Understanding K-Means Clustering: A Guide to Unsupervised Machine Learning

Machine learning algorithms can be broadly classified into two categories: supervised and unsupervised learning. The key difference lies in the presence of a target variable.

In unsupervised learning, there is no target variable; the dataset consists only of input variables that describe the data. This is where K-Means clustering, a popular unsupervised learning algorithm, comes into play.

What is K-Means Clustering?

K-Means clustering is used when we have unlabelled data, meaning data without defined categories or groups. The algorithm simplifies data classification into a certain number of clusters (denoted by 'K') that are fixed apriori. It achieves this by iteratively assigning each data point to one of the K groups based on their features' similarity. The primary goal is to group data points based on their feature similarity, aiming to minimize the within-cluster variance.

Understanding Clusters and Centroids

In the context of K-Means clustering, a **centroid** represents the center of a cluster. Each cluster is defined by its centroid, and the algorithm iteratively calculates the centroids during its execution.

However, determining the right number of clusters (K) can be challenging, especially in high-dimensional datasets. Here are steps to address this challenge:

- 1. Trial and Error (Trying Different K Values): Experiment with different values of K (the number of centroids) to find the most suitable one.
- 2. Initialization of Centroids: Start by initializing K centroids randomly in the feature space.
- 3. Centroid Update: Compute the average of all data points assigned to each centroid, updating the centroid's position accordingly.

The K-Means Clustering Algorithm: How it Works

1. Data Assignment Step:

 Each centroid defines a cluster. In this step, each data point is assigned to the nearest centroid based on the squared Euclidean distance.

2. Centroid Update Step:

Update the centroids by calculating the mean of all data points assigned to that centroid's cluster.

The algorithm iterates between these two steps until a stopping criterion is met. Common stopping criteria include no change in cluster assignments, minimizing the sum of distances, or reaching a maximum number of iterations.

Finding the Optimal Number of Clusters (K)

To see whether our clustering algorithm performs well, we need more than a scatter plot. The common metrics we used are:

Inertia is the within-cluster sum of square distance, which is used in k-means algorithm's objective function.

Silhouette Coefficient is a measure of how dense and separated are the clusters. The silhouette coefficient is a property assigned to each data point. The Silhouette value ranges from -1 to 1, where higher values (closer to 1) indicate better-defined clusters.

The elbow method is used to determine the optimal number of clusters in K-means clustering. The elbow method plots the value of the cost function produced by different values of K.

Practical implementation of K-Mean Clustering

Import Libraries

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
```

Load the Dataset: This dataset has been obtained from UCI ML Repository. https://archive.ics.uci.edu/ml/datasets/Facebook+Live+Sellers+in+Thailand

context: Live selling is becoming increasingly popular in Asian countries. Small vendors can now reach a wider audience and connect with many customers.

```
df = pd.read csv('/content/Live.csv')
df.shape
     (7050, 16)
df.info()
     <class 'pandas.core.frame.DataFrame'>
     RangeIndex: 7050 entries, 0 to 7049
    Data columns (total 16 columns):
        Column
                           Non-Null Count Dtype
                           -----
         status id
                           7050 non-null object
         status_type
                           7050 non-null
                                          object
         status_published 7050 non-null
                                          object
         num reactions
                           7050 non-null
                                          int64
         num comments
                           7050 non-null
                                          int64
         num shares
                           7050 non-null
                                          int64
         num likes
                           7050 non-null
                                          int64
         num loves
                           7050 non-null
                                          int64
         num wows
                           7050 non-null
                                          int64
         num hahas
                           7050 non-null
                                          int64
      10 num sads
                           7050 non-null
                                          int64
     11 num_angrys
                           7050 non-null
                                          int64
      12 Column1
                           0 non-null
                                          float64
                                          float64
      13 Column2
                           0 non-null
      14 Column3
                           0 non-null
                                          float64
      15 Column4
                           0 non-null
                                          float64
```

```
dtypes: float64(4), int64(9), object(3)
memory usage: 881.4+ KB
```

Explore

we want to make clusters using more than two features, but which of the features should we choose? Often times, this decision will be made for you. For example, a stakeholder could give you a list of the features that are most important to them. If you don't have that limitation, though, another way to choose the best features for clustering is to determine which numerical features have the largest variance. That's what we'll do here.

```
Drop Reduandant Columns

df.drop(['Column1', 'Column2', 'Column3', 'Column4'], axis=1, inplace=True)

Drop status_type, status_id and status_published variable from the dataset

df.drop(['status_type','status_id', 'status_published'], axis=1, inplace=True)

df.head()
```

What is Variance?

Variance (which is sometimes called volatility in finance), is a measurement of how spread out the points in a dataset are around the mean. It's calculated by first summing up the squared different between each data point and mean, then dividing by the number of data points minus 1.

 \blacksquare

Calculate the variance for all the features in df, and create a Series top_5_var with the 5 features with the largest variance.

```
242
                                                        201
                                                                                         \cap
df.var().sort values()
     num_angrys
                           0.528256
                           2.550907
     num sads
     num hahas
                          15.659301
     num_wows
                          76.032303
     num loves
                        1597.835141
     num shares
                       17318.550917
     num likes
                      202025.399758
     num reactions
                      214022.176652
                      791453.670644
     num comments
     dtype: float64
```

▼ Split

```
X = df
print("X type:", type(X))
print("X shape:", X.shape)
X.head()
```

```
X type: <class 'pandas.core.frame.DataFrame'>
X shape: (7050, 9)
                                                                                                            Ħ
   num reactions num comments num shares num likes num loves num wows num hahas num sads num angrys
0
             529
                           512
                                       262
                                                 432
                                                             92
                                                                        3
                                                                                  1
                                                                                            1
                                                                                                            d.
 1
             150
                             0
                                        0
                                                 150
                                                              0
                                                                        0
                                                                                  0
                                                                                            0
                                                                                                        0
 2
             227
                           236
                                                 204
                                                             21
                                                                                  1
                                        57
                                                                        1
                                                                                            0
                                                                                                        0
```

Standard Scaling:

Standardization

Standardization is a widely used scaling technique to transform features before fitting into models. Feature scaling changes all a dataset's continuous features to give us a more consistent range of values. Specifically, we subtract the mean from each data point and then divide by the standard deviation:

$$X = X - \mu \sigma$$

The goal of standardization is to improve model performance having all continuous features be on the same scale

```
from sklearn.preprocessing import StandardScaler
# Instantiate transformer
ss = StandardScaler()

# Transform `X`
X_scaled_data = ss.fit_transform(X)

# Put `X_scaled_data` into DataFrame
X_scaled = pd.DataFrame(X_scaled_data, columns=X.columns)
```

print("X_scaled type:", type(X_scaled))
print("X_scaled shape:", X_scaled.shape)
X_scaled.head()

X_scaled type: <class 'pandas.core.frame.DataFrame'>
X_scaled shape: (7050, 9)

	num_reactions	num_comments	num_shares	num_likes	num_loves	num_wows	num_hahas	num_sads	num_angrys
0	0.646104	0.323350	1.686879	0.482727	1.983266	0.196196	0.076713	0.473570	-0.155748
1	-0.173192	-0.252206	-0.304144	-0.144720	-0.318454	-0.147879	-0.176010	-0.152587	-0.155748
2	-0.006738	0.013089	0.129017	-0.024571	0.206938	-0.033187	0.076713	-0.152587	-0.155748
3	-0.257499	-0.252206	-0.304144	-0.231495	-0.318454	-0.147879	-0.176010	-0.152587	-0.155748
4	-0.037003	-0.252206	-0.304144	-0.024571	-0.093286	-0.147879	-0.176010	-0.152587	-0.155748

X_scaled_summary = X_scaled.aggregate(['mean', 'std']).astype(int)

```
print("X_scaled_summary type:", type(X_scaled_summary))
print("X_scaled_summary shape:", X_scaled_summary.shape)
X_scaled_summary
```

X_scaled_summary type: <class 'pandas.core.frame.DataFrame'>
X scaled summary shape: (2, 9)

	num_reactions	num_comments	num_shares	num_likes	num_loves	num_wows	num_hahas	num_sads	num_angrys	\blacksquare
mean	0	0	0	0	0	0	0	0	0	ıl.
std	1	1	1	1	1	1	1	1	1	

Build Model

First, Build a KMeans model, and fit it to the training data X, find centroid, intertia and silhouette score

Inertia Inertia is the within-cluster sum of square distance, which is used in k-means algorithm's objective function.

Basically, the inertia is the sum of the distance of each point to the centroid or center of its assigned cluster. A lower inertia means the points assigned to the clusters are closer to the centroid.

```
# find inertia
inertia = model.inertia_
print("Inertia (3 clusters):", inertia)

Inertia (3 clusters): 2735257865.1114435
```

Silhouette Score

Silhouette Coefficient is a measure of how dense and separated are the clusters. The silhouette coefficient is a property assigned to each data point

The silhouette coefficient ranges from -1 to 1. If a point is really close to the centroid of its assigned cluster, then $a \ll b$ and the silhouette coefficient will be approximately equal to 1. If the reverse is true, $a \gg b$, then the coefficient will be -1. If the point could have been assigned to either cluster, its coefficient will be 0.

Higher silhouette coefficient means higher density and highly separated clusters. This is because we want to have lower a (close to assigned cluster's centroid) and higher b (far away from unassigned cluster's centroid). A lower a value combined with higher b value will produce a higher silhouette score.

Interpret:

In the case of KMeans clustering with 3 clusters:

- 1. **Inertia (Within-Cluster Sum of Squares)**: Inertia represents the sum of squared distances of data points to their closest cluster center. For the given clustering with 3 clusters, the inertia is approximately 2,735,257,865.11. A lower inertia indicates that the data points are closer to the centroids of their respective clusters, suggesting a better fit of the clusters to the data.
- 2. **Silhouette Score**: The Silhouette Score is a metric that measures the separation distance between the resulting clusters. A higher silhouette score (ranging from -1 to 1) indicates that the clusters are well apart from each other and clearly distinguished. In this case, the Silhouette Score is approximately 0.812, which is a high score. It implies that the clusters are well-defined and distinct from each other, demonstrating a good clustering arrangement.

Overall, a lower inertia and a higher Silhouette Score in this context suggest that the KMeans algorithm successfully grouped the data into three clusters that are internally compact and well-separated from each other.

Goal KMean Clustering:

Here we Have High inertia,

A very high inertia value in the context of KMeans clustering may indicate that the clusters are widely spread or that the number of clusters (in this case, 3) might not be the optimal choice for the given data.

In KMeans clustering, the goal is to minimize the inertia. If you have a very high inertia, it could imply that the clusters are not compact, and there may be a suboptimal number of clusters for the given data.

To potentially improve the clustering and reduce the inertia, you could experiment with different values of the number of clusters (n_clusters) in the KMeans algorithm. You might try using methods like the Elbow Method or Silhouette Score to determine the optimal number of clusters for your specific dataset.

Here's an example of how you might use the Elbow Method to determine the optimal number of clusters:

```
inertia = []
for i in range(1, 11):
    kmeans = KMeans(n_clusters=i, random_state=0)
    kmeans.fit(X)
    inertia.append(kmeans.inertia_)

# Plot the Elbow Method
plt.plot(range(1, 11), inertia, 'bo-')
plt.xlabel('Number of Clusters')
plt.ylabel('Inertia')
plt.title('Elbow Method')
plt.show()
```

/usr/local/lib/python3.10/dist-packages/sklearn/cluster/ kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/ kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/ kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/ kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/ kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning

```
9
       8
       7 -
       6 -
     Inertia
       3 -
       2 -
# Initialize a range of potential cluster numbers (K)
k_range = range(2, 11)
silhouette scores = []
for k in k range:
    kmeans = KMeans(n_clusters=k, random_state=0)
    kmeans.fit(X)
    labels = kmeans.labels
    silhouette avg = silhouette score(X, labels)
    silhouette scores.append(silhouette avg)
# Plot the Silhouette Scores
plt.plot(k range, silhouette scores, 'bo-')
plt.xlabel('Number of Clusters (K)')
plt.ylabel('Silhouette Score')
plt.title('Silhouette Score for Each K')
```

plt.show()

```
/usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

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The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning /usr/local/lib/python3.10/dist-packages/sklearn/cluster/_kmeans.py:870: FutureWarning:

The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning
```

▼ Model Pipeline

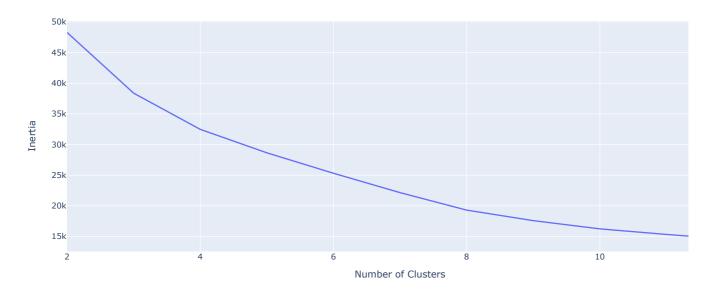
we could Use a **for loop** to build and train a K-Means model where n_clusters ranges from 2 to 12 (inclusive). Your model should include a StandardScaler. Each time a model is trained, calculate the inertia and add it to the list inertia_errors, then calculate the silhouette score and add it to the list silhouette scores.

```
/usr/local/lib/pvthon3.10/dist-packages/sklearn/cluster/ kmeans.pv:870: FutureWarning:
from sklearn.pipeline import make_pipeline

n_clusters = range(2,13)
inertia_errors = []
silhouette scores = []
```

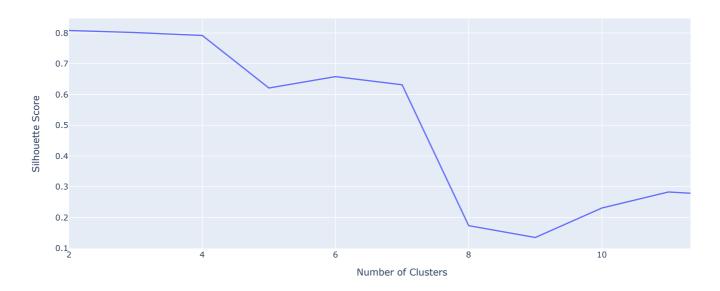
```
# Add `for` loop to train model and calculate inertia, silhouette score.
for k in n clusters:
    # model build
    model = make pipeline(StandardScaler(), KMeans(n clusters=k, random state=42))
    # train model
    model.fit(X)
    # calculate intertia
    inertia errors.append(model.named steps['kmeans'].inertia )
    #calculate silhouette score
    silhouette scores.append(silhouette score(X, model.named steps['kmeans'].labels ))
print("inertia errors type:", type(inertia errors))
print("inertia_errors len:", len(inertia errors))
print("Inertia:", inertia errors)
print()
print("silhouette scores type:", type(silhouette scores))
print("silhouette scores len:", len(silhouette scores))
print("Silhouette Scores:", silhouette scores)
import plotly.express as px
# Create line plot of `inertia errors` vs `n clusters`
fig = px.line(
    x=n clusters, y= inertia errors, title="K-Means Model: Inertia vs Number of Clusters"
fig.update layout(xaxis title="Number of Clusters", yaxis title="Inertia")
fig.show()
```

K-Means Model: Inertia vs Number of Clusters



```
# Create a line plot of `silhouette_scores` vs `n_clusters`
fig = px.line(
    x=n_clusters,
    y=silhouette_scores,
    title="K-Means Model: Silhouette Score vs Number of Clusters"
)
fig.update_layout(xaxis_title="Number of Clusters", yaxis_title="Silhouette Score")
fig.show()
```

K-Means Model: Silhouette Score vs Number of Clusters



▼ Final Model:

Build and train a new k-means model named final_model. Use the information you gained from the two plots above to set an appropriate value for the n_clusters argument. Once you've built and trained your model.

```
# Build model
final model = make pipeline(
    StandardScaler(),
    KMeans(n clusters=4, random state=42)
# Fit model to data
final model.fit(X)
final model
    /usr/local/lib/python3.10/dist-packages/sklearn/cluster/ kmeans.py:870: FutureWarning:
    The default value of `n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init` explicitly to suppress the warning
          Pipeline
      ▶ StandardScaler
          ▶ KMeans
```

Communicate with the Model

Extract the labels that your final_model created during training and assign them to the variable labels.

```
labels = final_model.named_steps['kmeans'].labels_
print("labels type:", type(labels))
print("labels len:", len(labels))
print(labels[:5])
```

```
labels type: <class 'numpy.ndarray'>
labels len: 7050
[0 0 0 0]
```

Create a DataFrame xgb that contains the mean values of the features in X for each of the clusters in your final_model

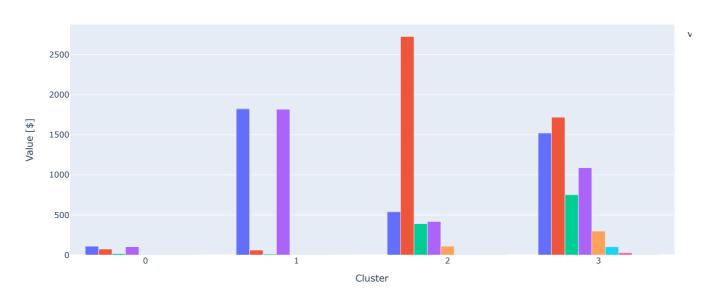
```
xgb = X.groupby(labels).mean()
print("xgb type:", type(xgb))
print("xgb shape:", xgb.shape)
xgb
    xgb type: <class 'pandas.core.frame.DataFrame'>
    xgb shape: (4, 9)
        num reactions num comments num shares
                                               num likes
                                                          num loves
                                                                      num wows num hahas num sads num angrys
                                                                                                               扁
           109.779374
                         74.045179
                                    16.552203
     0
                                               102.821999
                                                            5.996648
                                                                      0.522350
                                                                                0.286718
                                                                                          0.112069
                                                                                                     0.037516
                                                                                                               11.
     1
          1823.311828
                         61.333333
                                    11.645161 1817.534946
                                                            3.104839
                                                                      2.435484
                                                                                 0.198925
                                                                                          0.032258
                                                                                                     0.005376
     2
           538.492105 2728.015789 391.144737 418.002632 107.578947
                                                                      3.805263
                                                                                 5.400000 2.376316
                                                                                                     1.313158
     3
          1522.617647 1718.500000 750.264706 1088.617647 298.205882 101.941176 29.058824
                                                                                          2.970588
                                                                                                     1.823529
```

Use plotly express to create a side-by-side bar chart from xgb that shows the mean of the features in X for each of the clusters in your final_model.

```
# Create side-by-side bar chart of `xgb`
fig = px.bar(
    xgb,
    barmode='group',
    title="Mean Cluster"
)
```

fig.update_layout(xaxis_title="Cluster", yaxis_title="Value [\$]")
fig.show()

Mean Cluster



▼ PCA

Principal component analysis (PCA) is a dimension reduction technique that takes a data set characterized by a set of possibly correlated features and generates a new set of features that are uncorrelated.

It is used as a dimension reduction technique because the new set of uncorrelated features are chosen to be efficient in terms of capturing the variance in the data set.

In practice, PCA is rarely used when the dimension of the data set is already low. However, it is easier to illustrate the method when we have two or three dimensions.

Here, Create a PCA transformer, use it to reduce the dimensionality of the data in X to 2, and then put the transformed data into a DataFrame named X_pca

```
from sklearn.decomposition import PCA
# Instantiate transformer
pca = PCA(n_components=2, random_state=42)

# Transform `X`
X_t = pca.fit_transform(X)

# Put `X_t` into DataFrame
X_pca = pd.DataFrame(X_t, columns=['PC1', 'PC2'])

print("X_pca type:", type(X_pca))
print("X_pca shape:", X_pca.shape)
X_pca.head()
```

```
X pca type: <class 'pandas.core.frame.DataFrame'>
    X_pca shape: (7050, 2)
                       PC2
             PC1
     0 372 669904 308 269641
labels.astype(str)
    array(['0', '0', '0', ..., '0', '0'], dtype='<U11')
     2 252 700040 442 074050
# Create scatter plot of `PC2` vs `PC1`
fig = px.scatter(
    data frame=X pca,
    x= 'PC1',
    y= 'PC2',
    color=labels.astype(str),
    title="PCA Representation of Clusters"
fig.update_layout(xaxis_title="PC1", yaxis_title="PC2")
fig.show()
```

PCA Representation of Clusters

