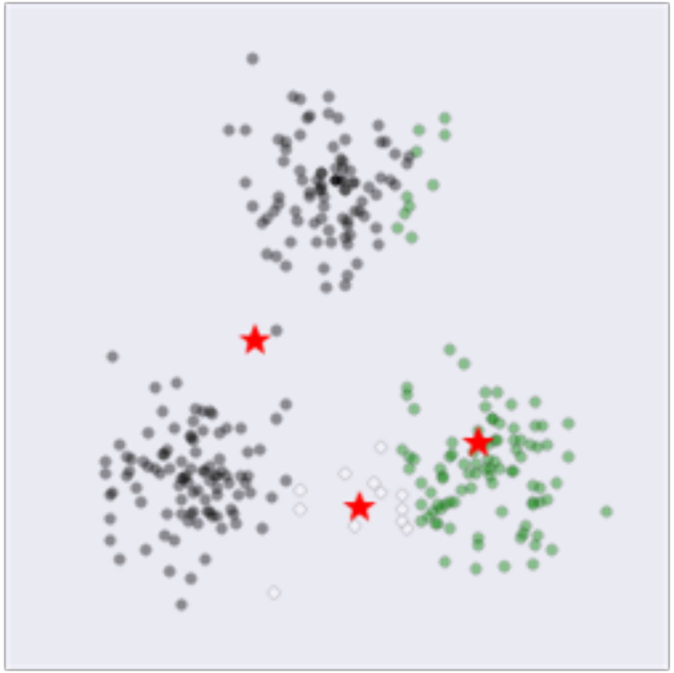


Steps of k-means algorithm

Start with k cluster centers chosen at random

1. *Compute distances from each point to centers*
2. *Label data according to their closest cluster*



Steps of k-means algorithm

Start with k cluster centers chosen at random

1. *Compute distances from each point to centers*
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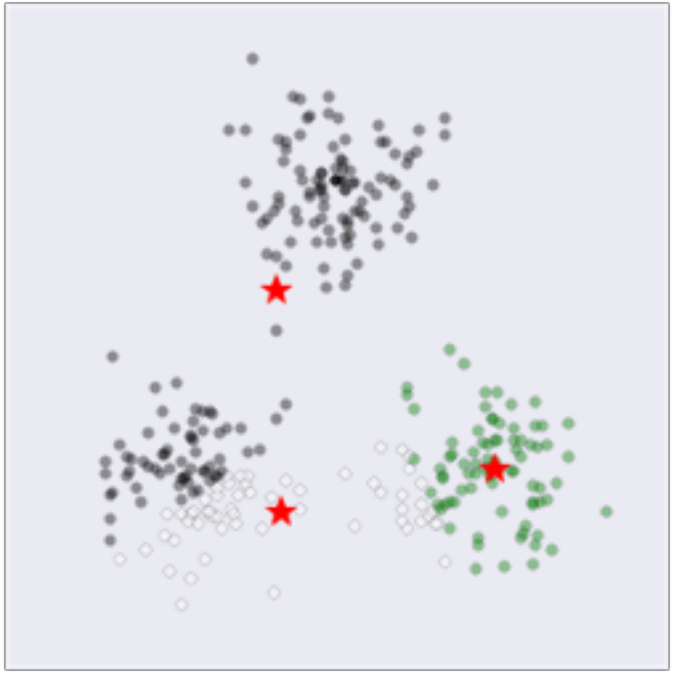
3. *Recompute cluster centers*



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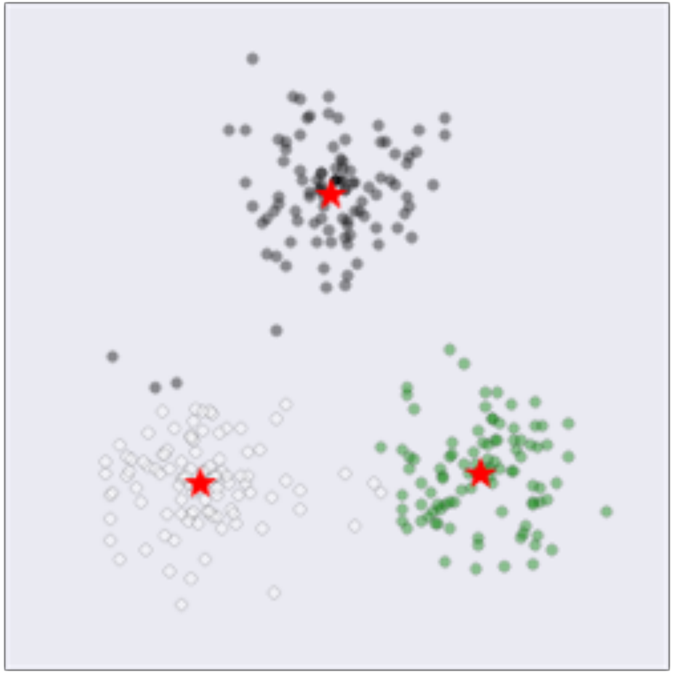

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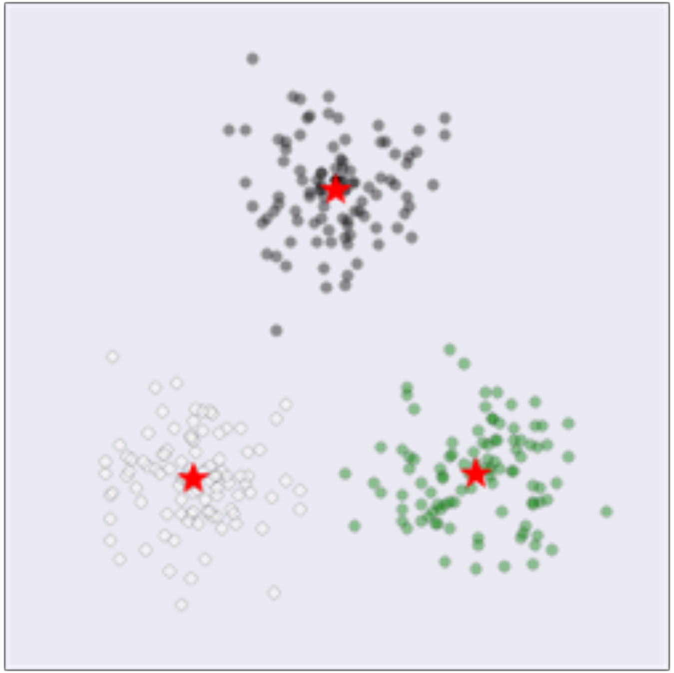

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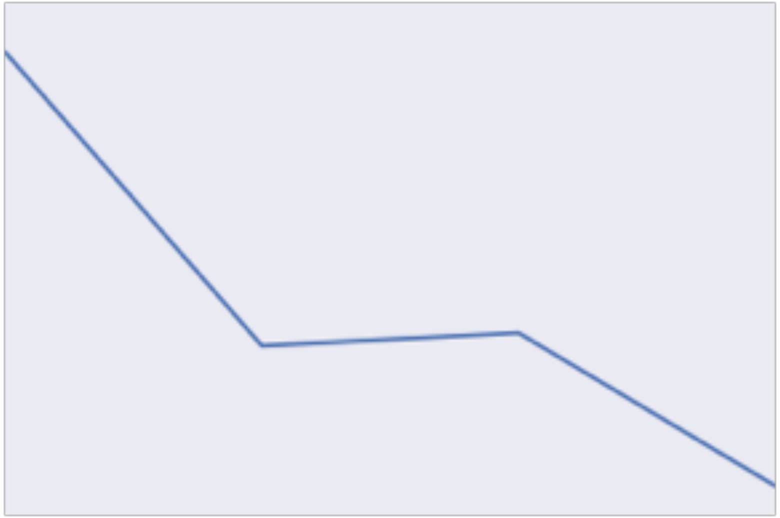
COST FUNCTION

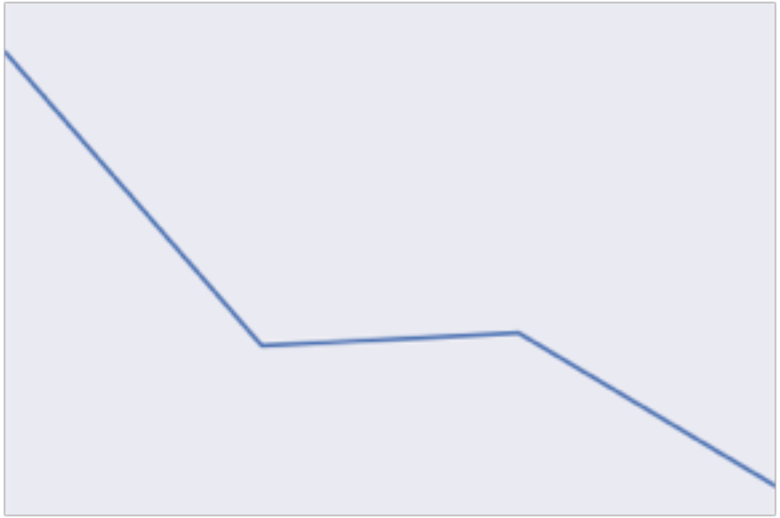
Average distance to closest cluster



Iterations →

At each step, we compute the **average distance** *to the closest cluster center as its 'cost'*

Average distance to closest cluster



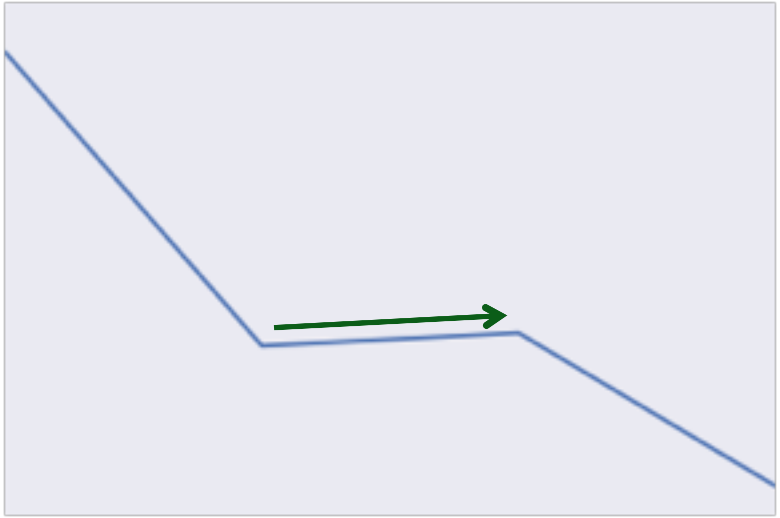
Iterations

At each step, we compute the **average distance** *to the closest cluster center as its 'cost'*

Sometimes you'd see the **sum of squared distances**, which optimizes identically

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} d(x, c_i)^2$$

Average distance to closest cluster



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As you see already, the cost function does **not** *necessarily always decrease*

III. CLUSTER VALIDATION

supervised	*test out your predictions*
unsupervised	*...*

supervised	*test out your predictions*
unsupervised	*can't really*

How do we choose k?

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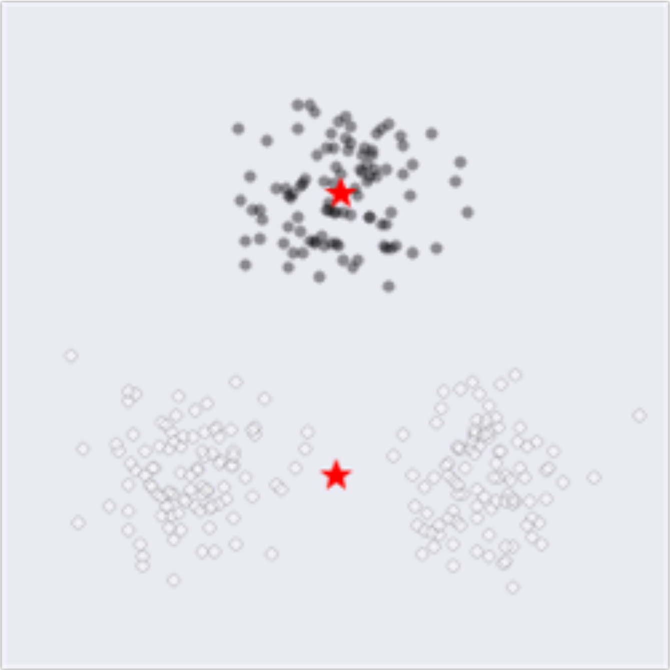

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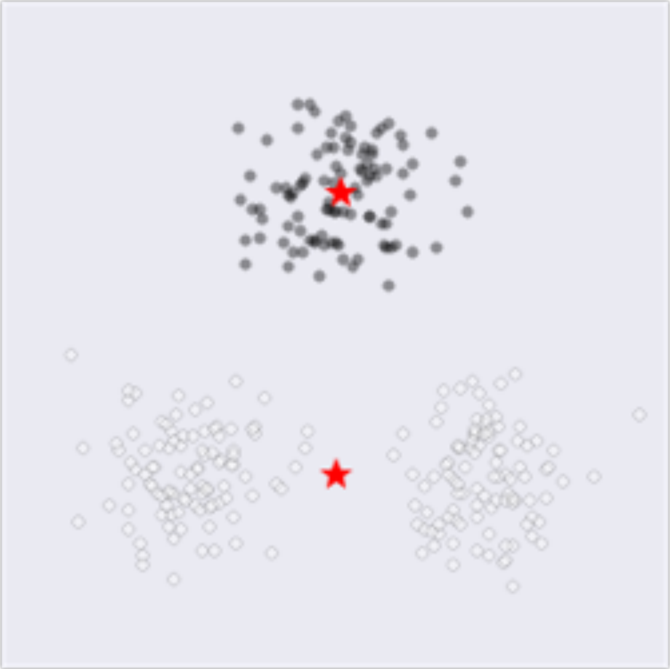

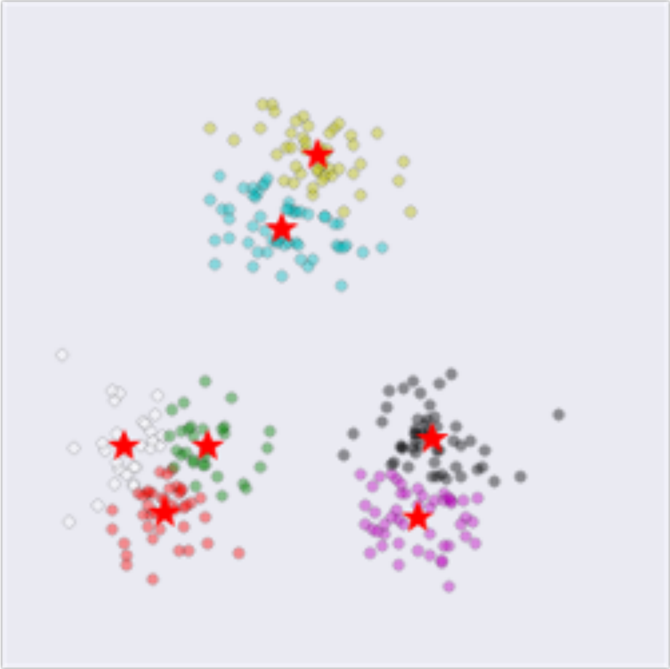

In general, k-means will converge to a solution and return a partition of k clusters, even if no natural clusters exist in the data.

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We will look at two validation metrics useful for partitional clustering, **cohesion** *and* **separation**.

Cohesion *measures clustering effectiveness within a cluster.*

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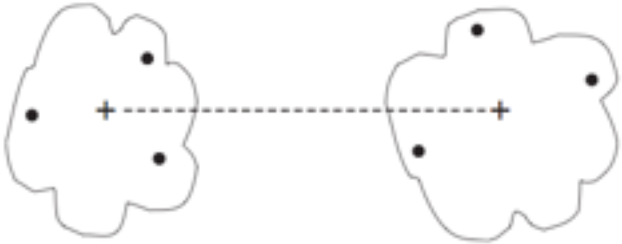

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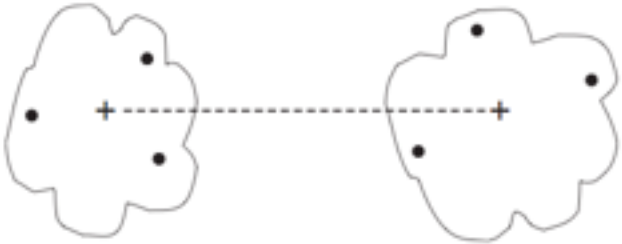

$$\hat{S}(C_i, C_j) = d(c_i, c_j)$$

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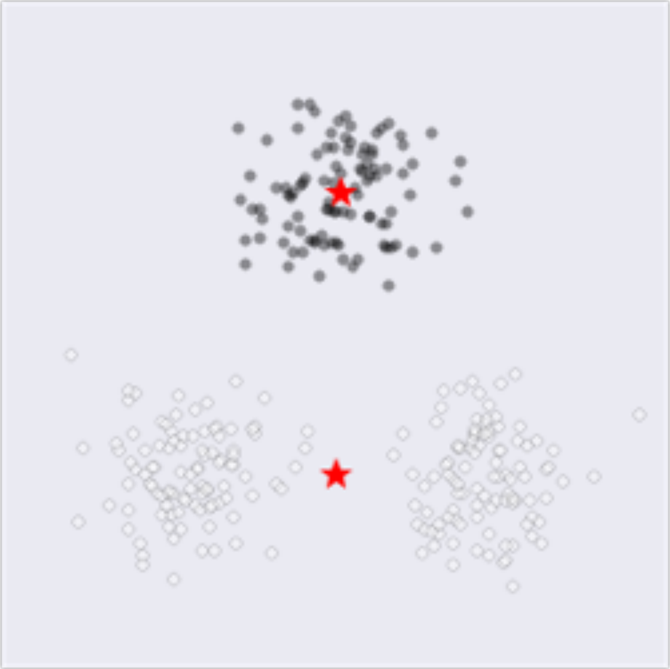

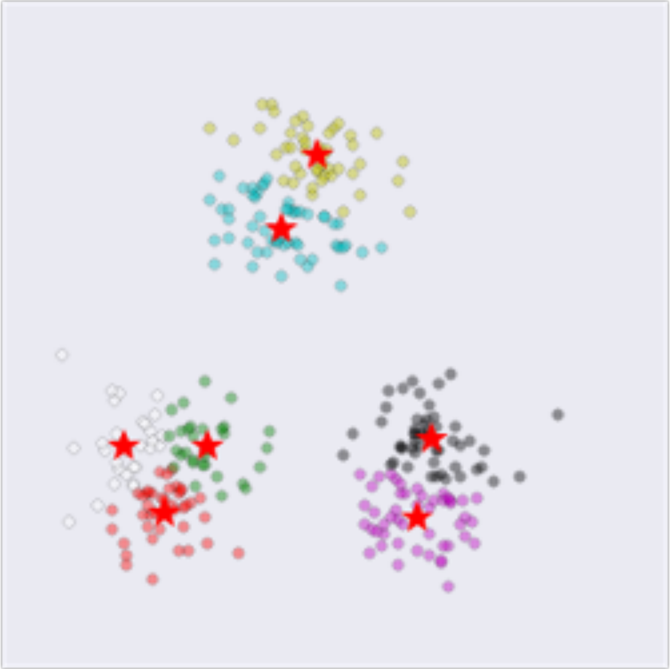

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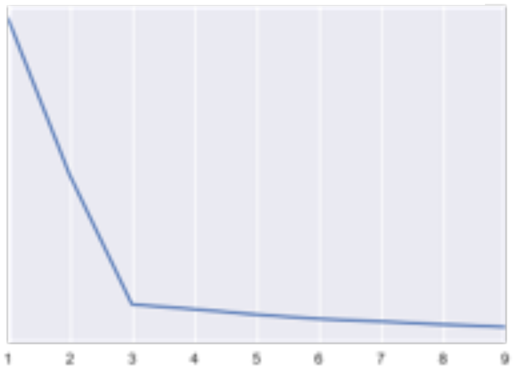
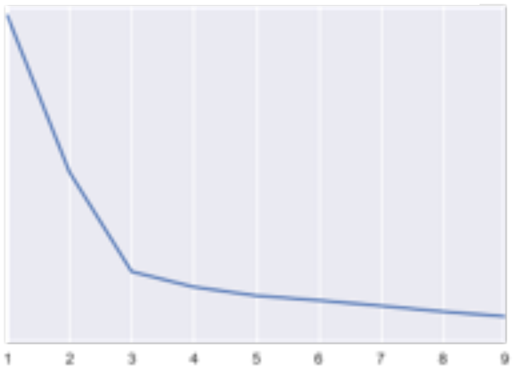
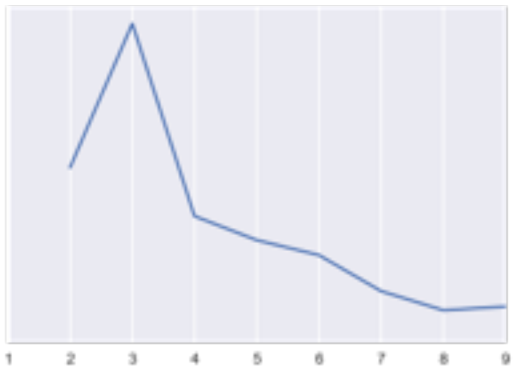


Average cohesion within clusters



Average separation between clusters



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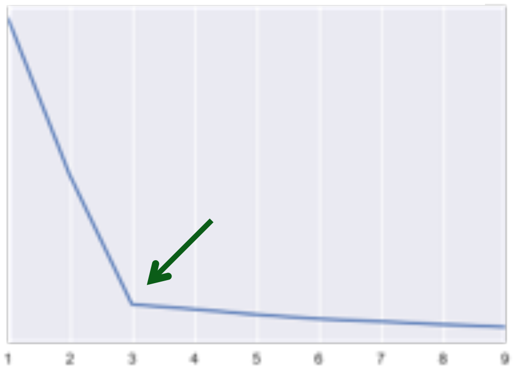

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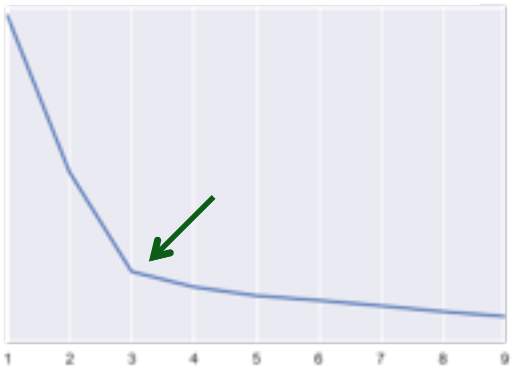
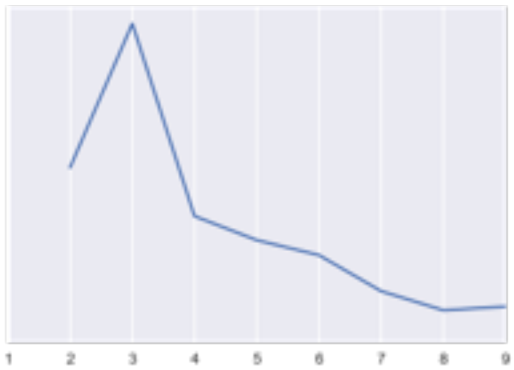


Average separation between clusters



Look for the **largest kink** *in the cost curve (this is called the* **elbow method***)*

How do we choose k?

Average distance to closest cluster

Average cohesion within clusters

Average separation between clusters

Look for the **largest kink** *in the cost curve (this is called the* **elbow method***)*

Or look for the **largest separation** *between clusters*

In practice, you'd choose k with a certain application in mind

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For example, you'd like to manufacture three sizes of clothing: small, medium or large

Ultimately, cluster validation and clustering in general are suggestive techniques that rely on human interpretation to be meaningful.

DISCUSSION