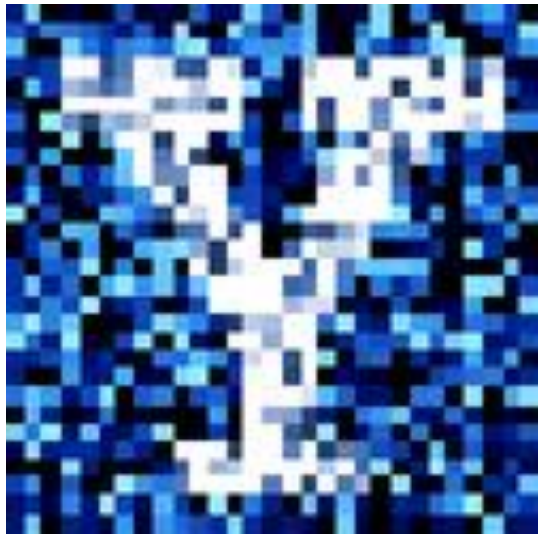
YData: Introduction to Data Science



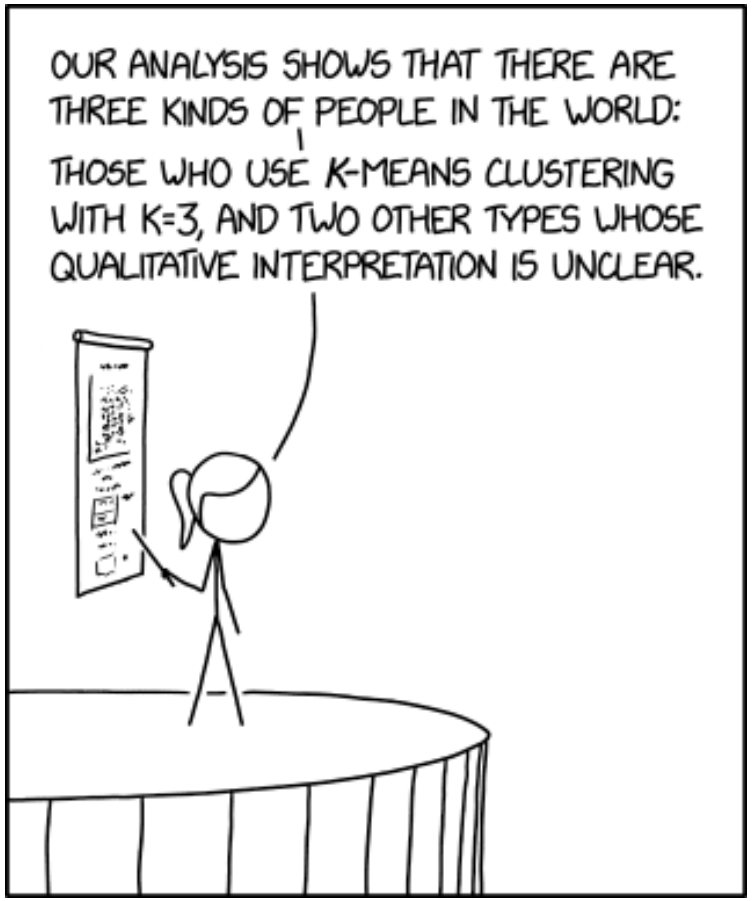
Lecture 24: Unsupervised learning

Overview

Unsupervised learning/clustering

- K-means cluster
- Hierarchical clustering

If there is time: objected oriented programming



Project timeline

~~Sunday, November 17th~~

- ~~Projects are due on Gradescope at 11pm~~
- Email a pdf of your project to your peer reviewers
  - A list of whose paper you will review is posted on Canvas
  - Fill out the draft reflection on Canvas

Sunday, November 24th

- Jupyter notebook files with your reviews need to be sent to the authors
- A template for doing your review has been posted

Sunday, December 8th

- Project is due on Gradescope
  - Add peer reviews to the Appendix of your project

Homework 9 has been posted

- It is due December 1st

Prediction: regression and classification

We “learn” a function f

- f(**x**) ⟶ y

Input: **x** is a data vector of "features"

Output:

- Regression: output is a real number (y ϵ R)
- Classification: output is a categorical variable y_k

Review: Regression

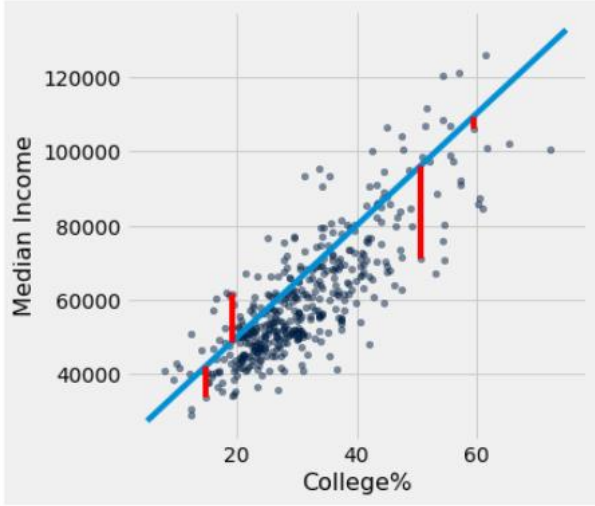
Regression is method of using one variable ***x*** *to predict* the value of a second variable ***y***

- i.e., $\hat{y} = f(x)$
- Linear regression: $\hat{y} = \text{intercept} + \text{slope} \cdot x$

$$\hat{y} = b_0 + b_1 \cdot x$$

The coefficients for these regression models are found by minimizing root mean square error (RMSE)

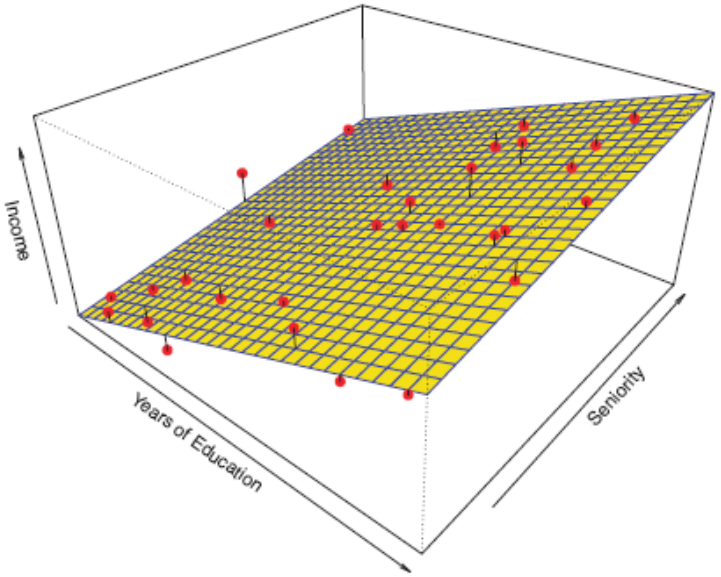
$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$



[Regression line app]

Review: Multiple regression

In multiple regression we try to predict a quantitative response variable *y* using several features $x_1, x_2, \ldots, x_k$



We estimate coefficients using a data set to make predictions ŷ

$$\hat{y} = b_0 + b_1 \cdot x_1 + b_2 \cdot x_2 + \ldots + b_k \cdot x_k$$

Learn the b_i's on the training set. Assess prediction accuracy on test set.

Review: Linear regression models in scikit-learn

We can use scikit-learn to create linear regression models

- You can also use the stats models package to do this

```
linear_model = LinearRegression()  # construct a linear regression model

linear_model.fit(X_train_features, y_train)      # train the classifier

y_preditions = linear_model.predict(X_test_features)   # make predictions

RMSE = np.sqrt(np.mean((y_test - y_predictions)**2))   # get the RMSE
```

"Learns" b_0, b_1, … by minimizing the RMSE on the training data

Numeric values to predict

Review: Inference for regression

We can run a hypothesis test to see if there is a linear relationship between a feature x, and a response variable y

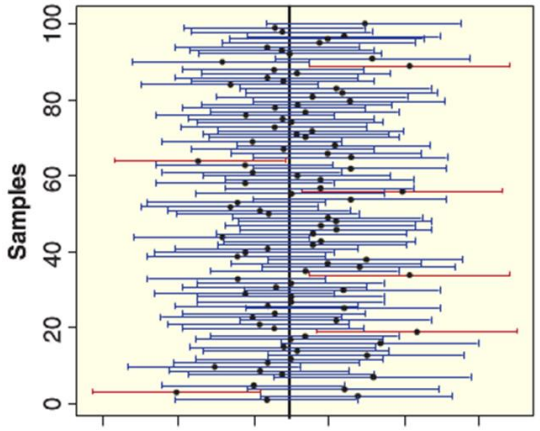
- H_0: $\beta_1 = 0$ (slope is 0, so no linear relationship between x and y
- H_A: $\beta_1 \neq 0$

The confidence interval for the slope coefficients:


```
import statsmodels.api as sm

sm_linear_model = sm.OLS(y_train, X_train_with_constant).fit()

sm_linear_model.summary()
```



Unsupervised learning

Supervised learning and unsupervised learning

In **supervised learning** we have a set of features X, along with a label y

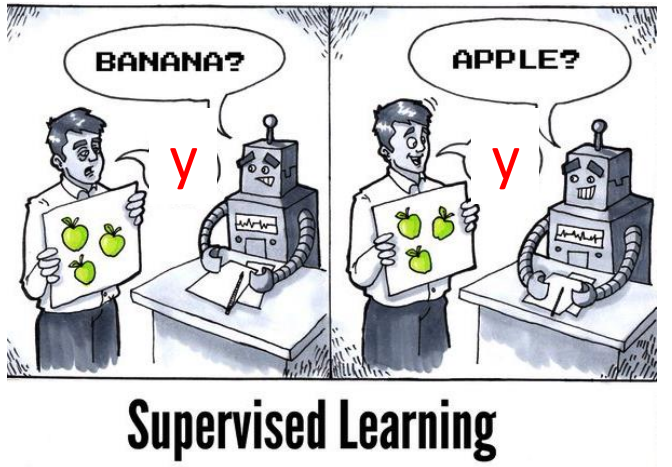
- We use the features X to predict y on new data

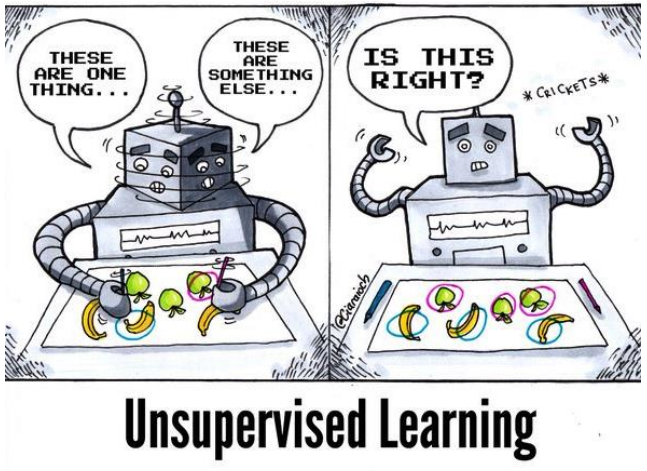
In **unsupervised learning**, we have features X, but **no** response variable y

Unsupervised learning can be useful in order to find structure in the data and to visualize patterns

A key challenge in unsupervised learning is that there is no real ground truth response variable y

- So we don't have measures like the mean prediction accuracy





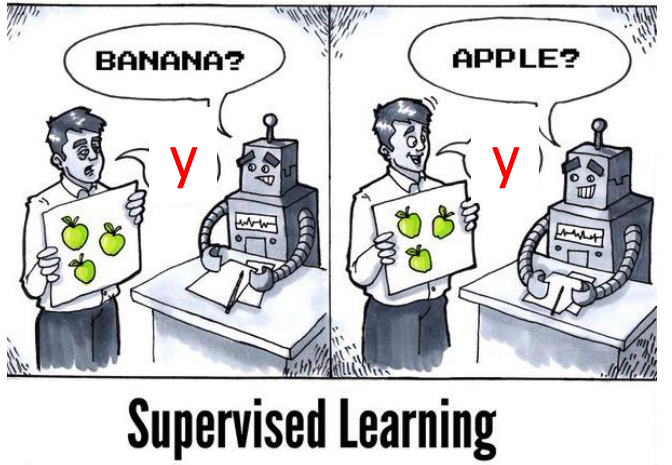
Unsupervised learning

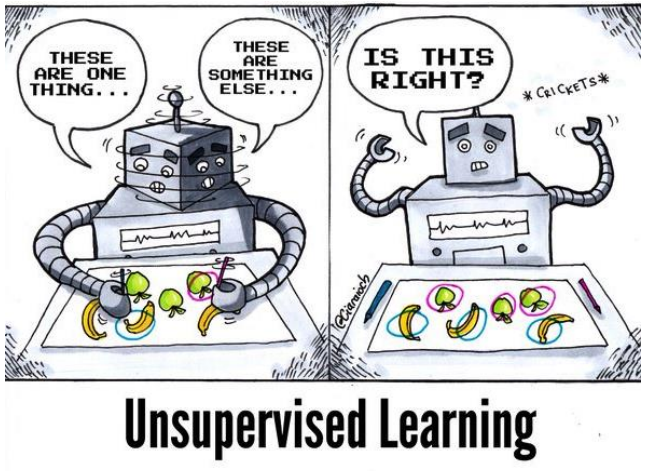
Given we are almost at the end of the semester, we will focus on clustering, which is one type of unsupervised learning:

In **clustering** we try to group similar data points together

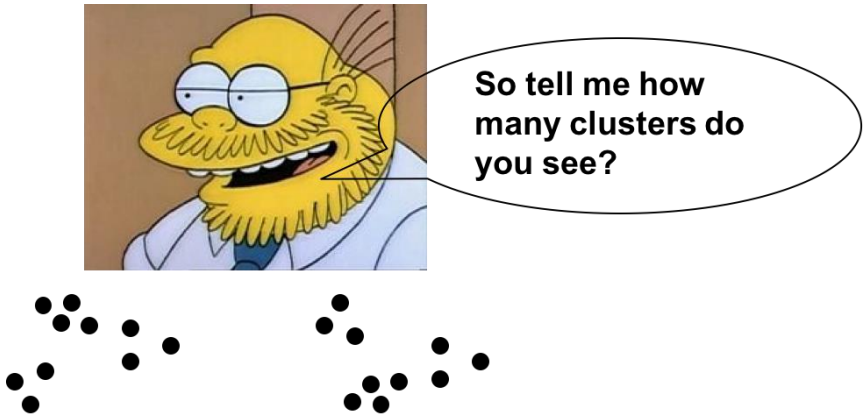
Another type of unsupervised learning:

- **Dimensionality reduction** where we try to find a smaller set of features that captures most of the variability original larger feature set
  - E.g., principal component analysis (PCA)

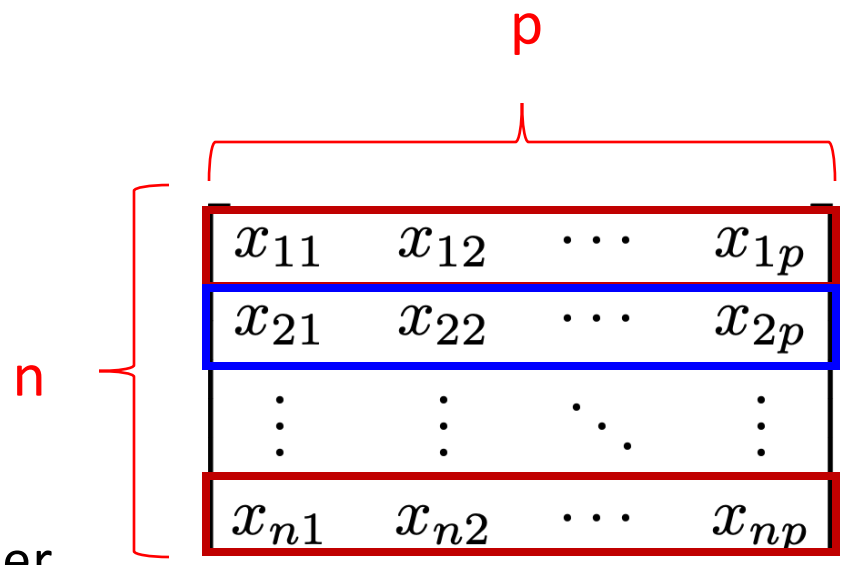




Clustering



Clustering



Clustering divides n data points x_i's into subgroups

- Data points in the same group are similar/homogeneous
- Data points in different groups are different from each other

Examples:

- Examining gene expression levels to group cancer types together
- Examining consumer purchasing behavior to perform market segmentation

Clustering can be:

- **Flat**: no structure beyond dividing points into groups
- **Hierarchical**: Population is divided into smaller and smaller groups (tree like structure)

K-means clustering

K-means clustering partitions the data into ***K*** distinct, non-overlapping clusters

- i.e., each data point x_i belongs to exactly one cluster C_k

The number of clusters, ***K***, needs to be specified prior to running the algorithm

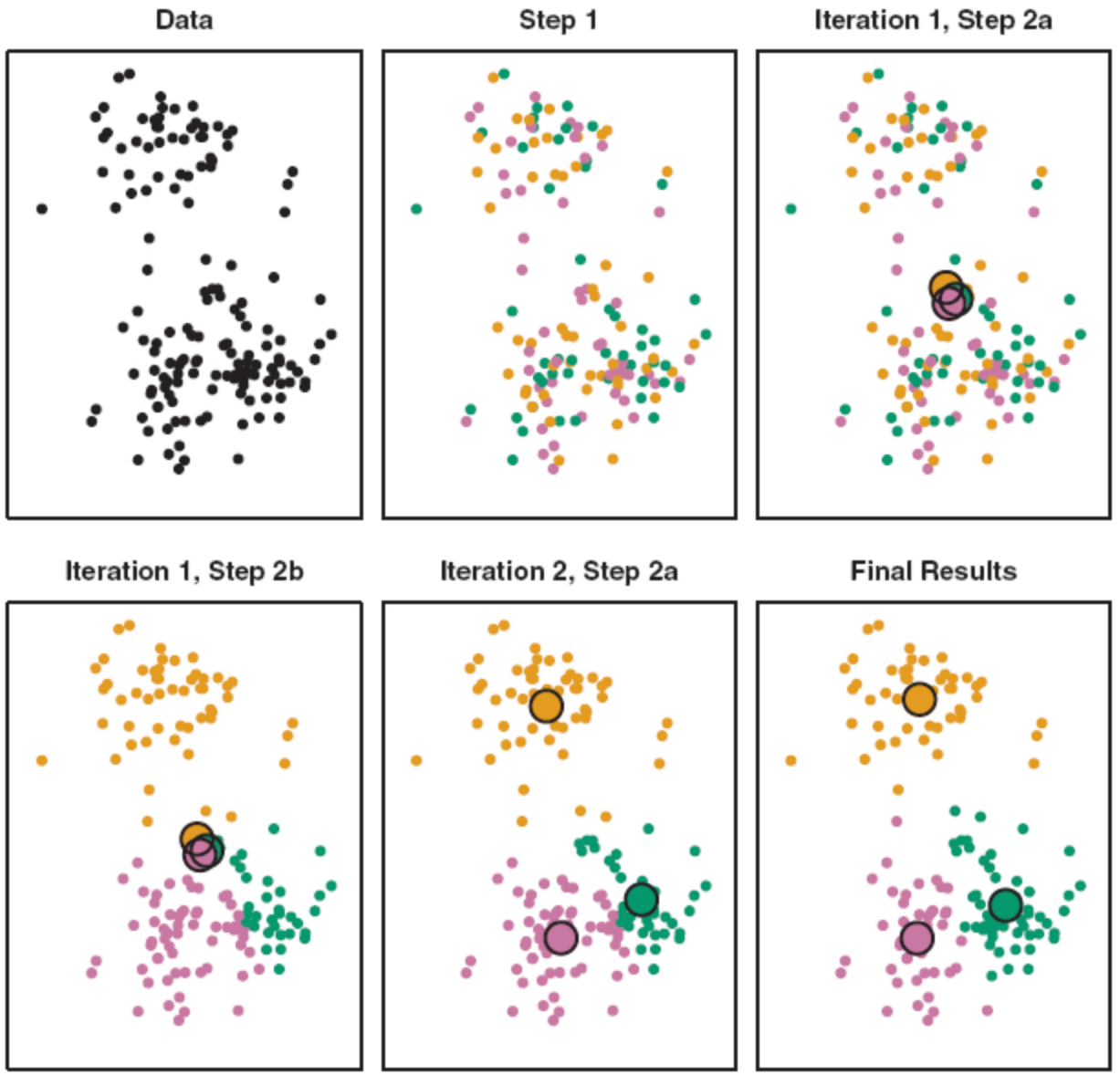
The goal is to minimize the within-cluster variation

- e.g., to make the Euclidean distance for all points within a cluster as small as possible

Finding the exact optimal solution is computationally intractable (there are k^n possible partitions), but a simple algorithm exists to find a local optimum which is often works well in practice.

K-means clustering

1. Randomly assign points to clusters C_k
2. Calculate cluster centers as means of points in each cluster
3. Assign points to the closest cluster center
4. Recalculate cluster center as the mean of points in each cluster
5. Repeat steps 3 and 4 until convergence



K-means clustering

Because only a local minimum is found, different random initializations will lead to different solutions

- One should run the algorithm multiple times to get better solutions

Let's explore this in Jupyter!

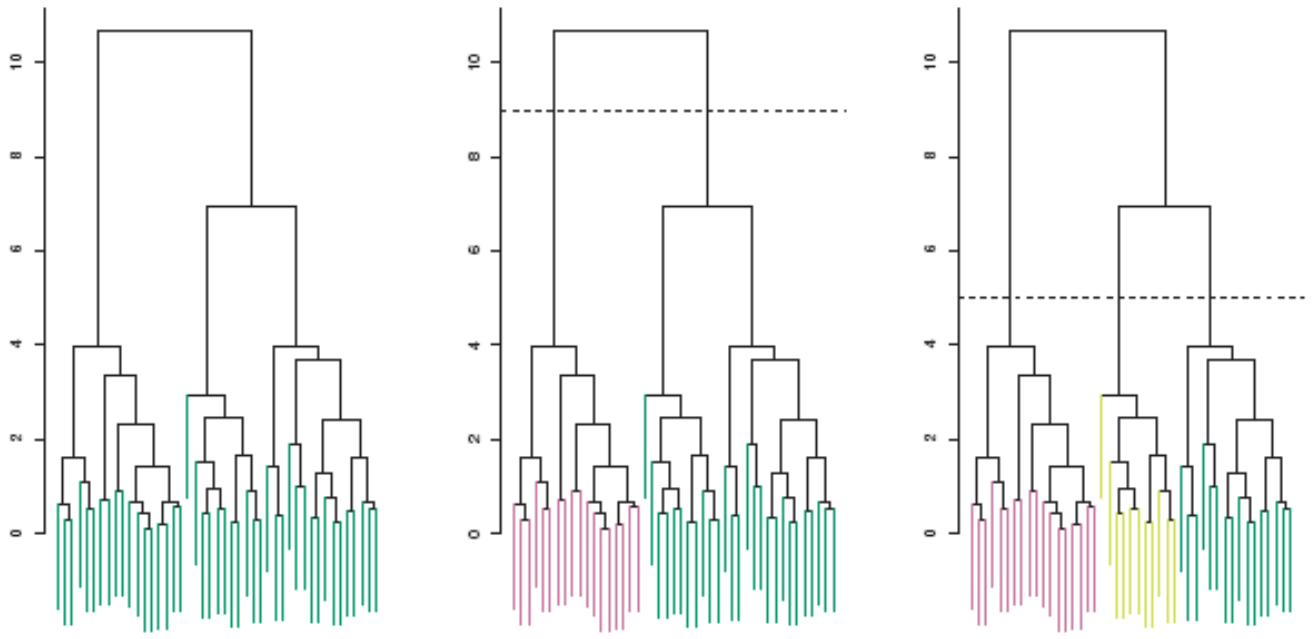
Hierarchical clustering

Hierarchical clustering

In **hierarchical clustering** we create a dendrogram which is a tree-based representation of successively larger clusters.

We can cut the dendrogram at any point to create as many clusters as desired

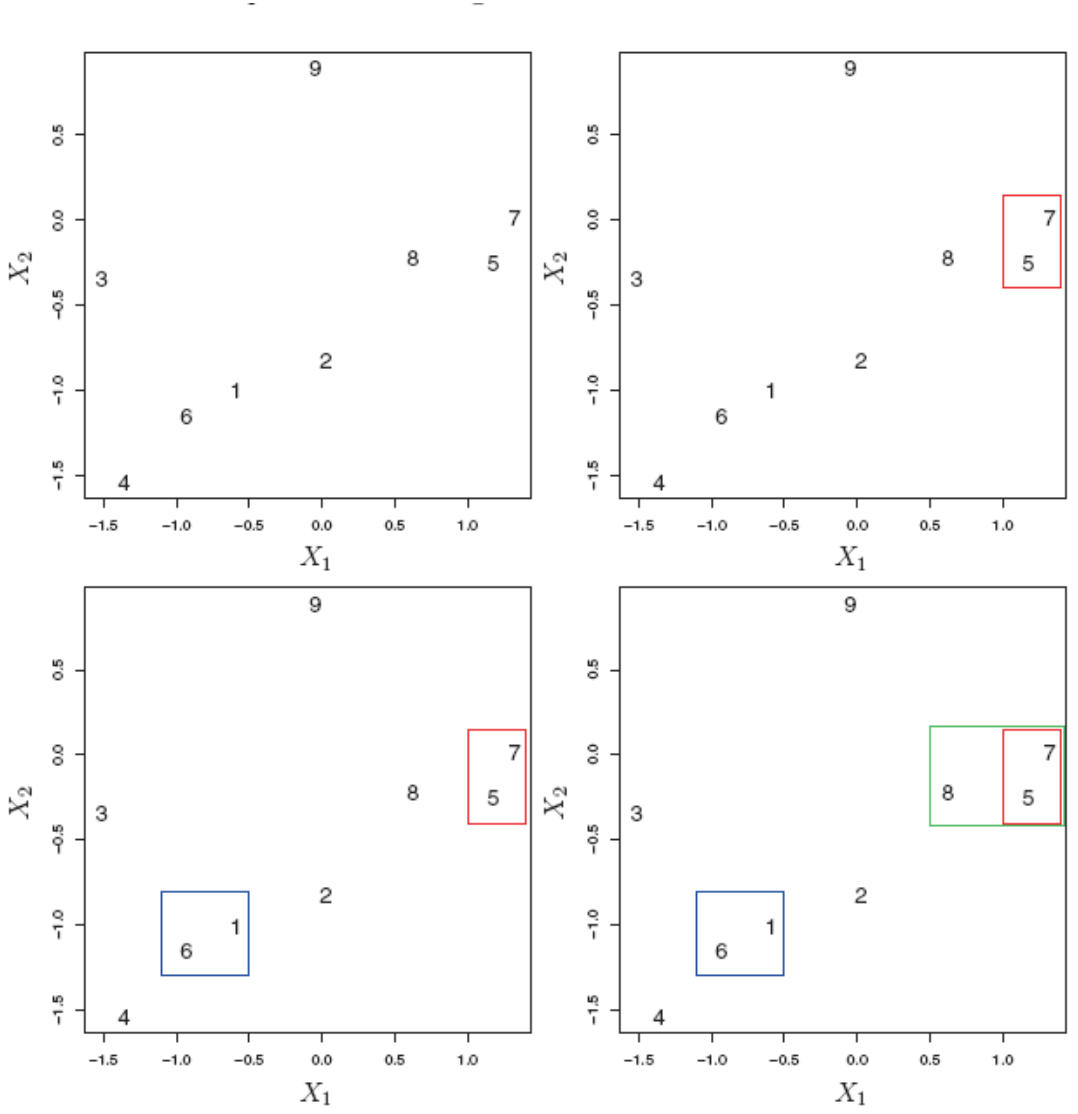
- i.e., don't need to specify the number of clusters, K, beforehand



Hierarchical clustering

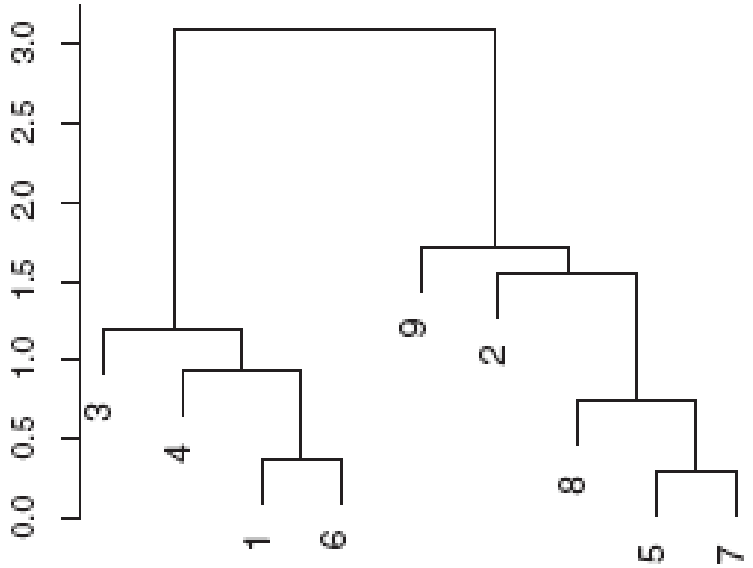
We can create a hierarchical clustering of the data using simple bottom-up agglomerative algorithm:

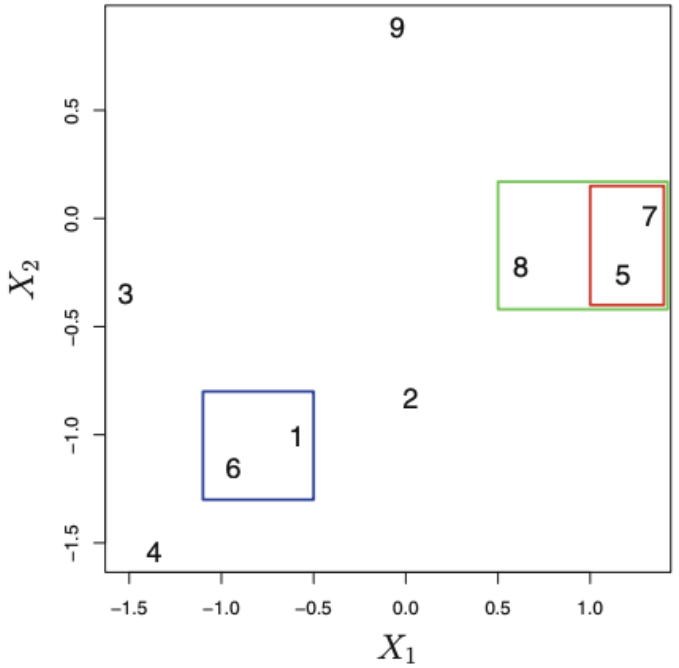
1. Choosing a (dis)similarity measure
   - E.g., The Euclidean distance
2. Initializing the clustering by treating each point as its own cluster
3. Successively merging the pair of clusters that are most similar
   - i.e., calculate the similarity between all pairs of clusters and merging the pair that is most similar
4. Stopping when all points have been merged into a single cluster



Hierarchical clustering

The vertical height that two clusters/points merge show how similar the two ***clusters*** are

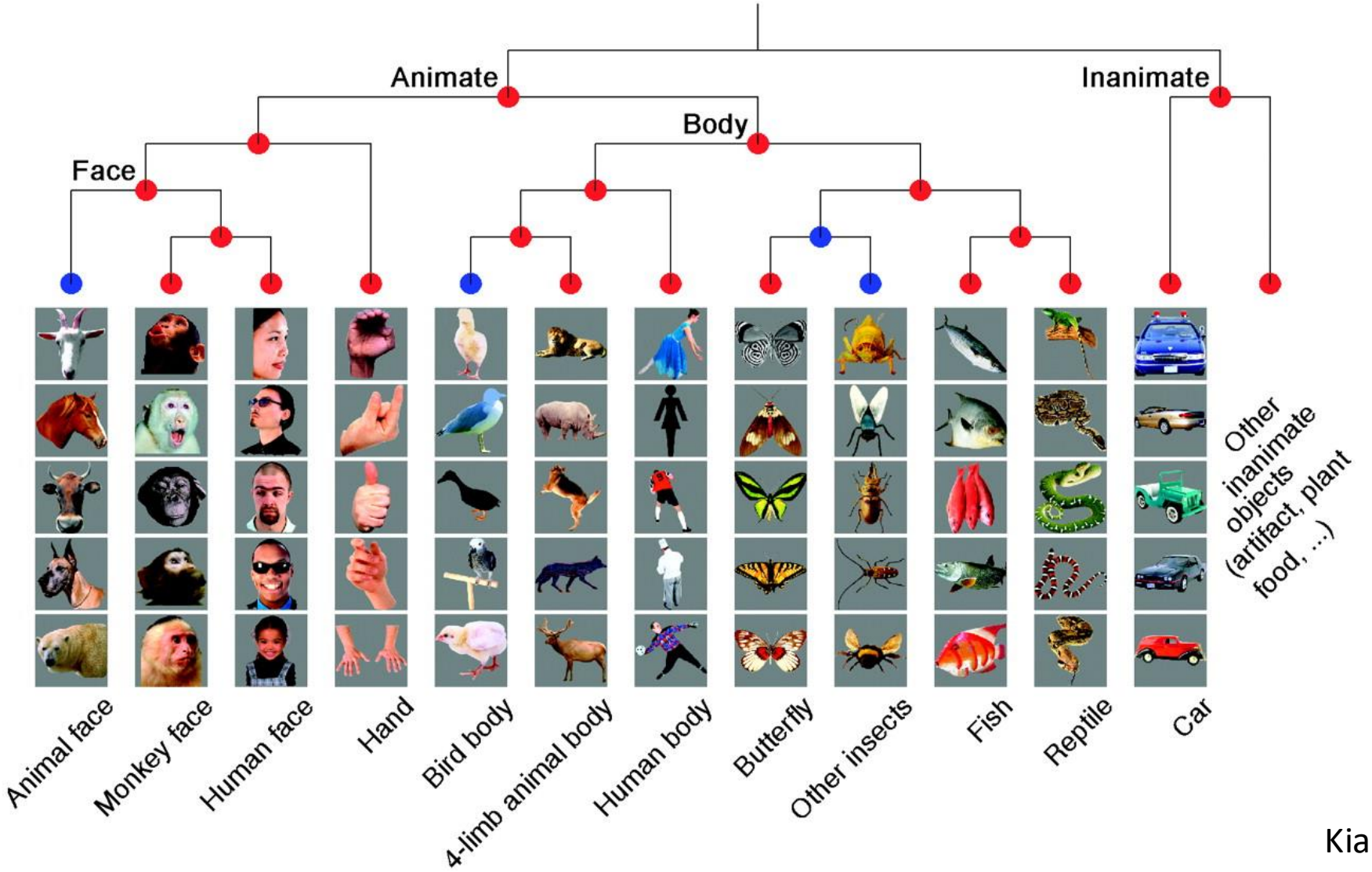




Note: horizontal distance between ***individual points*** is not important:

- point 9 is considered as similar to point 2 as it is to point 7

Hierarchical clustering example

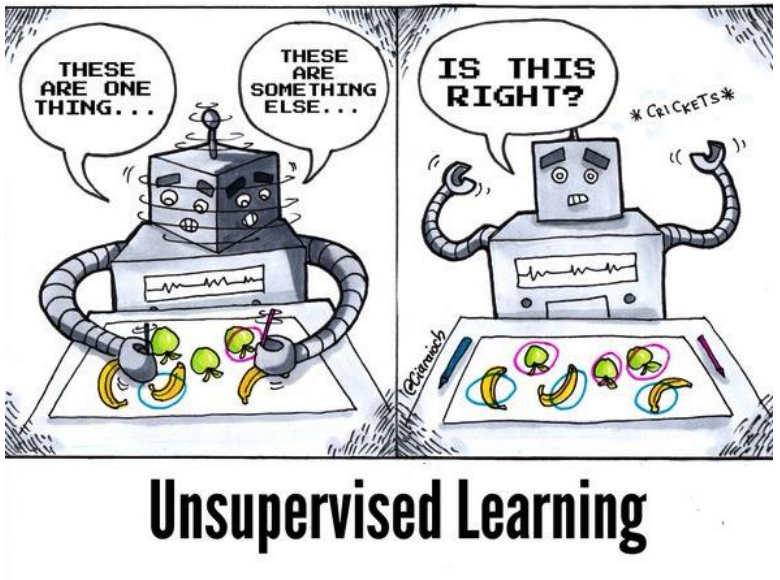


Kiani et al, 2007

Issues with clustering

Choices made can effect the results:

- Feature normalization and/or dissimilarity measure
- K-means: choice of K
- For hierarchical cluster: linkage and cut height



Potential approaches to deal with these issues:

- Try a few methods and see if one gives interesting/useful results
- Validate that you get similar results on a second set of data

Let's explore this in Jupyter!

Object oriented programming

Object-oriented programming

Object-oriented programming (OOP) is a programming paradigm based on the concept of "objects", which can contain:

1. **data**: in the form of fields
   - often known as attributes or properties

2. **methods**: functions that operate on the data

Have we seen any objects in this class yet?

```
knn = KNeighborsClassifier(n_neighbors = 1)        # constructor
knn.fit(X_train, y_train)                          # method
```

Using object-oriented programming makes it easier to design larger software systems

- E.g., useful for writing packages, such as the ones we have used in this class

Object-oriented programming

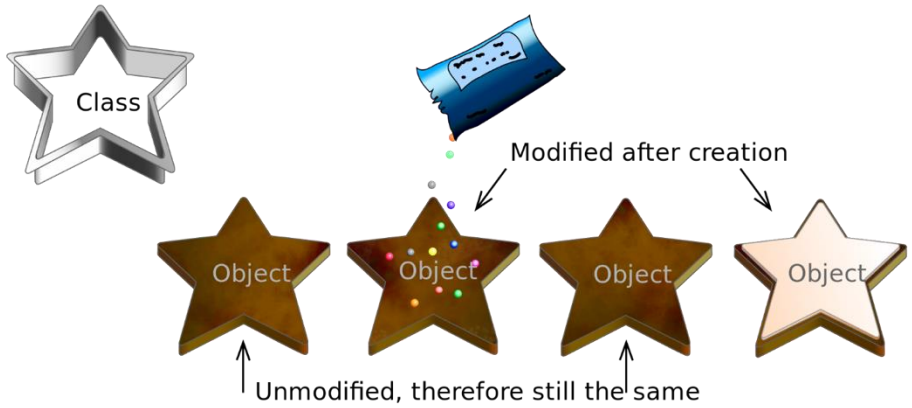
A **class** defines what the object is

- i.e., classes have code that lists the types of data stored and the methods

An **object** is a realization of classes (often called an instance of a class)

- Stores actual data that can be manipulated with methods

```
knn1 = KNeighborsClassifier(n_neighbors = 1)
knn5 = KNeighborsClassifier(n_neighbors = 5)
```



Useful because it allows us to have many object instances

- E.g., A KNN classifier trained on different data, different values of k, etc.

Object-oriented programming

A **constructor** defines what should happen when an object is created

- In Python the constructor is defined with the **__init__(self)** method

```
class KNN:

    # Constructor
    def __init__(self, n_neighbor):

        self.k = n_neighbor
```

```
# create an instance of an object
my_knn = KNN(n_neighbor = 5)

# get the stored value of k
my_knn.k
```

Object-oriented programming

Methods are functions that are applied to the data stored in the object

For example, the .fit() method in an KNN object would save training and test data

```
class KNN:

    …   # constructor, etc. above

    def fit(self, X_train, y_train):

        self.X_train = X_train
        self.y_train = y_train
```

```
# call the .fit() method
my_knn.fit(X_train, y_train)

# retrieve the training data
my_knn.X_train
```

Object-oriented programming

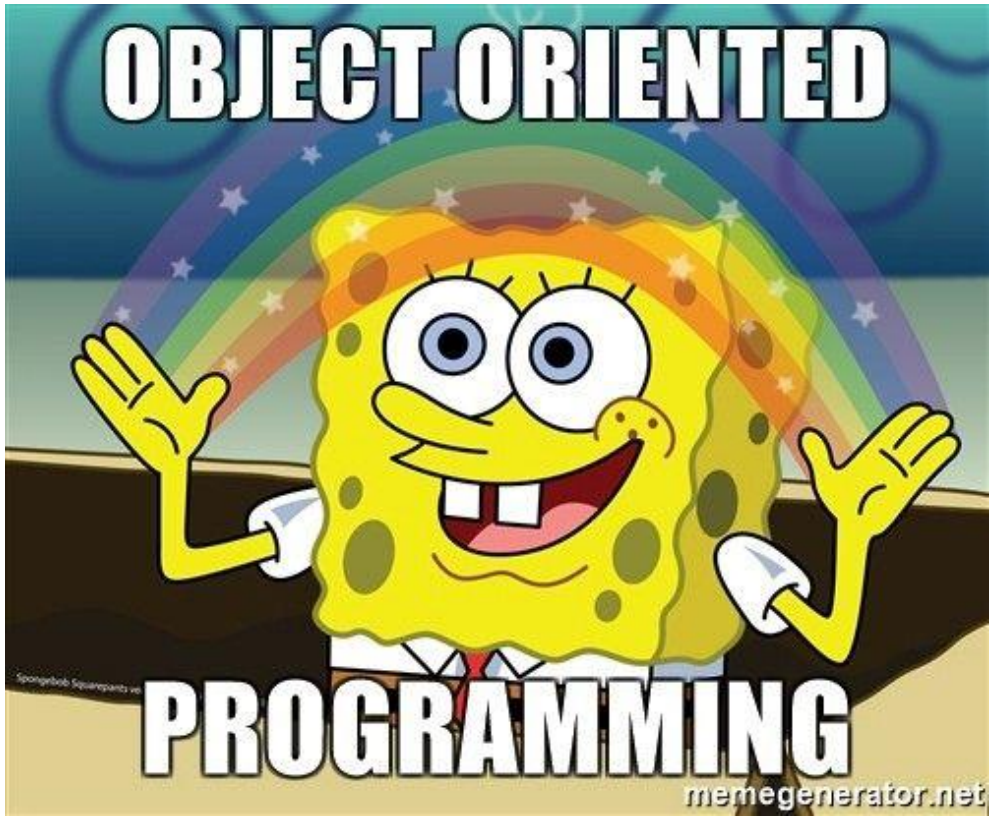
The __str__ method defines what should happen when the print() function is called on the object

```
# str method
def __str__(self):
    return 'I am an object’
```

```
# create an instance of an object
my_knn = KNN(n_neighbor = 5)

# print the object
print(my_knn)
```

Questions?



Let's explore this in Jupyter!