

# K MEANS CLUSTERING

Brian Chung

## SOMETHING COOL

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Is your model smarter than an 8th grader?



<https://www.kaggle.com/c/the-allen-ai-science-challenge>

<http://blog.talla.com/2016/01/how-we-approached-the-allen-ai-challenge-on-kaggle/>

### Why Deep Learning Won't Work On A Problem Like This

If you don't know much about machine learning other than what you read in the tech press, your first thought is probably "just throw deep learning at it." Right? Not exactly.

The Allen AI challenge is a difficult use case for deep learning because answering questions is highly dependent on the structure of natural language questions, as well as an accumulated knowledge base. Recently there has been an increased use of 'word vectors' that allow deep learning to effectively perform many NLP tasks. In this case, however, converting question [words to vectors](#) is insufficient because the resulting representation does not capture the *compositional* nature of language. For example, take the question "Which of the following is not a way that plants extract energy from their environment?". The usage of *not* changes the meaning of the sentence. "Their environment" is a unit in the sentence that also references the earlier "plants." Learning to parse sentences like these constitutes a learning task in its own right, and people can manually specify grammars for parsing language that are currently hard to beat statistically.

Compounding the difficulty of this task is the problem of using acquired knowledge. A person attempting to answer the questions on the test has an internal model of the facts that the question corresponds to. *Plants* exist in a given *environment* and *extract energy* in several ways. People are able to recall information relevant to the question and organize it in a way that helps answer the question. Research pairing deep learning with memory is an ongoing effort, but similar to natural language processing, shortcuts such as data retrieval are often still more efficient. For example, most search engines encode large bodies of facts in a regularly and easily processable form rather than trying to extract information from a representation in a neural network. Taken together, the problems of natural language processing and utilizing preexisting knowledge bases create a difficult challenge that is often easier to tackle with hand crafted modeling and engineering, rather than end-to-end deep learning. Maybe someday deep learning will solve this problem, but today is not that day.

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## **FROM LAST TIME**

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### **Questions:**

- L1 and L2 logistic regression comparison
- Do you tune C, and THEN the ROC curve? or do you do both? Or do you tune ROC and then C?
- clarity into C value and modulating C
- how do outliers affect logistic regression

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## RECAP

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Numpy Pandas

Data Exploration

**Data Skills**

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**Data Skills**

KNN

Naive Bayes

Logistic Regression

**Classification**

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Regularization

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Linear Regression

Regularization

K Means

**Regression**

**Clustering**

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## K MEANS CLUSTERING AGENDA

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- I. Cluster Analysis
- II. K-Means Clustering
- III. Validation

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## K MEANS CLUSTERING

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### I. CLUSTER ANALYSIS

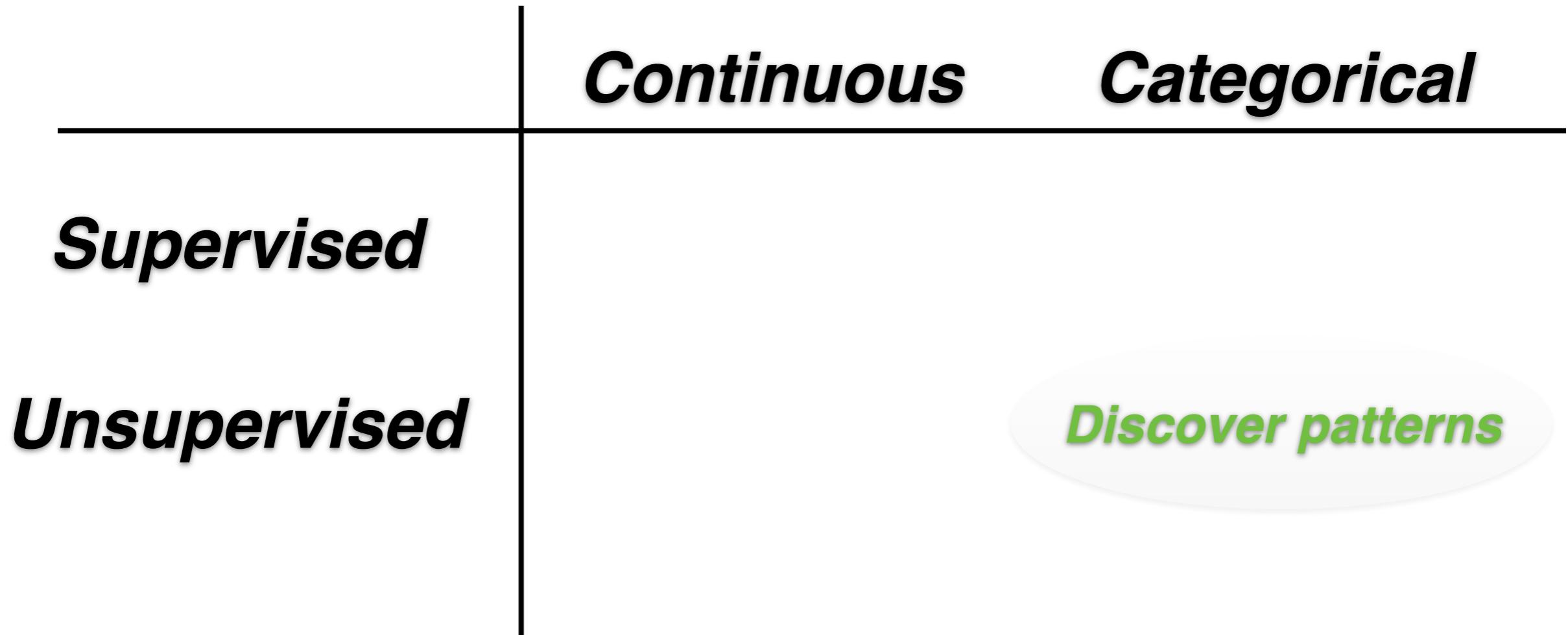
## TYPES OF ML SOLUTIONS

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	<i>Continuous</i>	<i>Categorical</i>
<i>Supervised</i>	<i>Regression</i>	<i>Classification</i>
<i>Unsupervised</i>	<i>Dimension Reduction</i>	<i>Clustering</i>

## TYPES OF ML SOLUTIONS

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## **CLUSTER ANALYSIS**

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**Q:** What is a cluster?

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

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

In general, greater similarity between points leads to better clustering

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*Ex: You sample 100 people's arm and chest measurements. Then you cluster these measurements into three groups in order to create three t-shirt sizes*

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## CLUSTER ANALYSIS

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**Q:** What is the purpose of cluster analysis?

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

*Ex: You have an image with 32-bit color but you want to reduce the file size of the image. You decide to cluster into 10 groups of colors, and assign each pixel the average of the colors in that group*

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## CLUSTER ANALYSIS

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**Q:** What is the purpose of cluster analysis?

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

*Ex: You're an owner of a pizza chain, and you want to open a few stores. You can analyze the **clusters** from where the pizza is being ordered frequently.*

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## CLUSTER ANALYSIS

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**Q:** What is the purpose of cluster analysis?

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

**Ex:** *Clustering can help marketers improve their customer base. They can target groups of people based on their similarity (i.e. purchasing preferences, purchasing power, etc.)*

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Clustering provides a *layer of abstraction* from the individual datapoints, and is one of many **prototype methods**. We define the data in terms of **prototypical points**.

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Clustering provides a *layer of abstraction* from the individual datapoint, and is one of many **prototype methods**. We define the data in terms of **prototypical points**.

The goal is to extract and enhance the natural structure of the data (and not to impose an arbitrary structure)

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## **CLUSTER ANALYSIS**

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**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

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The real purpose of clustering can be data exploration, so a solution is anything that contributes to your understanding.

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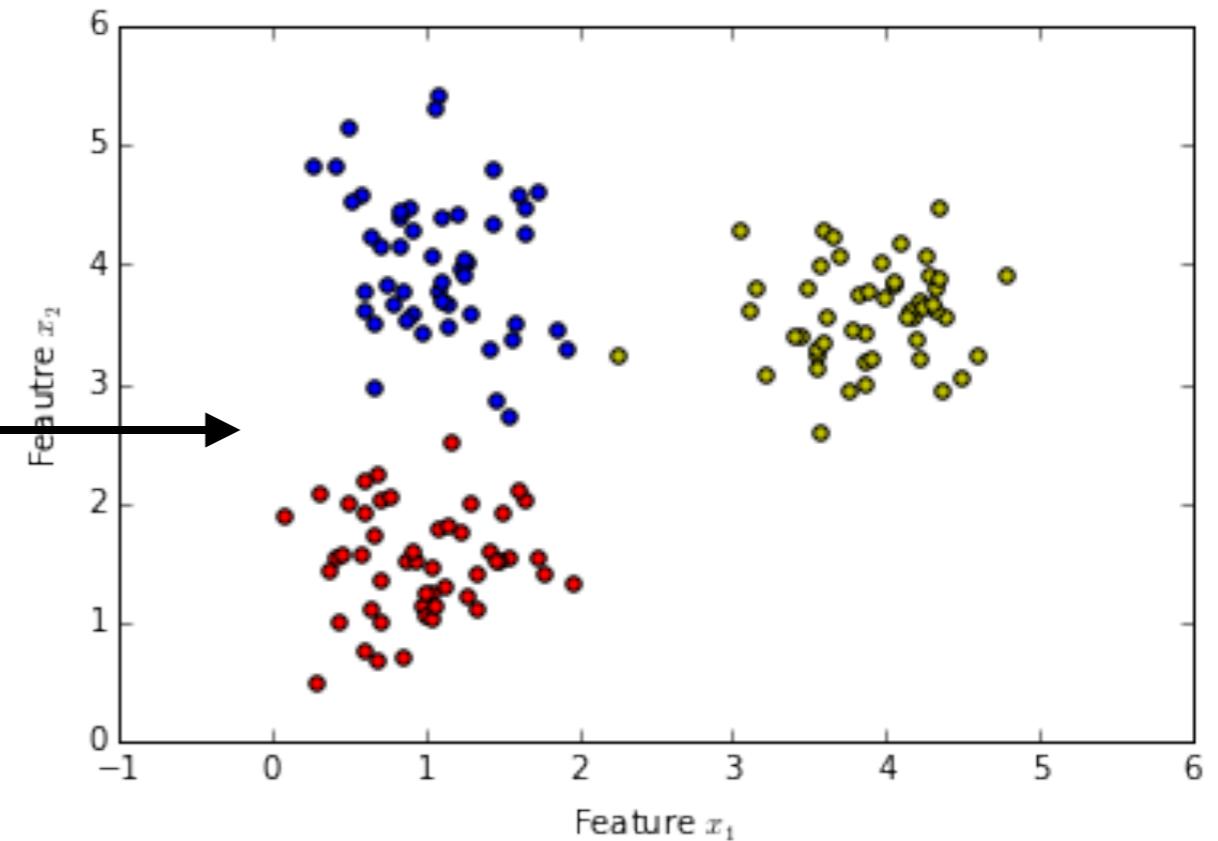
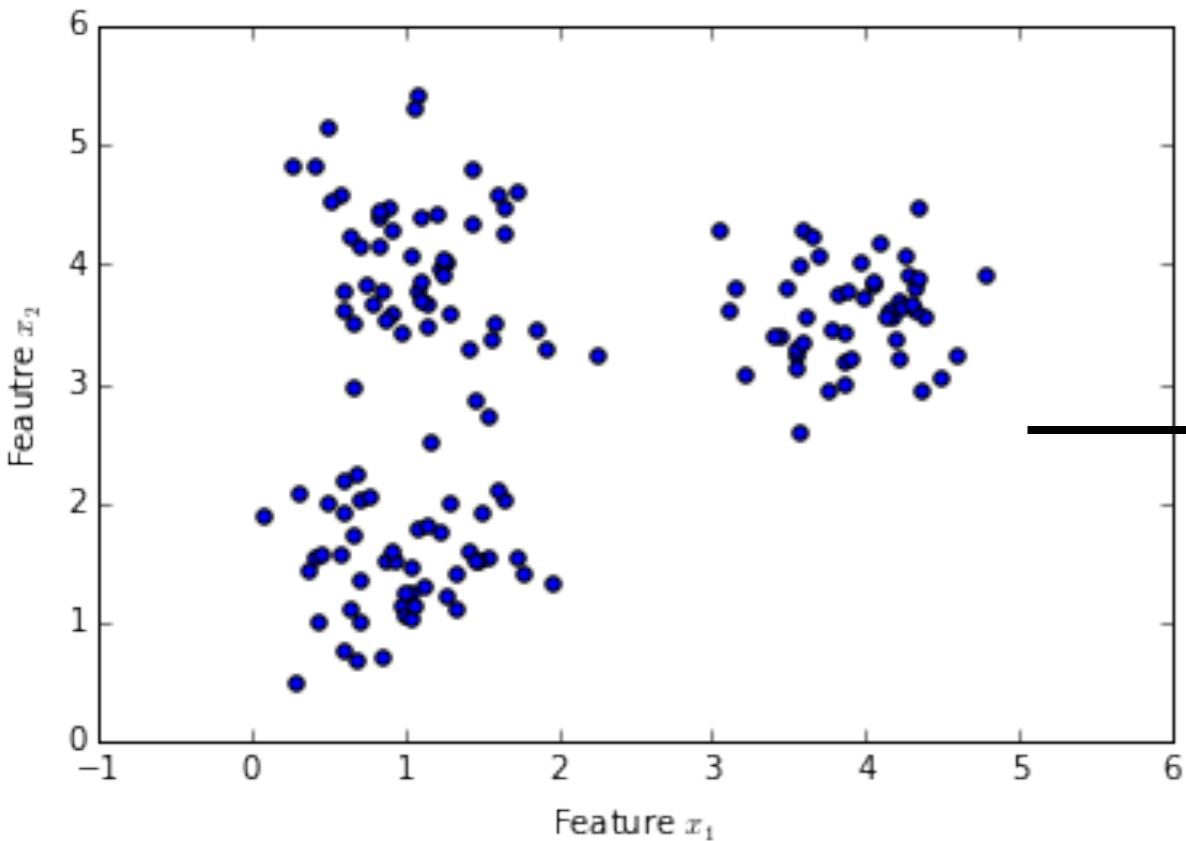
## K MEANS CLUSTERING

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- I. CLUSTER ANALYSIS
- II. K-MEANS CLUSTERING

## K-MEANS CLUSTERING

**K-Means Clustering** is a **greedy learner** that **partitions** a dataset into  $k$  clusters



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

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## K-MEANS CLUSTERING

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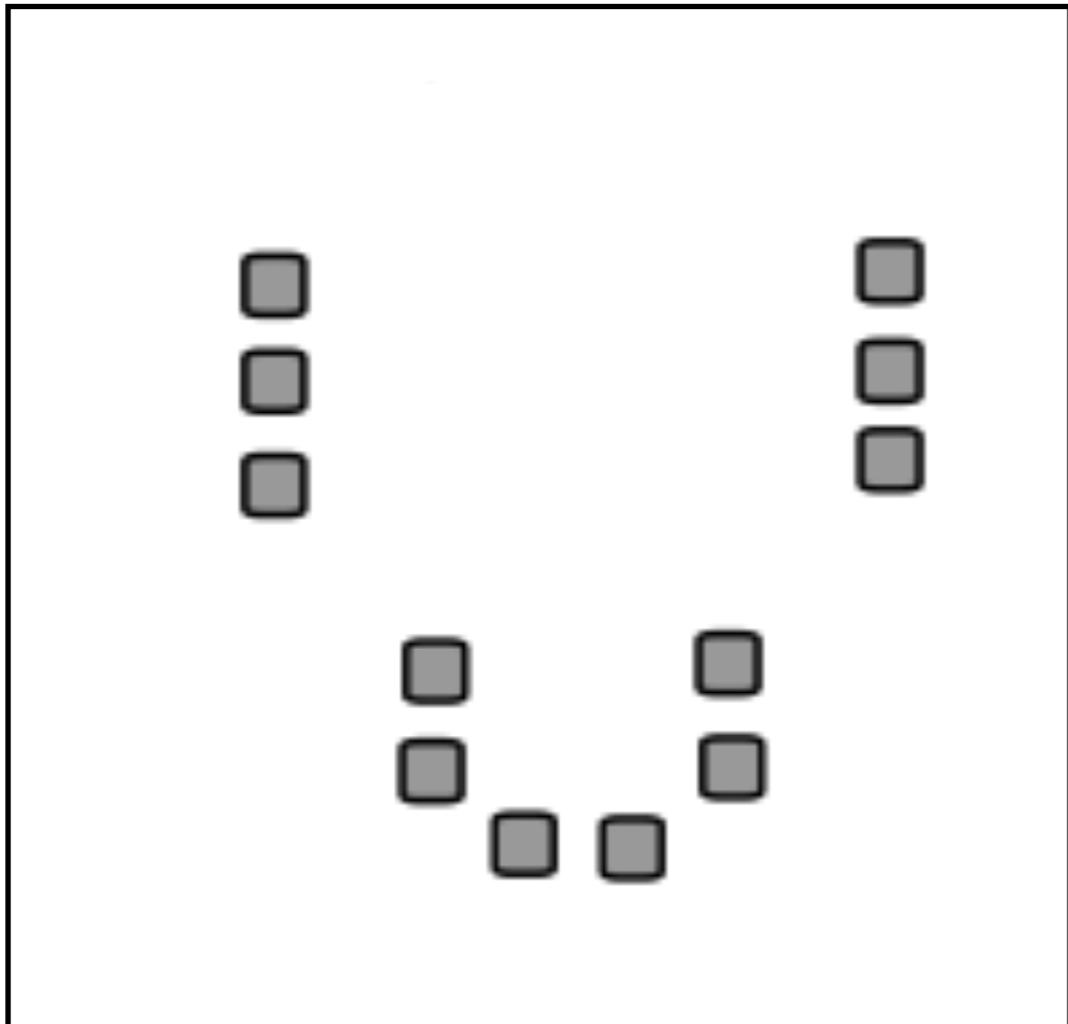
**K-Means Clustering** is a **greedy** learner that **partitions** a dataset into k clusters

**greedy** - captures local structure (*depends on initial conditions*)  
**partition** - each point belongs to exactly one cluster

*K-Means is algorithmically efficient  
(Linear in time and memory by number of records)*

## K-MEANS ALGORITHM

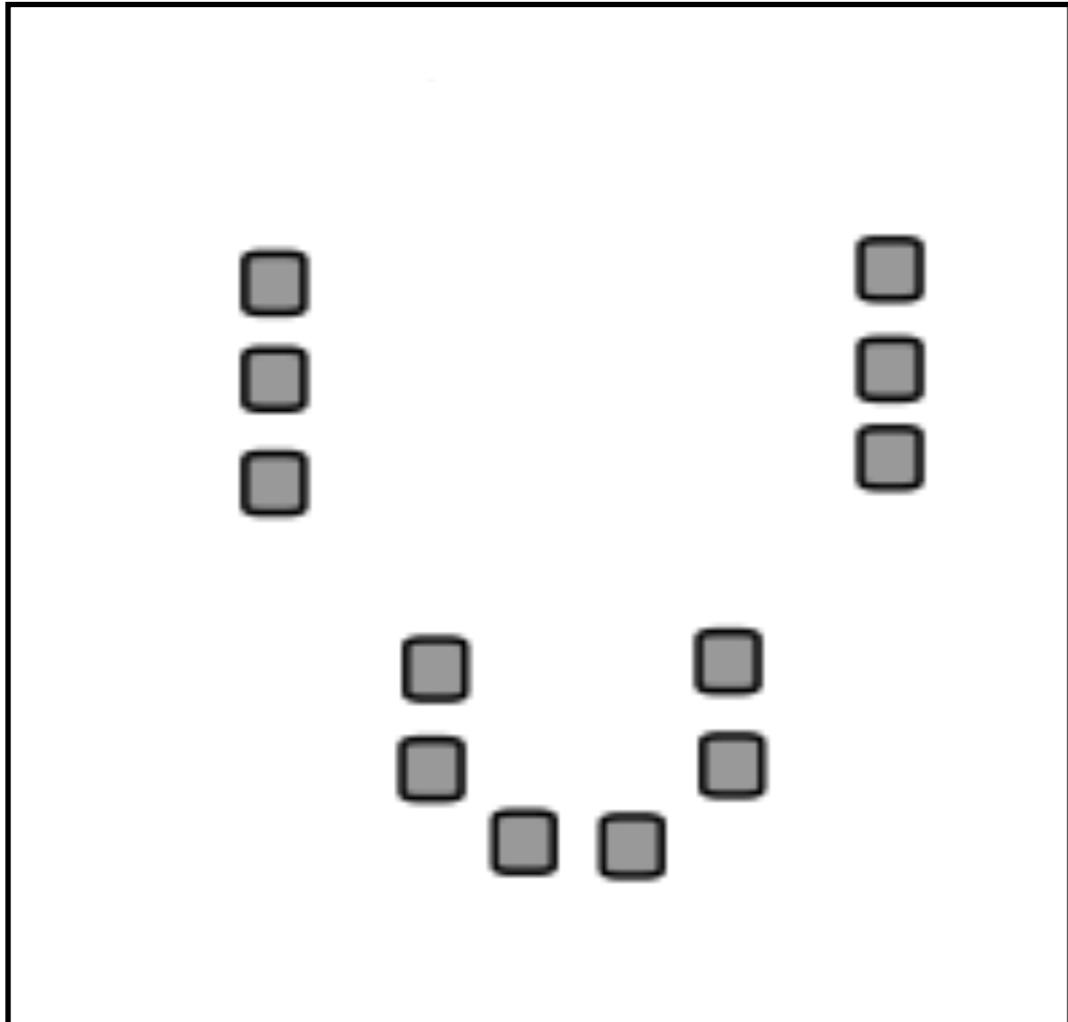
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Suppose we have data with no labels (i.e. unsupervised learning)

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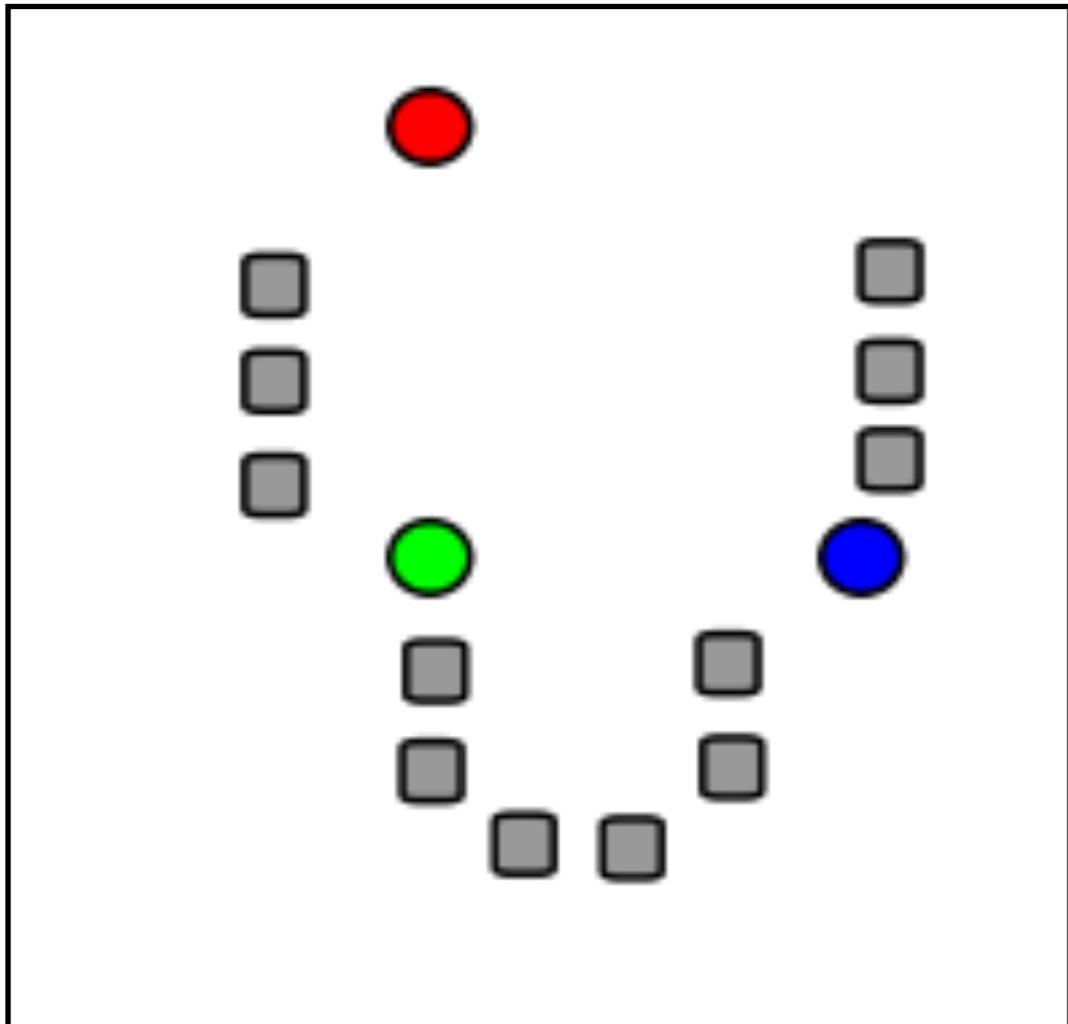


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We would like to infer class labels for the data, or assign each data point to a class label

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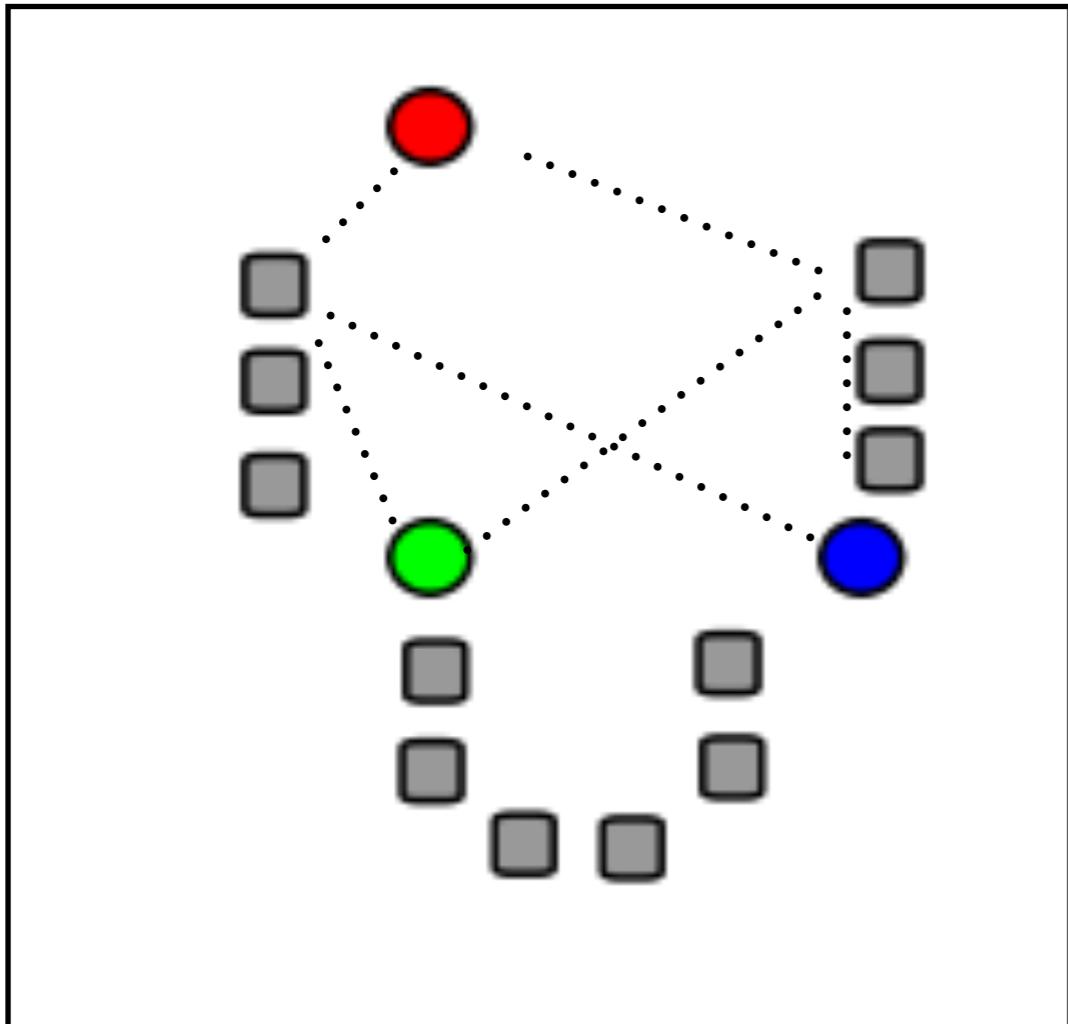
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1. Start with **k** cluster centers (centroids) chosen at random amongst the points

## K-MEANS ALGORITHM

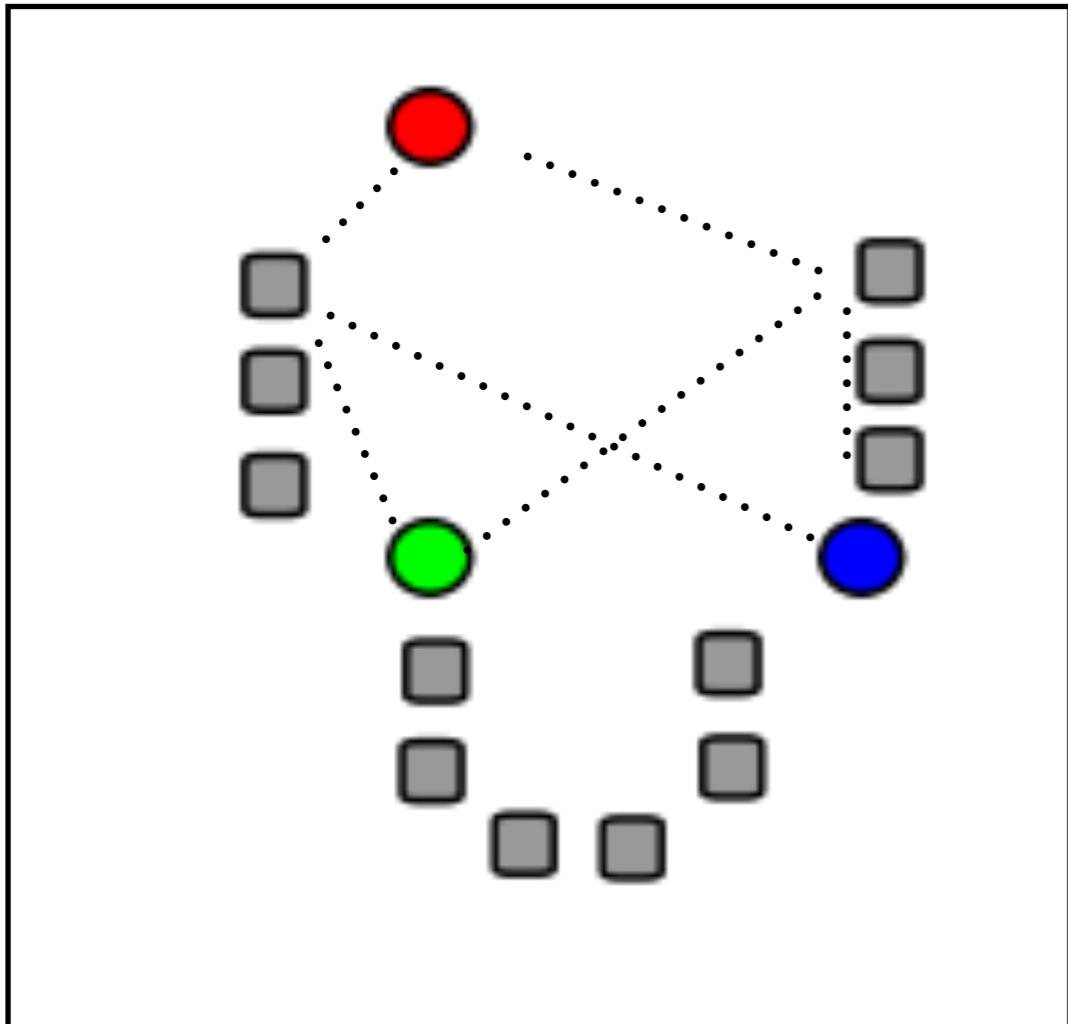
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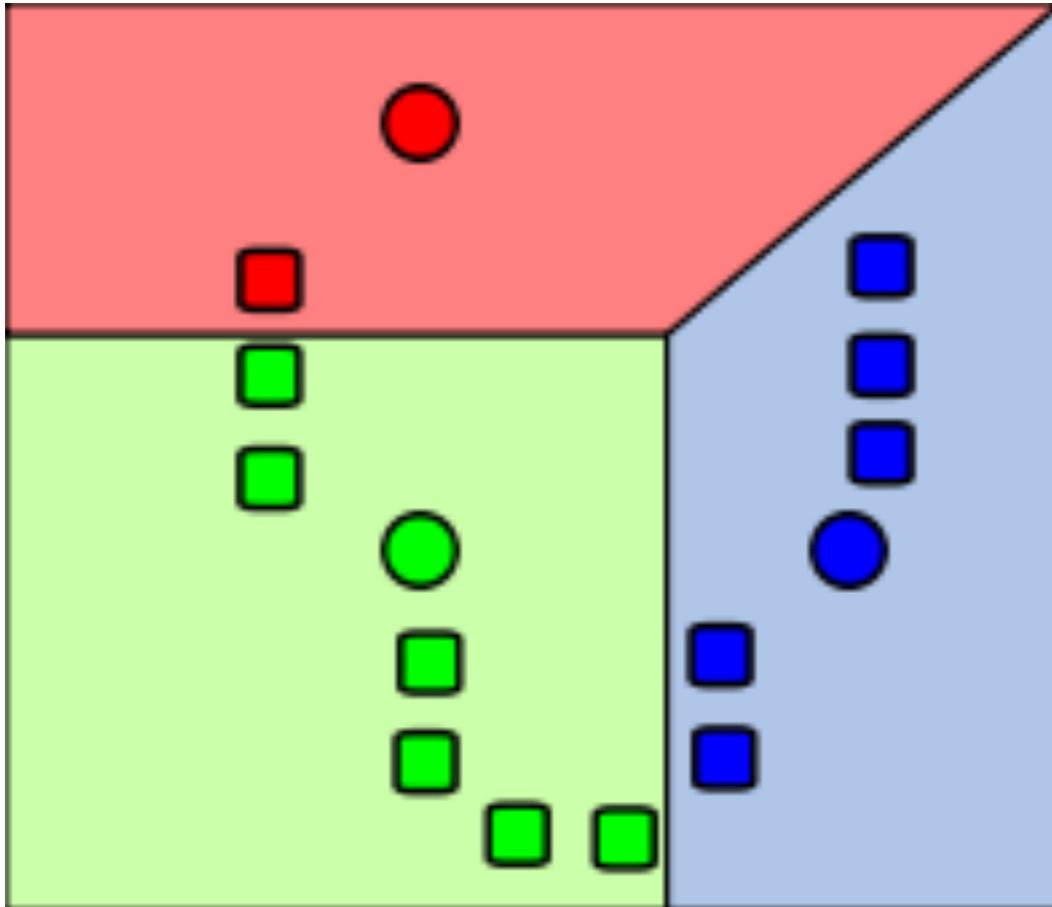
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1. Start with  $k$  cluster centers (centroids) chosen at random amongst the points
2. Compute distances to each centroid from every point **Just like KNN, we need to scale the features! (i.e.  $x / \text{sd}(x)$ )**

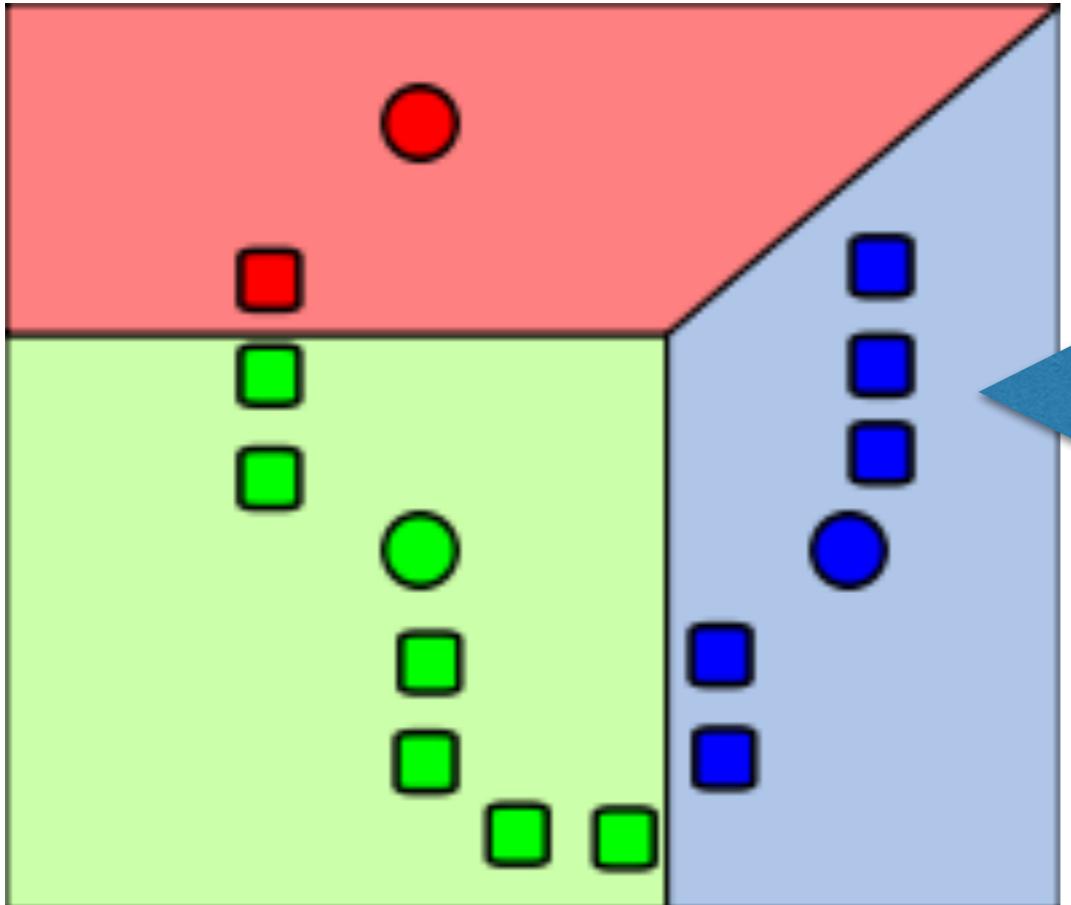
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3. Label each point according to its closest centroid

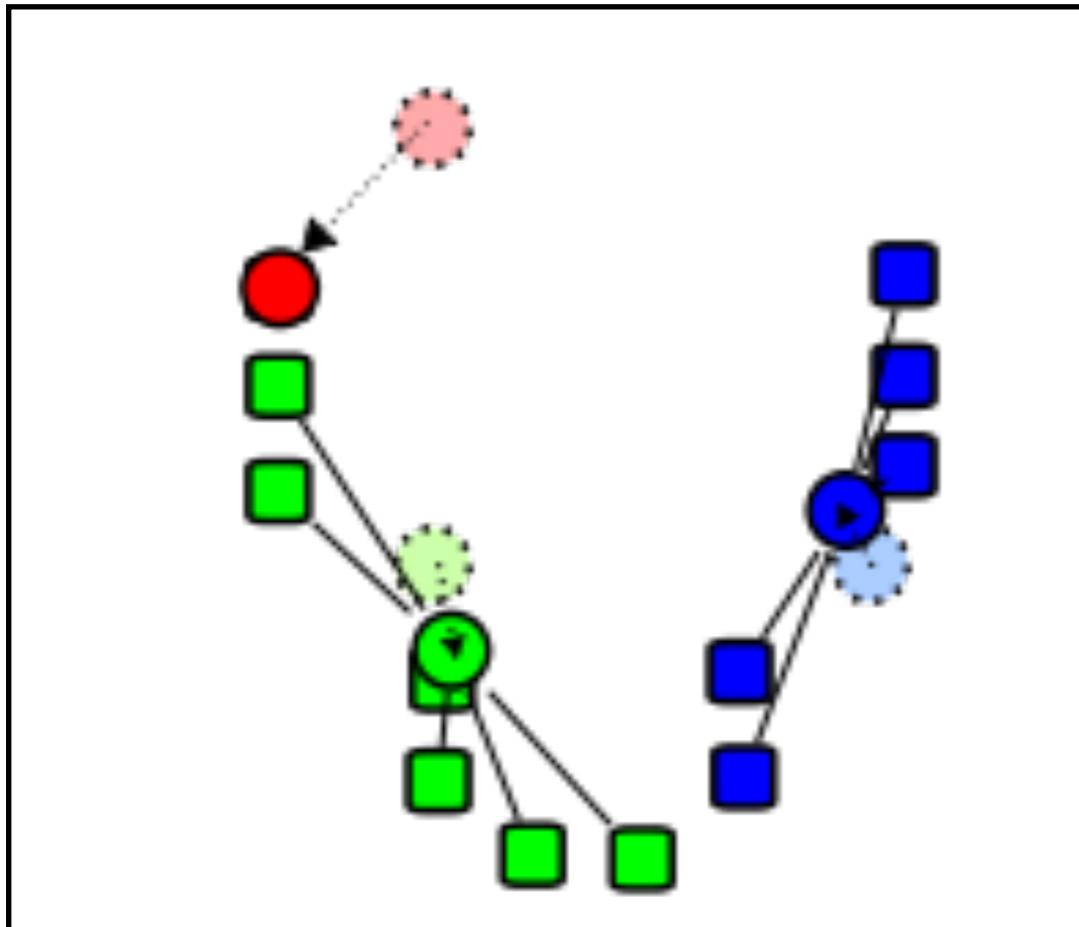
## K-MEANS ALGORITHM



This is called a Voronoi diagram, which indicates graphically the partitions of the feature space into their respective clusters

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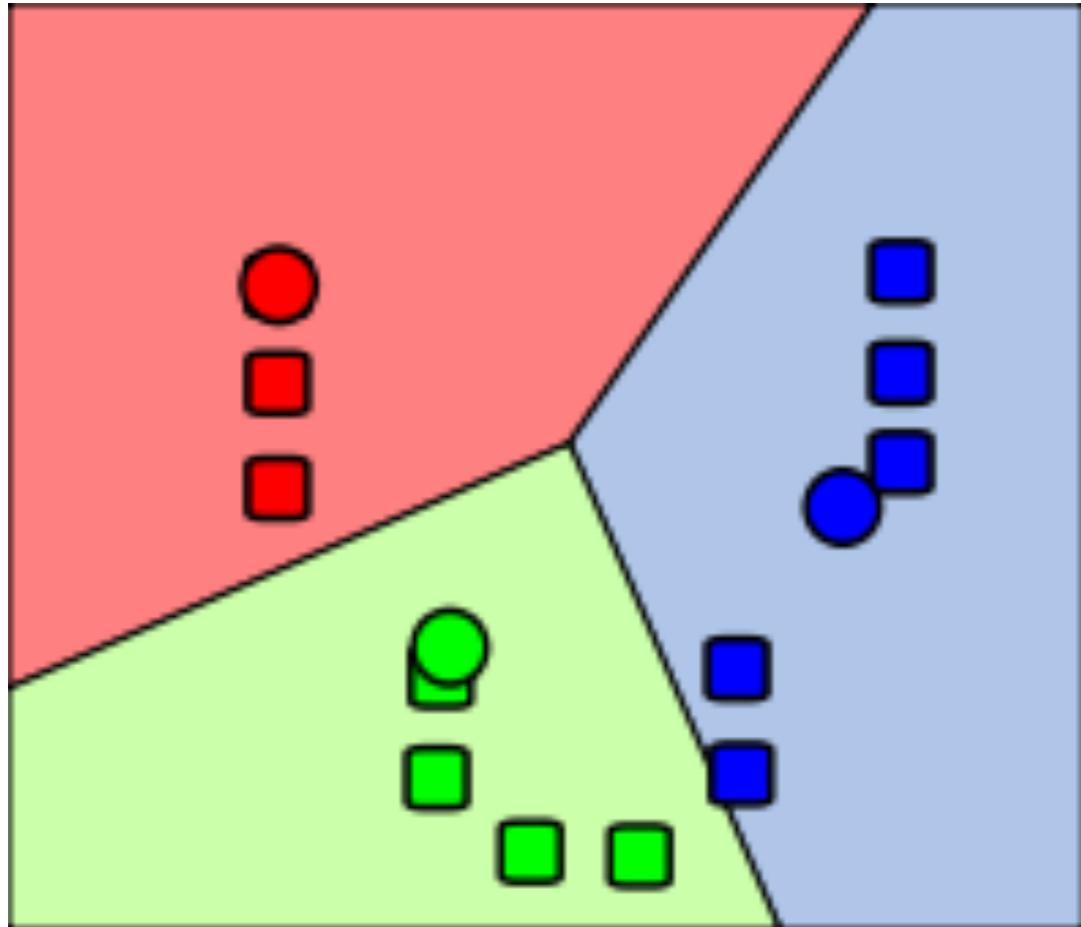
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5. Repeat steps 2-4 until convergence.  
i.e. For  $n$  iterations, or until the centroids do not change much

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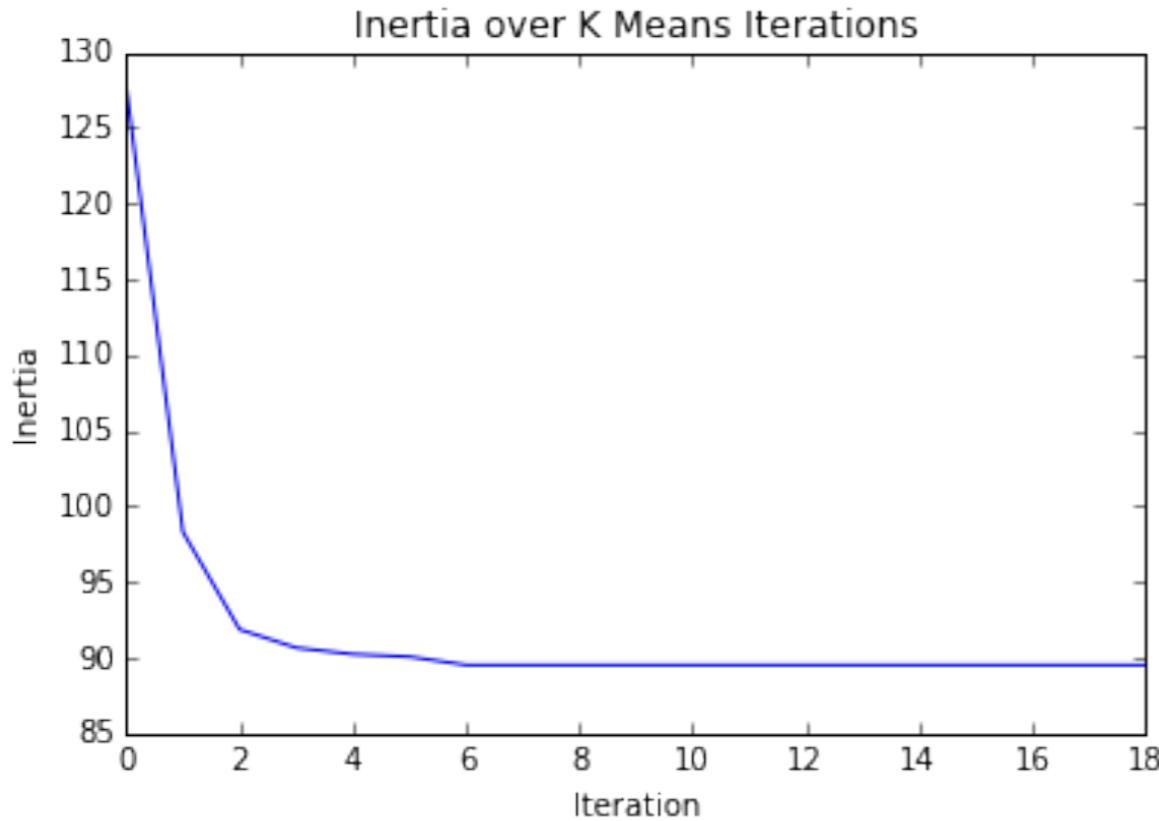
## K-MEANS EXAMPLE

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**Let's try an example...**

## K-MEANS - ANOTHER VIEW

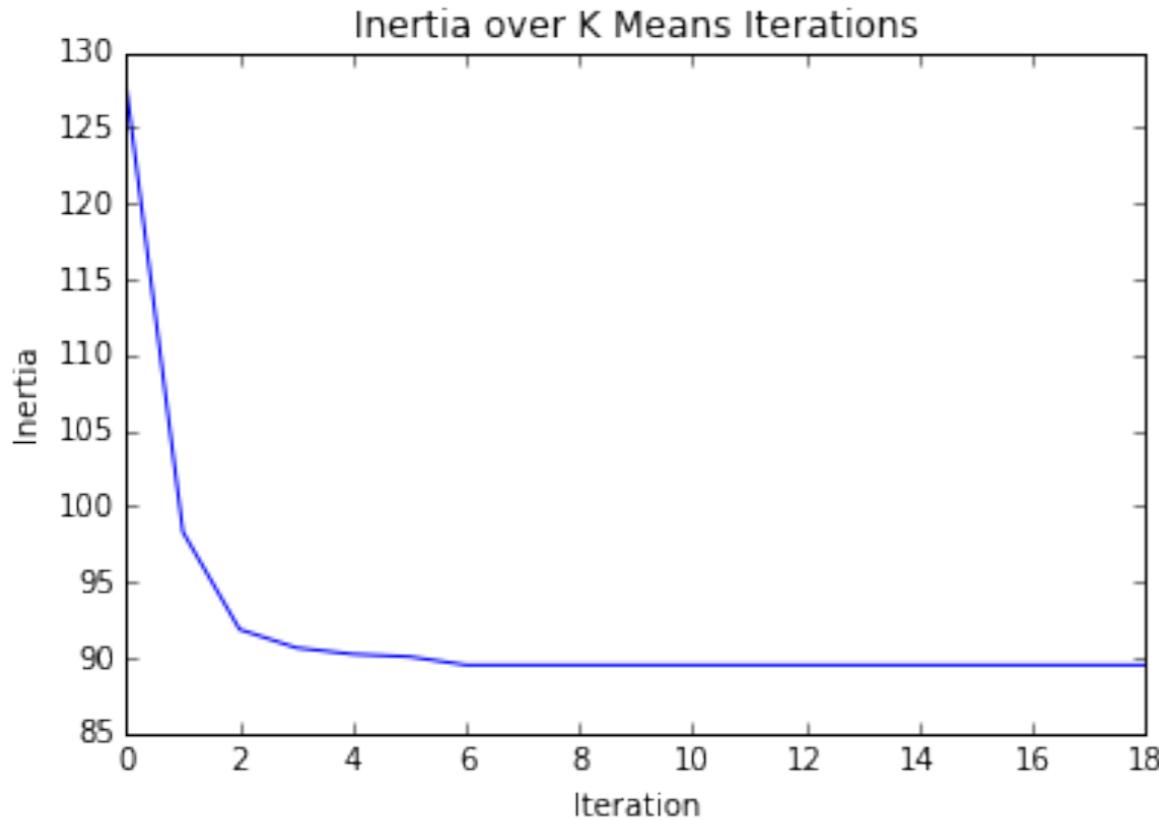
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K Means clustering could be thought of in a single line as minimizing the **squared euclidean distance** from within cluster points to the centroids (aka cluster means).

$$\sum_i^n \min_{\mu_j \in C} \left( \|x_j - \mu_i\|^2 \right)$$

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This is also called **inertia**

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## K-MEANS STRENGTHS AND WEAKNESSES

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- ✓ K Means is very efficient and is linear in time and space by the number of records

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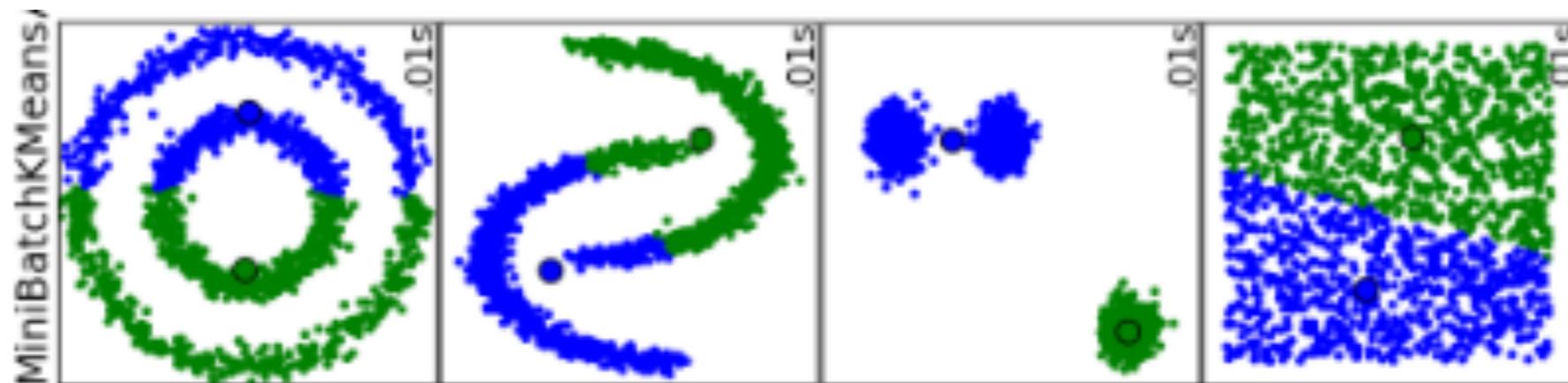
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(from sklearn documentation)

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Try preprocessing or k-medians

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Can try binarizing inputs, or Jaccard coefficient

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## K MEANS CLUSTERING

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- I. CLUSTER ANALYSIS
- II. K-MEANS CLUSTERING
- III. VALIDATION

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## ASSESSING ML PERFORMANCE

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**How do we assess *unsupervised* learning algorithms?**

## ASSESSING ML PERFORMANCE

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*We test our predictions and compare. We have quality measures such as R squared or accuracy*

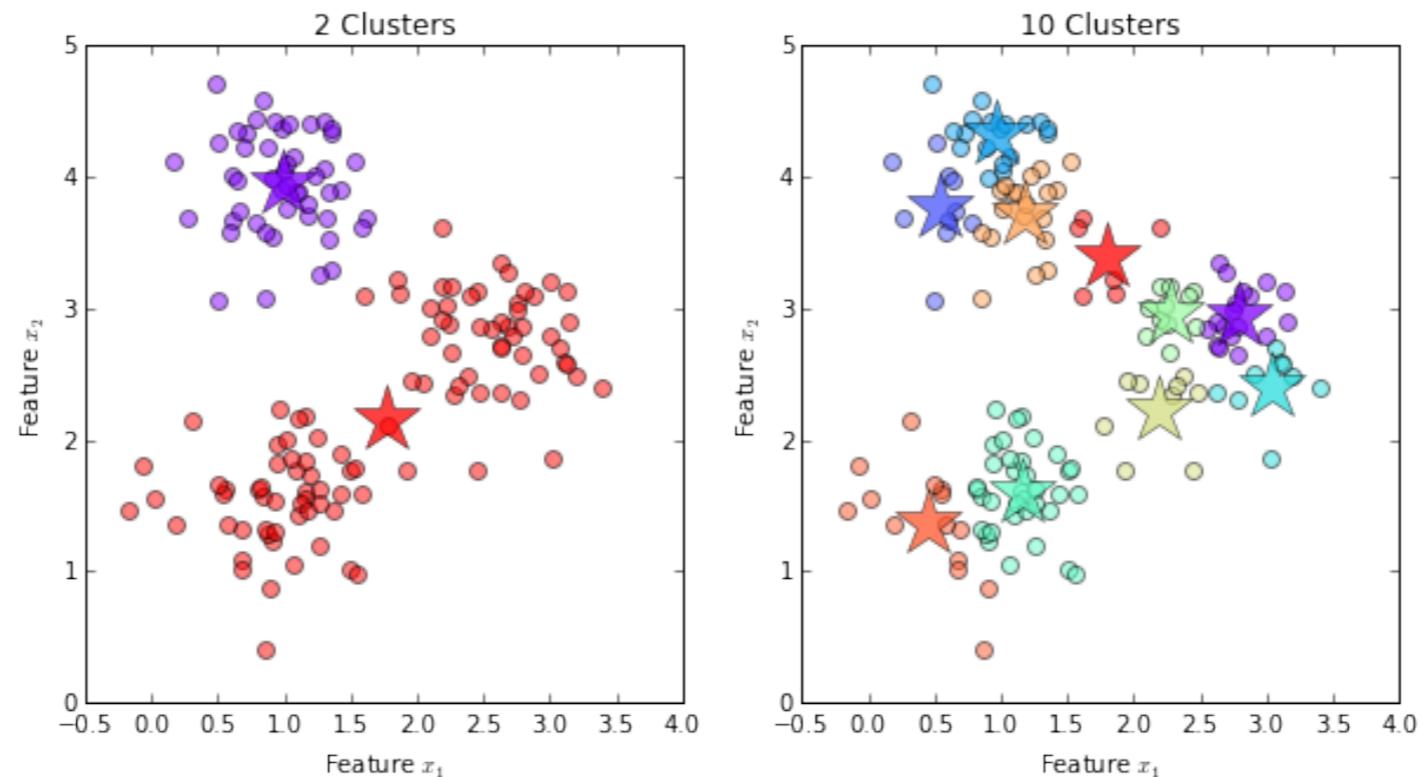
**How do we assess *unsupervised* learning algorithms?**

Sort of cant...



# ASSESSING ML PERFORMANCE

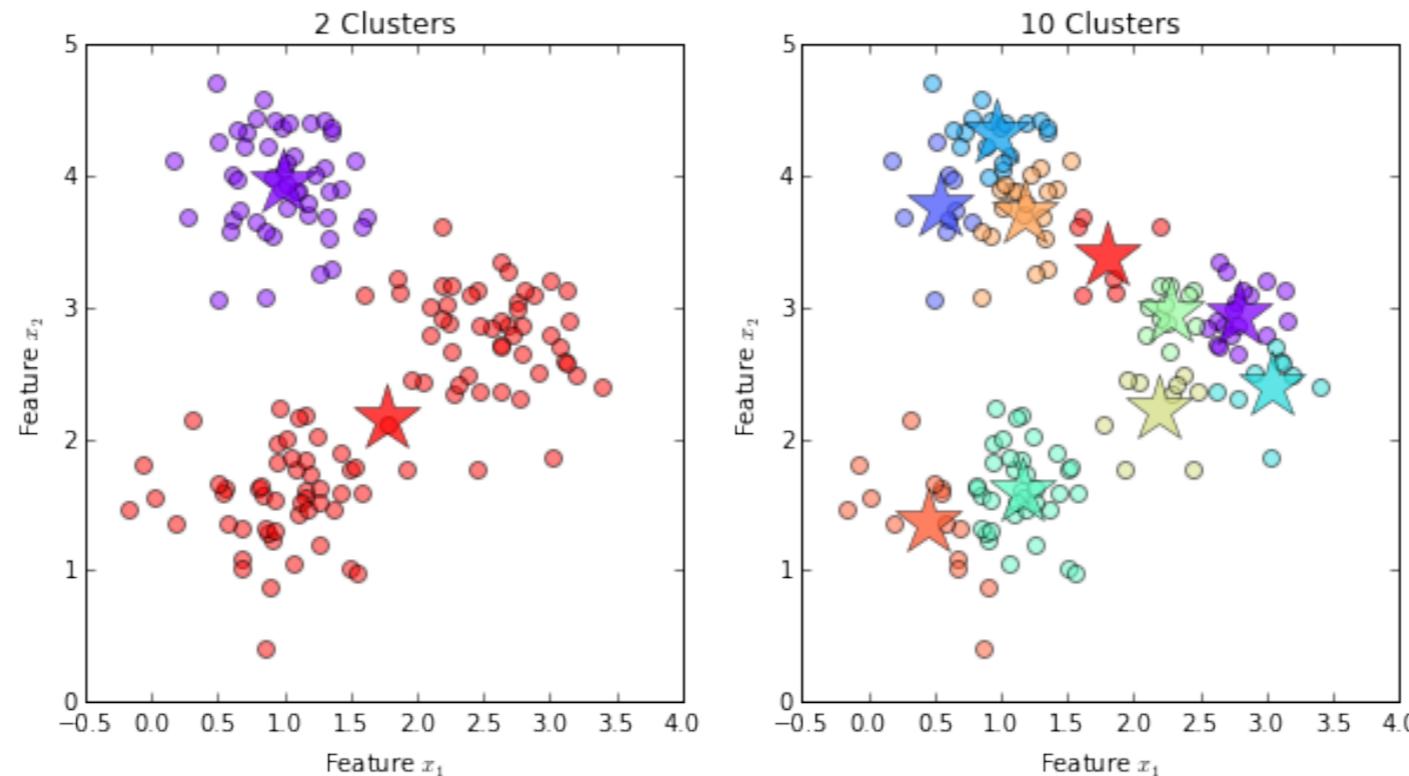
So then ... how do we choose k?



## ASSESSING ML PERFORMANCE

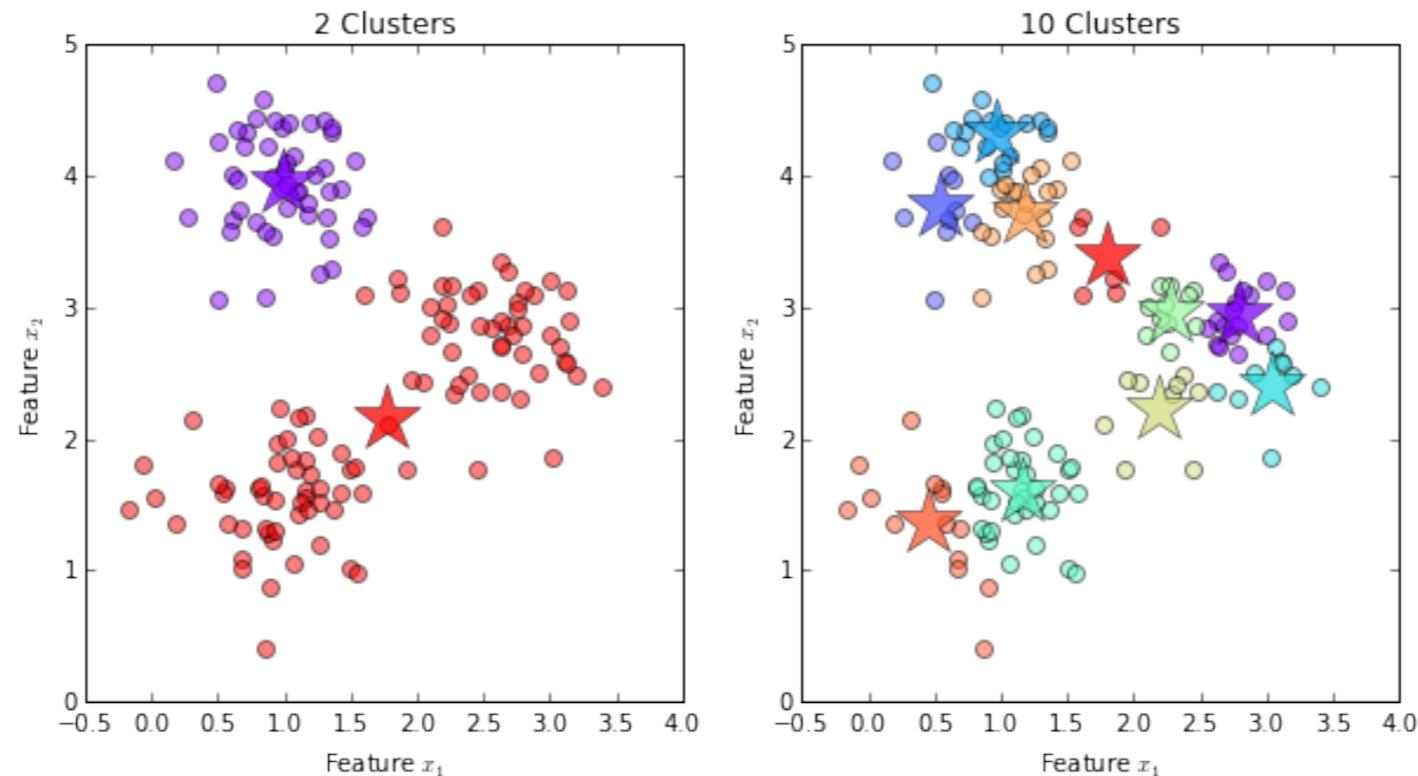
**Too few  $k$  clusters and you don't partition your data enough**

**Too many  $k$  clusters and you risk making clusters where no natural clusters exist in the data**



## ASSESSING ML PERFORMANCE

We will look at two metrics available to help assess the correct  $k$ , called **cohesion** and **separation**

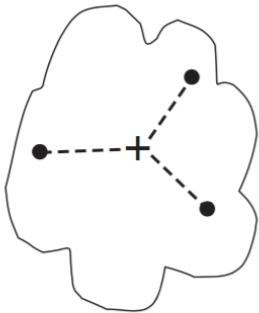


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## CLUSTER VALIDATION

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**Cohesion** measures clustering effectiveness within a cluster



$$\hat{C}(C_i) = \sum_{x \in C_i} d(x, c_i)$$

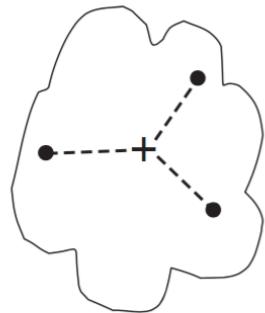
(a) Cohesion.

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## CLUSTER VALIDATION

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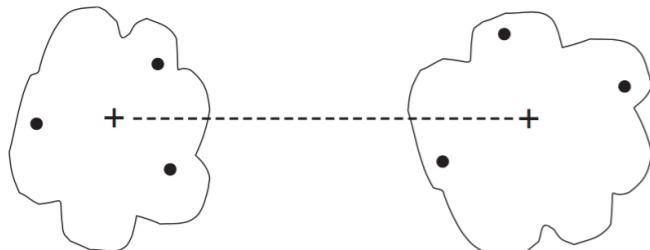
**Cohesion** measures clustering effectiveness within a cluster



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(a) Cohesion.

**Separation** measures clustering effectiveness between clusters

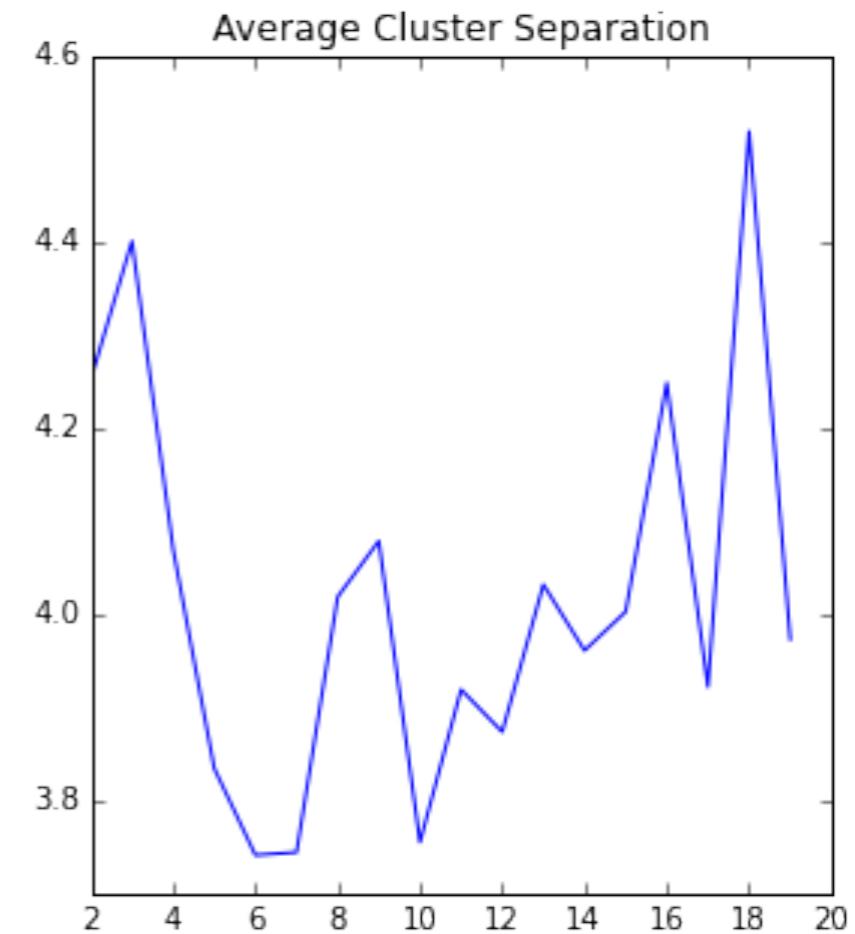
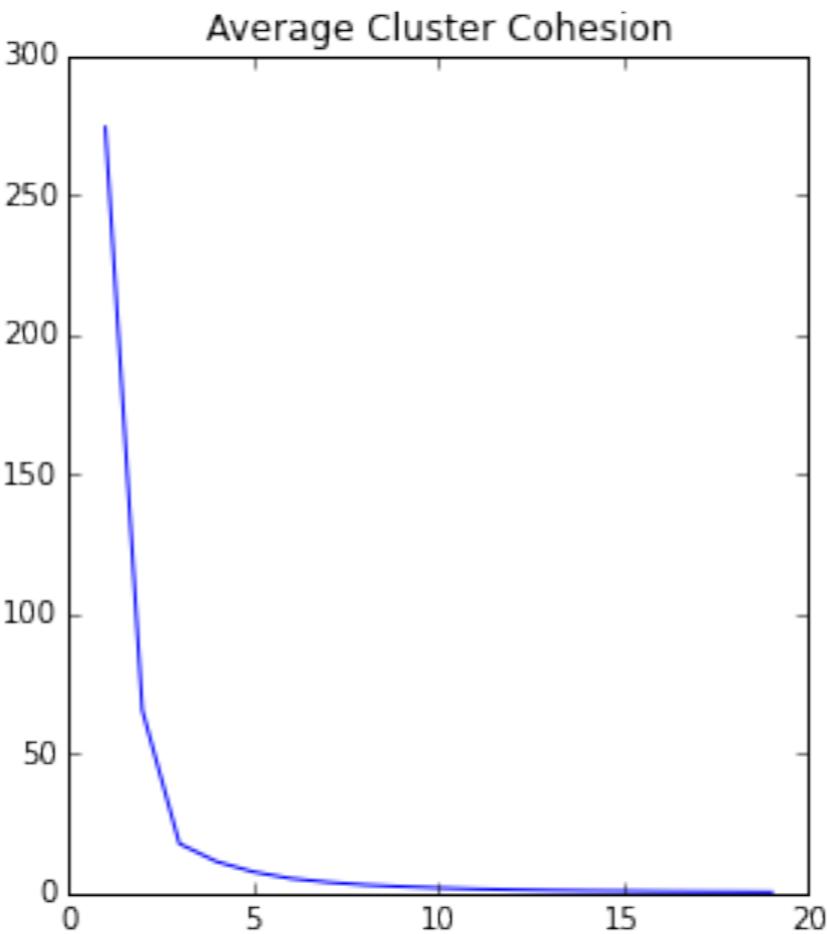
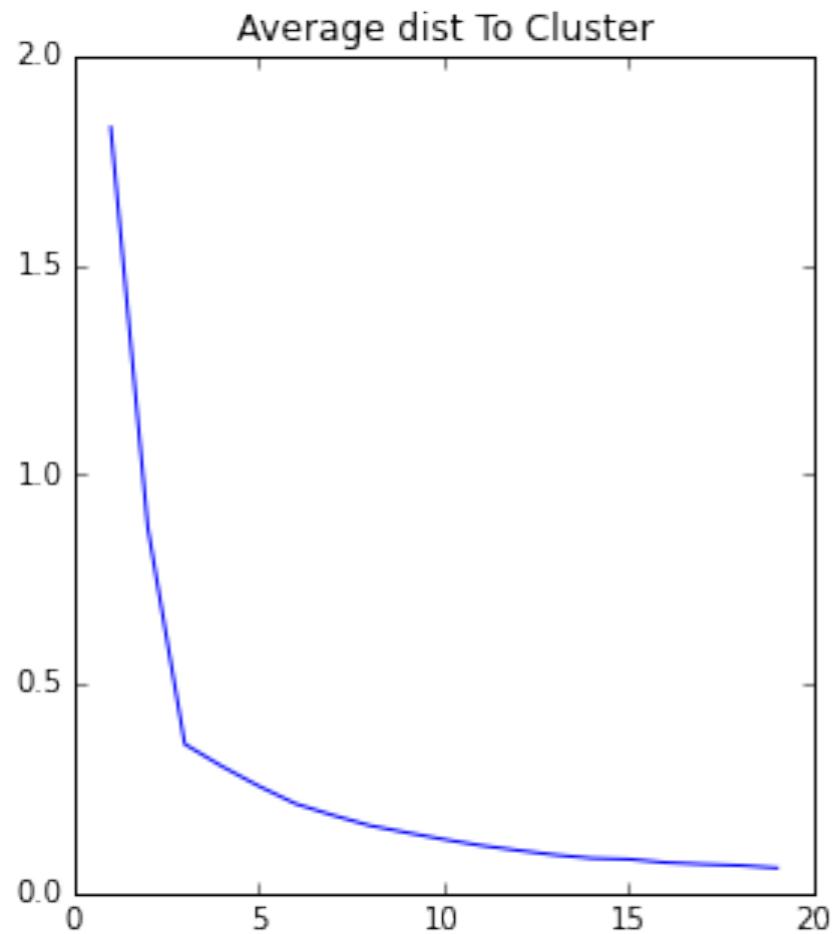


$$\hat{S}(C_i, C_j) = d(c_i, c_j)$$

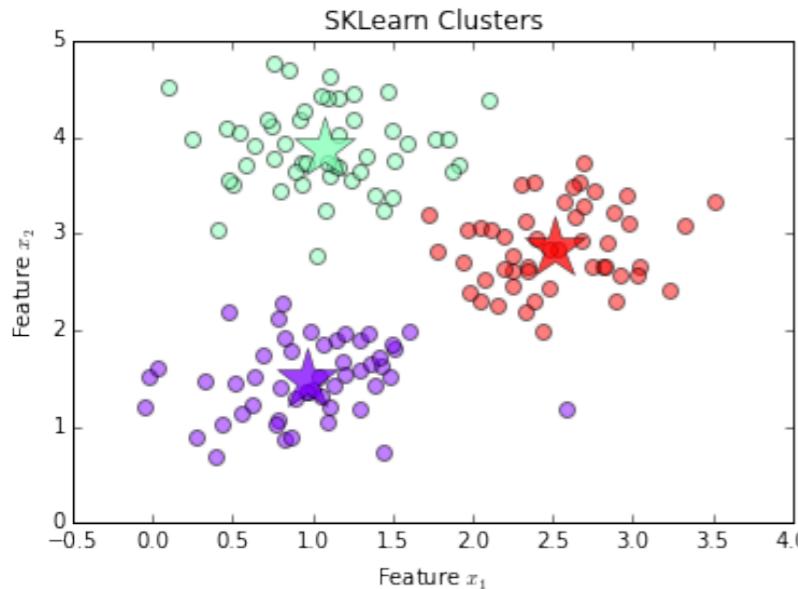
(b) Separation.

## CLUSTER VALIDATION

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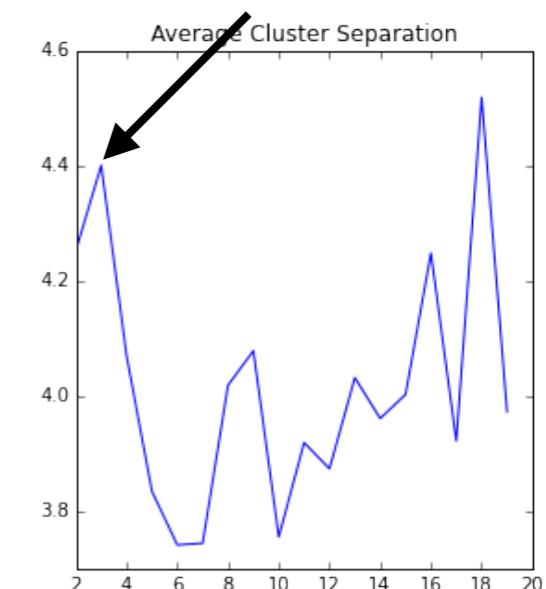
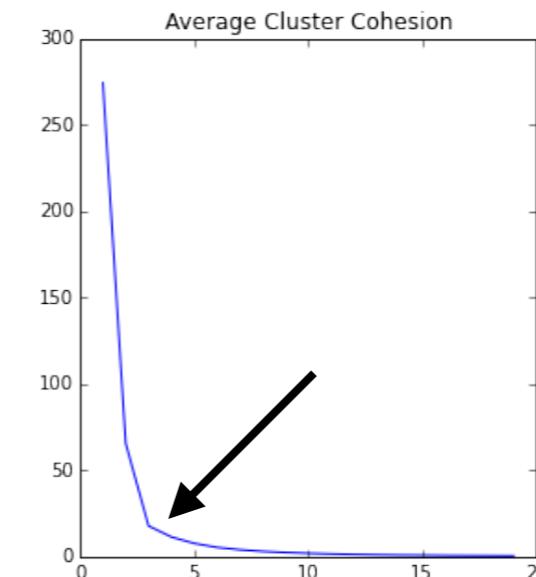
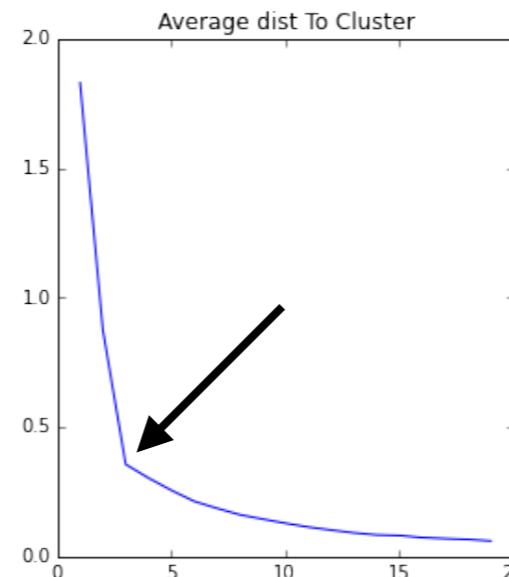


# CLUSTER VALIDATION

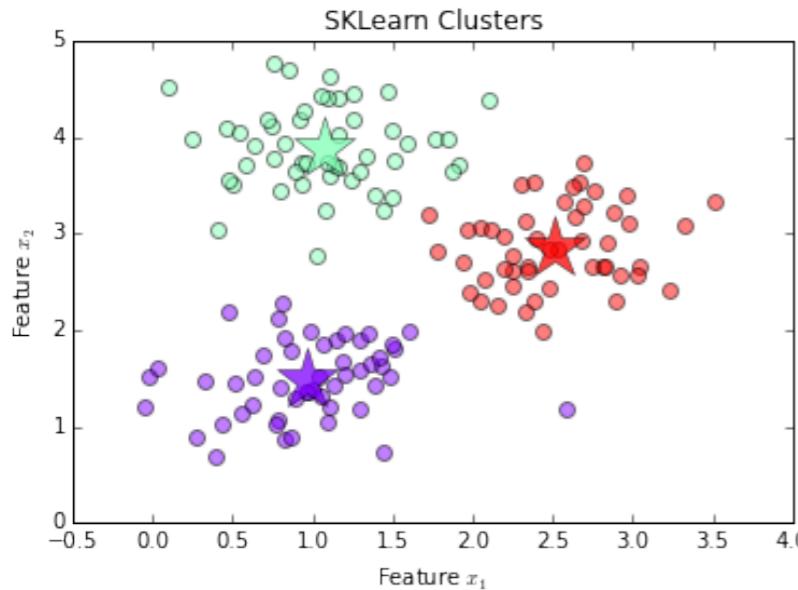


This example has been created from 3 natural clusters (3 fixed centroids plus gaussian noise)

Notice the shape of the curves below



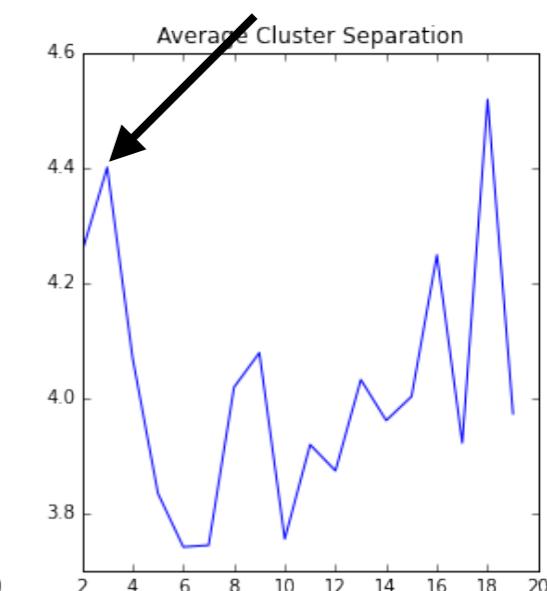
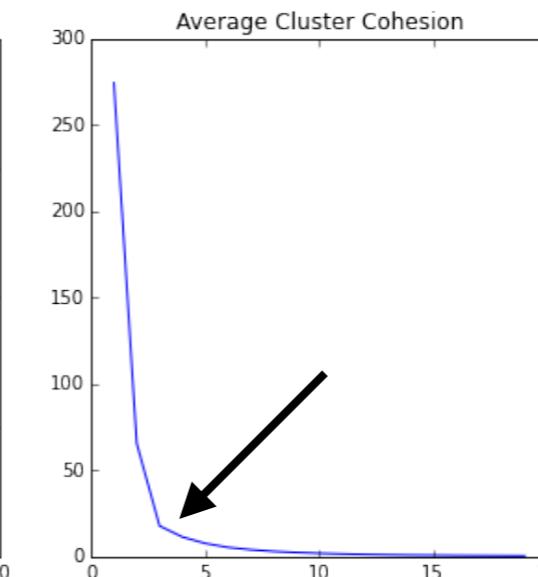
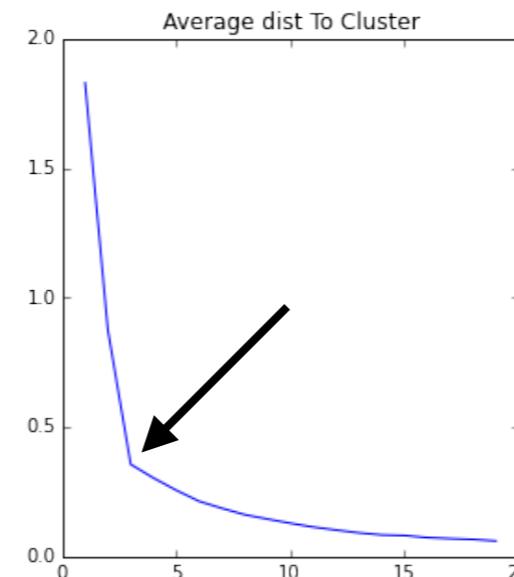
# CLUSTER VALIDATION



This example has been created from 3 natural clusters (3 fixed centroids plus gaussian noise)

Notice the shape of the curves below

**Choosing the k at which the curve kinks is called the “elbow method”**



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## **CLUSTER VALIDATION**

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Cluster validation is certainly an open problem. Since we don't have "labels", and it's hard to call one method right or wrong, many variants of "optimal k selection" have arisen.

<http://stats.stackexchange.com/questions/23472/how-to-decide-on-the-correct-number-of-clusters>

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**However, a good rule of thumb is to choose the number of clusters that intuition or requirements provide you**

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## CLUSTER VALIDATION

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- For instance, if you have three Dominos locations you could build in various locations, you could set  $k = 3$
- If you work for Armani and you want to create prototypical sizes for S, M, L, XL you would probably set  $k = 4$
- If you have a product dashboard, and you want to create 4 different templates for different types of users, you could set  $k = 5$ . Then you can view the average usage patterns within each cluster, and perhaps define them as “power users”, “beginners”, “light-weight” and “medium usage”.

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## **CLUSTER VALIDATION**

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Again, clustering requires human intervention and intuition to really provide strength

**Human intuition required**

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- III. VALIDATION
- IV. ADDITIONAL CONSIDERATIONS

---

## K-MEANS ADDITIONAL CONSIDERATIONS

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**Q:** *How do we define **distance** from a point to a centroid?*

**A:** *We've so far used the **euclidean distance** (squared euclidean distance to be exact). This is the typical metric, and is essentially the cluster variance. This is one of many **similarity metrics** that we can use to define closeness.*

$$d(x, c) = ||x - c||^2 = \sum_i (x_i - c_i)^2$$

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## K-MEANS ADDITIONAL CONSIDERATIONS

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**Q: How do we define *distance* from a point to a centroid?**

**A: There is also a variant that uses *binary features*, called the *Jaccard coefficient*. It is a metric useful for problems with sparse binary data, such as text mining, basket analysis, etc.**

$$J(x, c) = \frac{|x \cap c|}{|x \cup c|}$$

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## K-MEANS ADDITIONAL CONSIDERATIONS

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**Customer X has bought items A, B, C, D.**

**Customer Y has bought items B, B, C, E, F (bought B twice)**

**Their intersection of purchases is B, C**

**Their union of purchases is A, B, C, D, E, F**

$$J(x,y) = \frac{|x \cap y|}{|x \cup y|} = \frac{2}{6}$$

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## K-MEANS ADDITIONAL CONSIDERATIONS

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**Q:** *How do we define **distance** from a point to a centroid?*

**A:** *There's also manhattan distance, which is the sum of absolute values along each dimension from the point to the centroid. This is essentially an L1 variant of k means (minimize the within cluster median, rather than within cluster mean)*

$$d(x, c) = \left\| x - c \right\|_1 = \sum_i |x_i - c_i|$$

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## K-MEANS VARIATIONS

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- Select Different points
  - Random within space
  - Random within points
  - KMeans++ (Choose initial centroids far from each other)
- K Medians
- K Medoids

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## THAT'S IT!

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- Exit Tickets: DAT1 - Lesson 9 - K Means Clustering
  - Homework 5 is due Jan 20
  - Milestone 2 is due Jan 25
  - You'll have partial opportunity to work on it during class Jan 20th (as well as review)
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- For more info on kmeans read up on <http://www-users.cs.umn.edu/%7Ekumar/dmbook/ch8.pdf>
  - Check out more examples on the clustering user guide on sklearn website