GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 15: K-MEANS CLUSTERING

COURSE OUTLINE: COMPLETED

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?

COURSE OUTLINE

- 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

- DESCRIBE UNSUPERVISED LEARNING AND CLUSTERING
- DESCRIBE WHAT K-MEANS DOES
- APPLY K-MEANS IN SCLERA

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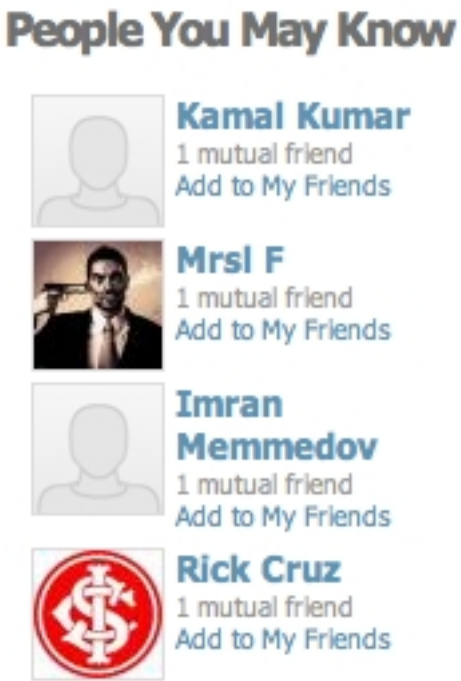
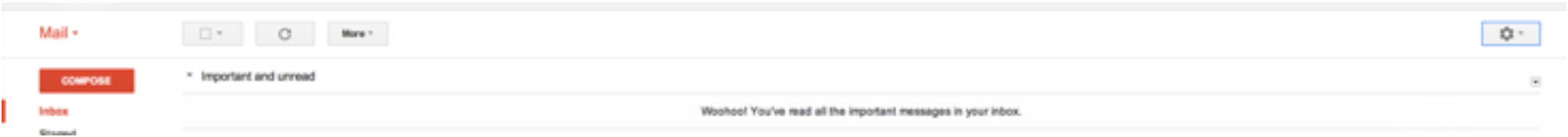
A: To enhance our understanding of a dataset by dividing the data into groups.


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 programatically 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)*
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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)

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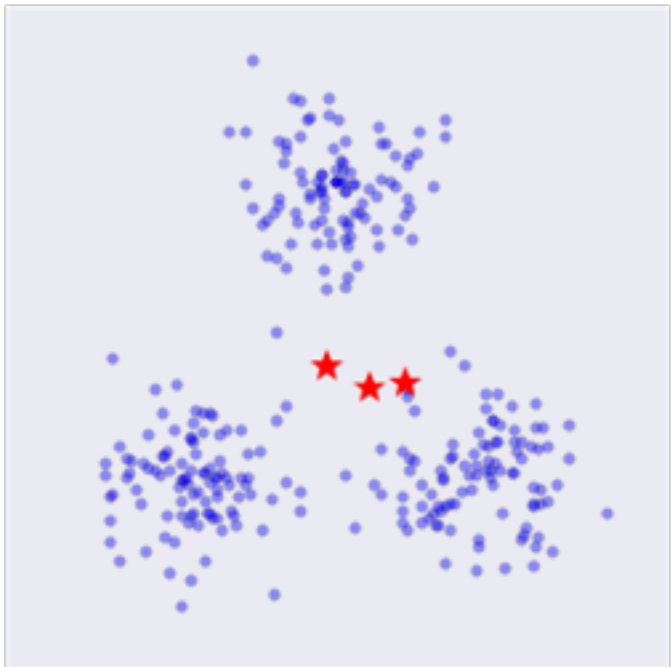
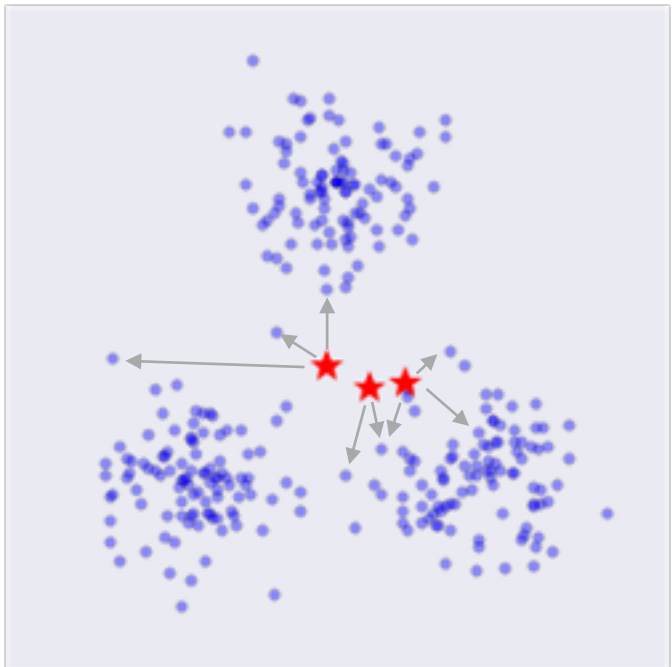
We could like to infer class labels from the data, i.e., cluster the data into similar groups

Steps of k-means algorithm



Steps of k-means algorithm

Start with k cluster centers chosen at random



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1. *Compute distances from each point to centers*

NOTE

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

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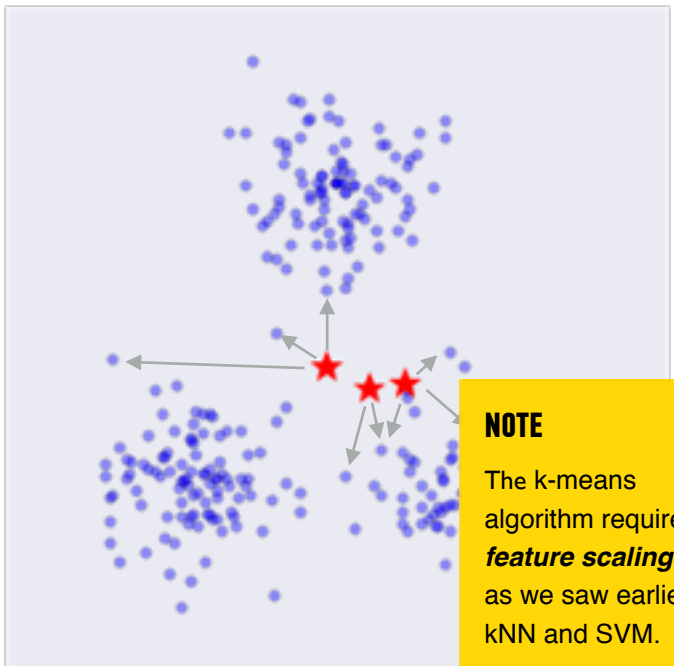

NOTE

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

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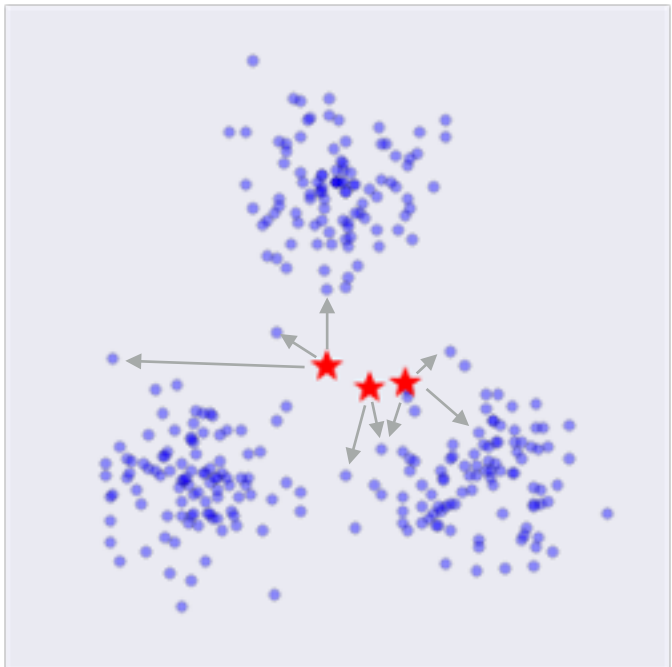

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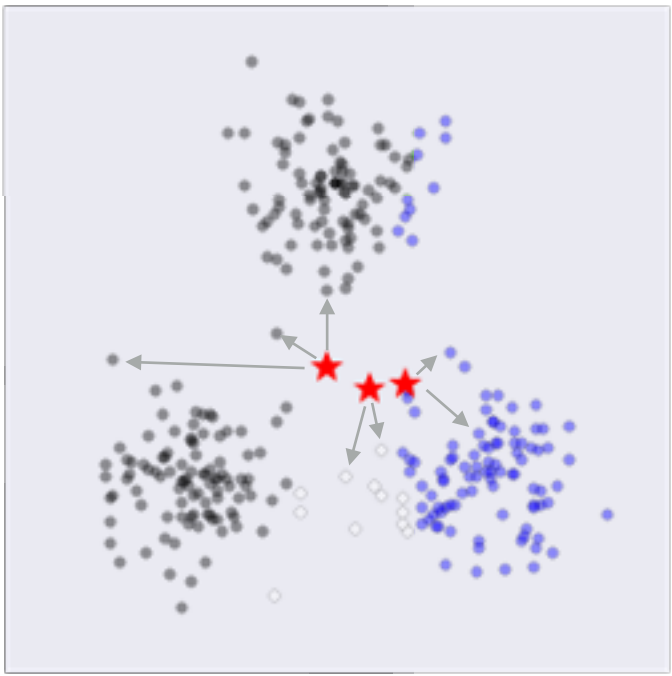
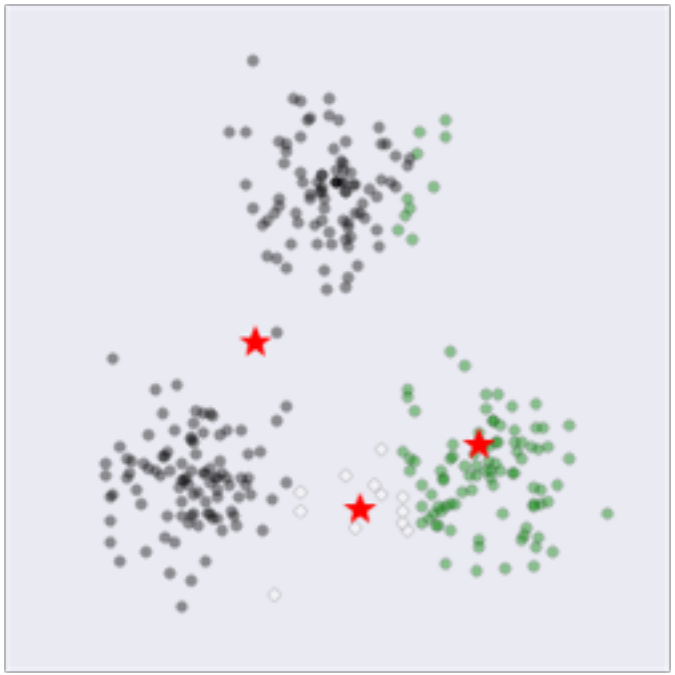


Steps of k-means algorithm

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

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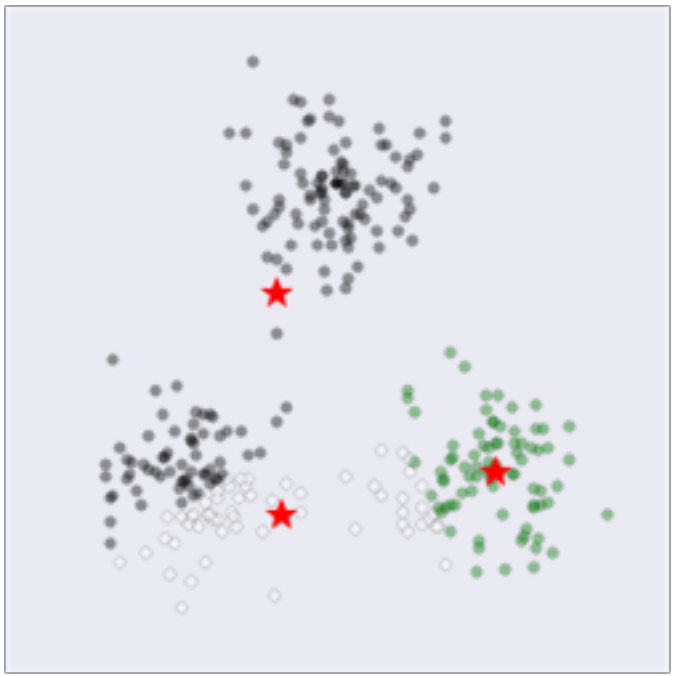

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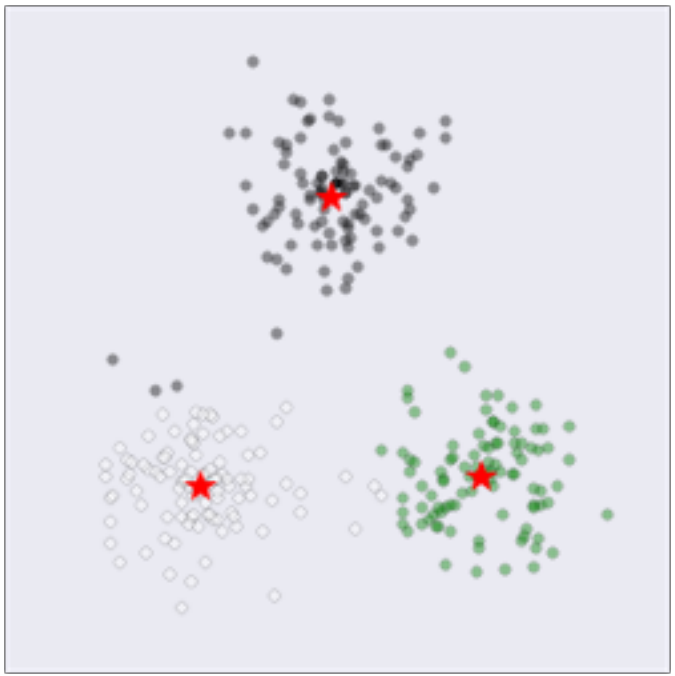
(or some maximum iteration has been reached)



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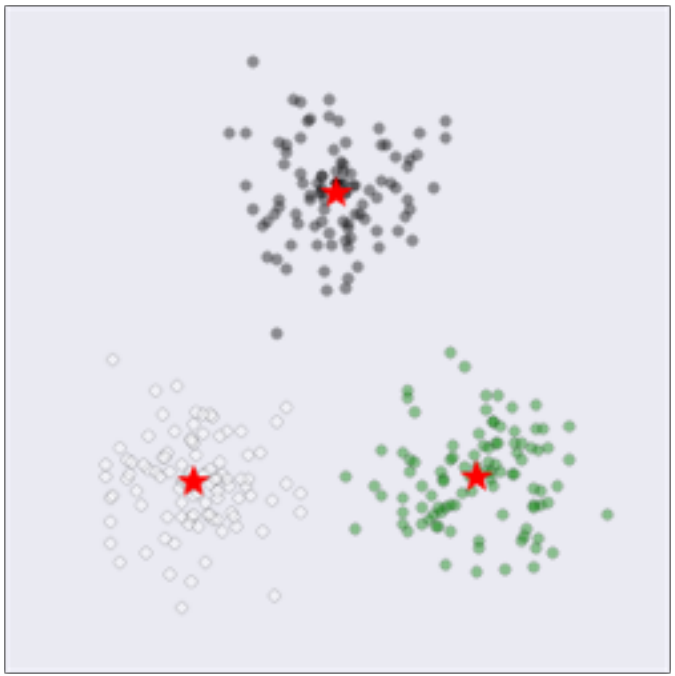

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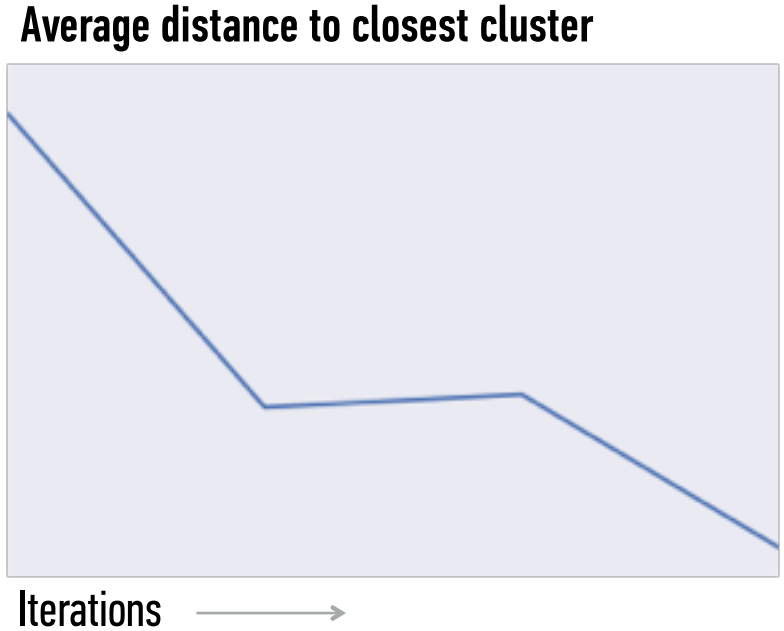
COST FUNCTION



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

Average distance to closest cluster

Iterations

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

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

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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	*can't really*

How do we choose k?

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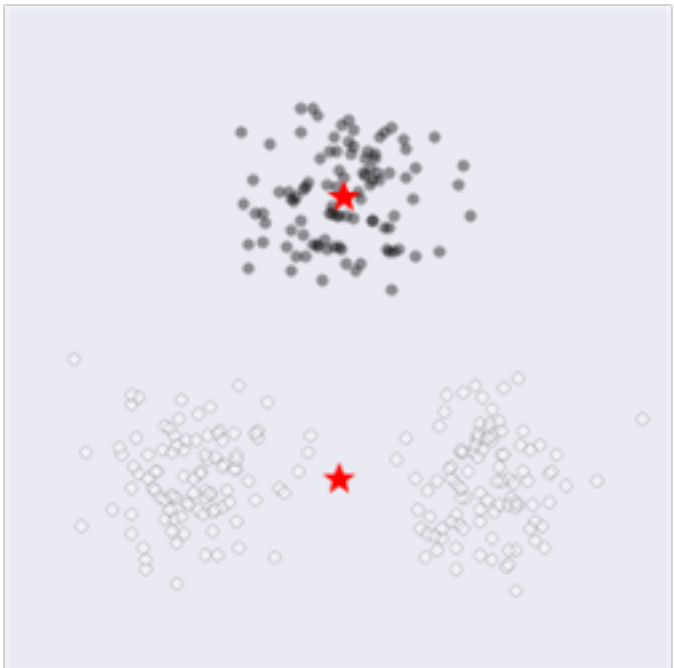

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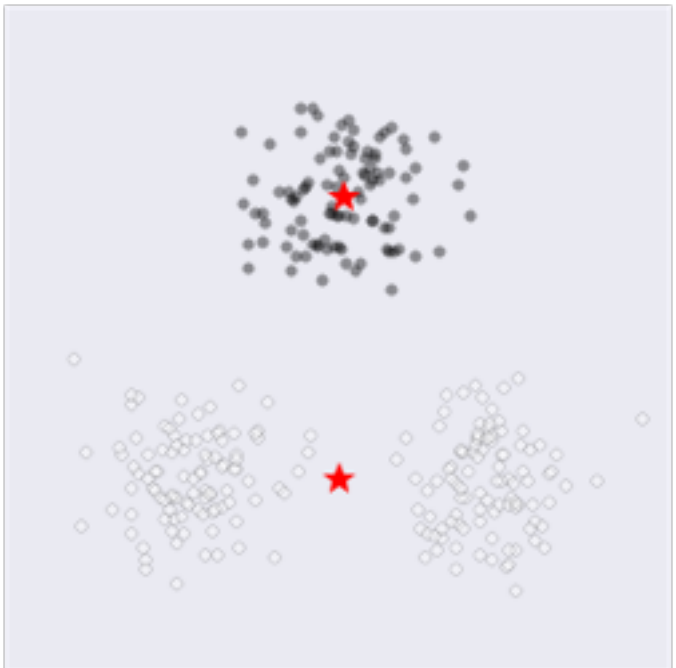

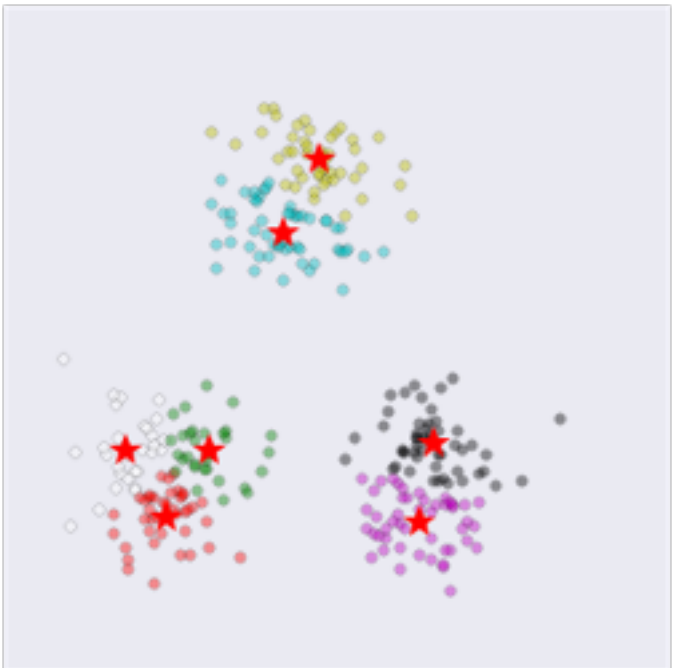

In general, k-means will converge to a solution and return a partition of k clusters, even if no natural clusters exist in the data.

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

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Separation *measures clustering effectiveness between clusters.*

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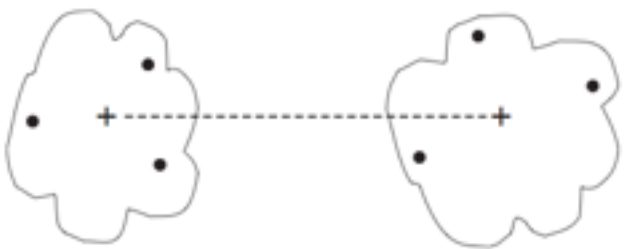

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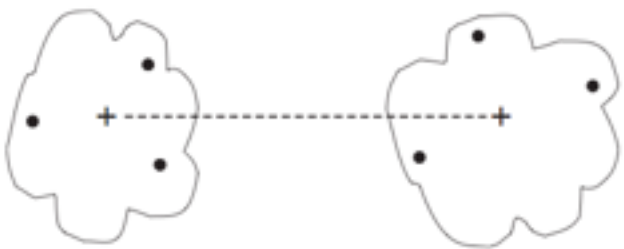
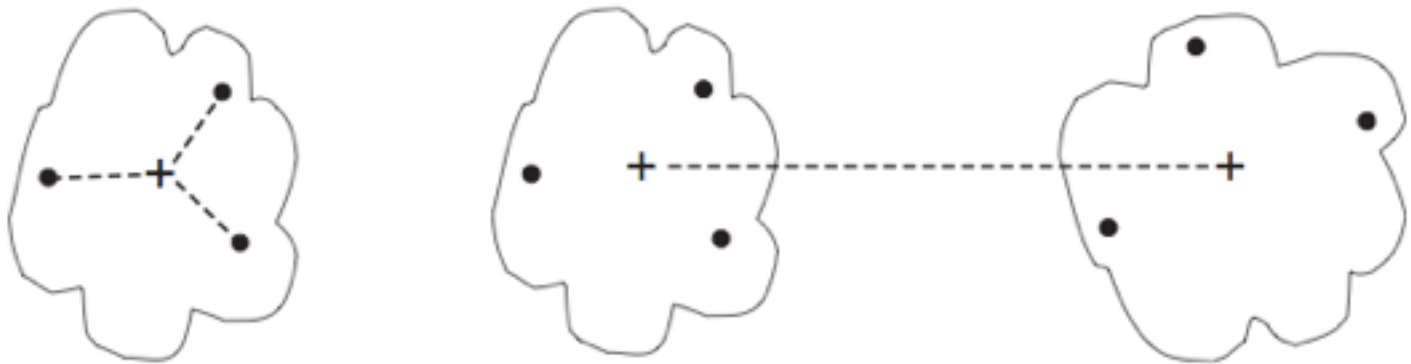


$$\hat{S}(C_i, C_j) = d(c_i, c_j)$$



(a) Cohesion.

(b) Separation.

source: http://www-users.cs.umn.edu/~kumar/dmbook/ch8.pdf

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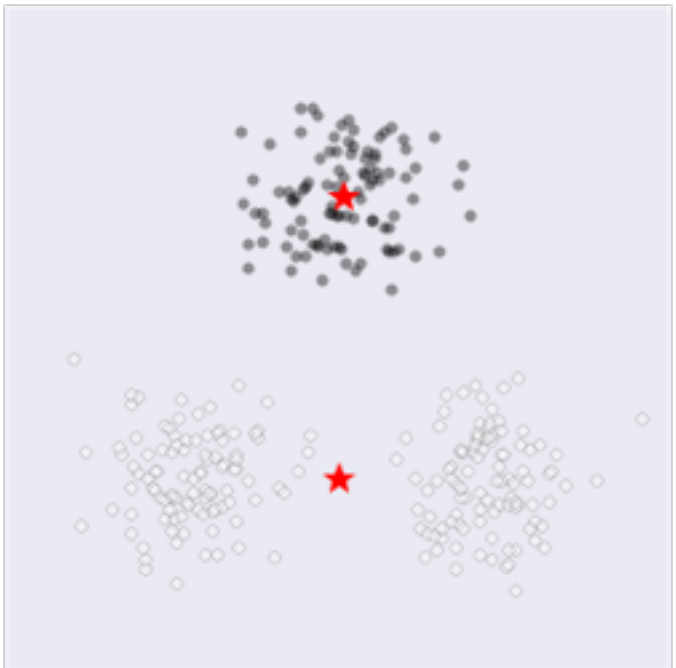
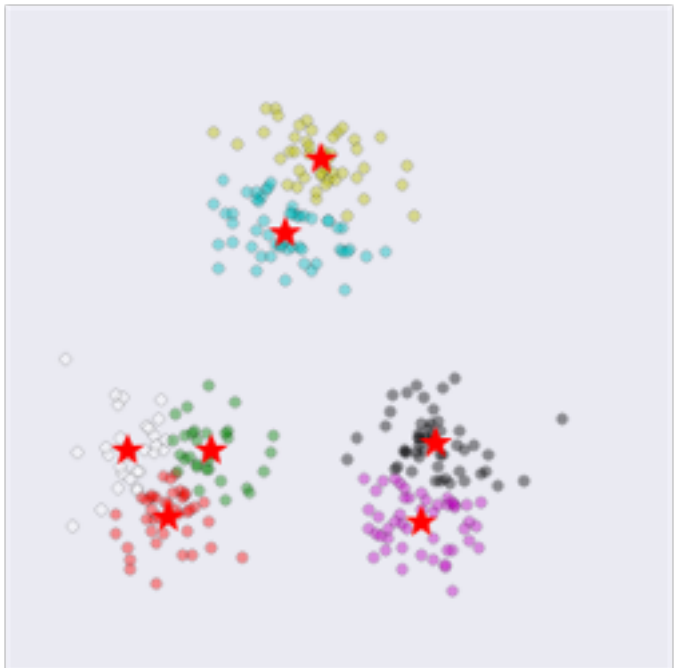
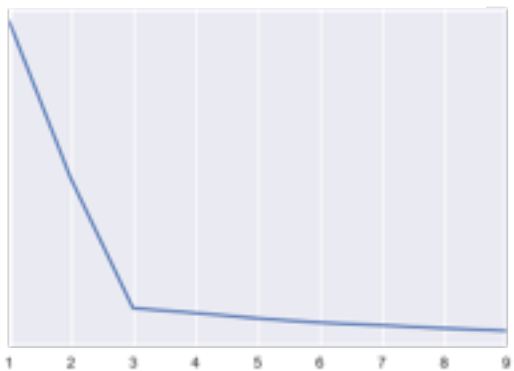


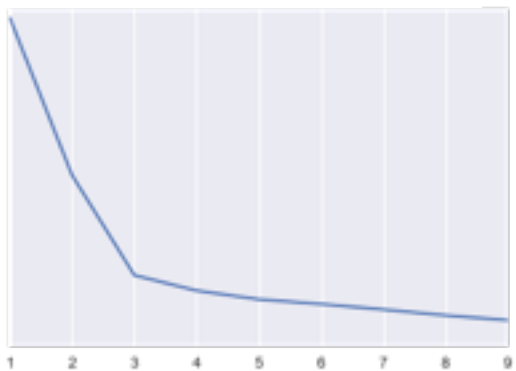


How do we choose k?

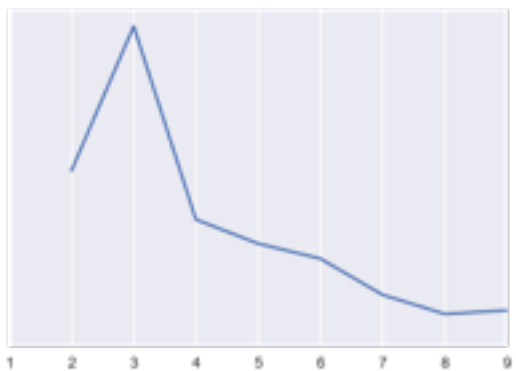
Average distance to closest cluster



Average cohesion within clusters



Average separation between clusters



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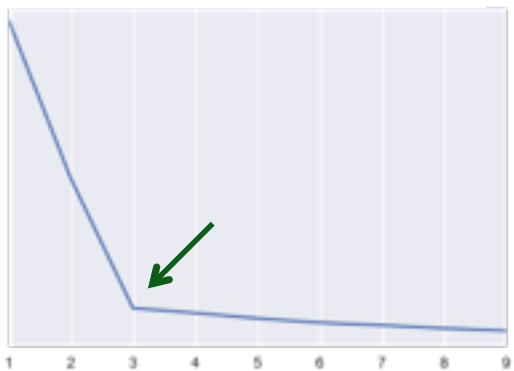

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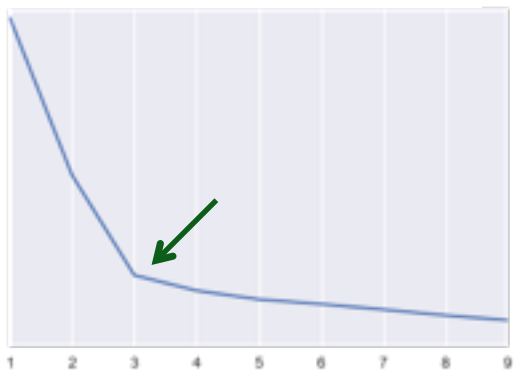

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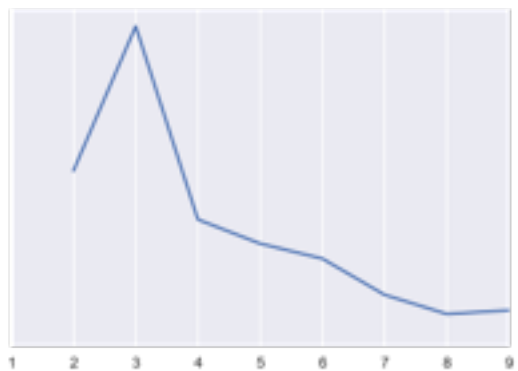

Look for the **largest kink** *in the cost curve (this is called the* **elbow method***)*

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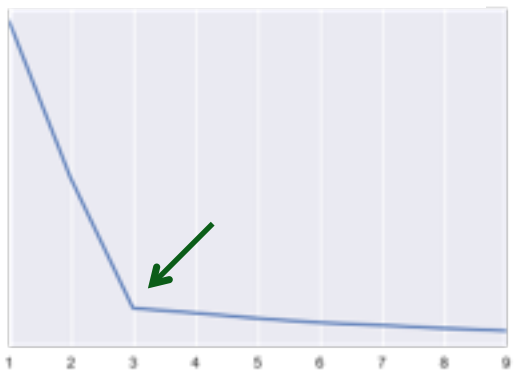

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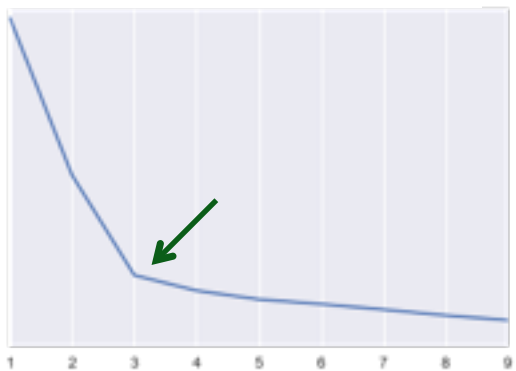

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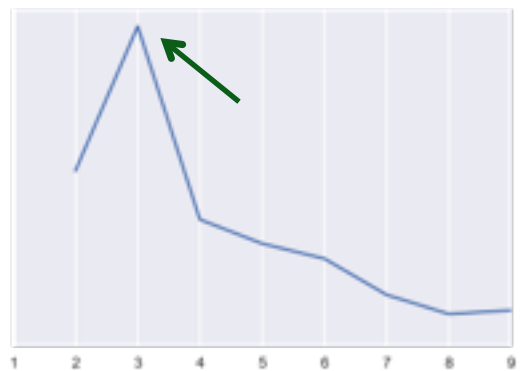

Look for the **largest kink** *in the cost curve (this is called the* **elbow method***)*

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