Cluster analysis in python

Wednesday, 17 June 2020 8:17 PM

Introduction to Cluster

Everyday example: Google news

- How does Google News classify articles?
- Unsupervised Learning Algorithm: Clustering
- Match frequent terms in articles to find similarity

Labeled and unlabeled data

Data with no labels

- Point 1: (1, 2)
- Point 2: (2, 2)
- Point 3: (3, 1)

Data with labels

- Point 1: (1, 2), Label: Danger Zone
- Point 2: (2, 2), Label: Normal Zone
- Point 3: (3, 1), Label: Normal Zone

What is unsupervised learning?

- A group of machine learning algorithms that find patterns in data
- Data for algorithms has not been labeled, classified or characterized
- The objective of the algorithm is to interpret any structure in the data
- Common unsupervised learning algorithms: clustering, neural networks, anomaly detection

What is clustering?

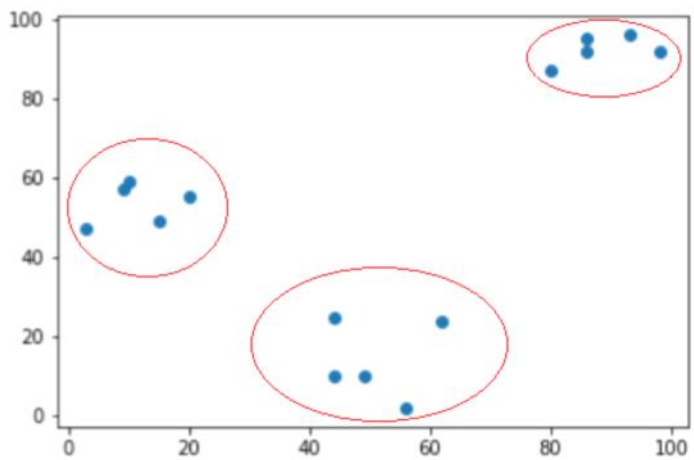
- The process of grouping items with similar characteristics
- Items in groups similar to each other than in other groups
- Example: distance between points on a 2D plane

Plotting data for clustering - Pokemon sightings

```
from matplotlib import pyplot as plt
```

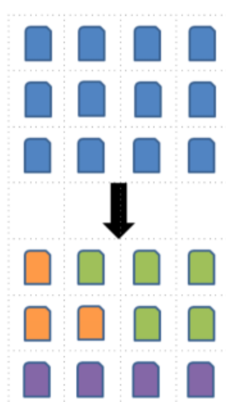
```
x_coordinates = [80, 93, 86, 98, 86, 9, 15, 3, 10, 20, 44, 56, 49, 62, 44]
y_coordinates = [87, 96, 95, 92, 92, 57, 49, 47, 59, 55, 25, 2, 10, 24, 10]
```

```
plt.scatter(x_coordinates, y_coordinates)
plt.show()
```



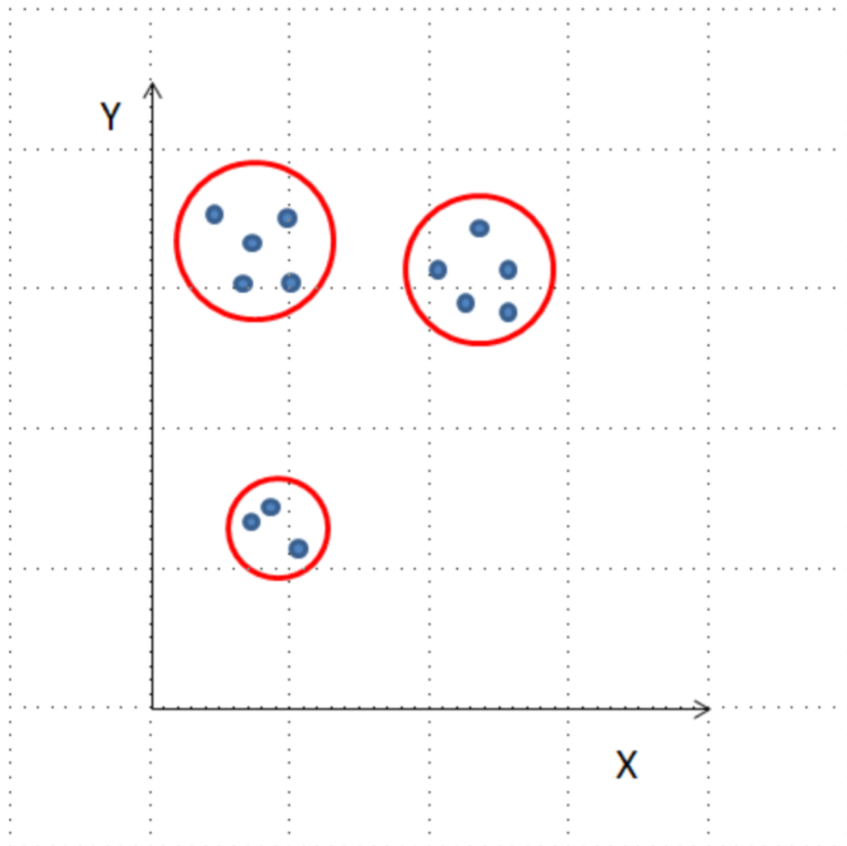
What is a cluster?

- A group of items with similar characteristics
- Google News: articles where similar words and word associations appear together
- Customer Segments



Clustering algorithms

- Hierarchical clustering
- K means clustering
- Other clustering algorithms: DBSCAN, Gaussian Methods



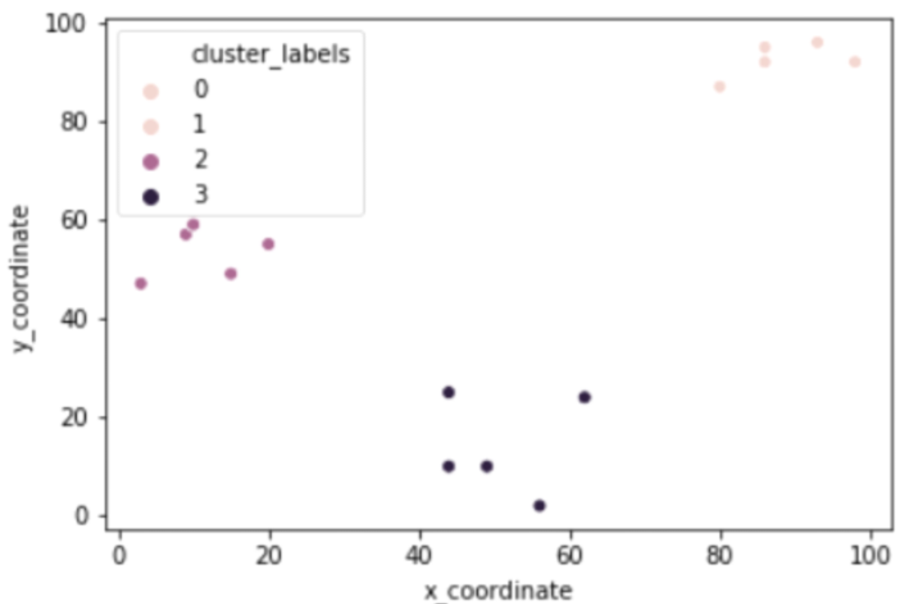
Hierarchical clustering in SciPy

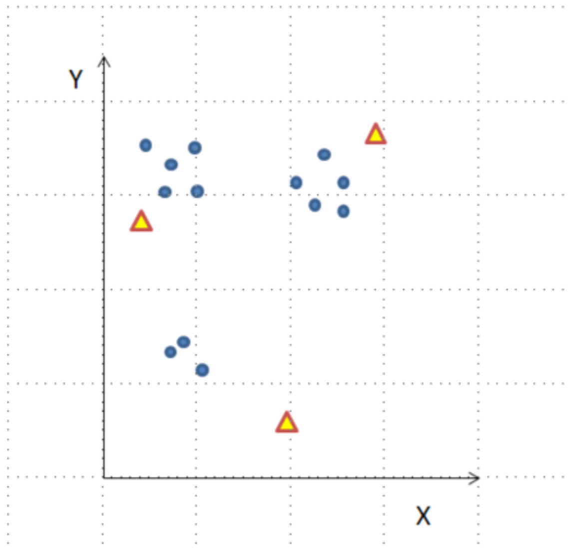
```
from scipy.cluster.hierarchy import linkage, fcluster
from matplotlib import pyplot as plt
import seaborn as sns, pandas as pd
```

```
x_coordinates = [80.1, 93.1, 86.6, 98.5, 86.4, 9.5, 15.2, 3.4,
                 10.4, 20.3, 44.2, 56.8, 49.2, 62.5, 44.0]
y_coordinates = [87.2, 96.1, 95.6, 92.4, 92.4, 57.7, 49.4,
                 47.3, 59.1, 55.5, 25.6, 2.1, 10.9, 24.1, 10.3]

df = pd.DataFrame({'x_coordinate': x_coordinates,
                   'y_coordinate': y_coordinates})
```

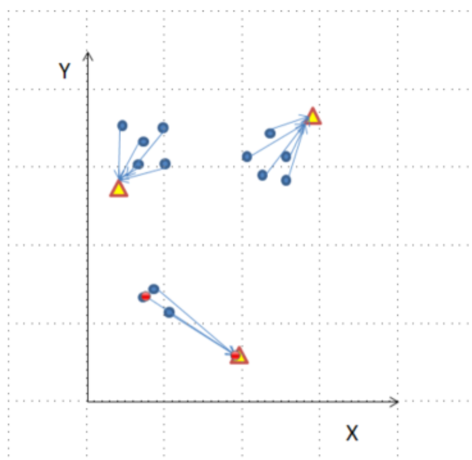
```
Z = linkage(df, 'ward')
df['cluster_labels'] = fcluster(Z, 3, criterion='maxclust')
```

```
sns.scatterplot(x='x_coordinate', y='y_coordinate',
                hue='cluster_labels', data = df)
plt.show()
```

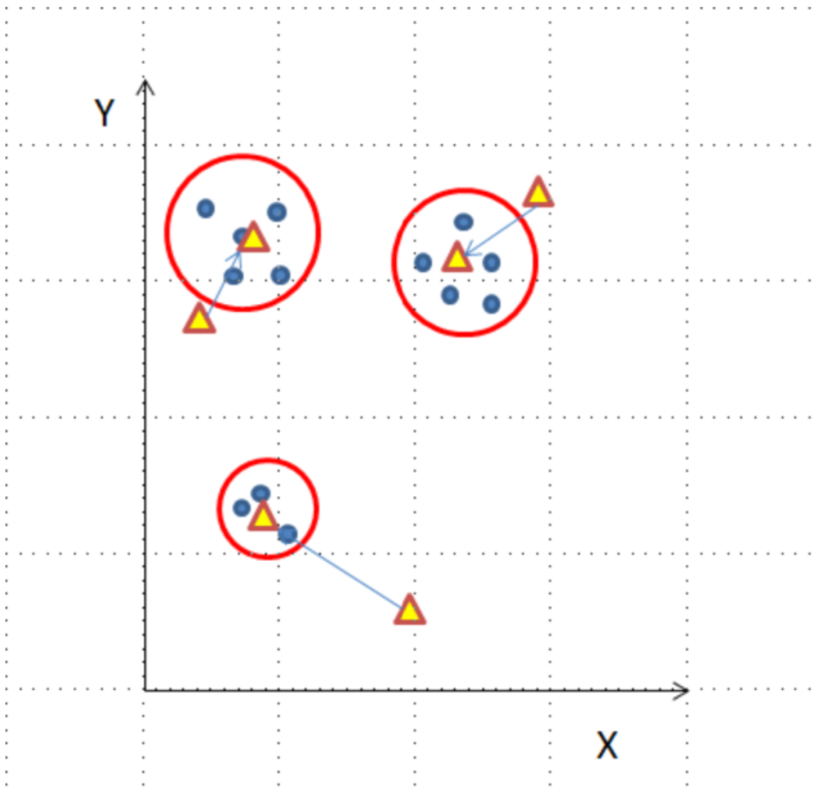




First, a random cluster center is generated for each of the three clusters.



Next, the distance to these cluster centers is computed for each point to assign to the closest cluster.



The cluster centers are recomputed.

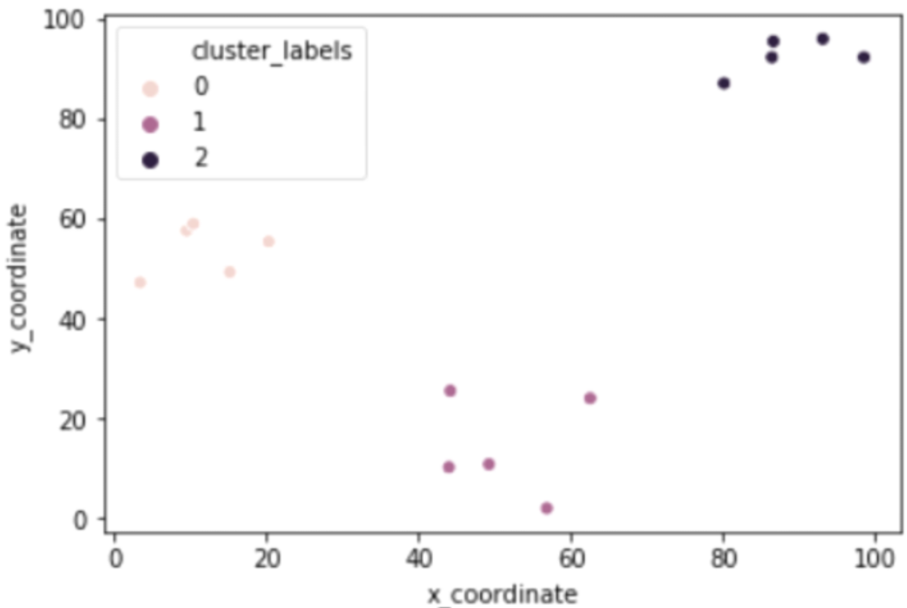
K-means clustering in SciPy

```
from scipy.cluster.vq import kmeans, vq
from matplotlib import pyplot as plt
import seaborn as sns, pandas as pd

import random
random.seed((1000,2000))
```

```
x_coordinates = [80.1, 93.1, 86.6, 98.5, 86.4, 9.5, 15.2, 3.4,
                 10.4, 20.3, 44.2, 56.8, 49.2, 62.5, 44.0]
y_coordinates = [87.2, 96.1, 95.6, 92.4, 92.4, 57.7, 49.4,
                 47.3, 59.1, 55.5, 25.6, 2.1, 10.9, 24.1, 10.3]

df = pd.DataFrame({'x_coordinate': x_coordinates, 'y_coordinate': y_coordinates})
```

```
centroids,_ = kmeans(df, 3)
df['cluster_labels'], _ = vq(df, centroids)
```

```
sns.scatterplot(x='x_coordinate', y='y_coordinate',
                hue='cluster_labels', data = df)
plt.show()
```



Why do we need to prepare data for clustering?

- Variables have incomparable units (product dimensions in cm, price in $)
- Variables with same units have vastly different scales and variances (expenditures on cereals, travel)
- Data in raw form may lead to bias in clustering
- Clusters may be heavily dependent on one variable
- Solution: normalization of individual variables

Normalization of data

Normalization: process of rescaling data to a standard deviation of 1

> x_new = x / std_dev(x)

```
from scipy.cluster.vq import whiten
```

```
data = [5, 1, 3, 3, 2, 3, 3, 8, 1, 2, 2, 3, 5]
```

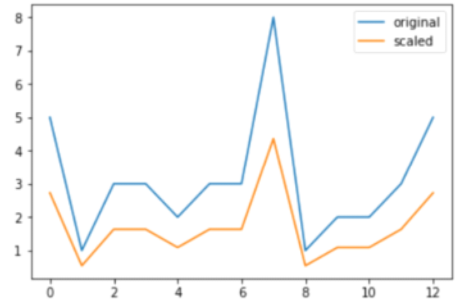
```
scaled_data = whiten(data)
print(scaled_data)
```

```
[2.73, 0.55, 1.64, 1.64, 1.09, 1.64, 1.64, 4.36, 0.55, 1.09, 1.09, 1.64, 2.73]
```

Illustration: normalization of data

```
# Import plotting library
from matplotlib import pyplot as plt

# Initialize original, scaled data
plt.plot(data,
         label="original")
plt.plot(scaled_data,
         label="scaled")
```

```
# Show legend and display plot
plt.legend()
plt.show()
```



Hierarchical Clustering

Creating a distance matrix using linkage

```
scipy.cluster.hierarchy.linkage(observations,
                                method='single',
                                metric='euclidean',
                                optimal_ordering=False
)
```

- `method` : how to calculate the proximity of clusters
- `metric` : distance metric
- `optimal_ordering` : order data points

Which method should use?

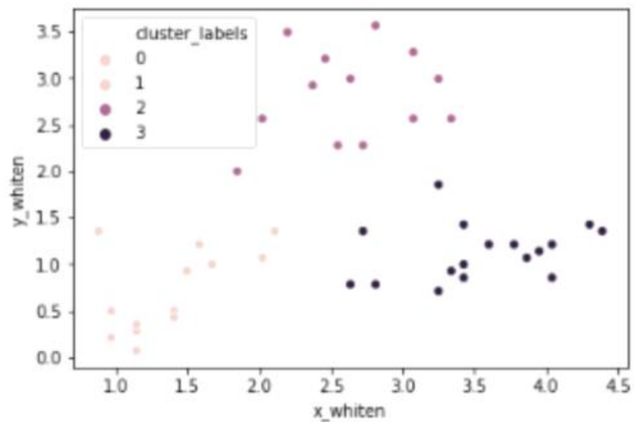
- single: based on two closest objects
- complete: based on two farthest objects
- average: based on the arithmetic mean of all objects
- centroid: based on the geometric mean of all objects
- median: based on the median of all objects
- ward: based on the sum of squares

Create cluster labels with fcluster

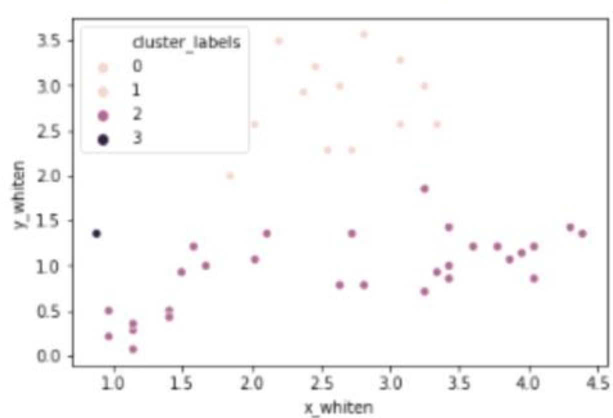
```
scipy.cluster.hierarchy.fcluster(distance_matrix,
                                 num_clusters,
                                 criterion
)
```

- `distance_matrix` : output of `linkage()` method
- `num_clusters` : number of clusters
- `criterion` : how to decide thresholds to form clusters

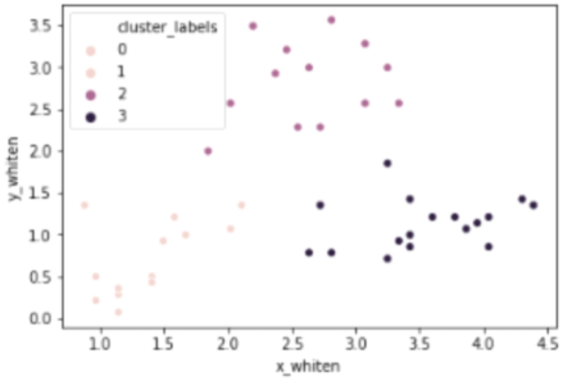
Hierarchical clustering with ward method



Hierarchical clustering with single method



Hierarchical clustering with complete method



Why visualize clusters?

- Try to make sense of the clusters formed
- An additional step in validation of clusters
- Spot trends in data

An introduction to seaborn

- `seaborn` : a Python data visualization library based on `matplotlib`
- Has better, easily modifiable aesthetics than matplotlib!
- Contains functions that make data visualization tasks easy in the context of data analytics
- Use case for clustering: `hue` parameter for plots

Visualize clusters with matplotlib

```
from matplotlib import pyplot as plt
```

```
df = pd.DataFrame({'x': [2, 3, 5, 6, 2],
                   'y': [1, 1, 5, 5, 2],
                   'labels': ['A', 'A', 'B', 'B', 'A']})
colors = {'A':'red', 'B':'blue'}
df.plot.scatter(x='x',
                y='y',
                c=df['labels'].apply(lambda x: colors[x]))
plt.show()
```

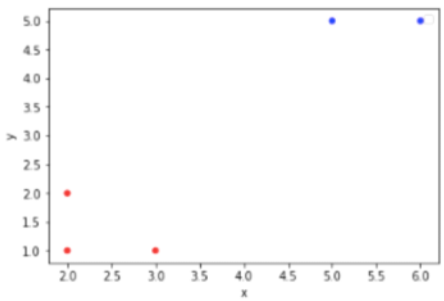
Visualize clusters with seaborn

```
from matplotlib import pyplot as plt
import seaborn as sns
```

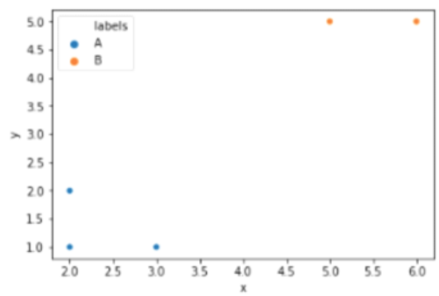
```
df = pd.DataFrame({'x': [2, 3, 5, 6, 2],
                   'y': [1, 1, 5, 5, 2],
                   'labels': ['A', 'A', 'B', 'B', 'A']})
sns.scatterplot(x='x',
                y='y',
                hue='labels',
                data=df)
plt.show()
```

Comparison of both methods of visualization

MATPLOTLIB PLOT

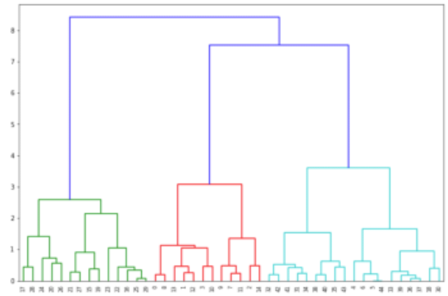


SEABORN PLOT



Introduction to dendrograms

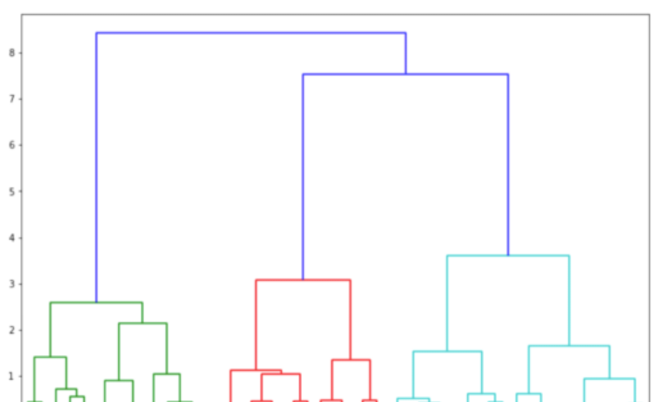
- Strategy till now - decide clusters on visual inspection
- Dendrograms help in showing progressions as clusters are merged
- A dendrogram is a branching diagram that demonstrates how each cluster is composed by branching out into its child nodes



Create a dendrogram in SciPy

```
from scipy.cluster.hierarchy import dendrogram
```

```
Z = linkage(df[['x_whiten', 'y_whiten']],
            method='ward',
            metric='euclidean')
dn = dendrogram(Z)
plt.show()
```



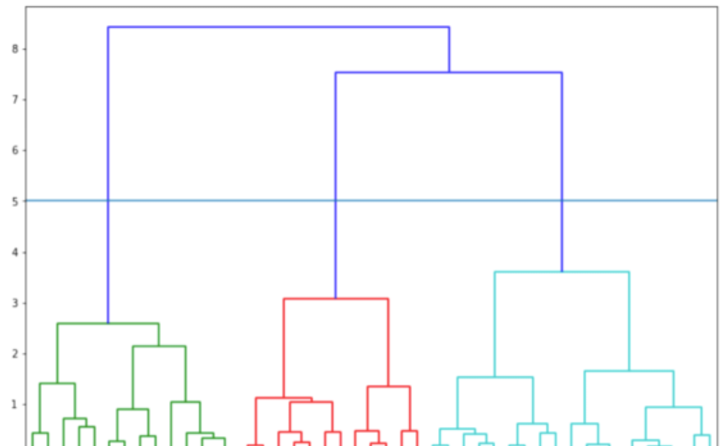
he x axis represents individual points, whereas the y axis represents the distance or dissimilarity between clusters.

In the dendrogram, each inverted U represents a cluster divided into its two child clusters.

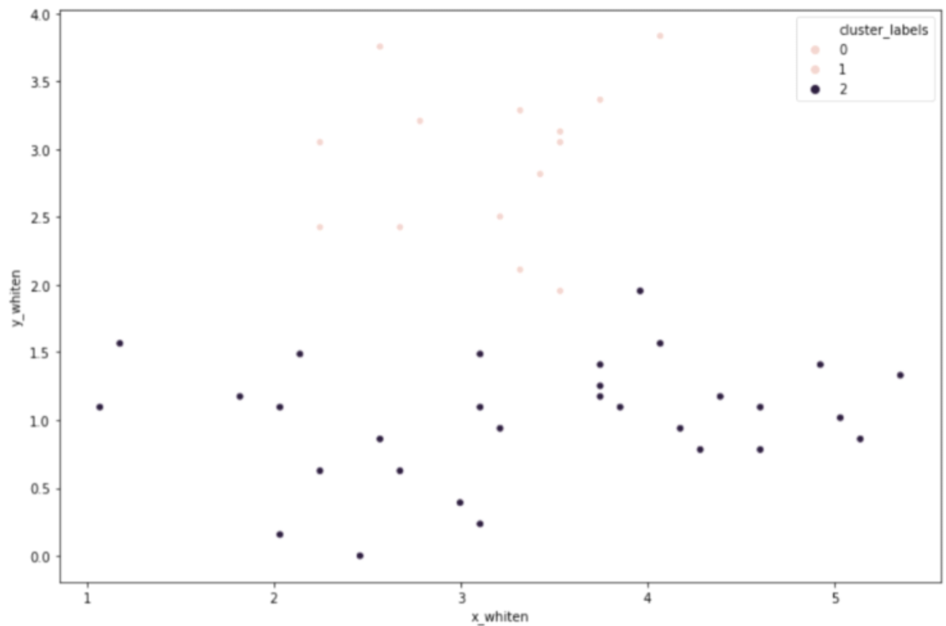
The inverted U at the top of the figure represents a single cluster of all the data points.

The width of the U shape represents the distance between the two child clusters.

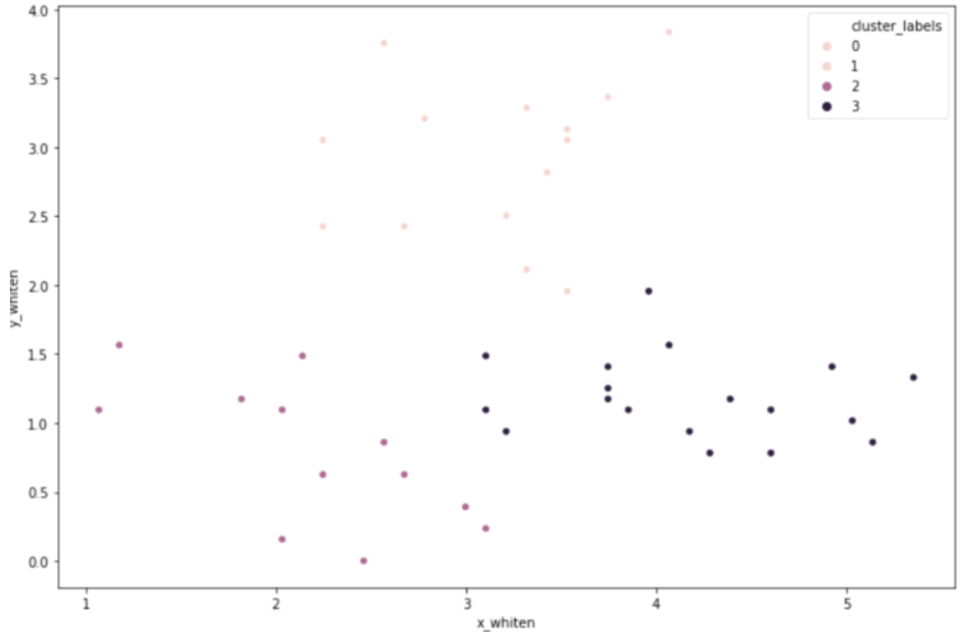
At the horizontal line drawn on the figure, we see that there are three clusters.



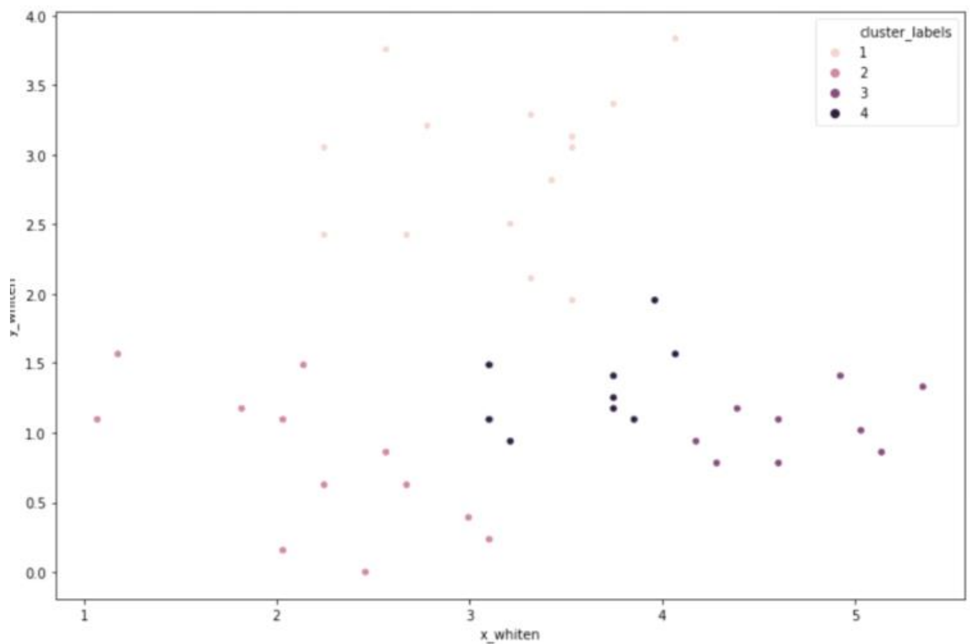
When you move the line below, the number of clusters increases but the inter-cluster distance decreases.



Here is the result of performing the clustering with two clusters.



Here is the result with three clusters.



And here is how 4 clusters look on the data.

Measuring speed in hierarchical clustering

- `timeit` module
- Measure the speed of `.linkage()` method
- Use randomly generated points
- Run various iterations to extrapolate

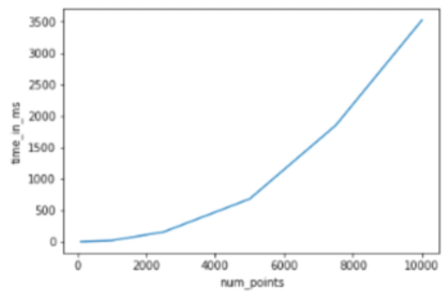
Use of timeit module

```
from scipy.cluster.hierarchy import linkage
import pandas as pd
import random, timeit
points = 100
df = pd.DataFrame({'x': random.sample(range(0, points), points),
                   'y': random.sample(range(0, points), points)})
%timeit linkage(df[['x', 'y']], method = 'ward', metric = 'euclidean')
```

```
1.02 ms ± 133 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

Comparison of runtime of linkage method

- Increasing runtime with data points
- Quadratic increase of runtime
- Not feasible for large datasets



K Means Clustering

Why k-means clustering?

- A critical drawback of hierarchical clustering: runtime
- K means runs significantly faster on large datasets

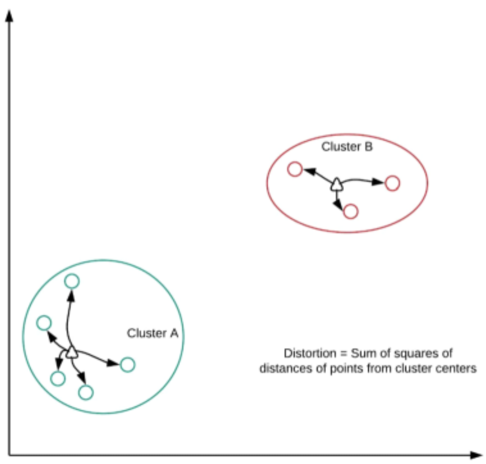
Step 1: Generate cluster centers

```
kmeans(obs, k_or_guess, iter, thresh, check_finite)
```

- `obs` : standardized observations
- `k_or_guess` : number of clusters
- `iter` : number of iterations (default: 20)
- `thres` : threshold (default: 1e-05)
- `check_finite` : whether to check if observations contain only finite numbers (default: True)

Returns two objects: cluster centers, distortion

How is distortion calculated?



Step 2: Generate cluster labels

```
vq(obs, code_book, check_finite=True)
```

- `obs` : standardized observations
- `code_book` : cluster centers
- `check_finite` : whether to check if observations contain only finite numbers (default: True)

Returns two objects: a list of cluster labels, a list of distortions

A note on distortions

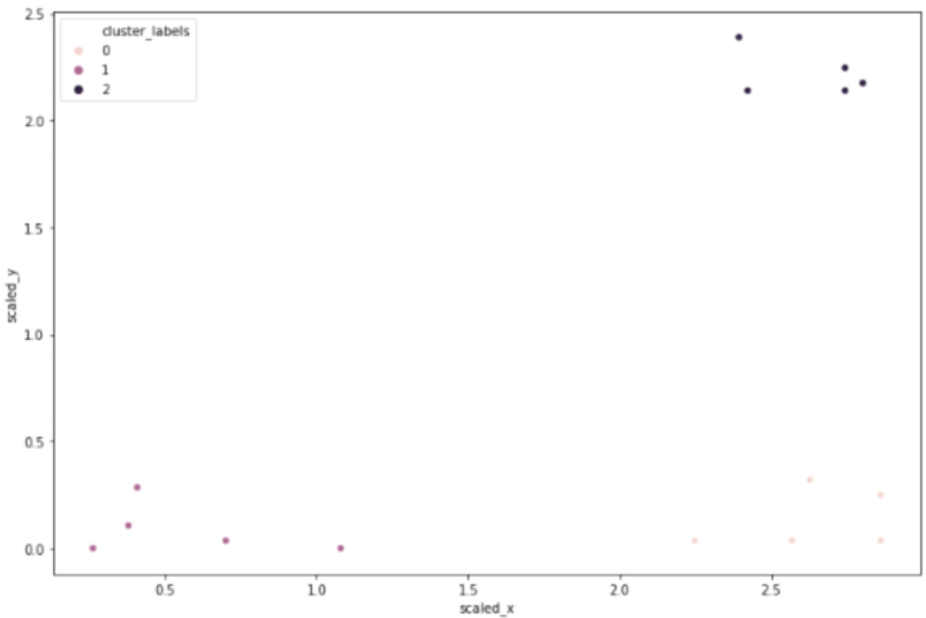
- `kmeans` returns a single value of distortions
- `vq` returns a list of distortions.

Running k-means

```
# Import kmeans and vq functions
from scipy.cluster.vq import kmeans, vq
```

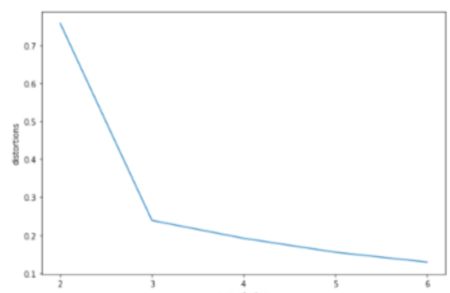
```
# Generate cluster centers and labels
cluster_centers, _ = kmeans(df[['scaled_x', 'scaled_y']], 3)
df['cluster_labels'], _ = vq(df[['scaled_x', 'scaled_y']], cluster_centers)
```

```
# Plot clusters
sns.scatterplot(x='scaled_x', y='scaled_y', hue='cluster_labels', data=df)
plt.show()
```



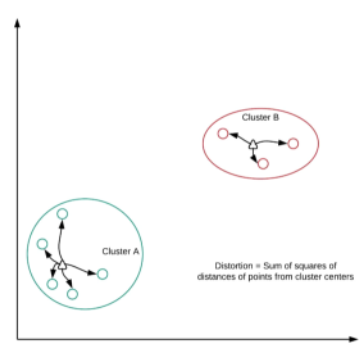
How to find the right k?

- No *absolute* method to find right number of clusters (k) in k-means clustering
- Elbow method



Distortions revisited

- Distortion: sum of squared distances of points from cluster centers
- Decreases with an increasing number of clusters
- Becomes zero when the number of clusters equals the number of points
- Elbow plot: line plot between cluster centers and distortion



Elbow method

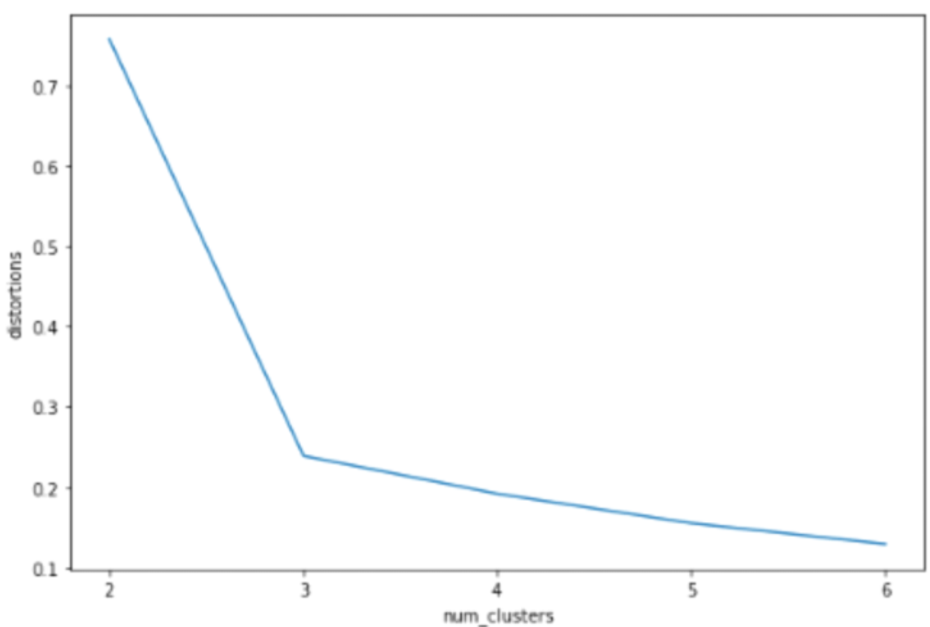
- Elbow plot: plot of the number of clusters and distortion
- Elbow plot helps indicate number of clusters present in data

Elbow method in Python

```
# Declaring variables for use
distortions = []

num_clusters = range(2, 7)
```

```
# Populating distortions for various clusters
for i in num_clusters:
    centroids, distortion = kmeans(df[['scaled_x', 'scaled_y']], i)
    distortions.append(distortion)
```

```
# Plotting elbow plot data
elbow_plot_data = pd.DataFrame({'num_clusters': num_clusters,
                                'distortions': distortions})

sns.lineplot(x='num_clusters', y='distortions',
             data = elbow_plot_data)
plt.show()
```



The ideal number of clusters here is therefore, 3.

Final thoughts on using the elbow method

- Only gives an indication of optimal _k_ (numbers of clusters)
- Does not always pinpoint how many _k_ (numbers of clusters)
- Other methods: average silhouette and gap statistic

Limitations of k-means clustering

- How to find the right _K_ (number of clusters)?
- Impact of seeds
- Biased towards equal sized clusters

Impact of seeds

Initialize a random seed

```
from numpy import random
random.seed(12)
```

Seed: `np.array(1000, 2000)`

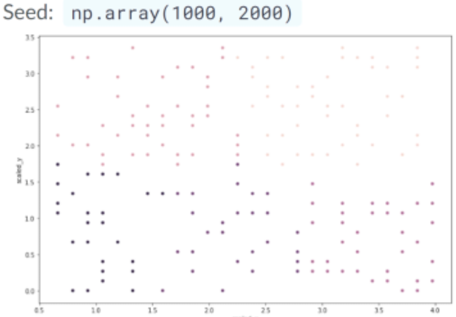
Cluster sizes: 29, 29, 43, 47, 52

Seed: `np.array(1,2,3)`

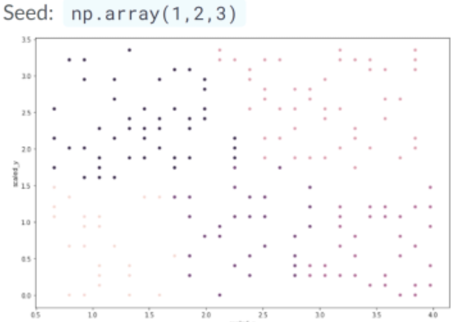
Cluster sizes: 26, 31, 40, 50, 53

Impact of seeds: plots

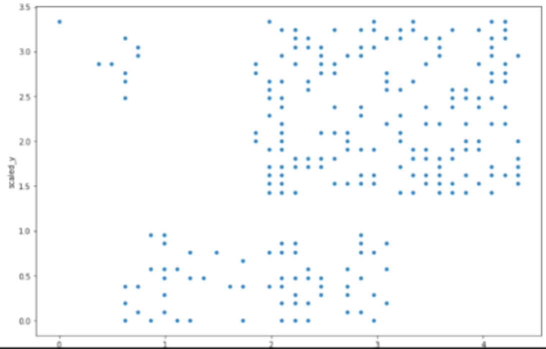
Seed: `np.array(1000, 2000)`



Seed: `np.array(1,2,3)`



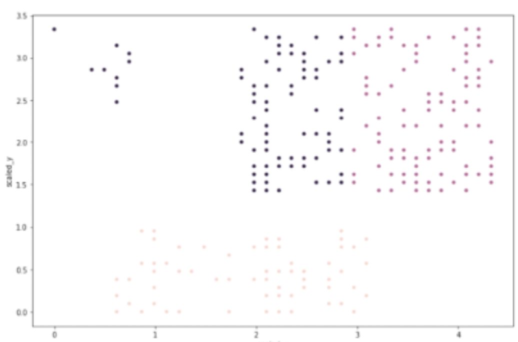
Uniform clusters in k means



us perform clustering on this set of 280 points, divided into non uniform groups of 200, 70 and 10.

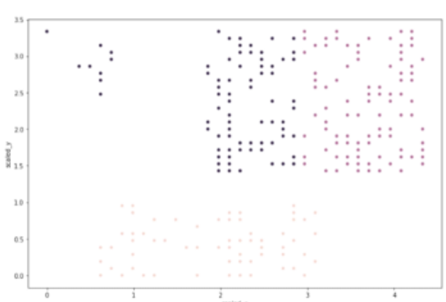
Uniform clusters in k-means: a comparison

K-means clustering with 3 clusters

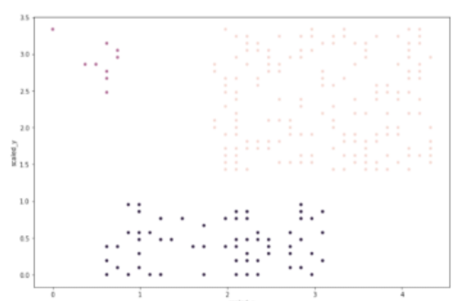


Uniform clusters in k-means: a comparison

K-means clustering with 3 clusters



Hierarchical clustering with 3 clusters



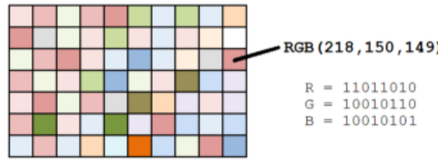
Final thoughts

- Each technique has its pros and cons
- Consider your data size and patterns before deciding on algorithm
- Clustering is exploratory phase of analysis

Clustering in Real World

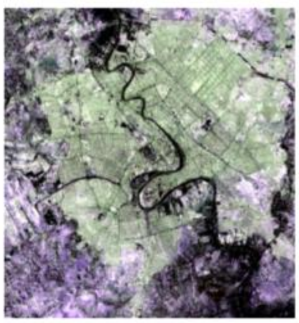
Dominant colors in images

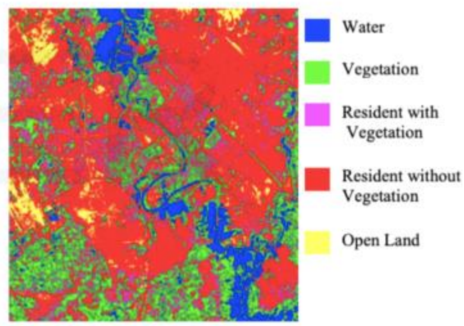
- All images consist of pixels
- Each pixel has three values: *Red*, *Green* and *Blue*
- Pixel color: combination of these RGB values
- Perform k-means on standardized RGB values to find cluster centers
- Uses: Identifying features in satellite images



Source

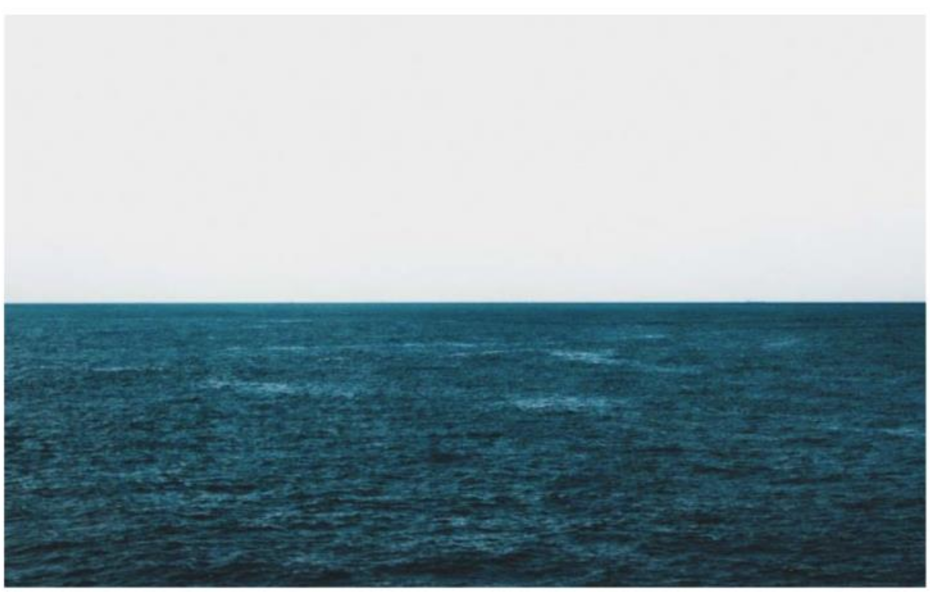
Feature identification in satellite images





Tools to find dominant colors

- Convert image to pixels: `matplotlib.image.imread`
- Display colors of cluster centers: `matplotlib.pyplot.imshow`



Convert image to RGB matrix

```
import matplotlib.image as img
image = img.imread('sea.jpg')
image.shape
```

```
(475, 764, 3)
```

```
r = []
g = []
b = []

for row in image:
    for pixel in row:
        # A pixel contains RGB values
        temp_r, temp_g, temp_b = pixel
        r.append(temp_r)
        g.append(temp_g)
        b.append(temp_b)
```

Data frame with RGB values

```
pixels = pd.DataFrame({'red': r,
                       'blue': b,
                       'green': g})
pixels.head()
```

red	blue	green
252	255	252
75	103	81
...	...	...

Find dominant colors

```
cluster_centers, _ = kmeans(pixels[['scaled_red', 'scaled_blue',
                                    'scaled_green']], 2)
```

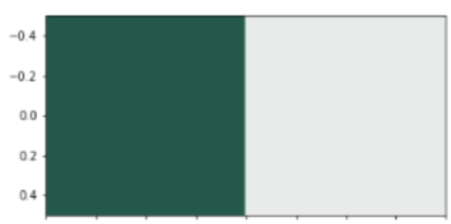
```
colors = []

# Find Standard Deviations
r_std, g_std, b_std = pixels[['red', 'blue', 'green']].std()

# Scale actual RGB values in range of 0-1
for cluster_center in cluster_centers:
    scaled_r, scaled_g, scaled_b = cluster_center
    colors.append((
        scaled_r * r_std/255,
        scaled_g * g_std/255,
        scaled_b * b_std/255
    ))
```

Display dominant colors

```
#Dimensions: 2 x 3 (N X 3 matrix)
print(colors)
```

```
[(0.08192923122023911, 0.34205845943857993, 0.2824002984155429),
 (0.893281510956742, 0.899818770315129, 0.8979114272960784)]
```

```
#Dimensions: 1 x 2 x 3 (1 X N x 3 matrix)
plt.imshow([colors])
plt.show()
```



Document clustering: concepts

1. Clean data before processing
2. Determine the importance of the terms in a document (in TF-IDF matrix)
3. Cluster the TF-IDF matrix
4. Find top terms, documents in each cluster

Clean and tokenize data

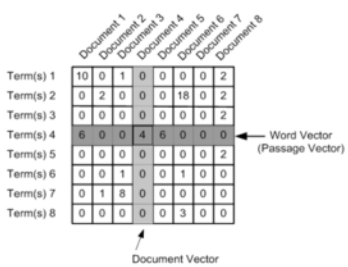
- Convert text into smaller parts called tokens, clean data for processing

```
from nltk.tokenize import word_tokenize
import re

def remove_noise(text, stop_words = []):
    tokens = word_tokenize(text)
    cleaned_tokens = []
    for token in tokens:
        token = re.sub('[^A-Za-z0-9]+', '', token)
        if len(token) > 1 and token.lower() not in stop_words:
            # Get lowercase
            cleaned_tokens.append(token.lower())
    return cleaned_tokens
remove_noise("It is lovely weather we are having.
              I hope the weather continues.")
```

```
['lovely', 'weather', 'hope', 'weather', 'continues']
```

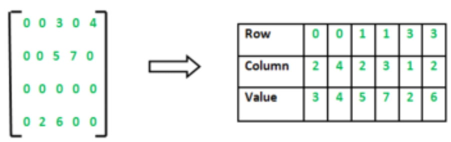
Document term matrix and sparse matrices

- Document term matrix formed
- Most elements in matrix are zeros



Source

- Sparse matrix is created



Source

TF-IDF (Term Frequency - Inverse Document Frequency)

- A weighted measure: evaluate how important a word is to a document in a collection

```
from sklearn.feature_extraction.text import TfidfVectorizer
tfidf_vectorizer = TfidfVectorizer(max_df=0.8, max_features=50,
                                   min_df=0.2, tokenizer=remove_noise)
tfidf_matrix = tfidf_vectorizer.fit_transform(data)
```

Clustering with sparse matrix

- `kmeans()` in SciPy does not support sparse matrices
- Use `.todense()` to convert to a matrix

```
cluster_centers, distortion = kmeans(tfidf_matrix.todense(), num_clusters)
```

Top terms per cluster

- Cluster centers: lists with a size equal to the number of terms
- Each value in the cluster center is its importance
- Create a dictionary and print top terms

```
terms = tfidf_vectorizer.get_feature_names()

for i in range(num_clusters):
    center_terms = dict(zip(terms, list(cluster_centers[i])))
    sorted_terms = sorted(center_terms, key=center_terms.get, reverse=True)
    print(sorted_terms[:3])
```

```
['room', 'hotel', 'staff']

['bad', 'location', 'breakfast']
```

More considerations

- Work with hyperlinks, emoticons etc.
- Normalize words (run, ran, running -> run)
- `.todense()` may not work with large datasets

Basic checks

```
# Cluster centers
print(fifa.groupby('cluster_labels')[['scaled_heading_accuracy',
    'scaled_volleys', 'scaled_finishing']].mean())
```

cluster_labels	scaled_heading_accuracy	scaled_volleys	scaled_finishing
0	3.21	2.83	2.76
1	0.71	0.64	0.58

```
# Cluster sizes
print(fifa.groupby('cluster_labels')['ID'].count())
```

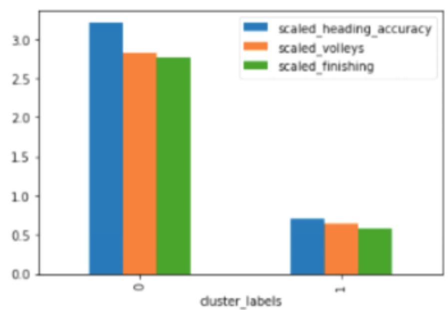
cluster_labels	count
0	886
1	114

This step assumes that you have created the elbow plot, performed the clustering process and generated cluster labels.

Visualizations

- Visualize cluster centers
- Visualize other variables for each cluster

```
# Plot cluster centers
fifa.groupby('cluster_labels') \
  [scaled_features].mean()
  .plot(kind='bar')
plt.show()
```



Top items in clusters

```
# Get the name column of top 5 players in each cluster
for cluster in fifa['cluster_labels'].unique():
    print(cluster, fifa[fifa['cluster_labels'] == cluster]['name'].values[:5])
```

Cluster Label	Top Players
0	['Cristiano Ronaldo' 'L. Messi' 'Neymar' 'L. Suárez' 'R. Lewandowski']
1	['M. Neuer' 'De Gea' 'G. Buffon' 'T. Courtois' 'H. Lloris']

Feature reduction

- Factor analysis
- Multidimensional scaling