In [1]:
```python
import warnings

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split

warnings.filterwarnings("ignore")
warnings.filterwarnings("ignore", category=DeprecationWarning)

pd.set_option("display.max_rows", 500)
pd.set_option("display.max_columns", 500)
pd.set_option("display.width", 1000)
```

Data Exploration and key features

In [2]:
```python
# Invoking the prepared data

df = pd.read_csv('all_data.csv')
```

We see the features:

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

Out[3]:

	CO(GT)_winsor	PT08.S1(CO)_winsor	PT08.S4(NO2)_winsor	T_winsor	RH_winsor	AH_winsor	day_winsor	year_winsor	quarter_winsor	weekday_winsor	NO2(GT)_winsor	CO(GT)	PT08.S1(CO)	C6H6(GT)	PT08.S2(NMHC)	NOx(GT)
5991	0.572233	0.240188	0.32157	0.457463	0.501059	0.142354	0.758688	0.0	1.0	0.0	0.838242	2.4	925.0	8.6	923.0	442.0

We now consider the relevant features, i. e., such features that are normalized and transformed as we did in the `exploration data` notebook, and the original data.

In [4]:
```python
key_features_original = [
    "CO(GT)",
    "PT08.S1(CO)",
    "NO2(GT)",
    "PT08.S4(NO2)",
    "T",
    "RH",
    "AH",
    "day",
    "year",
    "quarter",
    "weekday",]

key_features_winsor = [
    "CO(GT)_winsor",
    "PT08.S1(CO)_winsor",
    "PT08.S4(NO2)_winsor",
    "NO2(GT)_winsor",
    "T_winsor",
    "RH_winsor",
    "AH_winsor",
    "day_winsor",
    "year_winsor",
    "quarter_winsor",
    "weekday_winsor",
]
```

In [5]:
```python
df_clusters = df[key_features_original+key_features_winsor]
```

In [6]:
```python
df_clusters.sample(3)
```

Out[6]:

	CO(GT)	PT08.S1(CO)	NO2(GT)	PT08.S4(NO2)	T	RH	AH	day	year	quarter	weekday	CO(GT)_winsor	PT08.S1(CO)_winsor	PT08.S4(NO2)_winsor	NO2(GT)_winsor	T_winsor	RH_winsor	AH_winsor	day_winsor	year_
8016	1.9	1067.0	194.0	989.0	8.7	33.9	0.3832	7.0	2005.0	1.0	0.0	0.46965	0.441406	0.199005	0.939571	0.352892	0.423865	0.030810	0.505792	
6141	0.3	866.0	106.0	859.0	15.2	18.7	0.3214	21.0	2004.0	4.0	6.0	0.00000	0.147334	0.054984	0.600296	0.595488	0.035389	0.000000	0.874876	
4705	5.2	1387.0	194.0	2065.0	26.7	43.3	1.4881	22.0	2004.0	3.0	2.0	0.95968	0.811034	0.951642	0.939571	0.849216	0.585879	0.823688	0.891094	

K-means model

We first verify that our data satisfies normalization criteria:

In [7]:
```python
df_clusters[key_features_winsor].describe().T
```

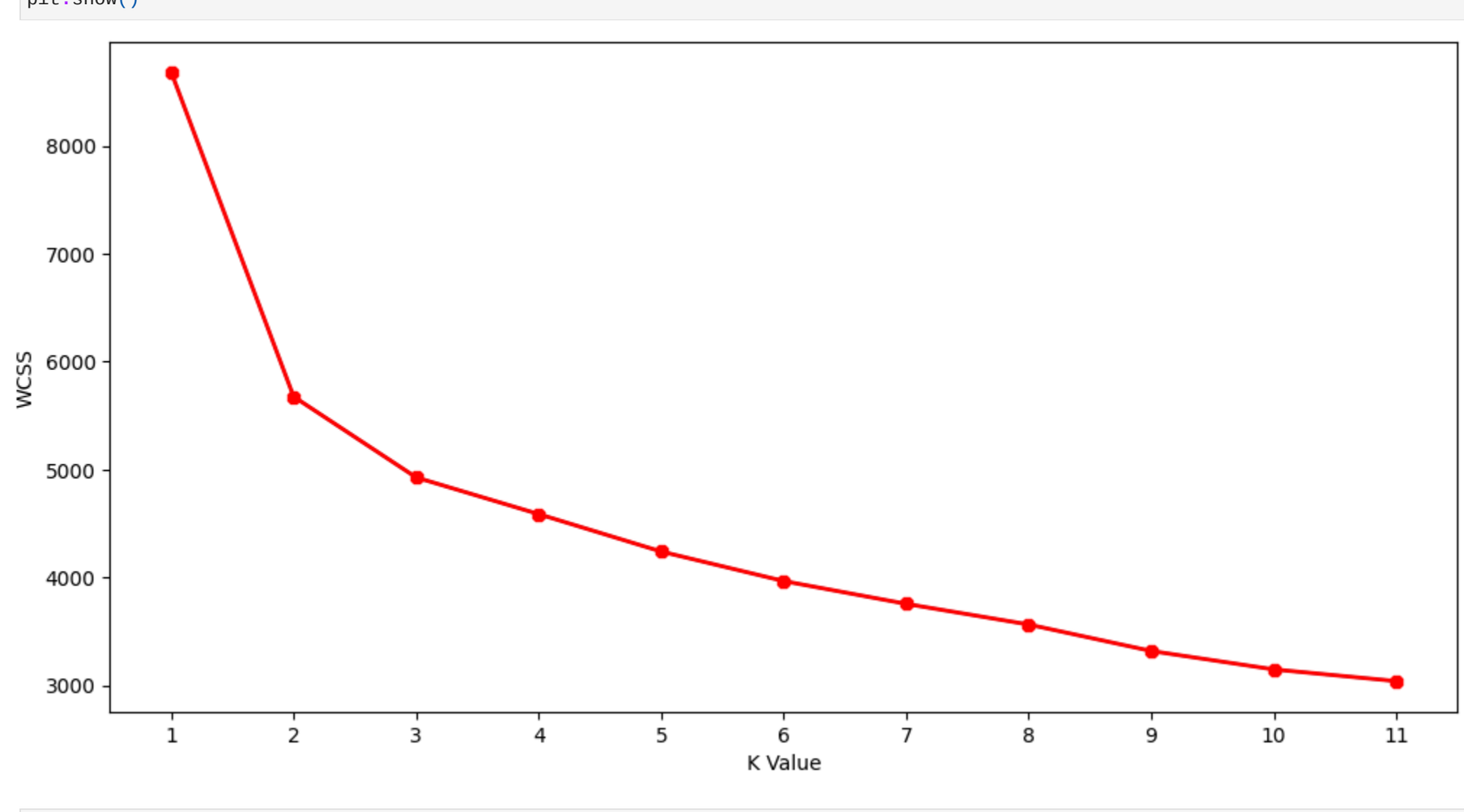
Out[7]:

	count	mean	std	min	25%	50%	75%	max
CO(GT)_winsor	9357.0	0.458918	0.241618	0.0	0.291491	0.447019	0.609095	1.0
PT08.S1(CO)_winsor	9357.0	0.456497	0.254699	0.0	0.264349	0.436113	0.631386	1.0
PT08.S4(NO2)_winsor	9357.0	0.565616	0.240293	0.0	0.431833	0.599253	0.729644	1.0
NO2(GT)_winsor	9357.0	0.589190	0.225316	0.0	0.483324	0.615927	0.727494	1.0
T_winsor	9357.0	0.622976	0.243586	0.0	0.491398	0.665892	0.802594	1.0
RH_winsor	9357.0	0.627853	0.255708	0.0	0.474486	0.676205	0.824020	1.0
AH_winsor	9357.0	0.519159	0.261592	0.0	0.345446	0.525677	0.715295	1.0
day_winsor	9357.0	0.704554	0.261762	0.0	0.548765	0.780807	0.906622	1.0
year_winsor	9357.0	0.240141	0.427192	0.0	0.000000	0.000000	0.000000	1.0
quarter_winsor	9357.0	0.521879	0.382349	0.0	0.000000	0.442507	0.756471	1.0
weekday_winsor	9357.0	0.627278	0.325847	0.0	0.356207	0.712414	0.920782	1.0

Since we are not dealing with other type of data types (besides of numeric), we then consider a K-means model:

In [8]:
```python
# Importing KMeans from sklearn
from sklearn.cluster import KMeans
```

In [9]:
```python
wcss=[]
RANGE = 12

for i in range(1,RANGE):
    km=KMeans(n_clusters=i, init='k-means++', random_state=1492)
    km.fit(df_clusters[key_features_winsor])
    wcss.append(km.inertia_)

#The elbow curve
plt.figure(figsize=(12,6))
plt.plot(range(1,RANGE),wcss)
plt.plot(range(1,RANGE),wcss, linewidth=2, color="red", marker ="8")
plt.xlabel("K Value")
plt.xticks(np.arange(1,RANGE,1))
plt.ylabel("WCSS")
plt.show()
```



In [10]:
```python
#Taking 5 clusters
km1=KMeans(n_clusters=4, init='random', random_state=1492)
#Fitting the input data
km1.fit(df_clusters[key_features_winsor])
```

Out[10]:

```
KMeans
KMeans(init='random', n_clusters=4, random_state=1492)
```

In [11]:
```python
#predicting the labels of the input data
y=km1.predict(df_clusters[key_features_winsor])
```

In [12]:
```python
#adding the labels to a column named label
df_clusters["label"] = y
```

In [13]:
```python
#The new dataframe with the clustering done
df_clusters.head()
```

Out[13]:

	CO(GT)	PT08.S1(CO)	NO2(GT)	PT08.S4(NO2)	T	RH	AH	day	year	quarter	weekday	CO(GT)_winsor	PT08.S1(CO)_winsor	PT08.S4(NO2)_winsor	NO2(GT)_winsor	T_winsor	RH_winsor	AH_winsor	day_winsor	year_win
0	2.6	1360.0	113.0	1692.0	13.6	48.9	0.7578	10.0	2004.0	1.0	2.0	0.609095	0.783328	0.747936	0.636118	0.546300	0.666742	0.354464	0.62198	
1	2.0	1292.0	92.0	1559.0	13.3	47.7	0.7255	10.0	2004.0	1.0	2.0	0.491514	0.711040	0.664232	0.521024	0.536480	0.650206	0.329419	0.62198	
2	2.2	1402.0	114.0	1555.0	11.9	54.0	0.7502	10.0	2004.0	1.0	2.0	0.533136	0.826194	0.661605	0.641056	0.487745	0.732847	0.348613	0.62198	
3	2.2	1376.0	122.0	1584.0	11.0	60.0	0.7867	10.0	2004.0	1.0	2.0	0.533136	0.799812	0.680497	0.679073	0.453538	0.803184	0.376487	0.62198	
4	1.6	1272.0	116.0	1490.0	11.2	59.6	0.7888	10.0	2004.0	1.0	2.0	0.399226	0.689053	0.617949	0.650802	0.461356	0.798715	0.378073	0.62198	

Analysis

In [14]:
```python
df_analysis = df_clusters[key_features_original+['label']]
```

In [15]:
```python
df_analysis.sample(3)
```

Out[15]:

	CO(GT)	PT08.S1(CO)	NO2(GT)	PT08.S4(NO2)	T	RH	AH	day	year	quarter	weekday	label
7393	5.7	1517.0	182.0	1902.0	14.1	57.8	0.9262	12.0	2005.0	1.0	2.0	0
4299	1.6	988.0	109.0	1341.0	27.1	26.9	0.9524	5.0	2004.0	3.0	6.0	2
5215	1.8	786.0	109.0	1123.0	15.0	56.4	0.9554	14.0	2004.0	4.0	3.0	2

In [16]:
```python
df_analysis.describe().T
```

Out[16]:

	count	mean	std	min	25%	50%	75%	max
CO(GT)	9357.0	2.089302	1.323024	0.1000	1.2000	1.8000	2.6000	11.900
PT08.S1(CO)	9357.0	1098.392433	212.911465	647.0000	941.0000	1063.0000	1221.0000	2040.000
NO2(GT)	9357.0	112.373303	43.948519	2.0000	86.0000	109.0000	133.0000	340.000
PT08.S4(NO2)	9357.0	1456.528054	339.370072	551.0000	1242.0000	1463.0000	1662.0000	2775.000
T	9357.0	18.297574	8.658221	-1.9000	12.0000	17.8000	24.1000	44.600
RH	9357.0	49.248509	16.974949	9.2000	36.6000	49.6000	61.9000	88.700
AH	9357.0	1.024352	0.395878	0.1847	0.7461	0.9954	1.2962	2.231
day	9357.0	15.876884	8.808653	1.0000	8.0000	16.0000	23.0000	31.000
year	9357.0	2004.240141	0.427192	2004.0000	2004.0000	2004.0000	2004.0000	2005.000
quarter	9357.0	2.422571	1.134365	1.0000	1.0000	2.0000	3.0000	4.000
weekday	9357.0	3.009939	2.000323	0.0000	1.0000	3.0000	5.0000	6.000
label	9357.0	1.638666	1.123581	0.0000	1.0000	2.0000	3.0000	3.000

In [17]:
```python
df_analysis[df_analysis['label']==0].describe().T
```

Out[17]:

	count	mean	std	min	25%	50%	75%	max
CO(GT)	2247.0	2.044192	1.335288	0.1000	1.1000	1.8000	2.70000	8.700
PT08.S1(CO)	2247.0	1107.112150	200.835137	715.0000	958.0000	1063.0000	1222.00000	1846.000
NO2(GT)	2247.0	141.070316	50.681205	17.0000	109.0000	138.0000	173.00000	340.000
PT08.S4(NO2)	2247.0	1163.965732	272.225393	551.0000	948.0000	1134.0000	1366.50000	2147.000
T	2247.0	10.495461	5.846498	-1.9000	5.6000	9.8000	14.30000	30.000
RH	2247.0	52.262127	16.029349	9.9000	40.8000	50.9000	64.75000	86.600
AH	2247.0	0.673987	0.259947	0.1847	0.4463	0.6604	0.89735	1.393
day	2247.0	15.022697	8.916698	1.0000	7.0000	15.0000	23.00000	31.000
year	2247.0	2005.000000	0.000000	2005.0000	2005.0000	2005.0000	2005.00000	2005.000
quarter	2247.0	1.038718	0.192966	1.0000	1.0000	1.0000	1.00000	2.000
weekday	2247.0	3.033378	2.021754	0.0000	1.0000	3.0000	5.00000	6.000
label	2247.0	0.000000	0.000000	0.0000	0.0000	0.0000	0.00000	0.000

In [18]:
```python
df_analysis[df_analysis['label']==1].describe().T
```

Out[18]:

	count	mean	std	min	25%	50%	75%	max
CO(GT)	1466.0	1.607503	0.766926	0.100	1.100000	1.8000	1.900000	6.6000
PT08.S1(CO)	1466.0	996.383356	147.832704	676.000	887.250000	988.0000	1088.000000	1520.0000
NO2(GT)	1466.0	93.009550	32.392852	5.000	71.000000	101.0000	109.000000	239.0000
PT08.S4(NO2)	1466.0	1431.698499	242.877678	698.000	1286.000000	1439.0000	1591.500000	2381.0000
T	1466.0	19.790109	7.928370	2.600	13.800000	19.1000	25.100000	41.7000
RH	1466.0	48.114734	17.284434	9.200	34.900000	48.0000	61.300000	87.2000
AH	1466.0	1.072660	0.367842	0.334	0.810075	1.0674	1.325725	2.0821
day	1466.0	17.047749	8.569119	1.000	10.000000	17.0000	25.000000	31.0000
year	1466.0	2004.000000	0.000000	2004.000	2004.000000	2004.0000	2004.000000	2004.0000
quarter	1466.0	2.893588	0.917557	1.000	2.000000	3.0000	4.000000	4.0000
weekday	1466.0	0.393588	0.492884	0.000	0.000000	0.0000	1.000000	2.0000
label	1466.0	1.000000	0.000000	1.000	1.000000	1.0000	1.000000	1.0000

In [19]:
```python
df_analysis[df_analysis['label']==2].describe().T
```

Out[19]:

	count	mean	std	min	25%	50%	75%	max
CO(GT)	3065.0	1.391648	0.567387	0.1000	0.9000	1.5000	1.8000	4.3000
PT08.S1(CO)	3065.0	965.854160	110.334591	647.0000	883.0000	969.0000	1052.0000	1332.0000
NO2(GT)	3065.0	85.251223	28.371168	2.0000	63.0000	88.0000	109.0000	216.0000
PT08.S4(NO2)	3065.0	1387.815334	206.355866	682.0000	1279.0000	1426.0000	1529.0000	1932.0000
T	3065.0	19.790310	7.775821	1.2000	14.4000	19.1000	24.7000	42.2000
RH	3065.0	50.049690	16.877328	10.0000	38.0000	49.8000	62.3000	88.7000
AH	3065.0	1.123784	0.382103	0.1988	0.8831	1.0592	1.3974	2.1806
day	3065.0	16.146493	8.684626	1.0000	9.0000	16.0000	24.0000	31.0000
year	3065.0	2004.000000	0.000000	2004.0000	2004.0000	2004.0000	2004.0000	2004.0000
quarter	3065.0	2.900163	0.899929	1.0000	2.0000	3.0000	4.0000	4.0000
weekday	3065.0	4.319413	1.436231	2.0000	3.0000	5.0000	6.0000	6.0000
label	3065.0	2.000000	0.000000	2.0000	2.0000	2.0000	2.0000	2.0000

In [20]:
```python
df_analysis[df_analysis['label']==3].describe().T
```

Out[20]:

	count	mean	std	min	25%	50%	75%	max
CO(GT)	2579.0	3.231601	1.436817	1.4000	2.1000	2.9000	4.00000	11.900
PT08.S1(CO)	2579.0	1306.295463	179.938259	934.0000	1168.0000	1282.0000	1420.00000	2040.000
NO2(GT)	2579.0	130.610702	32.872330	27.0000	109.0000	122.0000	148.00000	288.000
PT08.S4(NO2)	2579.0	1807.203567	256.311212	1086.0000	1635.0000	1782.0000	1954.00000	2775.000
T	2579.0	22.472858	7.764322	1.4000	16.8000	21.8000	27.50000	44.600
RH	2579.0	46.315161	17.191819	9.3000	32.4000	47.1000	58.70000	86.500
AH	2579.0	1.183983	0.337500	0.3003	0.9295	1.1381	1.45105	2.231
day	2579.0	15.635130	8.910547	1.0000	8.0000	16.0000	23.00000	31.000
year	2579.0	2004.000000	0.000000	2004.0000	2004.0000	2004.0000	2004.00000	2004.000
quarter	2579.0	2.792943	0.996392	1.0000	2.0000	3.0000	4.00000	4.000
weekday	2579.0	2.920512	1.559115	0.0000	2.0000	3.0000	4.00000	6.000
label	2579.0	3.000000	0.000000	3.0000	3.0000	3.0000	3.00000	3.000

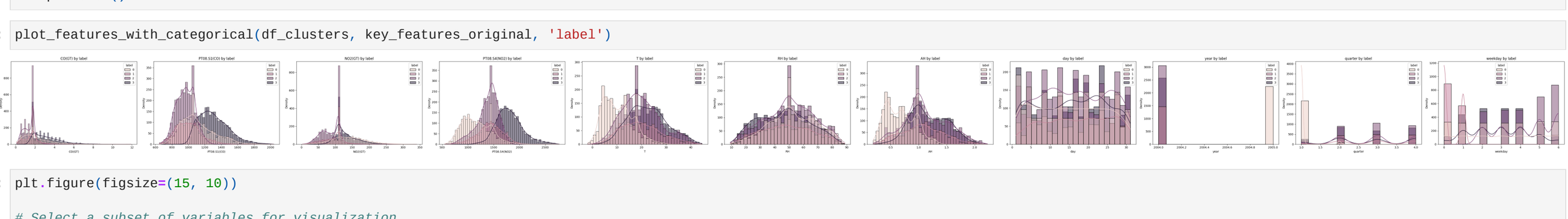
In [21]:
```python
analysis = 'analysis.csv'
```

In [22]:
```python
df_analysis.to_csv(analysis, index=False)
```

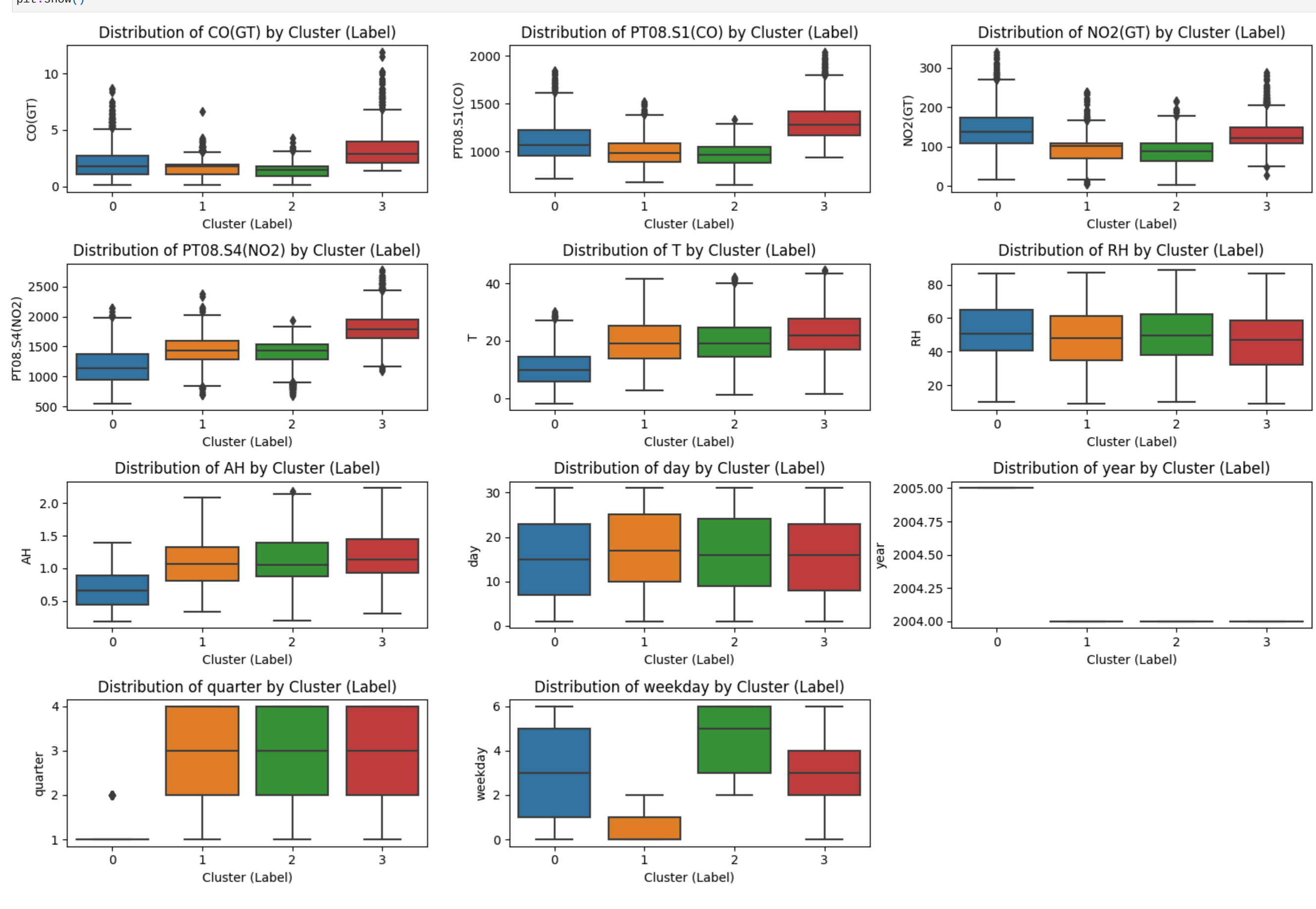
In [ ]:

In [23]:
```python
import seaborn as sns
import matplotlib.pyplot as plt

def plot_features_with_categorical(df, features, categorical_var):
    size = len(features)

    # Create a figure with subplots in a single row
    fig, axes = plt.subplots(1, size, figsize=(7 * size, 5), dpi=100)

    # Ensure axes is iterable, even if there's only one subplot
    if size == 1:
        axes = [axes]

    # Loop through each feature and create a displot
    for i, feature in enumerate(features):
        sns.histplot(df, x=feature, hue=categorical_var, kde=True, fill=True, ax=axes[i])

        # Set the title and labels for each subplot
        axes[i].set_title(f'{feature} by {categorical_var}')
        axes[i].set_xlabel(feature)
        axes[i].set_ylabel('Density')

    # Adjust the layout to avoid overlap
    plt.tight_layout()
    plt.show()
```

In [24]:
```python
plot_features_with_categorical(df_clusters, key_features_original, 'label')
```



In [25]:
```python
plt.figure(figsize=(15, 10))

# Select a subset of variables for visualization
variables_to_plot = key_features_original

# Create a boxplot for each variable, showing distribution by label (cluster)
for i, var in enumerate(variables_to_plot, 1):
    plt.subplot(4, 3, i)
    sns.boxplot(x='label', y=var, data=df_clusters)
    plt.title(f'Distribution of {var} by Cluster (Label)')
    plt.xlabel('Cluster (Label)')
    plt.ylabel(var)

plt.tight_layout()
plt.show()
```



PCA Visualizations

Now we visualize the segmentation of the data via principal components. In this case, for simplicity, we take the two principal components that contain the most information about the total variance. The first principal component captures the maximum possible variance in the data, while the second captures the next highest amount of variance. Both are orthogonal to each other.

In [26]:
```python
list_labels = list(df_clusters['label'].drop_duplicates())
```

In [27]:
```python
for number in range(len(list_labels)):
    print(df_clusters[df_clusters['label']==number].shape[0])
```

```
2247
1466
3065
2579
```

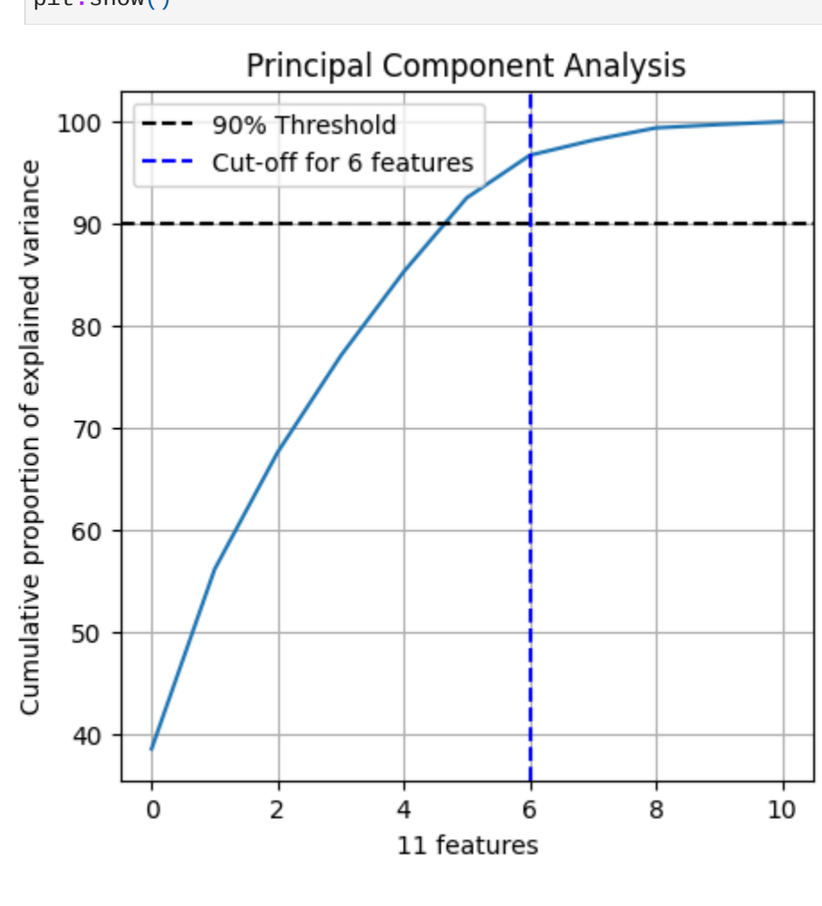
In [28]:
```python
from sklearn.decomposition import PCA
```

In [29]:
```python
components = df_clusters[key_features_winsor].shape[1]
```

In [30]:
```python
pca = PCA(components)
data = pca.fit_transform(df_clusters[key_features_winsor])
```

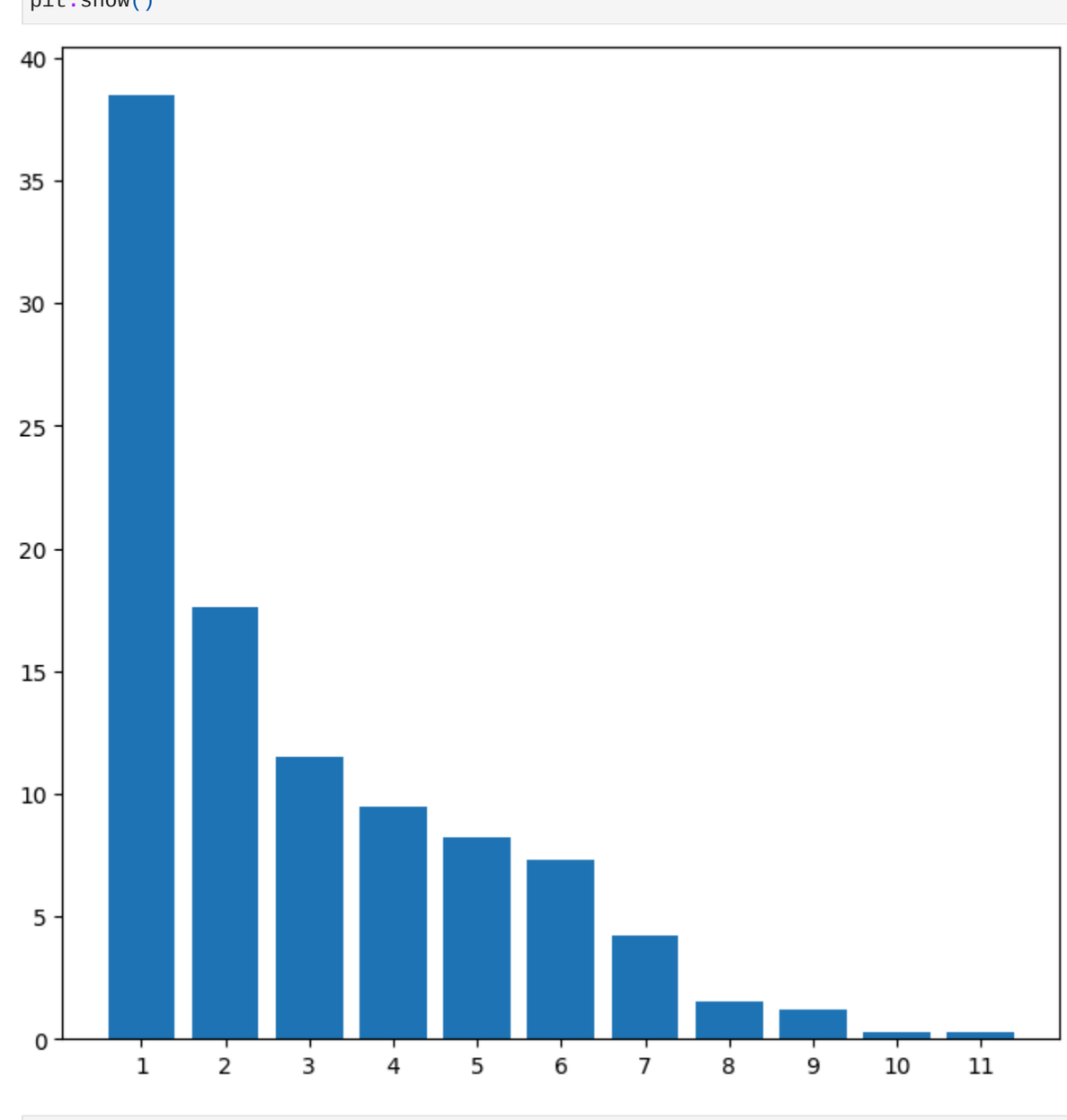
In [31]:
```python
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.90) + 1
```

In [32]:
```python
# Plot the graph
plt.figure(figsize=(5, 5))
plt.plot(cumsum*100)

# Add horizontal lines
plt.axhline(y=90, color='black', linestyle='--', label='90% Threshold')

# Add vertical lines
plt.axvline(x=d, color='b', linestyle='--', label=f'Cut-off for {d} features')

# Add labels and legend
plt.xlabel(f'{components} features')
plt.ylabel('Cumulative proportion of explained variance')
plt.title('Principal Component Analysis')
plt.legend()

# Show plot
plt.grid(True)
#plt.savefig('pca.png', dpi=100, bbox_inches="tight")
plt.show()
```

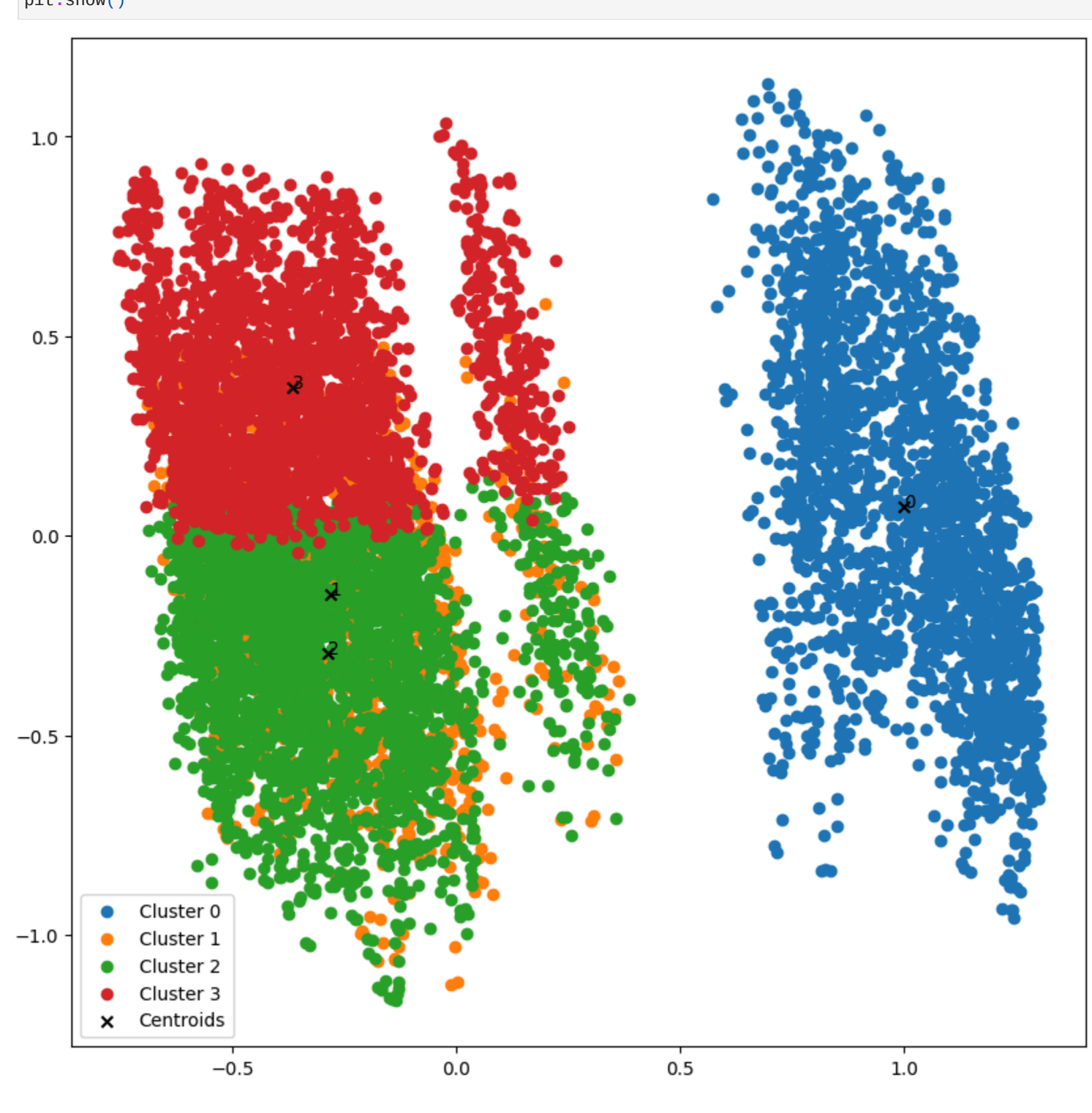


Then, it is only necessary to consider 5 features in order to have at least 90% of the information associated to the variance of the original data

In [33]:
```python
plt.figure(figsize=(8,8))
var = np.round(pca.explained_variance_ratio_*100, decimals = 1)
lbls = [str(x) for x in range(1, len(var)+1)]
plt.bar(x=range(1,len(var)+1), height = var, tick_label = lbls)
plt.show()
```



In [34]:
```python
centers = np.array(km1.cluster_centers_)
# KMeans clustering
#model = KMeans(n_clusters=7, init="k-means++")
model = KMeans(n_clusters=len(list_labels), init="random", random_state=1492)

label = model.fit_predict(data)
centers = np.array(model.cluster_centers_)

# Plotting
plt.figure(figsize=(10, 10))
uniq = np.unique(label)

for i in uniq:
    plt.scatter(data[label == i, 0], data[label == i, 1], label=f'Cluster {i}')

plt.scatter(centers[:, 0], centers[:, 1], marker="x", color='k', label='Centroids')

# Annotating cluster points with labels
for i, txt in enumerate(uniq):
    plt.annotate(txt, (centers[i, 0], centers[i, 1]), fontsize=10, color='k')

plt.legend()
plt.show()
```



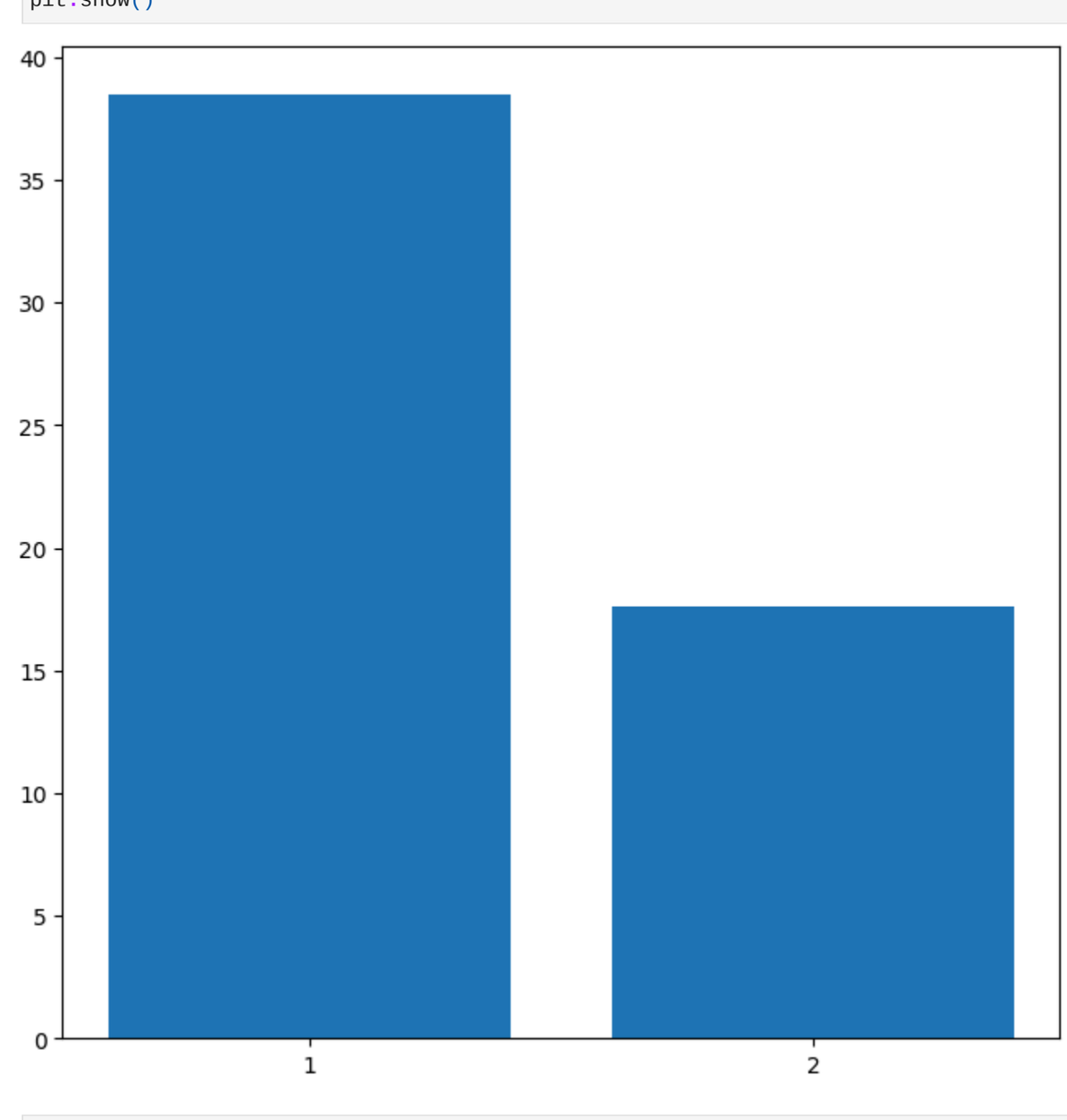
Two Principal Components

In [35]:
```python
pca = PCA(2)
data = pca.fit_transform(df_clusters[key_features_winsor])
```

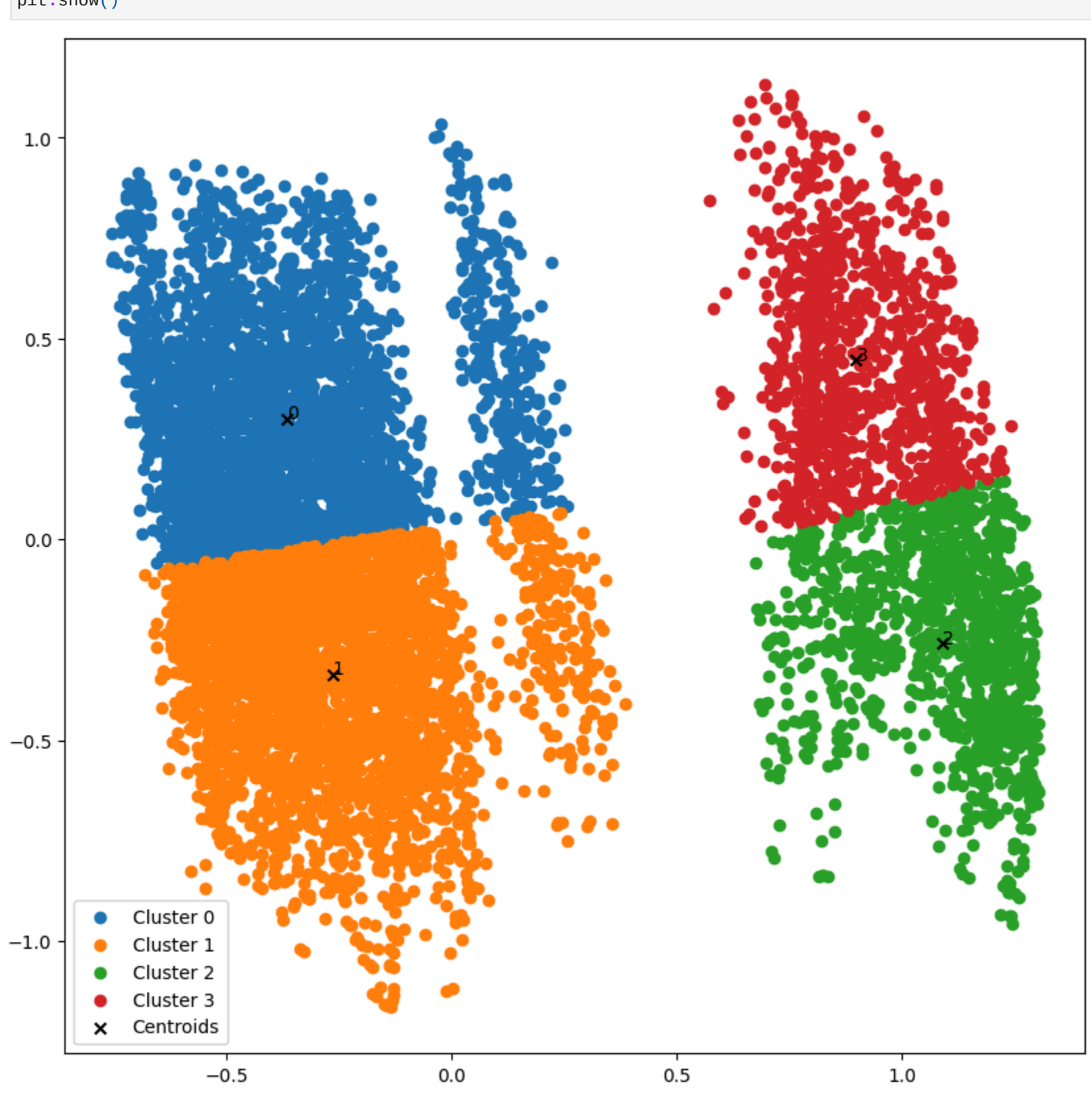
In [36]:
```python
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.90) + 1
```

Then, it is only necessary to consider 5 features in order to have at least 90% of the information associated to the variance of the original data

In [37]:
```python
plt.figure(figsize=(8,8))
var = np.round(pca.explained_variance_ratio_*100, decimals = 1)
lbls = [str(x) for x in range(1, len(var)+1)]
plt.bar(x=range(1,len(var)+1), height = var, tick_label = lbls)
plt.show()
```



In [38]:
```python
centers = np.array(km1.cluster_centers_)
# KMeans clustering
#model = KMeans(n_clusters=7, init="k-means++")
model = KMeans(n_clusters=len(list_labels), init="random", random_state=1492)

label = model.fit_predict(data)
centers = np.array(model.cluster_centers_)

# Plotting
plt.figure(figsize=(10, 10))
uniq = np.unique(label)

for i in uniq:
    plt.scatter(data[label == i, 0], data[label == i, 1], label=f'Cluster {i}')

plt.scatter(centers[:, 0], centers[:, 1], marker="x", color='k', label='Centroids')

# Annotating cluster points with labels
for i, txt in enumerate(uniq):
    plt.annotate(txt, (centers[i, 0], centers[i, 1]), fontsize=10, color='k')

plt.legend()
plt.show()
```



Limitations of Air Quality Models

Data Quality and Availability:

1. Incomplete data, for example, respect geolocation or vehicular traffic, or devices errors/calibrations can limit the accuracy of predictions.
2. Lack of real-time data integration might affect the responsiveness of the model to sudden changes in air quality.
3. Models might not adequately represent local variations if the spatial resolution is too coarse.

Possible Improvements

1. Increase the spatial and temporal resolution of models to capture microclimates and rapid changes better.
2. Use localized models for areas with significant human activity to get more accurate predictions for those regions.
3. Include traffic data, industrial output, and even social media data for real-time incident reporting.
4. Use advanced meteorological modeling to better understand and predict the impact of weather conditions.
5. Develop an integrated system that combines air quality data with public health data to directly correlate pollution levels with health outcomes. Different data sources APIs, etc.
6. Implement real-time data processing and predictive analytics to provide immediate warnings and updates.
7. Leverage IoT and edge computing to process data closer to the source, reducing latency.

Technical requirements

1. We would require BI-Dat Netherlands to put in production such type of models.
2. It would be important to consider a machine learning architecture to integrate the different data sources with the different stages of the production phase.
3. Data from the production phase should be collected in real time.
4. Hard time in need to exercise responses, depending of the final businesses goal, e.g. reduce the lead quantity of wo by moderns, hours, etc.
5. Data from different sources, such as machine sensors, ERP, MES, PLM, etc.
6. API, having to write, from different models, that presence scalable realms to real-world scenarios.
7. Integration of different data sources:traffic, industrial outputs, and social media.