CCSS Workshop Series

Unsupervised Learning Workshop

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- Respect differing viewpoints and ideas
- Share your own perspectives and ask any questions
- Accept constructive criticism
- Use welcoming and inclusive language
- Show courtesy and respect for all instructors and attendees

If you believe that an instructor or attendee has violated the code of conduct, please report the violation to CCSS-ResearchSupport@cornell.edu. We take all reported incidents seriously.

Land Acknowledgement

Cornell University is located on the traditional homelands of the Gayogohó:nọ' (the Cayuga Nation). The Gayogohó:nọ' are members of the Haudenosaunee Confederacy, an alliance of six sovereign Nations with a historic and contemporary presence on this land. The Confederacy precedes the establishment of Cornell University, New York state, and the United States of America. We acknowledge the painful history of Gayogohó:nọ' dispossession, and honor the ongoing connection of Gayogohó:nọ' people, past and present, to these lands and waters.

Here are additional links for more on the <u>history of Cornell's violent, colonial formation, the</u> <u>movement to return native lands</u>, and about the <u>AIISP program at Cornell.</u>

Consider donating to the Gayogohó:no sovereignty initiative here.

Today's Agenda

LECTURE

- Supervised vs. Unsupervised Learning
- Intro to Clustering
- K-Means Essentials
- Common Challenges

HANDS-ON WORKSHOP

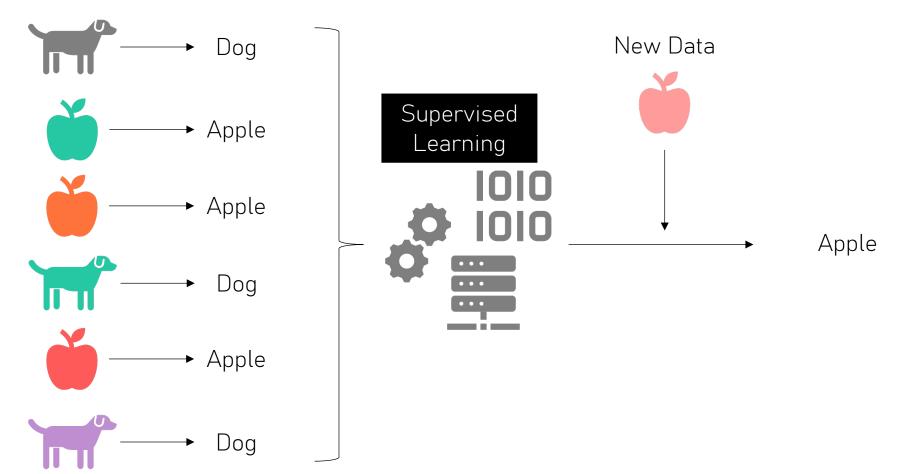
 Mini Case Study: Clustering houses in Boston

Supervised Learning vs. Unsupervised Learning

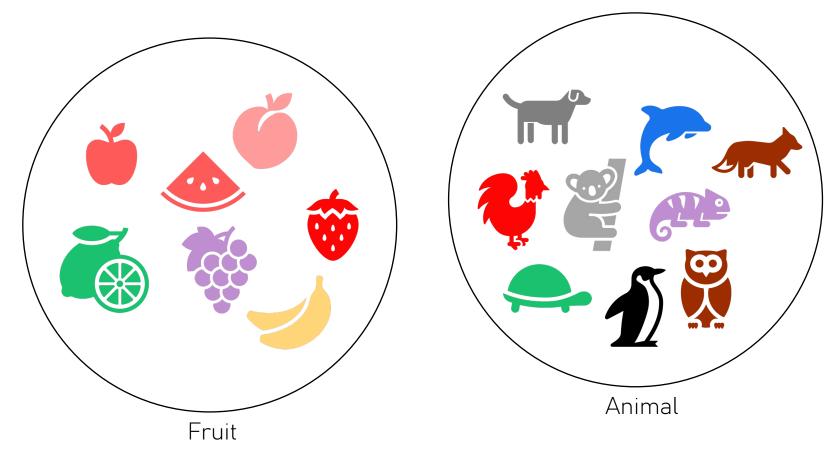
Learning from labeled data

Learning from unlabeled data

Supervised Learning vs. Unsupervised Learning

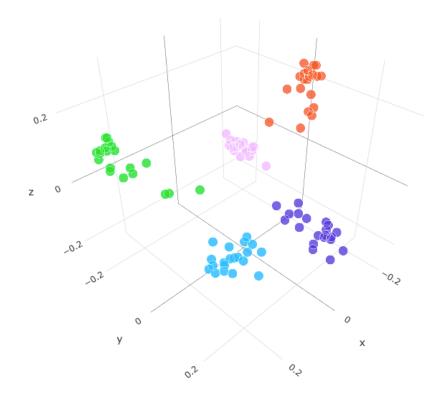


Supervised Learning vs. Unsupervised Learning



Intro to Clustering

- Data in the real world are often unlabeled
- The goal of unsupervised learning is to find patterns and/or structure in such data
- Clustering is the most commonly used unsupervised learning technique
- Clustering identifies similar "groups" (i.e., clusters) in unlabeled data



Credit: https://openai.com/blog/introducing-text-and-code-embeddings/

Intro to Clustering

Some applications of clustering...

- Recommendation systems
- Search results
- Market segmentation



Credit: https://medium.com/intro-to-artificial-intelligence/semantic-segmentation-udaitys-self-driving-car-engineer-nanodegree-c01eb6eaf9d

Data Structure

```
Var. 1 Var. 2 Var. 3 Var. 4

[[ 5.1, 3.5, 1.4, 0.2 ... ]
  [ 4.9, 3. , 1.4, 0.2 ... ]
  [ 4.7, 3.2, 1.3, 0.2 ... ]
  [ 4.6, 3.1, 1.5, 0.2 ... ]
  [ 5.9, 3. , 5.1, 1.8 ... ]]
```

Data Structure

```
Var. 1 Var. 2 Var. 3 Var. 4 Cluster

[[ 5.1, 3.5, 1.4, 0.2 ... ] ?
[ 4.9, 3. , 1.4, 0.2 ... ] ?
[ 4.7, 3.2, 1.3, 0.2 ... ] ?
[ 4.6, 3.1, 1.5, 0.2 ... ] ?
[ 5.9, 3. , 5.1, 1.8 ... ]] ?
```

K-Means Clustering

The goal of clustering is to separate data so that data similar to one another are in the same group, while data different from one another are in different groups. So, two questions arise:

How many groups do we choose?

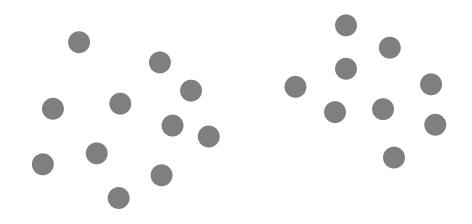
How do we define similarity?

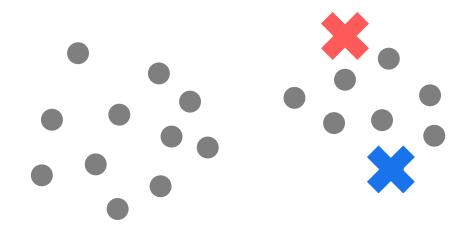
K-Means Clustering

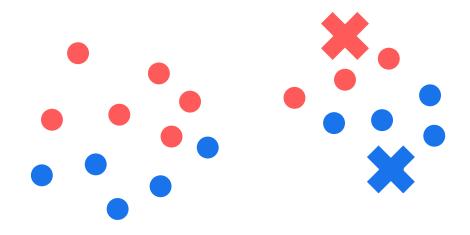
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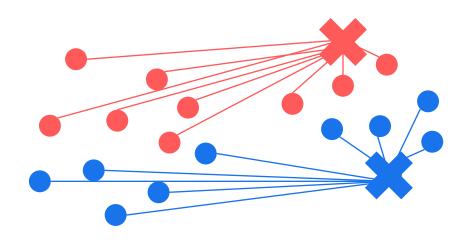
How many groups do we choose? —— The "K" refers to the number of clusters (groups) we expect to find in a dataset

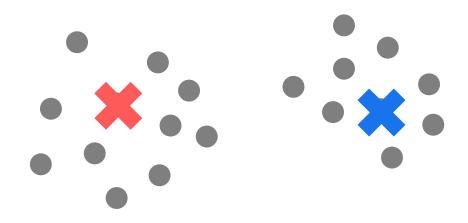
The "Means" refers to the average distance of data to each cluster center, also known as the *centroid*, which we are trying to minimize.

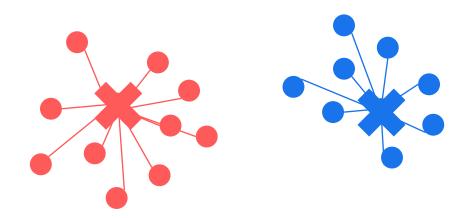












Implement K-Means Clustering

K-Means Clustering is conducted through an iterative process:

1. Place k centroids for the initial clusters

model = KMeans(n_clusters = k)

2. Assign data samples to the nearest centroid

3. Update centroids based on the above-assigned data samples

model.fit(X)

4. Assign each data point to a cluster

model.predict(X)

Let's work on a mini case study in Google Colab

A few unresolved questions ...

How do I determine the # of clusters for k-means?

- Data exploration & visualization
- Theory & domain knowledge
- Other practical reasons (e.g., budget)
- ..

Do I really need all these features for clustering?

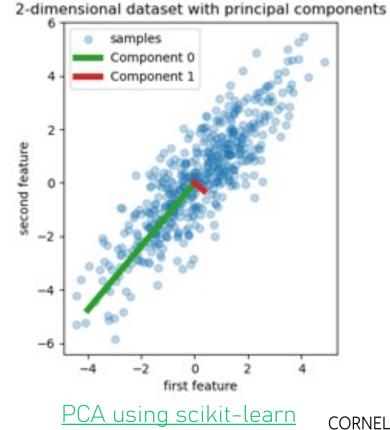
- Dimension scaling/reduction
 - Understand your data in a simpler way
 - Not all features are equally important
 - Multiple features may provide repetitive information
- Principal component analysis (PCA)

Do my clustering results make sense?

- Examine clustering results
- Visualization after clustering

Principal Component Analysis (PCA)

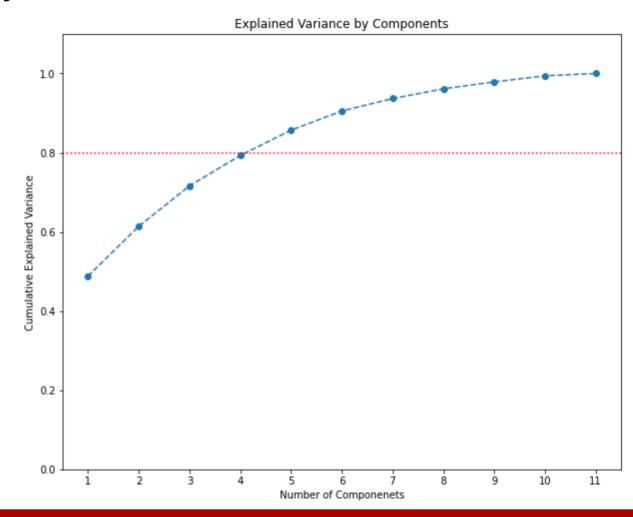
- Not all of the features in your dataset will be equally helpful for clustering
- PCA is a technique for dimension reduction (i.e., to reduce your dataset from higher to lower dimensions)
- Each "component" is a linear combination of your features



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Principal Component Analysis (PCA)

 To choose the number of component we need, we want to make sure we are explaining sufficient variances in the data when we scale down its dimensions.



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• ...

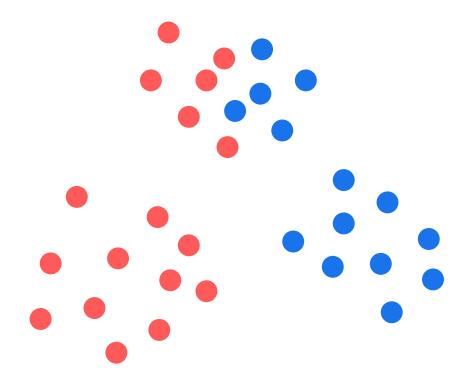
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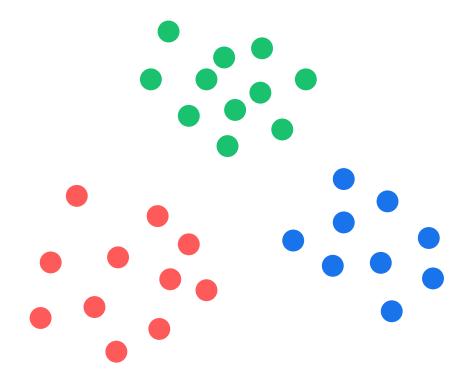
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- Examine clustering results
- Visualization after clustering

Examine & Visualize Clustering Results



Examine & Visualize Clustering Results



Summary: The Full Process of Unsupervised Learning

Visualize before k-means

Explore the data – Does it even make sense to cluster?

Dimension reduction using PCA

Do we need all the variables to help us cluster the data?

Determine the # of clusters

How many clusters should we group the data into?

Fit the k-means model

How do we implement k-means clustering?

Examine the clustering results

What are some unique characteristics of each cluster?

(Handle new data)

When we get new data, which cluster does each instance belong to?

Beyond this current workshop...

- Unsupervised learning is more than just K-Means Check out unsupervised learning on Scikit-Learn
- In research, exploration is often just the first step!
- Stay tuned CCSS is rolling out an interactive Machine Learning for Social Sciences Handbook in May

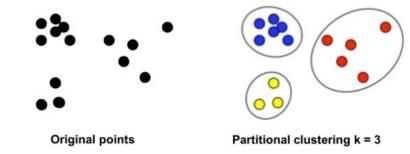


FIGURE 1. Example of clustering based on partitional methods.

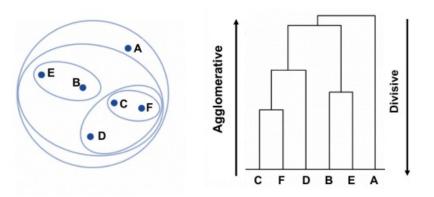


FIGURE 2. Example of clustering based on hierarchical methods.

Luna-Romera et al., 2019

