Python Programming

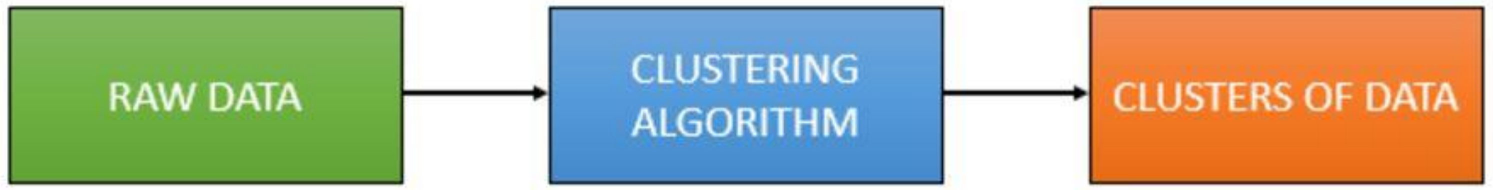
Clustering

Feedback is greatly appreciated!

Clustering

Clustering

Clustering is the grouping of objects together so that objects belonging in the same group (cluster) are more similar to each other than those in other groups (clusters)



Clustering

Clustering is an unsupervised learning algorithm that will attempt to group similar clusters together in your data.

So what does a typical clustering problem look like?

- Cluster Similar Documents
- Cluster Customers based on Features
- Market Segmentation
- Identify similar physical groups

Contd.

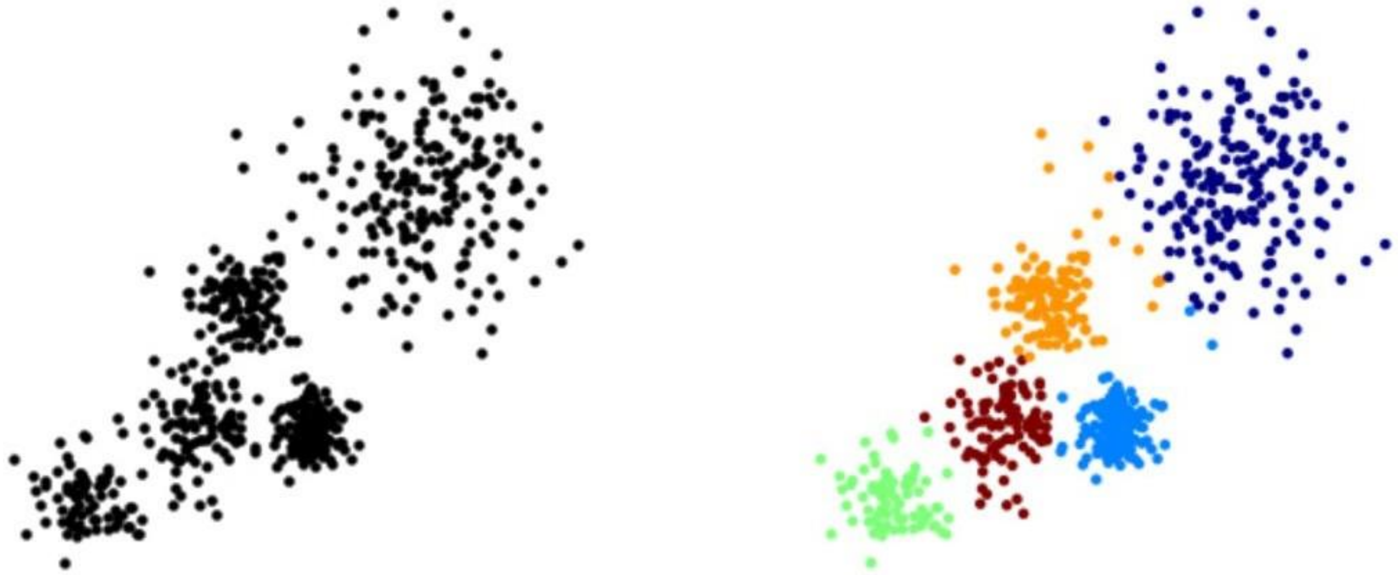
Method name	Parameters	Scalability	Use case	Geometry (metric used)
K-Means	number of clusters	Very large n_samples, medium n_clusterswith MiniBatch code	General-purpose, even cluster size, flat geometry, not too many clusters	Distances between points
Affinity propagation	damping, sample preference	Not scalable with n_samples	Many clusters, uneven cluster size, non-flat geometry	Graph distance (e.g. nearest-neighbor graph)
Mean-shift	bandwidth	Not scalable with n_samples	Many clusters, uneven cluster size, non-flat geometry	Distances between points
Spectral clustering	number of clusters	Medium n_samples, small n_clusters	Few clusters, even cluster size, non-flat geometry	Graph distance (e.g. nearest-neighbor graph)
Ward hierarchical clustering	number of clusters	Large n_samples and n_clusters	Many clusters, possibly connectivity constraints	Distances between points
Agglomerative clustering	number of clusters, linkage type, distance	Large n_samples and n_clusters	Many clusters, possibly connectivity constraints, non Euclidean distances	Any pairwise distance
DBSCAN	neighborhood size	Very large n_samples, medium n_clusters	Non-flat geometry, uneven cluster sizes	Distances between nearest points
Gaussian mixtures	many	Not scalable	Flat geometry, good for density estimation	Mahalanobis distances to centers
Birch	branching factor, threshold, optional global clusterer.	Large n_clustersand n_samples	Large dataset, outlier removal, data reduction.	Euclidean distance between points

http://scikit-learn.org/stable/modules/clustering.html

UMKC

Clustering

The overall goal is to divide data into distinct groups such that observations within each group are similar



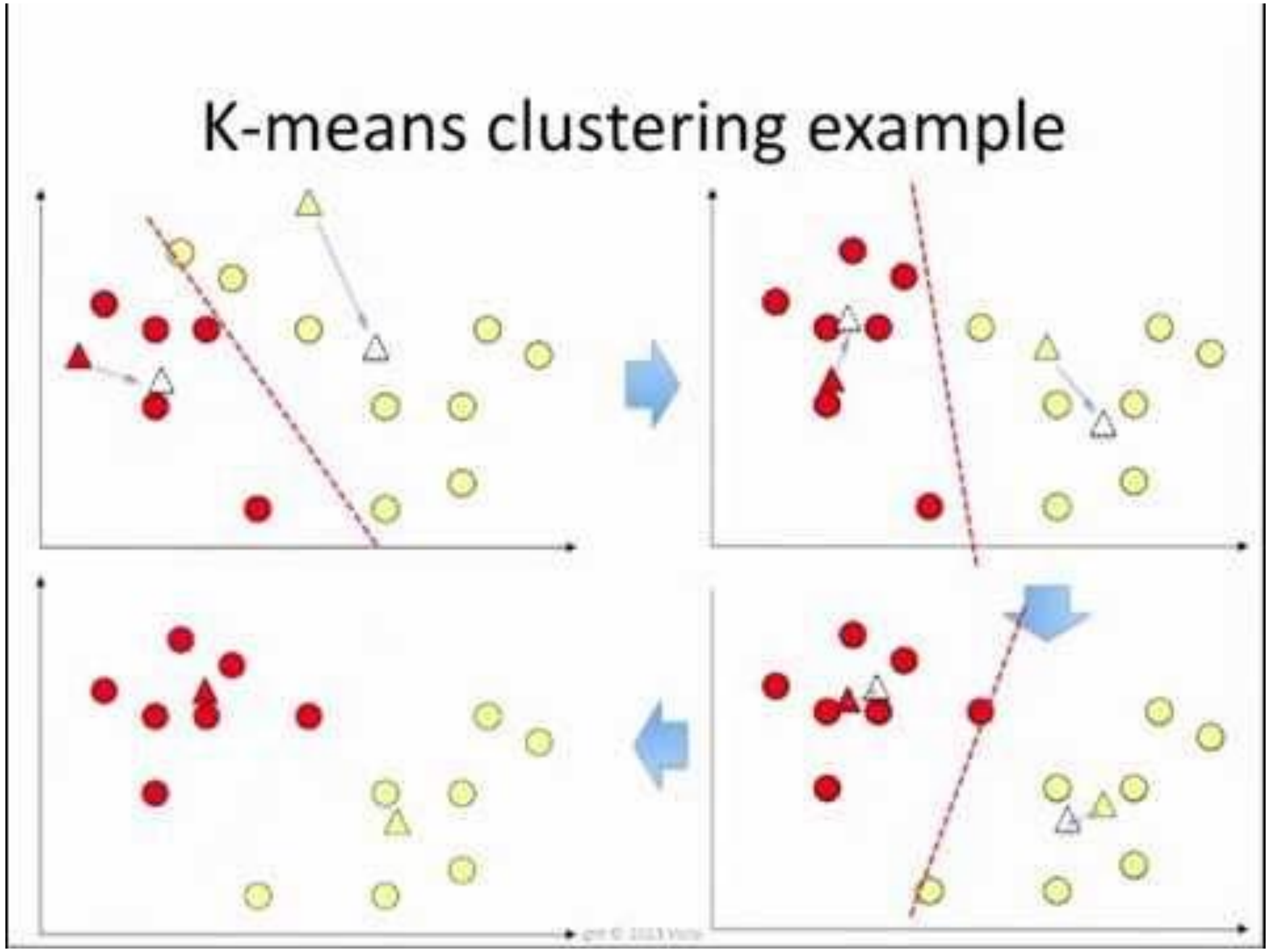
K Means Clustering

K Means Clustering

The K Means Algorithm

- Choose a number of Clusters “K”
- Randomly assign each point to a cluster
- Until clusters stop changing, repeat the following:
    - For each cluster, compute the cluster centroid by taking the mean vector of points in the cluster
    - Assign each data point to the cluster for which the centroid is the closest

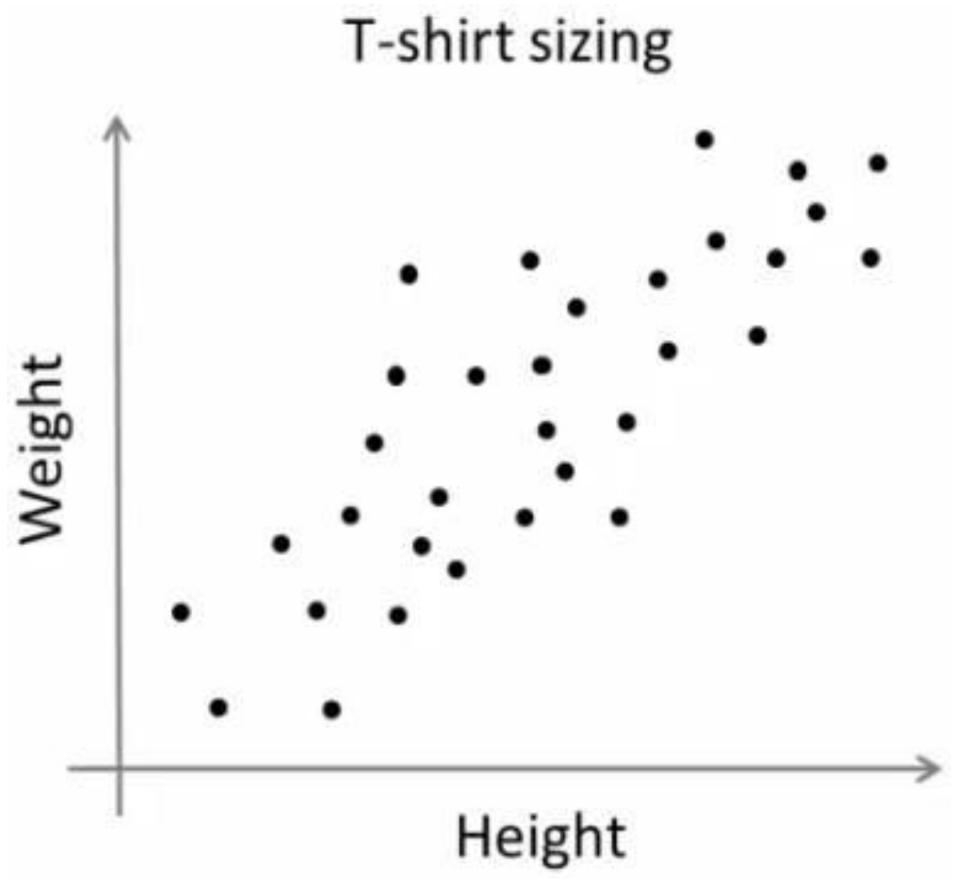
K Means Clustering



K-Means

T-shirt size problem
Consider a company, which is going to release a new model of T-shirt to market.
Obviously, they will have to manufacture models in different sizes to satisfy people of all sizes.
So the company make a data of people's height and weight, and plot them on to a graph.

Company can't create t-shirts with all the sizes. Instead, they divide people to Small, Medium and Large, and manufacture only these 3 models which will fit into all the people.



As a first step in finding a sensible initial partition(k=2)

Subject	A	B
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

	Individual	Mean Vector (centroid)
Group 1	1	(1.0, 1.0)
Group 2	4	(5.0, 7.0)

Steps to do clustering

	Cluster 1		Cluster 2	
Step	Individual	Mean Vector (centroid)	Individual	Mean Vector (centroid)
1	1	(1.0, 1.0)	4	(5.0, 7.0)
2	1, 2	(1.2, 1.5)	4	(5.0, 7.0)
3	1, 2, 3	(1.8, 2.3)	4	(5.0, 7.0)
4	1, 2, 3	(1.8, 2.3)	4, 5	(4.2, 6.0)
5	1, 2, 3	(1.8, 2.3)	4, 5, 6	(4.3, 5.7)
6	1, 2, 3	(1.8, 2.3)	4, 5, 6, 7	(4.1, 5.4)

- The remaining individuals are now examined in sequence and allocated to the cluster to which they are closest, in terms of Euclidean distance to the cluster mean.
- The mean vector is recalculated each time a new member is added.

Steps to do clustering

- Now the initial partition has changed, and the two clusters at this stage having the following characteristics

	Individual	Mean Vector (centroid)
Cluster 1	1, 2, 3	(1.8, 2.3)
Cluster 2	4, 5, 6, 7	(4.1, 5.4)

Steps to do clustering

Individual	Distance to mean (centroid) of Cluster 1	Distance to mean (centroid) of Cluster 2
1	1.5	5.4
2	0.4	4.3
3	2.1	1.8
4	5.7	1.8
5	3.2	0.7
6	3.8	0.6
7	2.8	1.1

- But we cannot yet be sure that each individual has been assigned to the right cluster.
- So, we compare each individual’s distance to its own cluster mean and to
  that of the opposite cluster.

Steps to do clustering

	Individual	Mean Vector (centroid)
Cluster 1	1, 2	(1.3, 1.5)
Cluster 2	3, 4, 5, 6, 7	(3.9, 5.1)

- Only individual 3 is nearer to the mean of the opposite cluster (Cluster 2) than its own (Cluster 1).
- In other words, each individual's distance to its own cluster mean should be smaller that the distance to the other cluster's mean (which is not the case with individual 3).
- Thus, individual 3 is relocated to Cluster 2

Web tools for kmeans clustering

- https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

Kmeans Evaluation

- ***Silhouette Coefficient = (x-y)/ max(x,y)***
  - where, **y** is the mean intra cluster distance: mean distance to the other instances in the same cluster
  - **x** depicts mean nearest cluster distance i.e. mean distance to the instances of the next closest cluster.

Evaluation

- Silhouette score can be used to study the separation distance between the resulting clusters
- The silhouette plot displays a measure of how close each point in one cluster is to points in the neighboring clusters and thus provides a way to assess parameters like number of clusters visually
- This measure has a range of [-1, 1]
- Silhouette coefficients near +1 indicate that the sample is far away from the neighboring clusters
- A value of 0 indicates that the sample is on or very close to the decision boundary between two neighboring clusters
- Negative values indicate that samples might have been assigned to the wrong cluster.

Dimensionality Reduction

- dimension reduction is the process of reducing the number of random variables under consideration by obtaining a set of principal variables.
- It can be divided into <u>feature selection</u> and <u>feature extraction</u>

Why do we need Dimension reduction

- In machine learning, to catch useful indicators and obtain a more accurate result, we tend to add as many features as possible at first.
- However, after a certain point, the performance of the model will decrease with the increasing number of elements
- This phenomenon is often referred to as “The Curse of Dimensionality.”

https://web.stanford.edu/~schmit/cme193/lec/lec5.pdf

Why do we need Dimension reduction

- In addition to avoiding overfitting and redundancy, dimensionality reduction also leads to better human interpretations and less computational cost with simplification of models

Feature selection and feature extraction

- Feature selection tries to select a subset of the original features for use in the machine learning model.
- In this way, we could remove redundant and irrelevant features without incurring much loss of information
- Feature extraction creates new features by projecting the data in the high-dimensional space to a space of fewer dimensions.

Principal Component Analysis(PCA)

- The main linear technique for dimensionality reduction
- principal component analysis, performs a linear mapping of the data to a lower-dimensional space in such a way that the variance of the data in the low-dimensional representation is maximized.

Feature scaling

- It refers to putting the values in the same range or same scale so that no variable is dominated by the other.
- It is mostly used in the categorical data where the categories are assigned simple integers such as 0,1,2…which might represent different categories.
- Or when we have different unit in our dataset like KG and GRAM, COUNT
- But the problem is that when we put this through a machine learning model, it may interpret it as the weightage or something else .
- For instance, it may use 0 as the least preference and 2 as a high preference

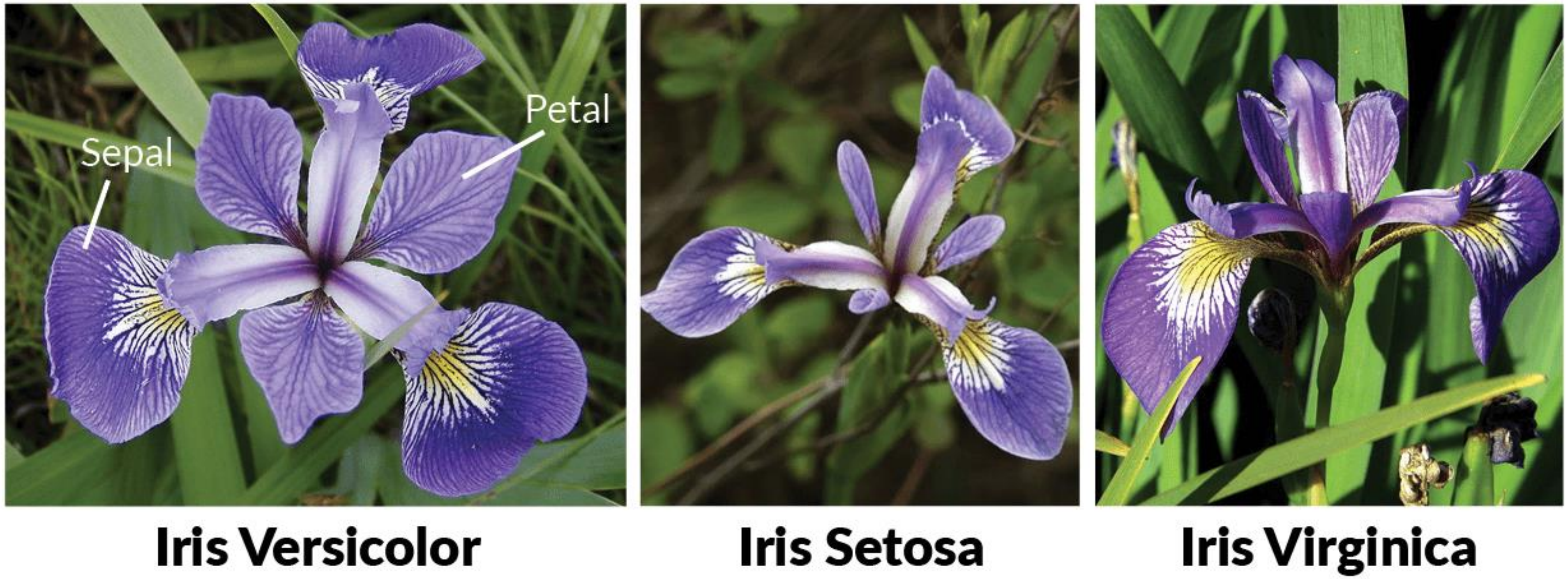
Various methods of feature scaling

- Standardization: It is also called Z-score normalization

$$z = \frac{x - \mu}{\sigma}$$

- Min-Max Scaling: It is also referred to as Normalization The features are scaled between 0 and 1

Use Case: Clustering and Dimension Reduction on Iris data set



Clustering

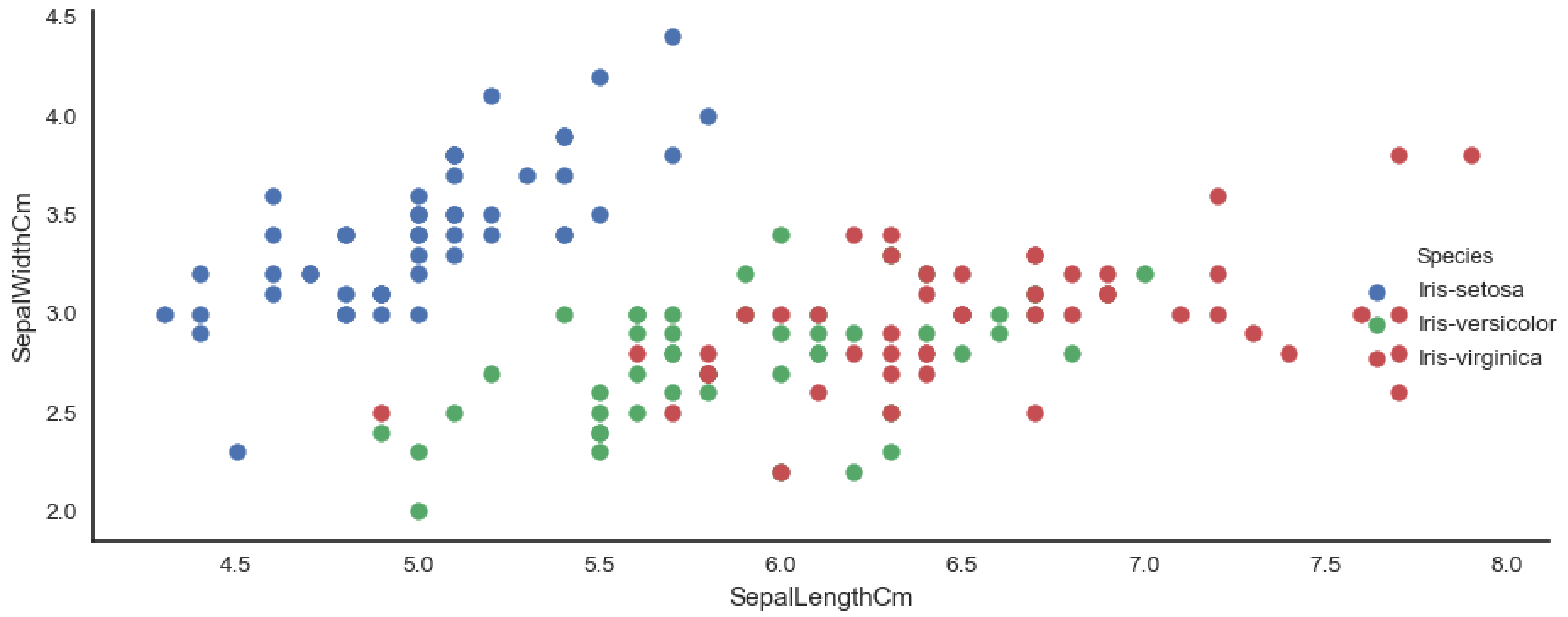
- Reading data:

```
dataset = pd.read_csv('Iris.csv')
x = dataset.iloc[:,[1,2,3,4]]
y = dataset.iloc[:-1]
# see how many samples we have of each species
dataset["Species"].value_counts()
```

```
Iris-versicolor    50
Iris-setosa        50
Iris-virginica     50
```

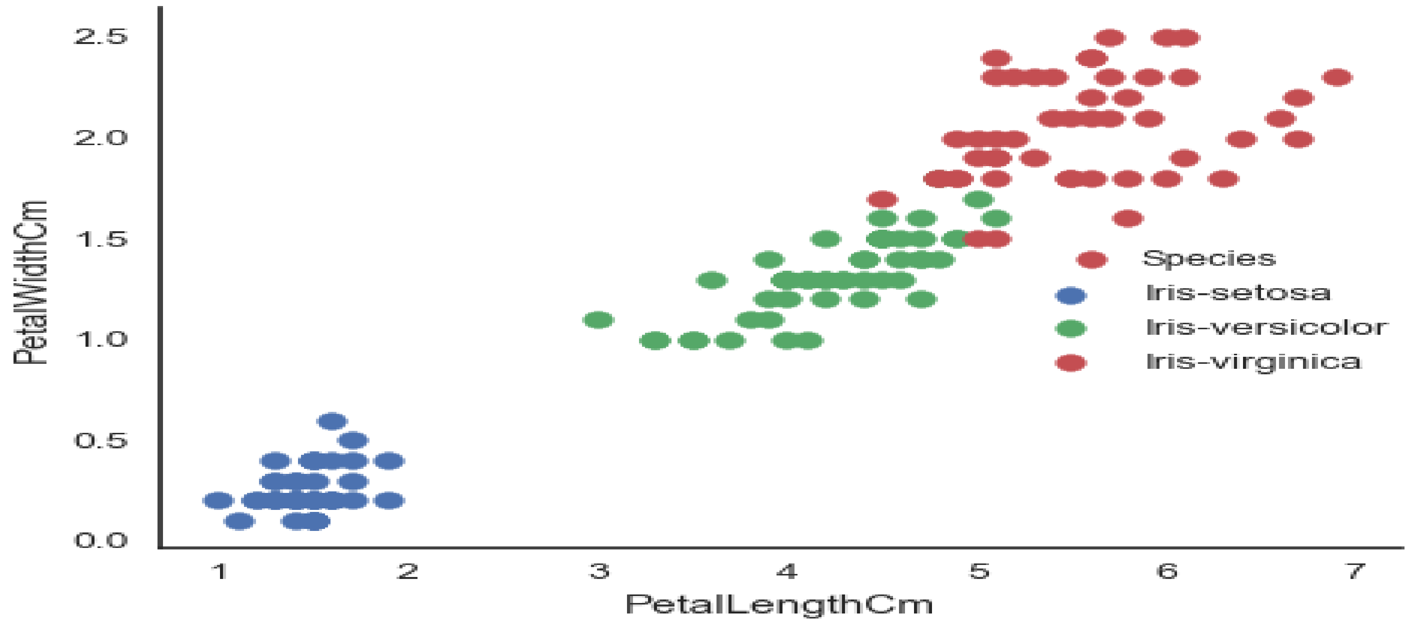
Visualize data

```
sns.FacetGrid(dataset, hue="Species", size=4).map
(plt.scatter,"SepalLengthCm",SepalWidthCm").add_legend()
```



Visualize data

- *# do same for petals*
  sns.FacetGrid(dataset, hue="**Species**", size=4).map(plt.scatter, "**PetalLengthCm**","**PetalWidthCm**").add_legend()



observations

- Note that the species are nearly linearly separable with **petal** size, but **sepal** sizes are more mixed.
- A clustering algorithm might have a hard time realizing that there were three separate species

Standardization

- .

```
from sklearn import preprocessing
scaler = preprocessing.StandardScaler()
scaler.fit(X)
X_scaled_array = scaler.transform(X)
X_scaled = pd.DataFrame(X_scaled_array, columns = X.columns)
```

https://web.stanford.edu/~schmit/cme193/lec/lec5.pdf

UMKC

K-Means Clustering

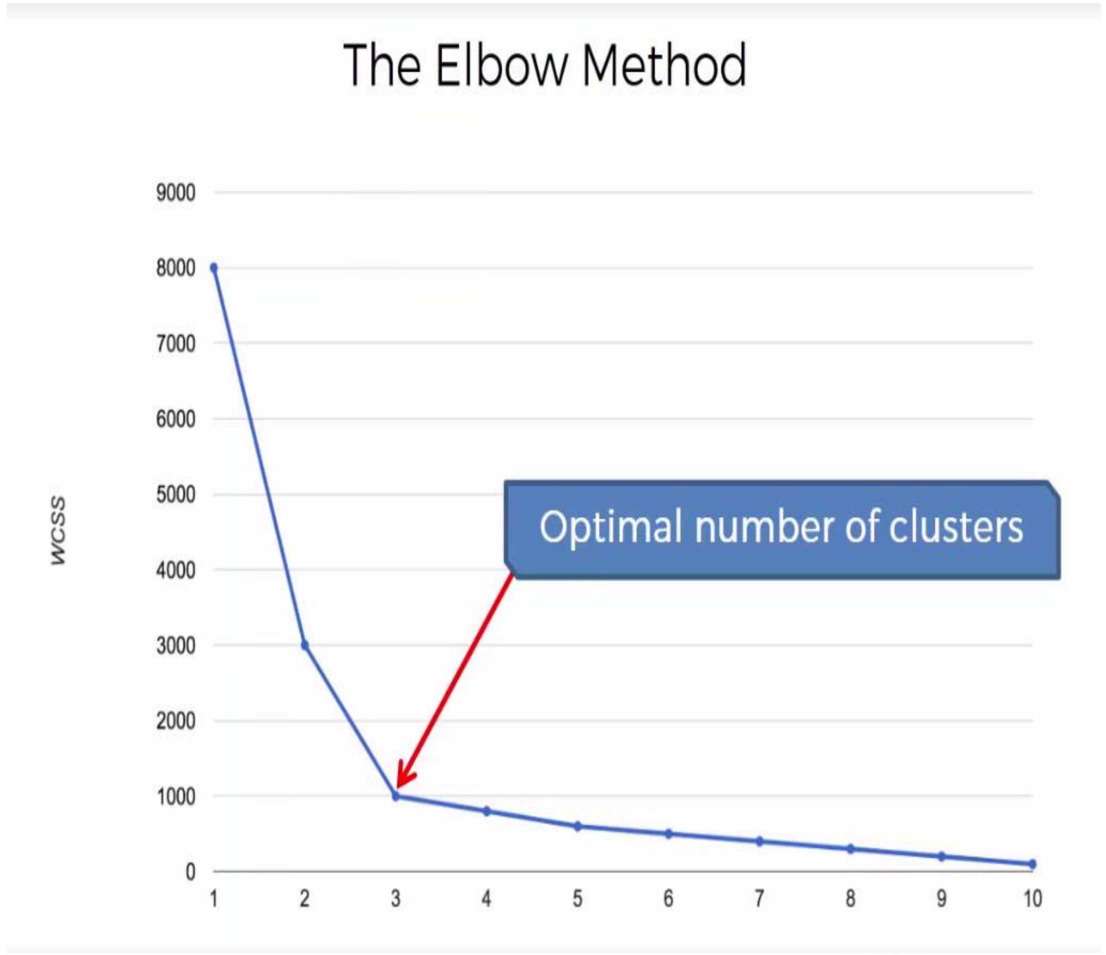
```
from sklearn.cluster import Kmeans
 nclusters = 3 # this is the k in kmeans
seed = 0
km = KMeans(n_clusters=nclusters, random_state=seed)
km.fit(X_scaled) # predict the cluster for each data point
y_cluster_kmeans = km.predict(X_scaled)
```

Silhouette score

```
# predict the cluster for each data point
y_cluster_kmeans = km.predict(x)
from sklearn import metrics
score = metrics.silhouette_score(x, y_cluster_kmeans)
```

Elbow plot: number of clusters

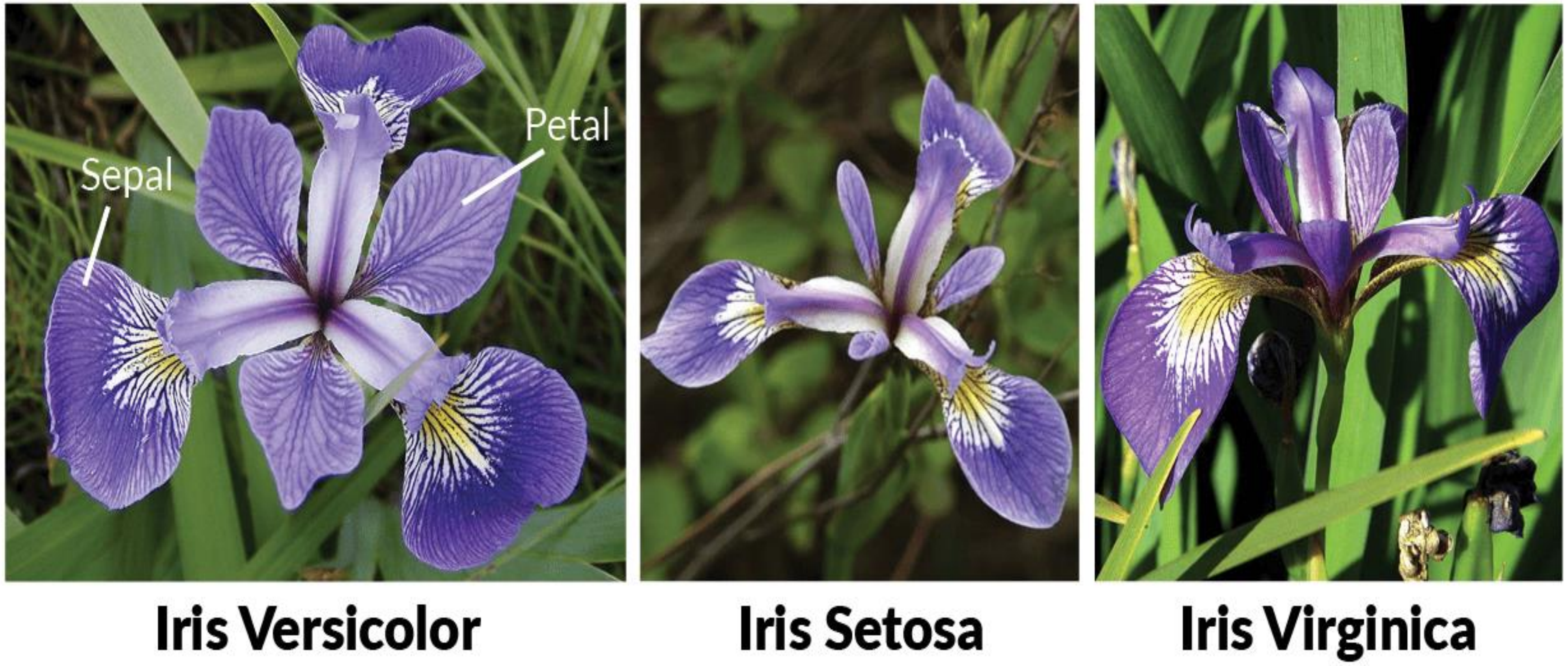
```
wcss = []  ##Within Cluster Sum of Squares
##elbow method to know the number of clusters
for i in range(1,11):
    kmeans = KMeans(n_clusters=i,
                            max_iter=300,random_state=0)
    kmeans.fit(x)
    wcss.append(kmeans.inertia_)

plt.plot(range(1,11),wcss)
plt.title('the elbow method')
plt.xlabel('Number of Clusters')
plt.ylabel('Wcss')
plt.show()
```



https://web.stanford.edu/~schmit/cme193/lec/lec5.pdf

Sum of squared distances of samples to their closest cluster center.

Dimensionality reduction on IRIS data



Read data and Standardize

- PCA is effected by scale
- you need to scale the features in the data before applying PCA
- You can transform the data onto unit scale (mean = 0 and variance = 1)

```
dataset = pd.read_csv('Iris.csv')
x = dataset.iloc[:,[1,2,3,4]]
y = dataset.iloc[:,-1]
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
# Fit on training set only.
scaler.fit(x)
# Apply transform to both the training set and the test set.
x_scaler = scaler.transform(x)
```

Apply PCA

- Notice the code below has 2 for the number of components parameter.
- It means that scikit-learn choose 2 of principal components

```
from sklearn.decomposition import PCA# Make an instance of the Model
pca = PCA(2)
X_pca = pca.fit_transform(x_scaler)
```

References

http://www-bcf.usc.edu/~gareth/ISL/ISLR%20Sixth%20Printing.pdf
https://web.stanford.edu/~schmit/cme193/lec/lec5.pdf
http://machinelearningmastery.com/machine-learning-in-python-step-by-step/
http://scikit-learn.org/stable/auto_examples/linear_model/plot_ols.html
https://www.analyticsvidhya.com/blog/2015/08/comprehensive-guide-regression/
http://scikit-learn.org/stable/modules/clustering.html
http://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_digits.html
http://www.kdnuggets.com/2015/11/seven-steps-machine-learning-python.html/2
http://beancoder.com/linear-regression-stock-prediction/
https://github.com/tarlen5/coursera_ml/blob/master/unit6/ex2_sklearn
https://www.kaggle.com/bburns/iris-exploration-pca-k-means-and-gmm-clustering
https://towardsdatascience.com/pca-using-python-scikit-learn-e653f8989e60

Filling null values with mean

```
data_new.apply(lambda x: x.fillna(x.mean()),axis=0)
```