IN PROGRESS - Clustering the NASA Exoplanet Archive With K-Means to Find New-Earth Candidates

In [1]:
```python
import numpy as np
import pandas as pd
from sklearn.cluster import KMeans
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.metrics import silhouette_samples, silhouette_score
import plotly.express as px
import plotly.graph_objects as go
import matplotlib.cm as cm
import matplotlib.pyplot as plt
from sklearn.datasets import make_blobs
import warnings
warnings.filterwarnings('ignore')
```

In [2]:
```python
### load exoplanet dataset ###
df = pd.read_excel('/Users/shaner/Desktop/nasa_exoplanets.xlsx')
df.head()
```

Out[2]:

	pl_name	hostname	pl_orbper	pl_orbpererr1	pl_orbpererr2	pl_orbperlim	pl_orbsmax	pl_orbsmaxerr1	pl_orbsmaxerr2	pl_orbsmaxlim	...	pl_masseerr2	pl_masselim	pl_orbeccen	pl_orbeccenerr1
0	11 Com b	11 Com	NaN	NaN	NaN	NaN	1.21	0.06	-0.05	0.0	...	NaN	NaN	NaN	NaN
1	11 Com b	11 Com	326.03000	0.32	-0.32	0.0	1.29	0.05	-0.05	0.0	...	NaN	NaN	0.231	0.005
2	11 UMi b	11 UMi	NaN	NaN	NaN	NaN	1.51	0.06	-0.05	0.0	...	NaN	NaN	NaN	NaN
3	11 UMi b	11 UMi	516.21997	3.20	-3.20	0.0	1.53	0.07	-0.07	0.0	...	NaN	NaN	0.080	0.030
4	11 UMi b	11 UMi	516.22000	3.25	-3.25	0.0	1.54	0.07	-0.07	0.0	...	NaN	NaN	0.080	0.030

5 rows × 26 columns

In [3]:
```python
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 34979 entries, 0 to 34978
Data columns (total 26 columns):
 #   Column           Non-Null Count  Dtype
---  ------           --------------  -----
 0   pl_name          34979 non-null  object
 1   hostname         34979 non-null  object
 2   pl_orbper        31918 non-null  float64
 3   pl_orbpererr1    30584 non-null  float64
 4   pl_orbpererr2    30583 non-null  float64
 5   pl_orbperlim     31918 non-null  float64
 6   pl_orbsmax       19324 non-null  float64
 7   pl_orbsmaxerr1   5031 non-null   float64
 8   pl_orbsmaxerr2   5030 non-null   float64
 9   pl_orbsmaxlim    22103 non-null  float64
 10  pl_rade          24108 non-null  float64
 11  pl_radeerr1      23387 non-null  float64
 12  pl_radeerr2      23387 non-null  float64
 13  pl_radelim       26853 non-null  float64
 14  pl_masse         3515 non-null   float64
 15  pl_masseerr1     3264 non-null   float64
 16  pl_masseerr2     3264 non-null   float64
 17  pl_masselim      3547 non-null   float64
 18  pl_orbeccen      17533 non-null  float64
 19  pl_orbeccenerr1  3011 non-null   float64
 20  pl_orbeccenerr2  3010 non-null   float64
 21  pl_orbeccenlim   20279 non-null  float64
 22  pl_eqt           16029 non-null  float64
 23  pl_eqterr1       1793 non-null   float64
 24  pl_eqterr2       1793 non-null   float64
 25  pl_eqtlim        18774 non-null  float64
dtypes: float64(24), object(2)
memory usage: 6.9+ MB
```

In [4]:
```python
### drop rows with null values ###
df.dropna(inplace=True)

### keep only relevant columns ###
columns_to_keep = ['pl_name','hostname','pl_orbper','pl_orbsmax',
                   'pl_rade','pl_masse','pl_orbeccen','pl_eqt']
df = df[columns_to_keep]

df.head()
```

Out[4]:

	pl_name	hostname	pl_orbper	pl_orbsmax	pl_rade	pl_masse	pl_orbeccen	pl_eqt
103	55 Cnc e	55 Cnc	0.736544	0.01544	2.080	7.8100	0.061	1958.0
205	CoRoT-1 b	CoRoT-1	1.508977	0.02590	15.917	340.0781	0.071	1834.0
213	CoRoT-10 b	CoRoT-10	13.240600	0.10550	10.870	874.0000	0.530	600.0
222	CoRoT-12 b	CoRoT-12	2.828042	0.04016	16.140	291.4380	0.070	1442.0
248	CoRoT-19 b	CoRoT-19	3.897130	0.05180	14.460	352.7800	0.047	2000.0

In [5]:
```python
### new row of data for earth ###
new_row = {'pl_name': 'Earth', 'hostname': 'Sol','pl_orbper': 365,'pl_orbsmax': 1,
           'pl_rade': 1,'pl_masse': 1,'pl_orbeccen': 0.0167, 'pl_eqt': 255}

### add the new row using the loc indexer ###
df.loc[len(df)] = new_row

df.tail()
```

Out[5]:

	pl_name	hostname	pl_orbper	pl_orbsmax	pl_rade	pl_masse	pl_orbeccen	pl_eqt
34703	WASP-89 b	WASP-89	3.356423	0.04270	11.657	1875.19700	0.1930	1120.0
34783	Wolf 503 b	Wolf 503	6.001270	0.05712	2.043	6.27000	0.4090	789.0
34785	Wolf 503 b	Wolf 503	6.001270	0.05706	2.043	6.26000	0.4100	790.0
34854	XO-7 b	XO-7	2.864142	0.04421	15.390	225.34147	0.0380	1743.0
328	Earth	Sol	365.000000	1.00000	1.000	1.00000	0.0167	255.0

In [6]:
```python
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 329 entries, 103 to 328
Data columns (total 8 columns):
 #   Column       Non-Null Count  Dtype
---  ------       --------------  -----
 0   pl_name      329 non-null    object
 1   hostname     329 non-null    object
 2   pl_orbper    329 non-null    float64
 3   pl_orbsmax   329 non-null    float64
 4   pl_rade      329 non-null    float64
 5   pl_masse     329 non-null    float64
 6   pl_orbeccen  329 non-null    float64
 7   pl_eqt       329 non-null    float64
dtypes: float64(6), object(2)
memory usage: 23.1+ KB
```

In [7]:
```python
### select features for clustering and pca ###
features = ['pl_orbper','pl_orbsmax','pl_rade','pl_masse','pl_orbeccen','pl_eqt']
```

In [8]:
```python
### standardize the data ###
scaler = StandardScaler()
scaled_data = scaler.fit_transform(df[features])
```

In [9]:
```python
### perform pca ###
pca = PCA(n_components=6)
pca_result = pca.fit_transform(scaled_data)
```

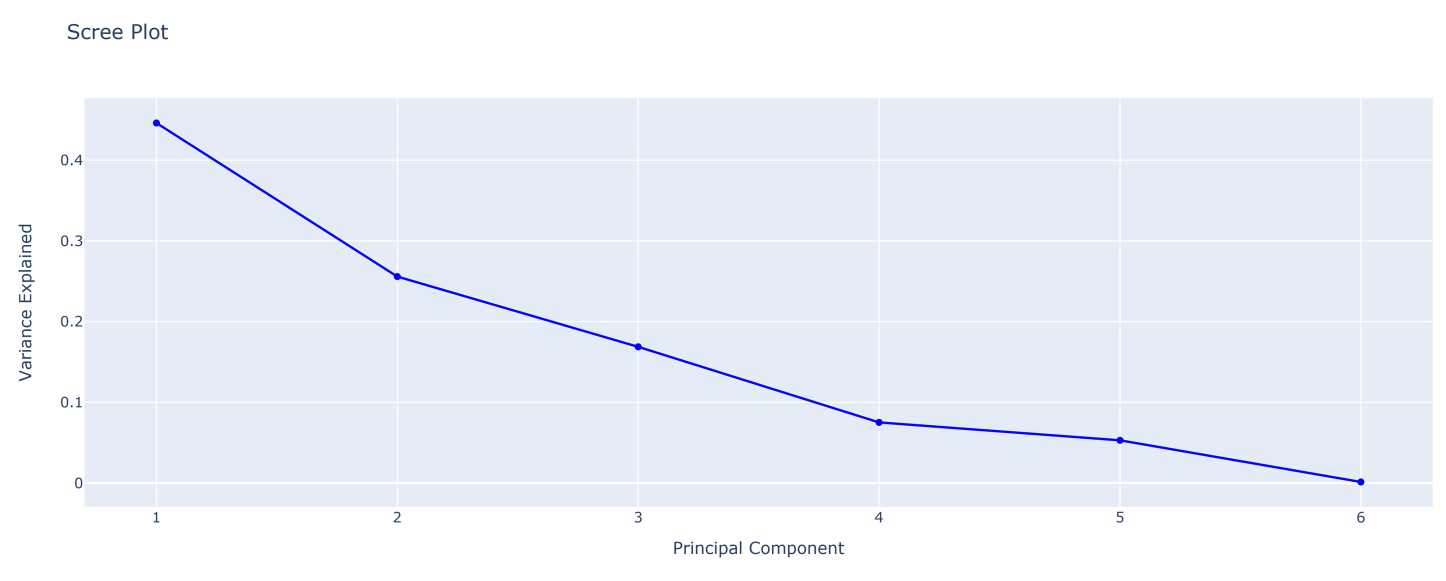
In [10]:
```python
### add pca results to the original dataframe ###
df['PC1'] = pca_result[:, 0]
df['PC2'] = pca_result[:, 1]
```

In [11]:
```python
df.tail()
```

Out[11]:

	pl_name	hostname	pl_orbper	pl_orbsmax	pl_rade	pl_masse	pl_orbeccen	pl_eqt	PC1	PC2
34703	WASP-89 b	WASP-89	3.356423	0.04270	11.657	1875.19700	0.1930	1120.0	0.855620	-0.361257
34783	Wolf 503 b	Wolf 503	6.001270	0.05712	2.043	6.27000	0.4090	789.0	-0.512051	1.559456
34785	Wolf 503 b	Wolf 503	6.001270	0.05706	2.043	6.26000	0.4100	790.0	-0.510312	1.560056
34854	XO-7 b	XO-7	2.864142	0.04421	15.390	225.34147	0.0380	1743.0	0.435594	-1.828709
328	Earth	Sol	365.000000	1.00000	1.000	1.00000	0.0167	255.0	-0.982863	1.822467

In [12]:
```python
### scree with plotly ###
pc_values = np.arange(pca.n_components_) + 1

fig = px.line(x=pc_values, y=pca.explained_variance_ratio_, markers=True,
             title='Scree Plot', labels={'x': 'Principal Component', 'y': 'Variance Explained'})
fig.update_traces(line=dict(color='blue', width=2))

fig.show()
```



In [13]:
```python
print(pca.explained_variance_ratio_)
```

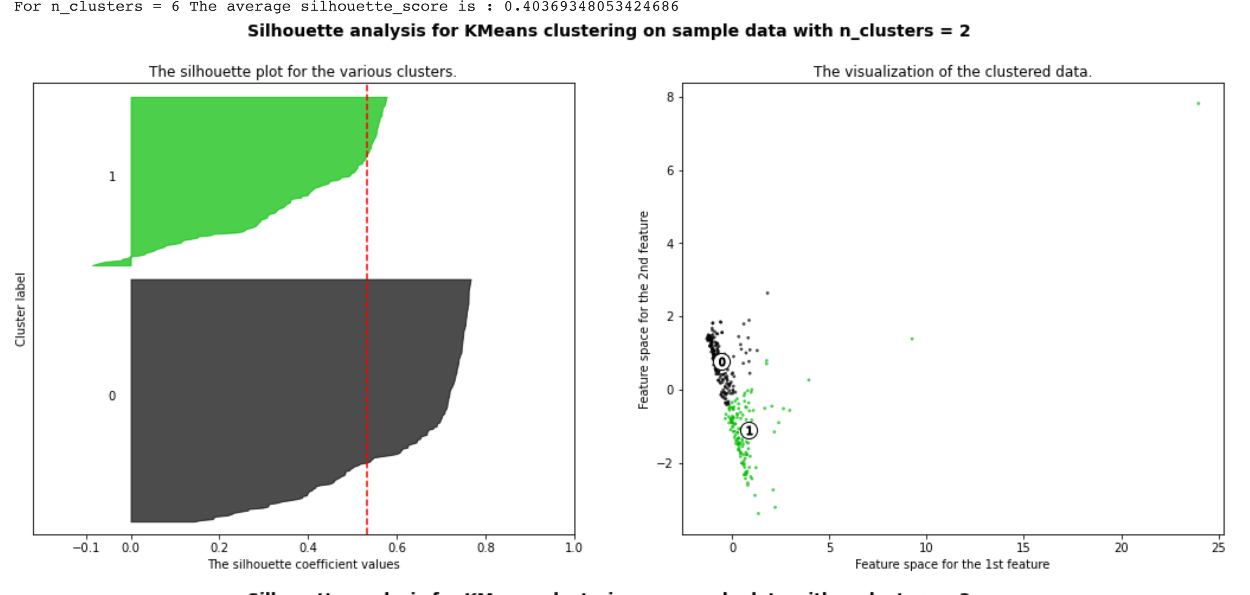
```
[0.44611392 0.25580946 0.16874826 0.07510377 0.05292132 0.00130326]
```

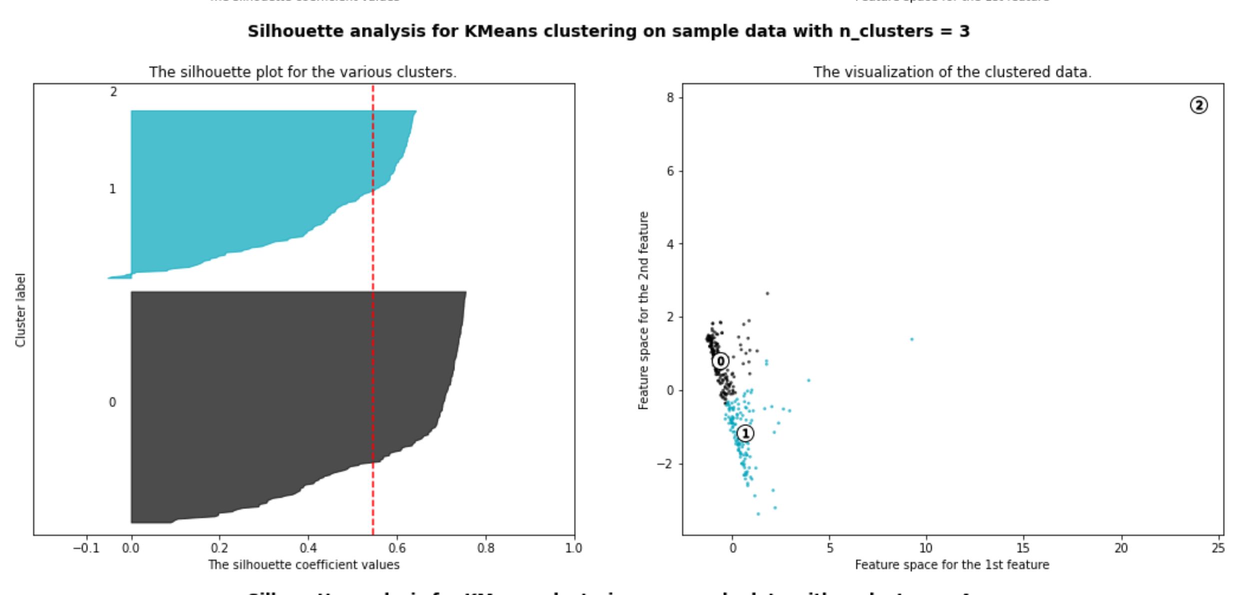
In [14]:
```python
### calculate cumulative explained variance ###
cumulative_explained_variance = np.cumsum(pca.explained_variance_ratio_)

print(cumulative_explained_variance)
```

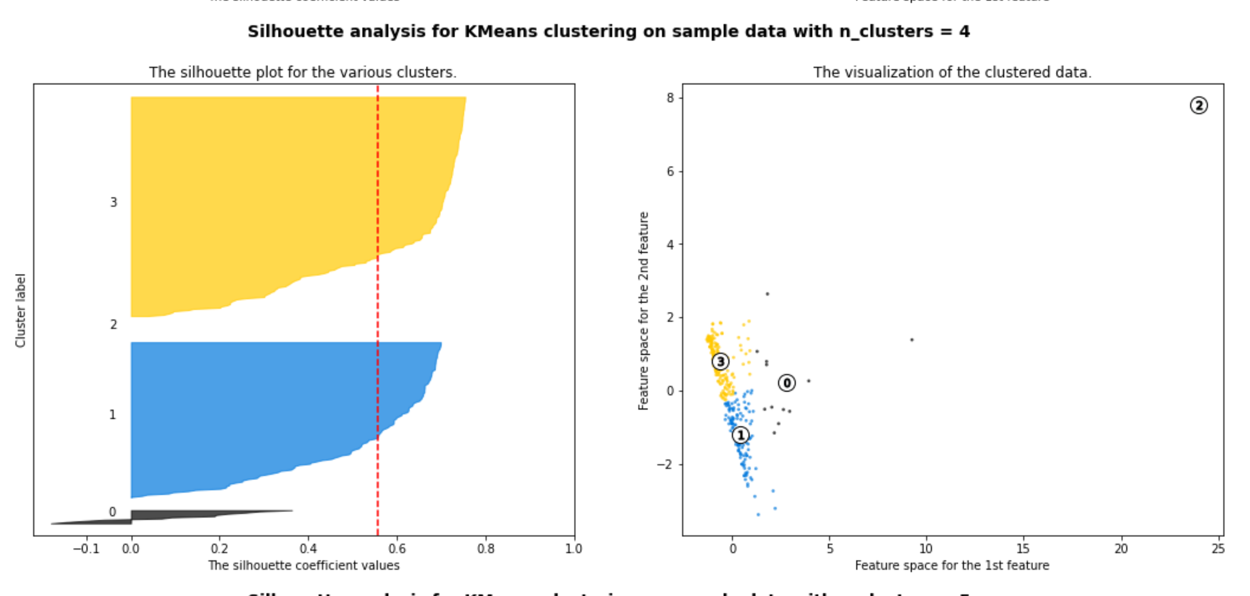
```
[0.44611392 0.70192338 0.87067164 0.94577542 0.99869674 1.        ]
```

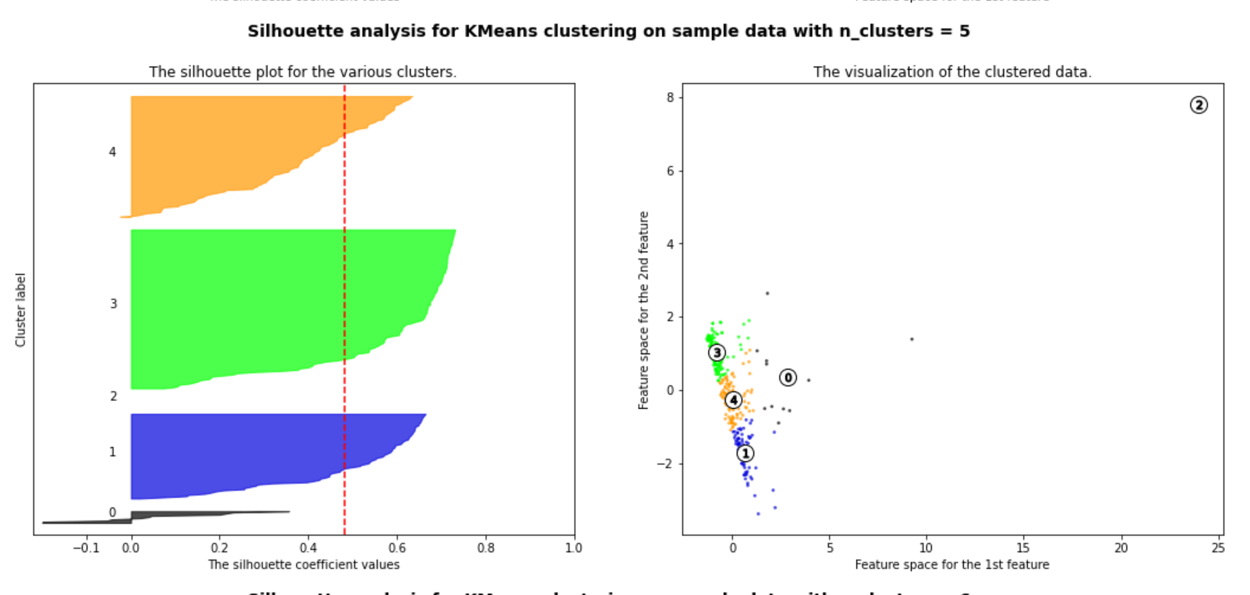
In [15]:
```python
### silhouette ###
range_n_clusters = [2, 3, 4, 5, 6]

X = np.array(df)[:, -2:]

for n_clusters in range_n_clusters:
    ### create a subplot with 1 row and 2 columns ###
    fig, (ax1, ax2) = plt.subplots(1, 2)
    fig.set_size_inches(18, 7)

    ### the 1st subplot is the silhouette plot ###
    ### the silhouette coefficient can range from -1, 1 but in this example all ###
    ### lie within [-0.22, 1] ###
    ax1.set_xlim([-0.22, 1])
    ### the (n_clusters+1)*10 is for inserting blank space between silhouette ###
    ### plots of individual clusters, to demarcate them clearly ###
    ax1.set_ylim([0, len(X) + (n_clusters + 1) * 10])

    ### initialize the clusterer with n_clusters value and a random generator ###
    ### seed of 10 for reproducibility ###
    clusterer = KMeans(n_clusters=n_clusters, n_init="auto", random_state=10)
    cluster_labels = clusterer.fit_predict(X)

    ### the silhouette_score gives the average value for all the samples ###
    ### this gives a perspective into the density and separation of the formed ###
    ### clusters ###
    silhouette_avg = silhouette_score(X, cluster_labels)
    print(
        "For n_clusters =",
        n_clusters,
        "The average silhouette_score is :",
        silhouette_avg,
    )

    ### compute the silhouette scores for each sample ###
    sample_silhouette_values = silhouette_samples(X, cluster_labels)

    y_lower = 10
    for i in range(n_clusters):
        ### aggregate the silhouette scores for samples belonging to ###
        ### cluster i, and sort them ###
        ith_cluster_silhouette_values = sample_silhouette_values[cluster_labels == i]

        ith_cluster_silhouette_values.sort()

        size_cluster_i = ith_cluster_silhouette_values.shape[0]
        y_upper = y_lower + size_cluster_i

        color = cm.nipy_spectral(float(i) / n_clusters)
        ax1.fill_betweenx(
            np.arange(y_lower, y_upper),
            0,
            ith_cluster_silhouette_values,
            facecolor=color,
            edgecolor=color,
            alpha=0.7,
        )

        ### label the silhouette plots with their cluster numbers at the middle ###
        ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))

        ### compute the new y_lower for next plot ###
        y_lower = y_upper + 10  ### 10 for the 0 samples ###

    ax1.set_title("The silhouette plot for the various clusters.")
    ax1.set_xlabel("The silhouette coefficient values")
    ax1.set_ylabel("Cluster label")

    ### the vertical line for average silhouette score of all the values ###
    ax1.axvline(x=silhouette_avg, color="red", linestyle="--")

    ax1.set_yticks([])  ### clear the yaxis labels / ticks ###
    ax1.set_xticks([-0.1, 0, 0.2, 0.4, 0.6, 0.8, 1])

    ### 2nd plot showing the actual clusters formed ###
    colors = cm.nipy_spectral(cluster_labels.astype(float) / n_clusters)
    ax2.scatter(
        X[:, 0], X[:, 1], marker=".", s=30, lw=0, alpha=0.7, c=colors, edgecolor="k"
    )

    ### labeling the clusters ###
    centers = clusterer.cluster_centers_
    ### draw white circles at cluster centers ###
    ax2.scatter(
        centers[:, 0],
        centers[:, 1],
        marker="o",
        c="white",
        alpha=1,
        s=200,
        edgecolor="k",
    )

    for i, c in enumerate(centers):
        ax2.scatter(c[0], c[1], marker="$%d$" % i, alpha=1, s=50, edgecolor="k")

    ax2.set_title("The visualization of the clustered data.")
    ax2.set_xlabel("Feature space for the 1st feature")
    ax2.set_ylabel("Feature space for the 2nd feature")

    plt.suptitle(
        "Silhouette analysis for KMeans clustering on sample data with n_clusters = %d"
        % n_clusters,
        fontsize=14,
        fontweight="bold",
    )

plt.show()
```

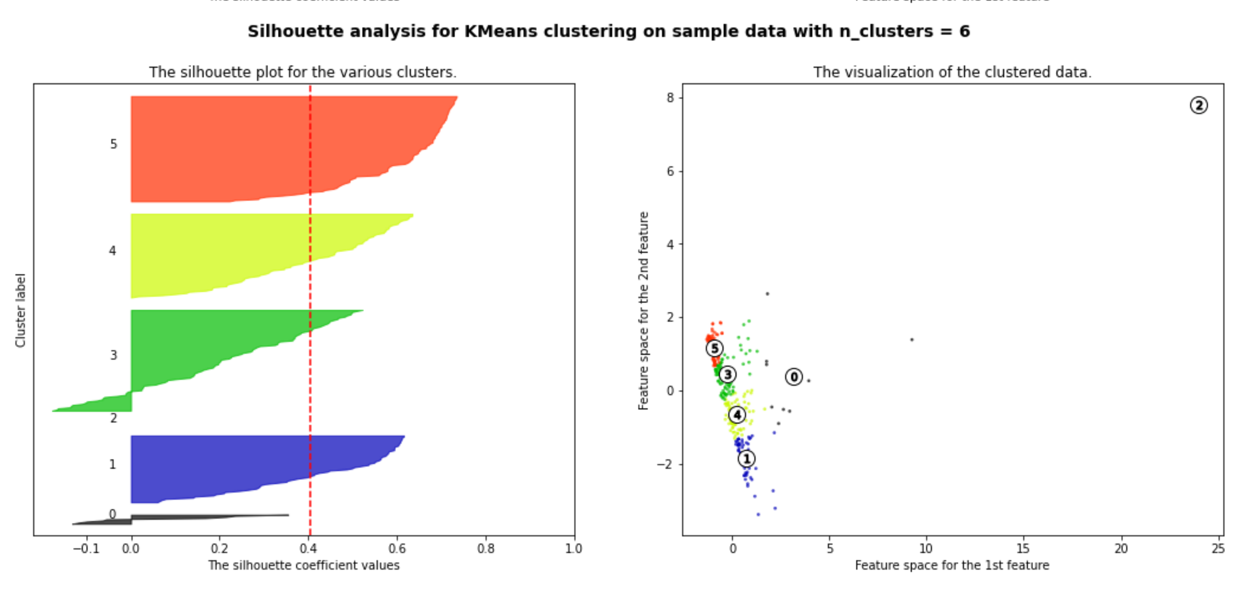
```
For n_clusters = 2 The average silhouette_score is : 0.5318041858857563
For n_clusters = 3 The average silhouette_score is : 0.546039188889465
For n_clusters = 4 The average silhouette_score is : 0.5562891187374129
For n_clusters = 5 The average silhouette_score is : 0.48258324553568516
For n_clusters = 6 The average silhouette_score is : 0.40369348053424686
```











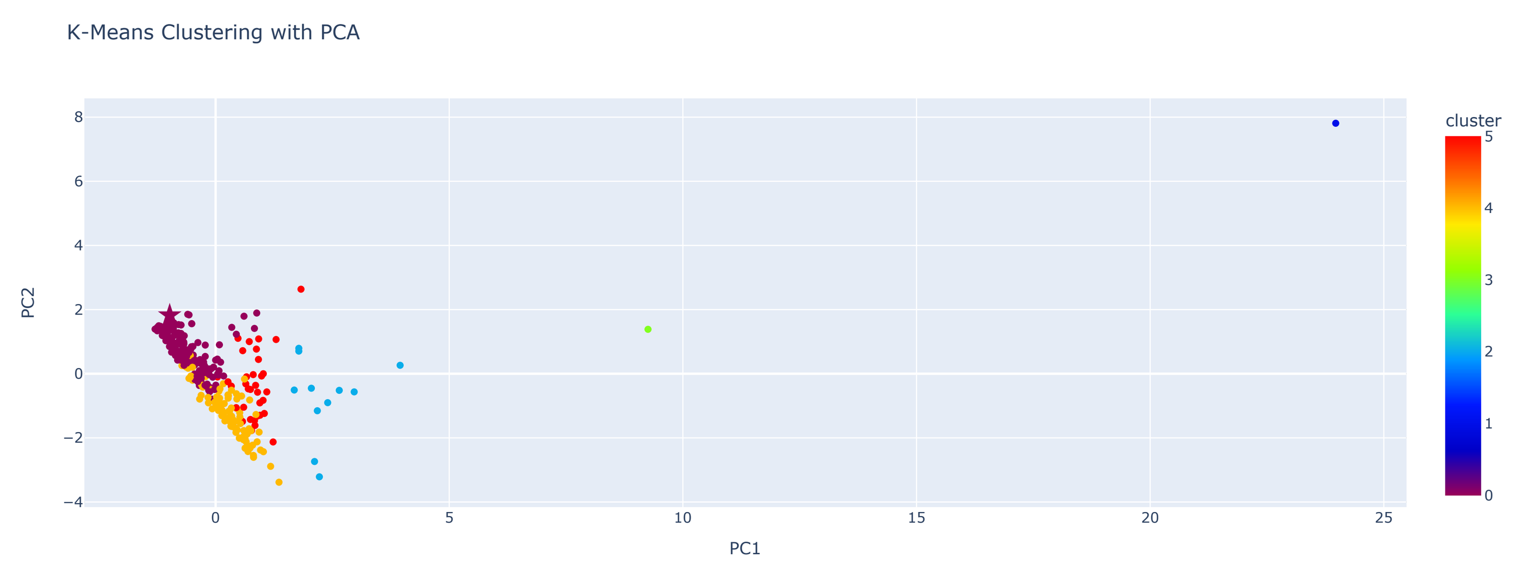
In [16]:
```python
### number of clusters ###
num_clusters = 6

### initialize kmeans model ###
kmeans = KMeans(n_clusters=num_clusters, random_state=42)

### fit the model to main dataset ###
kmeans.fit(df[features])
```

Out[16]:

```
KMeans
KMeans(n_clusters=6, random_state=42)
```

In [17]:
```python
### predict clusters ###
df['cluster'] = kmeans.predict(df[features])
```

In [18]:
```python
### create a scatter plot with plotly ###
fig = px.scatter(df, x='PC1', y='PC2', color='cluster',
    color_continuous_scale = 'rainbow', title='K-Means Clustering with PCA')

### select the trace to mark with 'x' ###
trace_to_mark = 328  ### earth row (0-based index)

### add a new trace with 'x' marker ###
marked_trace = px.scatter(df.iloc[trace_to_mark:trace_to_mark + 1], x='PC1', y='PC2',
                          color='cluster', color_continuous_scale='rainbow',
                          title='K-Means Clustering with PCA')
marked_trace.update_traces(marker=dict(symbol='star', size=15))

### add the new marked trace to the existing figure ###
fig.add_trace(marked_trace.data[0])

fig.show()
```



In [19]:
```python
### create a scatter plot with plotly ###
fig = px.scatter(df, x='PC1', y='PC2', color='cluster',
    color_continuous_scale = 'rainbow', title='K-Means Clustering with PCA')

### select the eaerth trace to mark with 'x' ###
trace_to_mark = 328  ### EARTH (0-based index) ###

### add a new trace with 'x' marker ###
marked_trace = px.scatter(df.iloc[trace_to_mark:trace_to_mark + 1], x='PC1', y='PC2',
                          color='cluster', color_continuous_scale='rainbow',
                          title='K-Means Clustering with PCA')
marked_trace.update_traces(marker=dict(symbol='star', size=15))

### calculate cluster centroids ###
centroids = df.groupby('cluster')['PC1', 'PC2'].mean().reset_index()

### add centroids as markers ###
centroid_trace = px.scatter(centroids, x='PC1', y='PC2', color='cluster',
                            color_continuous_scale='rainbow')
centroid_trace.update_traces(marker=dict(symbol='diamond', size=10, color='black'))

fig.add_trace(centroid_trace.data[0])

### add the new marked trace to the existing figure ###
fig.add_trace(marked_trace.data[0])

### update x and y axis ranges ###
x_range = [-1.5, 4]  ### replace xmin and xmax with desired range ###
y_range = [-4, 3]  ### replace ymin and ymax with desired range ###
fig.update_layout(xaxis_range=x_range, yaxis_range=y_range)

fig.show()
```