YData: Introduction to Data Science

Lecture 24: Linear regression and unsupervised learning

Overview

Quick review of classification and the KNN classifier

Feature normalization

Linear regression

Unsupervised learning/clustering

- K-means cluster
- If there is time: hierarchical clustering

Project timeline

~~Sunday, November 16th~~

- ~~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 23rd

- A template for doing your review has been posted
- Jupyter notebook files with your reviews need to be emailed to the authors
- A pdf containing all three reviews needs to be uploaded Gradescope

Sunday, December 7th

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

Homework 9 has been posted

- It is due Monday December 1st

Prediction: regression and classification

We “learn” a function f

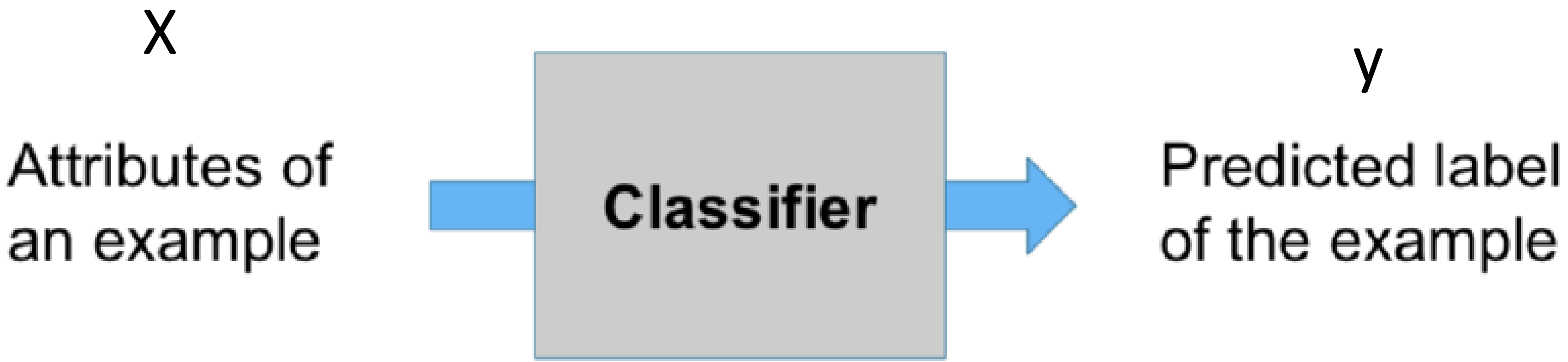
- $f(\mathbf{x}) \longrightarrow y$

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

Output:

- <u>Regression</u>: output is a real number ($y \in R$)
- <u>Classification</u>: output is a categorical variable y_k

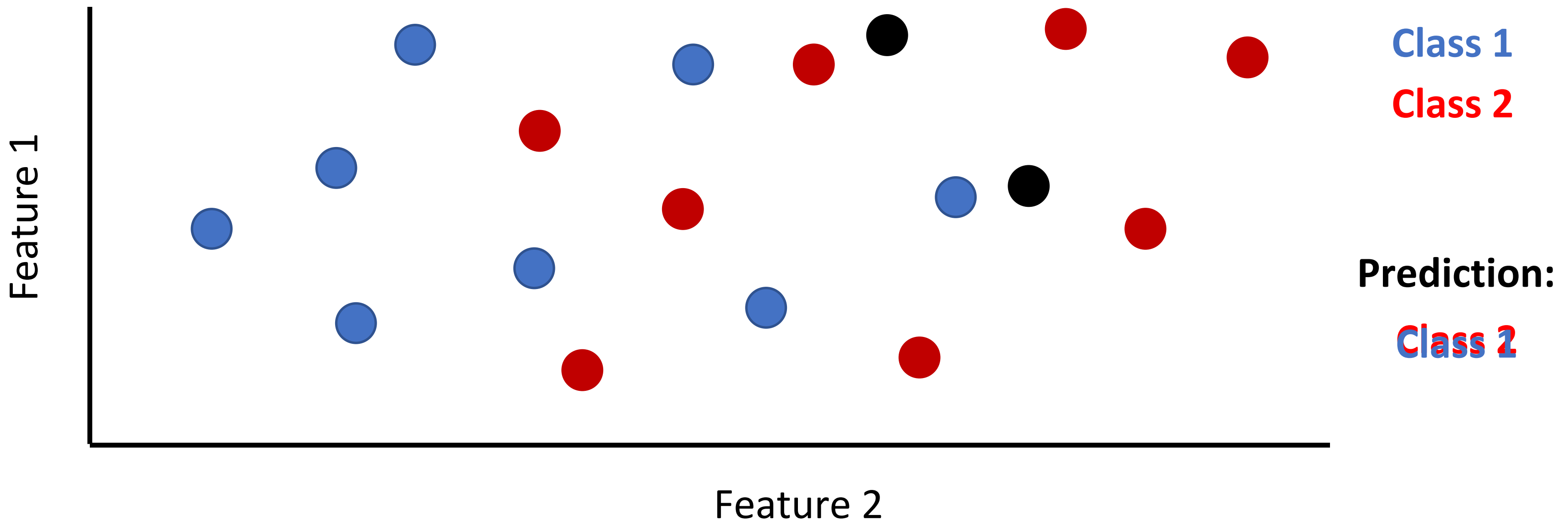
Training a classifier



K-Nearest Neighbor Classifier (KNN)

Training the classifier: Store all the features with their labels

Making predictions: The label of closest k training points is returned



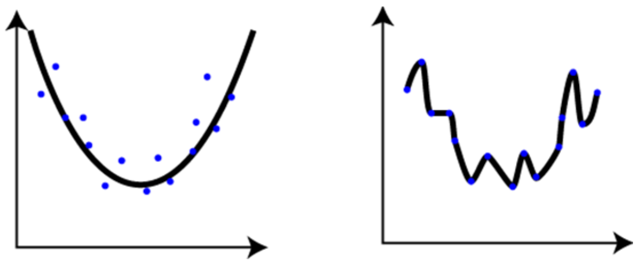
KNN classifiers using scikit-learn

We can fit and evaluate the performance of a KNN classifier using:

```
knn = KNeighborsClassifier(n_neighbors = 1)        # construct a classifier

knn.fit(X_features, y_labels)       # train the classifier

penguin_preditions = knn.predict(X_penguin_features)  # make predictions

np.mean(penguin_preditions == y_penguin_labels)       # get accuracy
```

Review: overfitting

Overfitting occurs when our classifier matches too close to the training data and doesn't capture the true underlying patterns

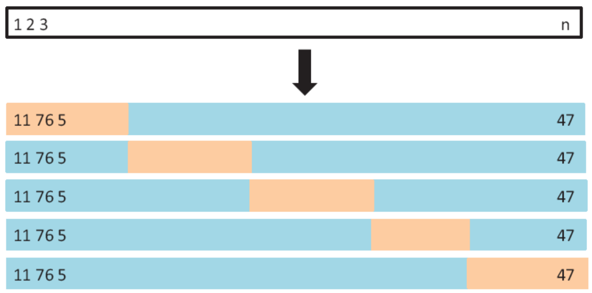


[Overfitting song…](#)

To avoid overfitting we split our data into a training and test set

- Classifier learns relationship on training data
- Classifier's performance is evaluated on the test data

We can use k-fold cross-validation to get a better estimate of the test accuracy



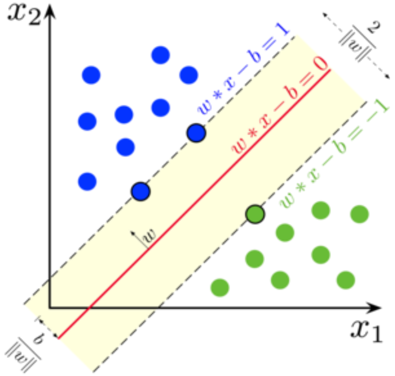
Review: Other classifiers

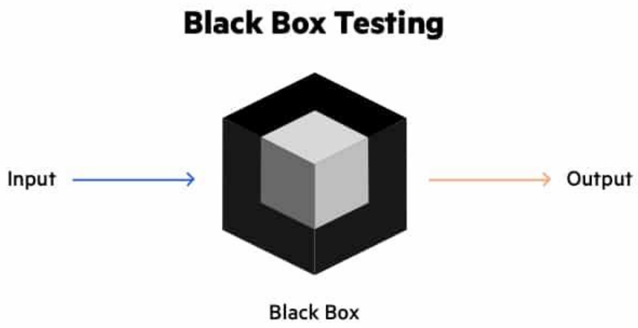
We also built our own KNN classifier

Scikit-learn makes it easy to try out different classifiers get their cross-validation performance

- E.g., SVM, random forests, neural networks, etc.

```
svm = LinearSVC()

scores = cross_val_score(svm,
    X_features,  y_labels, cv = 5)

scores.mean()
```





Review: steps to build a KNN classifier

We build our KNN classifier by creating a series of functions…

1. euclid_dist(x1, x2)
   - Calculates the Euclidean distance between two points x1 and x2

$$D = \sqrt{(x_0 - x_1)^2 + (y_0 - y_1)^2 + (z_0 - z_1)^2}$$

2. get_labels_and_distances(test_point, X_train_features, y_train_labels)
   - Finds the distance between a test point and all the training points

3. classify_point(test_point, k, X_train_features, y_train_labels)
   - Classifies one test point by returning the majority label of the k closest points

4. classify_all_test_data(X_test_data, k, X_train_features, y_train_labels)
   - Classifiers all test points

Feature normalization

Review: Distance between two points

Two features x and y: $D = \sqrt{(x_0 - x_1)^2 + (y_0 - y_1)^2}$

Three features x, y, and z: $D = \sqrt{(x_0 - x_1)^2 + (y_0 - y_1)^2 + (z_0 - z_1)^2}$

- And so on for more features…

It's important the features are standardized

- If not, features that typically have larger values will dominate the distance measurement

Feature normalization

bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g
46.1	15.1	215.0	5100.0
37.3	17.8	191.0	3350.0
51.3	18.2	197.0	3750.0
39.5	16.7	178.0	3250.0
48.7	15.1	222.0	5350.0

$\bar{x}$

s

In order to deal with features that are measured on very different scales, we can normalize the features

With a z-score normalization, we normalize each feature to have:

- A mean of 0
- A standard deviation of 1

$$z_i = \frac{x_i - \bar{x}}{s}$$

We can do this in Python using:

```
scalar = StandardScaler()
scalar.fit(X_train)
X_train_transformed = scalar.transform(X_train)
X_test_transformed = scalar.transform(X_test)
```

Feature normalization

To avoid overfitting ("data leakage") we can:

- Calculate the mean and standard deviation on the training
- Apply these means and standard deviations to normalize the training and test sets

To do this in a cross-validation loop, we can use a pipeline:

```
scalar = StandardScaler()
knn = KNeighborsClassifier(n_neighbors = 1)
cv = KFold(n_splits=5)

pipeline = Pipeline([('transformer', scalar), ('estimator', knn)])

scores = cross_val_score(pipeline, X_penguin_features, y_penguin_labels, cv = cv)
```

Let's explore this in Jupyter!

Linear regression

Prediction: regression and classification

We “learn” a function f

- f(**x**) $\longrightarrow$ y

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

Output:

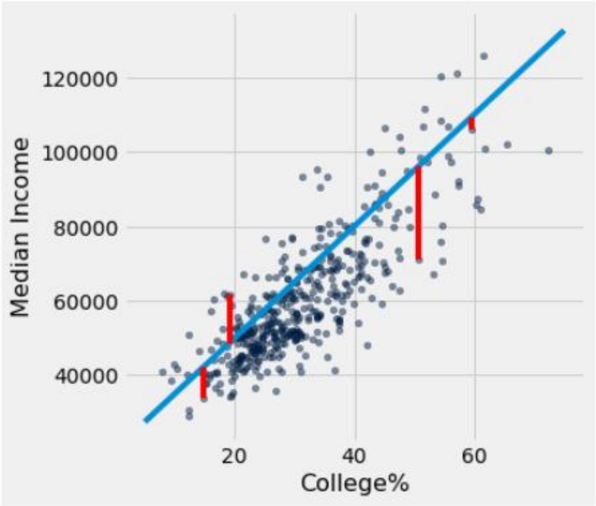
- <u>Regression</u>: output is a real number (y ϵ R)
- <u>Classification</u>: output is a categorical variable y_k

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: $\hat{y}$ = intercept + slope $\cdot$ x

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



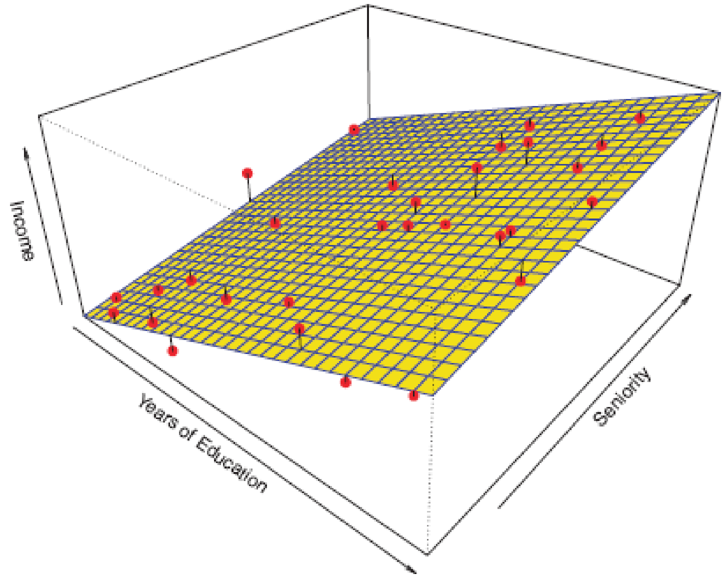
The coefficients for these regression models are found by minimizing root mean square error (RMSE)

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

Regression line app

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 $\hat{y}$

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

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

Multiple regression

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

There are many uses for multiple regression models including:

- To make predictions as accurately as possible
- To understand which predictors (x) are related to the response variable (y)

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
```

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

Numeric values to predict

```
y_preditions = linear_model.predict(X_test_features)   # make predictions

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

Real world example

Rather than predicting stock prices…

Let’s try this in Jupyter!

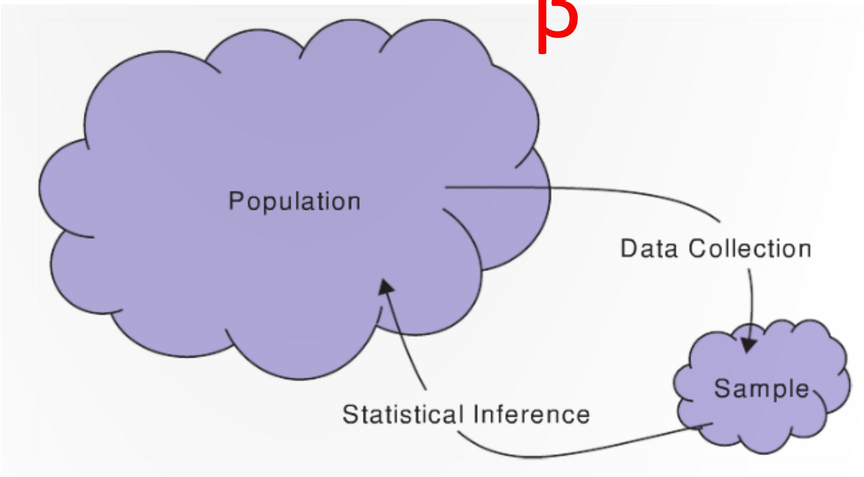
Inference for simple linear regression

Inference for simple linear regression

The Greek letter **β** is used to denote the slope ***of the population***

The letter **b** is used to denote the slope ***of the sample***

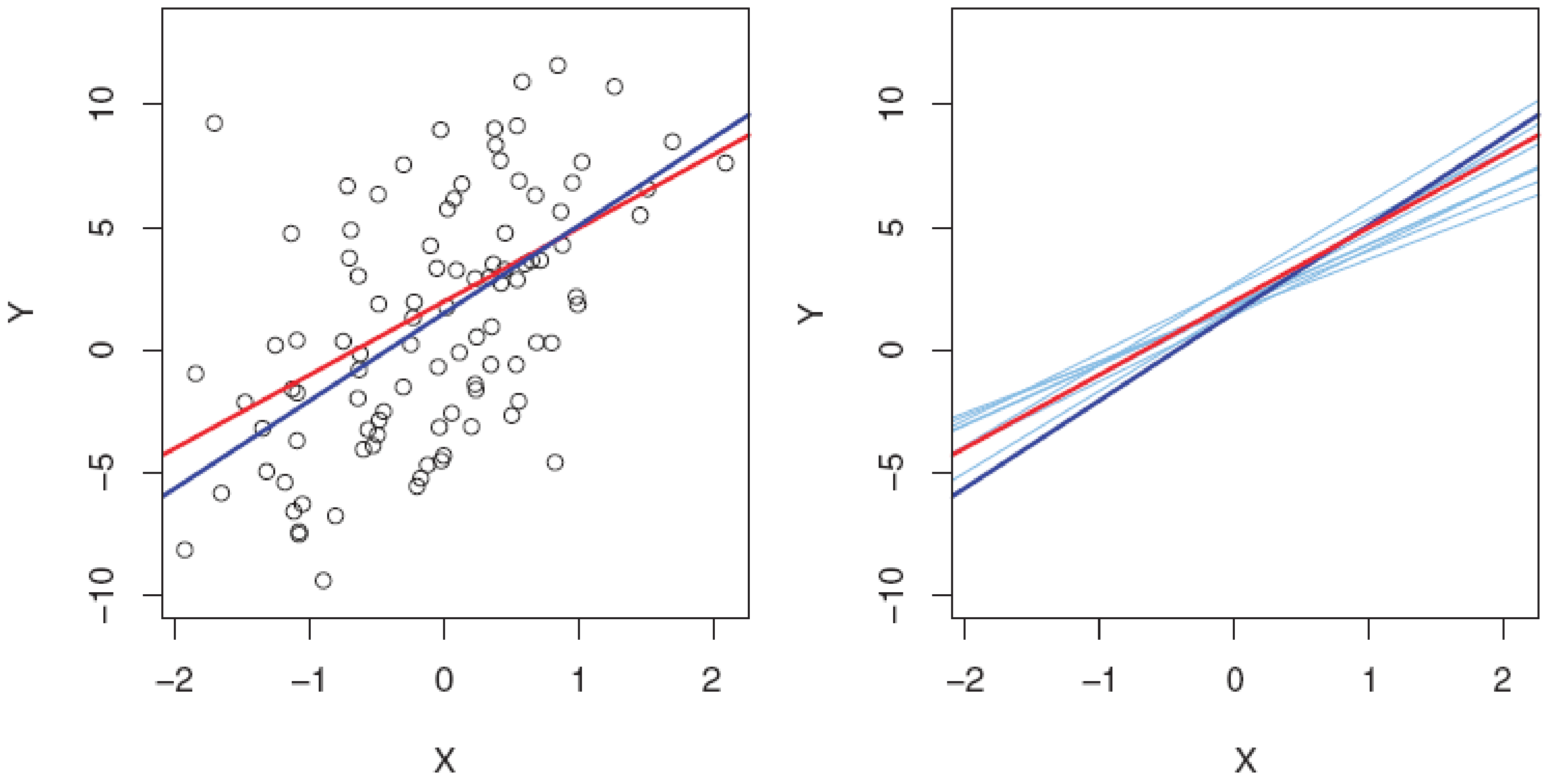
β



b

Population: β_o and β_1

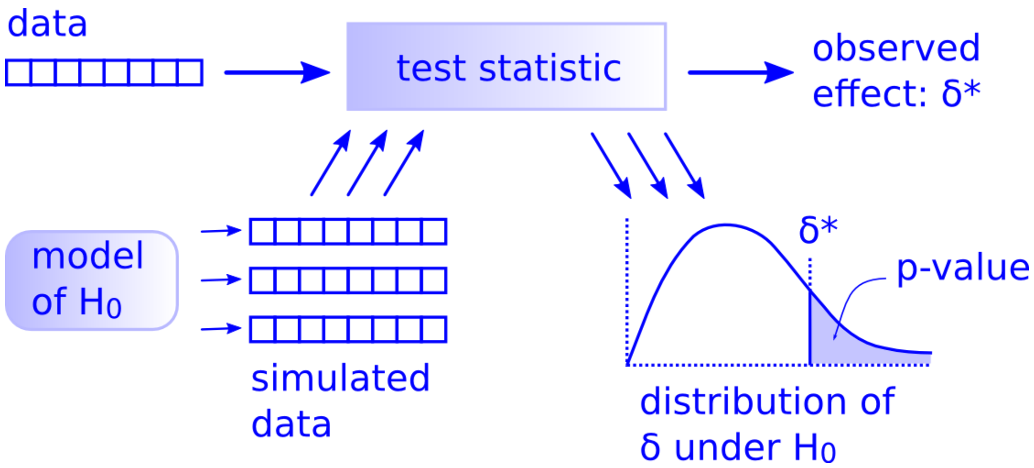
Sample estimates: b_0 and b_1

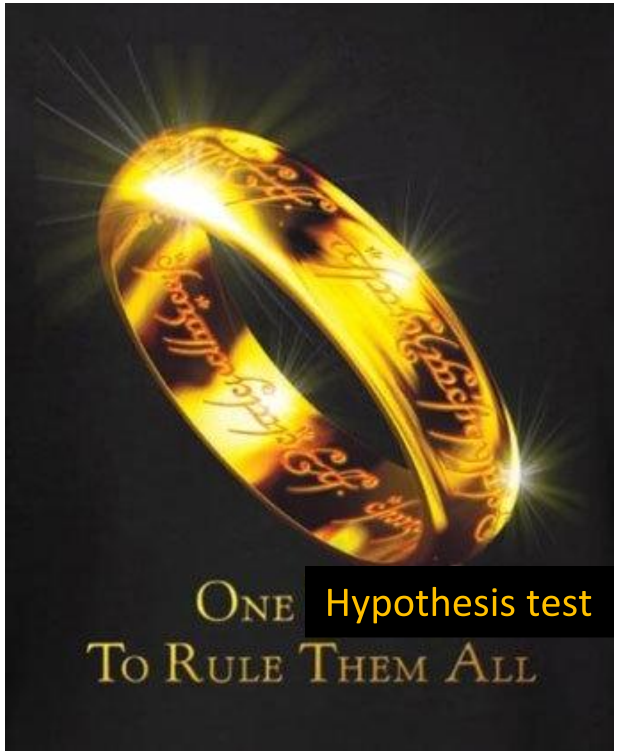


Hypothesis test for regression coefficients

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

There is only one hypothesis test!





Hypothesis test for regression coefficients

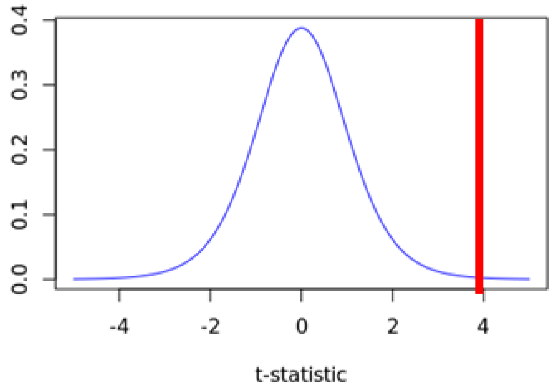
We can run a hypothesis test to see if there is a linear relationship between a feature x, and a response variable y

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

One type of hypothesis test we can run is based on a t-statistic: $t = \frac{b_1 - 0}{\hat{SE}_{b_1}}$

- The t-statistic comes from a t-distribution with n - k degrees of freedom
  - (If a few conditions are met)

We could also shuffle our data, fit models, and extract b_1 coefficients to create a null distribution



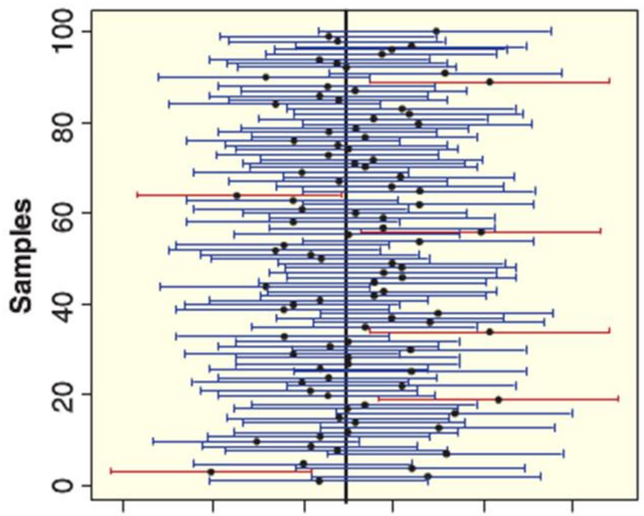
Confidence intervals for regression coefficients

The confidence interval for the slope coefficients:

β_1

We can use the statsmodels package to run hypothesis tests and create confidence intervals using "parametric" methods based on t-distributions

```
import statsmodels.api as sm

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

sm_linear_model.summary()
```



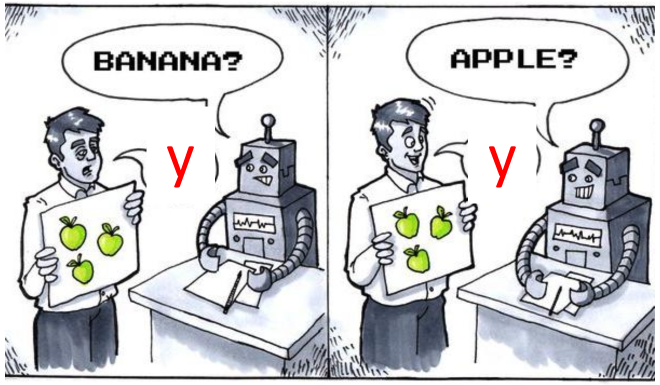
Let's try this in Jupyter!

Unsupervised learning

Supervised learning and unsupervised learning

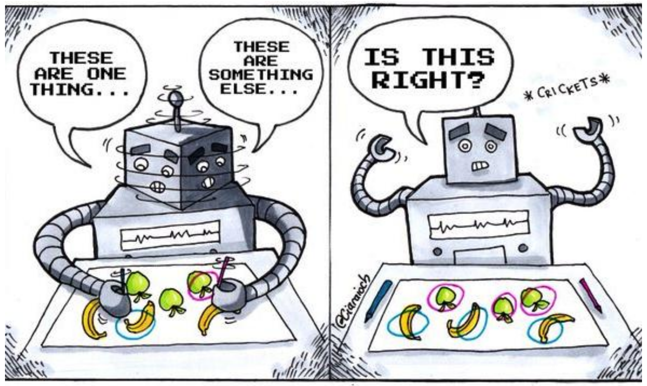
In **supervised learning** we have a set of features X, along with a label y

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



Supervised Learning

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



Unsupervised Learning

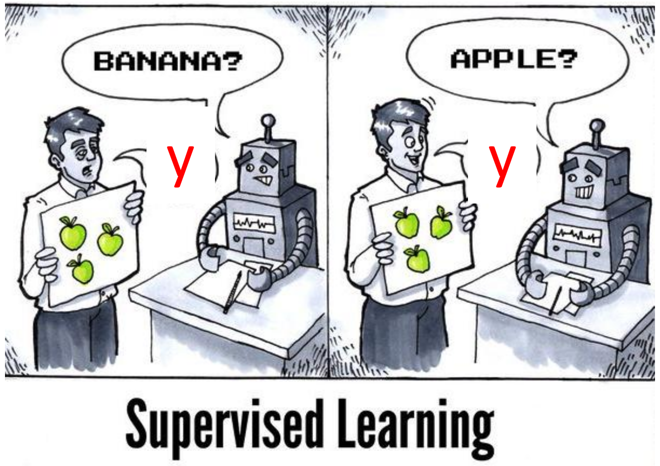
Unsupervised learning can be useful in order to find structure in the data and to visualize patterns

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

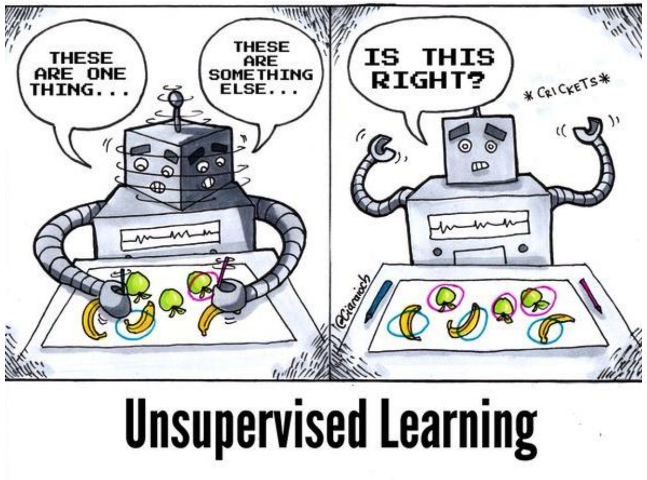
Given we are almost at the end of the semester, we will focus on clustering, which is one type of unsupervised learning



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

$$n\left\{\overbrace{\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}}^{p}\right.$$

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

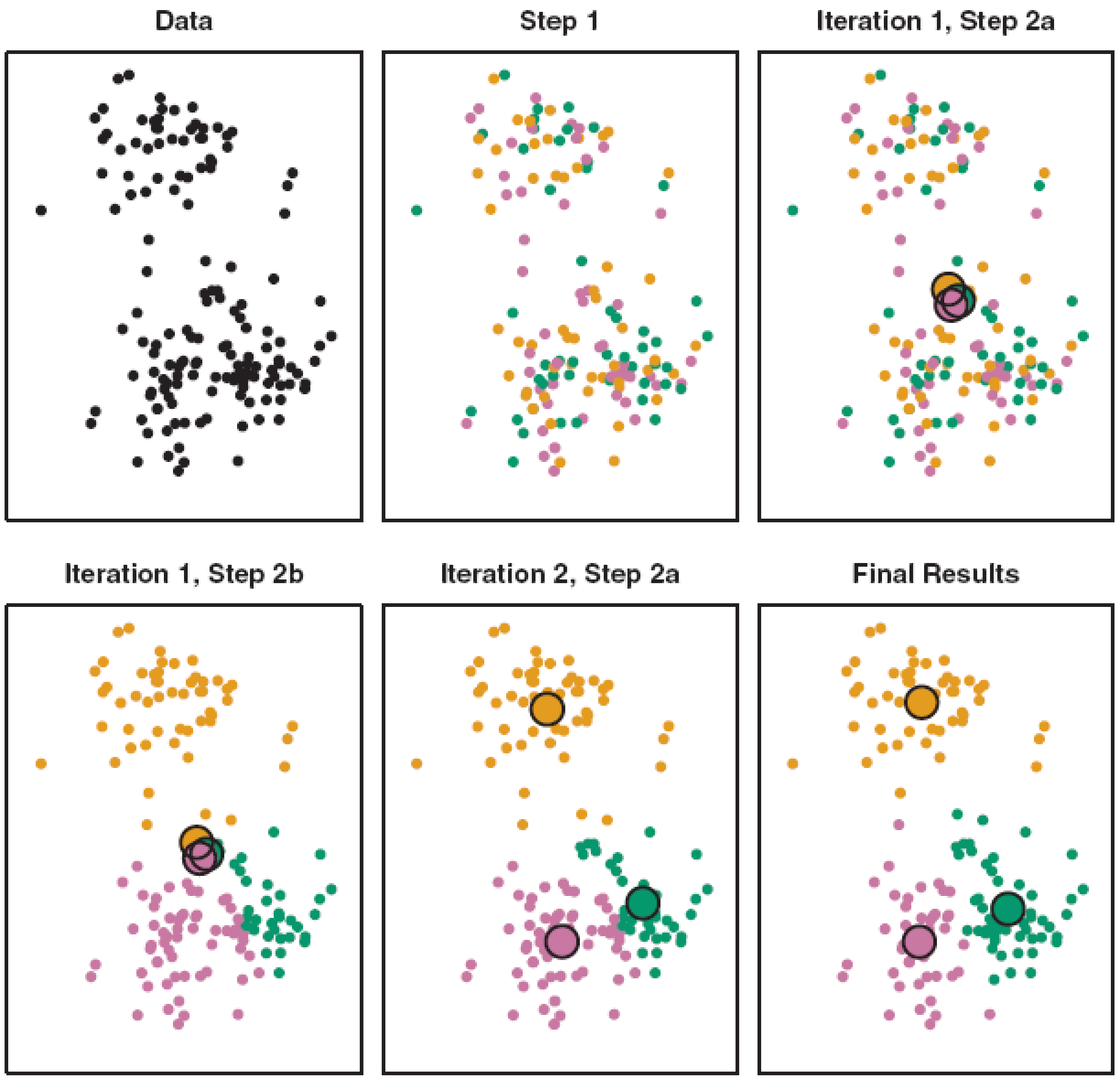
The goal is to minimize the within-cluster variation

- 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!

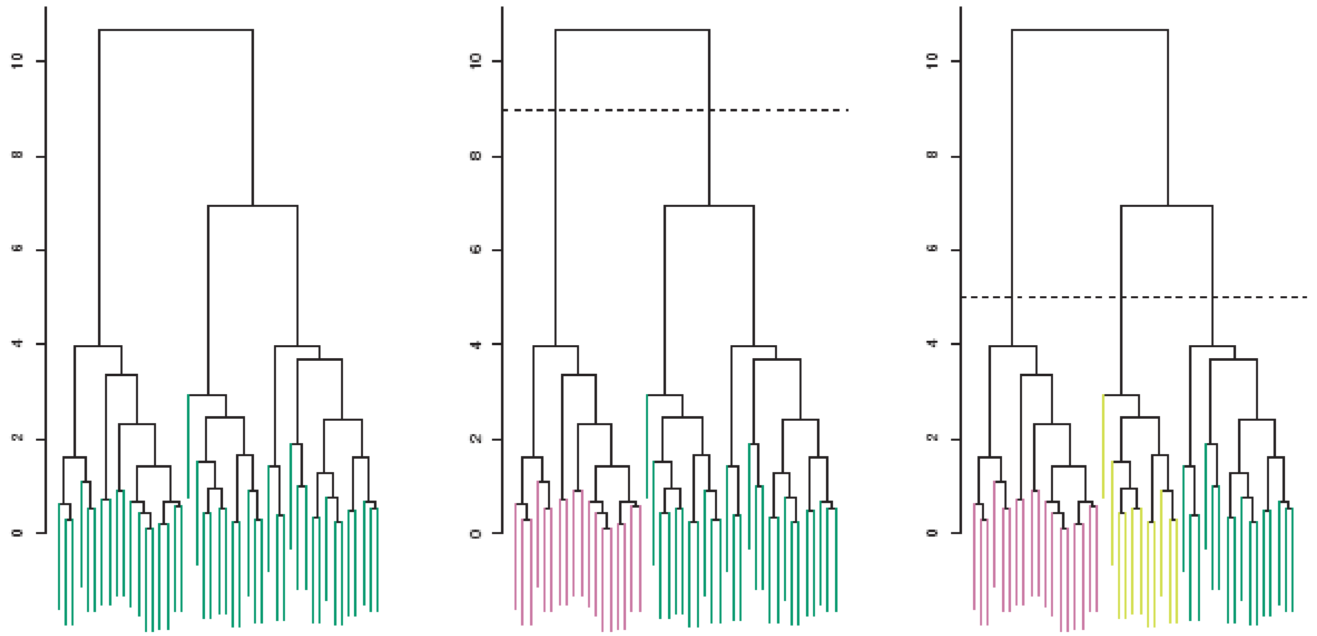
Hierarchical clustering

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

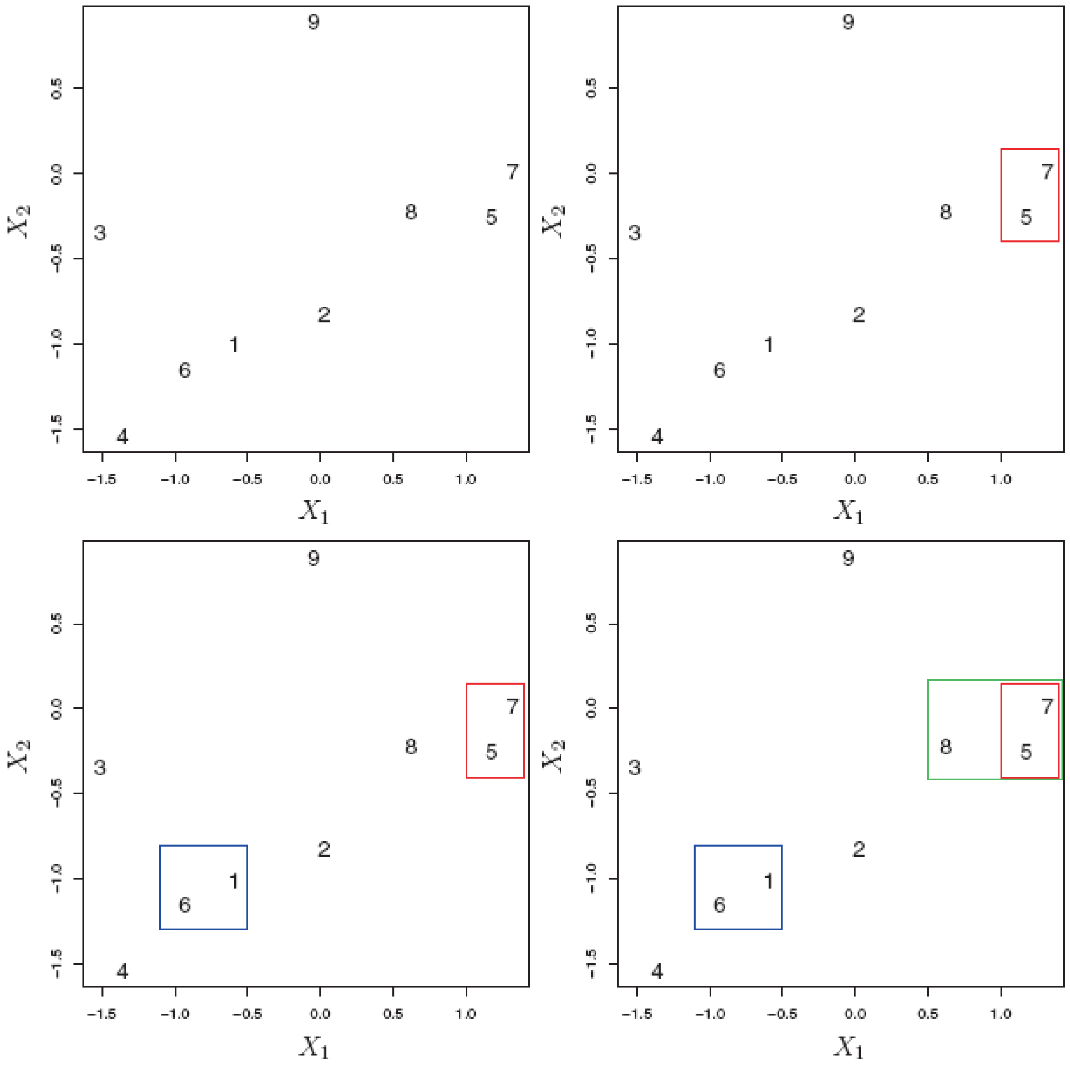
We can create a hierarchical clustering of the data using simple bottom-up agglomerative algorithm:

1. Choosing a (dis)similarity measure
   - E.g., The Euclidean distance

2. Initializing the clustering by treating each point as its own cluster

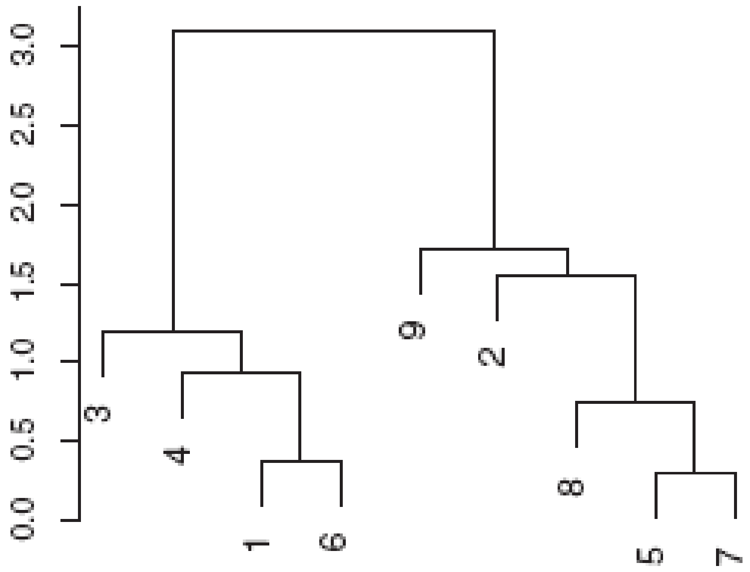
3. Successively merging the pair of clusters that are most similar
   - i.e., calculate the similarity between all pairs of clusters and merging the pair that is most similar

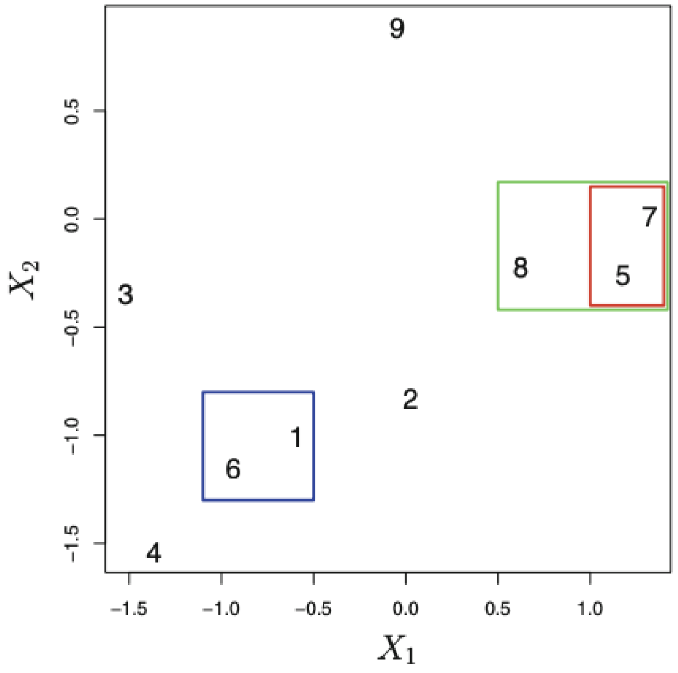
4. Stopping when all points have been merged into a single cluster



Hierarchical clustering

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

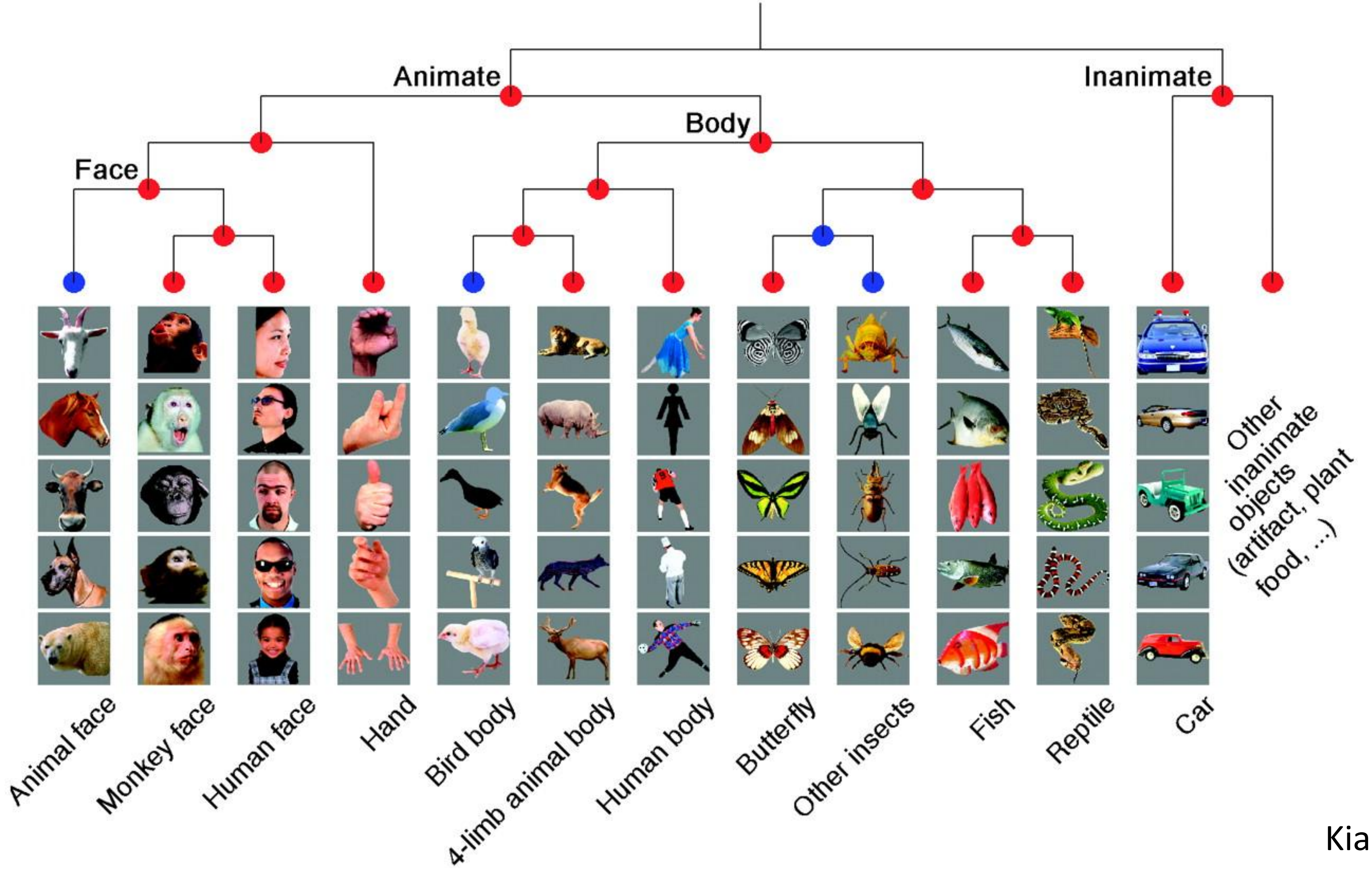




Note: horizontal distance between ***individual points*** is not important:

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

Hierarchical clustering example

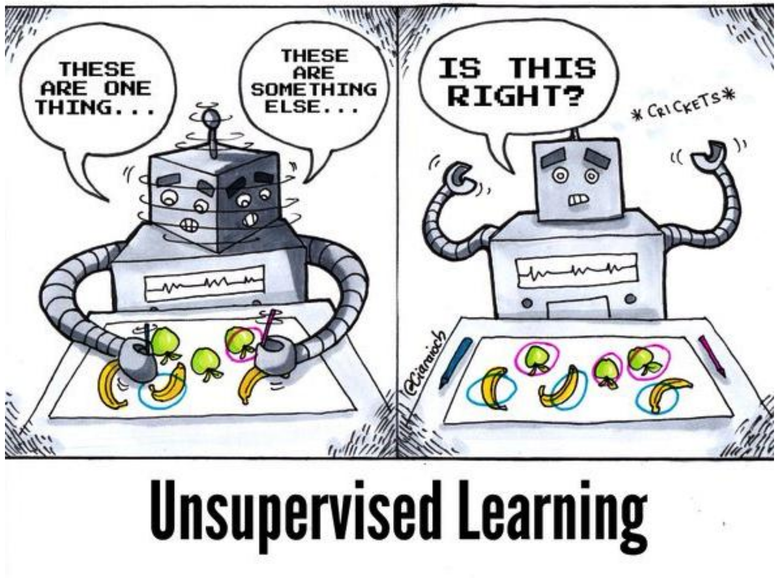


Kiani et al, 2007

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!