

EDA_lab_7_March

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3 EDA lab

3.1 7 March, 2025

4 Outlier detection in Iris dataset

4.0.1 Using KNN method

4.0.2 Importing the necessary libraries

```
[1]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.datasets import load_iris
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
```

4.0.3 Loading the dataset

```
[2]: iris = load_iris()

## Creating dataframe with feature names
df = pd.DataFrame(iris.data, columns = iris.feature_names)
df['target'] = iris.target

df
```

```
[2]:      sepal length (cm)  sepal width (cm)  petal length (cm)  petal width (cm)  \
0                5.1             3.5             1.4             0.2
1                4.9             3.0             1.4             0.2
2                4.7             3.2             1.3             0.2
3                4.6             3.1             1.5             0.2
```

4	5.0	3.6	1.4	0.2
..
145	6.7	3.0	5.2	2.3
146	6.3	2.5	5.0	1.9
147	6.5	3.0	5.2	2.0
148	6.2	3.4	5.4	2.3
149	5.9	3.0	5.1	1.8

	target
0	0
1	0
2	0
3	0
4	0
..	...
145	2
146	2
147	2
148	2
149	2

[150 rows x 5 columns]

```
[3]: from sklearn.neighbors import NearestNeighbors

k = 5

nbrs = NearestNeighbors(n_neighbors=k+1)
nbrs.fit(df[['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)', 'petal_
↪width (cm)']])

distances, indices = nbrs.kneighbors(df[['sepal length (cm)', 'sepal width_
↪(cm)', 'petal length (cm)', 'petal width (cm)']])
avg_distance = distances[:,1:].mean(axis = 1)
df['Avg_Distance'] = avg_distance
threshold_knn = np.percentile(avg_distance, 95)
df['Outlier_KNN'] = df['Avg_Distance'] > threshold_knn
print("KNN method detected outliers(Without PCA):", df['Outlier_KNN'].sum())
```

KNN method detected outliers(Without PCA): 8

```
[4]: i1 = df[df['Outlier_KNN']== True].index
i1
```

```
[4]: Index([41, 98, 106, 109, 117, 118, 131, 135], dtype='int64')
```

4.1 Applying PCA to the dataset and checking the results

```
[5]: features = iris.feature_names
x = df.loc[:,features].values

scaler = StandardScaler()
x_std = scaler.fit_transform(x)

pca = PCA(n_components=2)
principalcomponents = pca.fit_transform(x_std)

principaldf = pd.DataFrame(data = principalcomponents, columns=['PC1', 'PC2'])
```

4.2 Detecting the outliers using KNN

```
[6]: k = 5

nbrs = NearestNeighbors(n_neighbors=k+1)
nbrs.fit(principaldf[['PC1', 'PC2']])

distances, indices = nbrs.kneighbors(principaldf[['PC1', 'PC2']])
avg_distance = distances[:,1:].mean(axis = 1)

principaldf['Avg_Distance'] = avg_distance

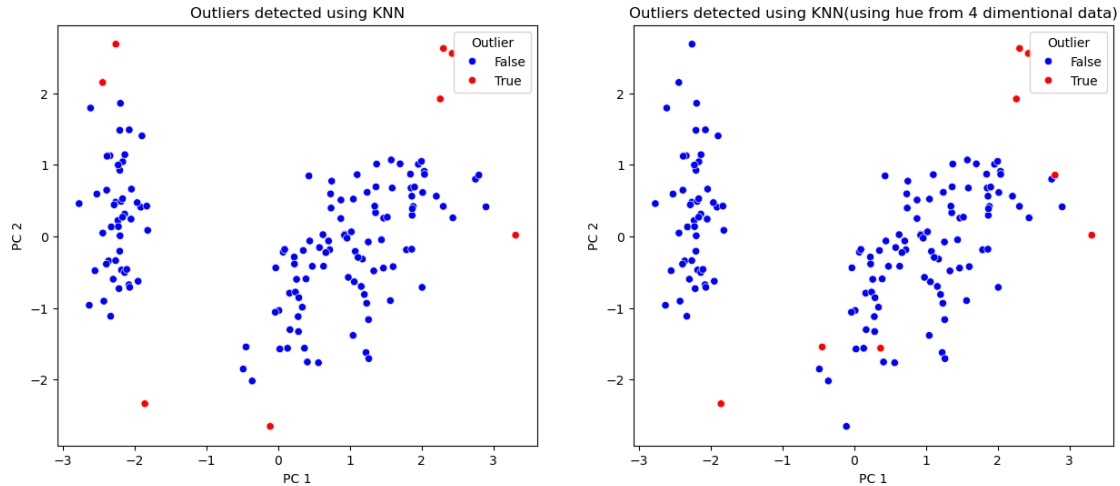
threshold_knn = np.percentile(avg_distance, 95)

principaldf['Outlier_KNN'] = principaldf['Avg_Distance'] > threshold_knn

#plot the KNN outlier detection results
plt.figure(figsize=(15,6))
plt.subplot(1,2,1)
sns.
    ↪scatterplot(x='PC1',y='PC2',data=principaldf,hue='Outlier_KNN',palette={False:
    ↪'blue',True:'red'})
plt.title("Outliers detected using KNN")
plt.xlabel("PC 1")
plt.ylabel("PC 2")
plt.legend(title='Outlier')
plt.subplot(1,2,2)
sns.
    ↪scatterplot(x='PC1',y='PC2',data=principaldf,hue=df['Outlier_KNN'],palette={False:
    ↪'blue',True:'red'})
plt.title("Outliers detected using KNN(using hue from 4 dimentional data)")
plt.xlabel("PC 1")
plt.ylabel("PC 2")
plt.legend(title='Outlier')
```

```
plt.show()

print("KNN method detected outliers(With PCA):",principaldf['Outlier_KNN'].
      ↪sum())
```



KNN method detected outliers(With PCA): 8

```
[7]: i2 = principaldf[principaldf['Outlier_KNN']== True].index
      print(i1)
      print(i2)
```

Index([41, 98, 106, 109, 117, 118, 131, 135], dtype='int64')

Index([15, 33, 41, 60, 109, 117, 118, 131], dtype='int64')

4.2.1 Inference:

- We have detected same number of outliers using KNN with and without applying PCA
- Though the total number of outlier is the same but, the index of the outlier is not exactly the same, i.e different data points are outlier before and after applying PCA

4.3 Using Mahalanobis Distance for outlier detection

```
[8]: from scipy.stats import chi2
      cov_matrix = np.cov(df[['sepal length (cm)', 'sepal width (cm)', 'petal length_
      ↪(cm)', 'petal width (cm)']].values.T)
      cov_inv = np.linalg.inv(cov_matrix)

      #Compute Mahalanobis distances for all observations.
      m_dist = []

      #Calculate the mean of the features to center the data.
```

```

mean_df = df[['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)', 'petal_
↳width (cm)']].mean().values

#Iterate through each row (observation) in the DataFrame.
for i, row in df[['sepal length (cm)', 'sepal width (cm)', 'petal length_
↳(cm)', 'petal width (cm)']].iterrows():
    #Calculate the difference between the observation and the mean.
    diff = row.values - mean_df

    #Compute the Mahalanobis distance for the observation.
    md = np.sqrt(np.dot(np.dot(diff.T, cov_inv), diff))

    m_dist.append(md)

#Add the Mahalanobis distances to the DataFrame.
df['Mahalanobis_dist'] = m_dist

#Determine the threshold from the chi-square distribution.
#dof: degrees of freedom, which is equal to the number of features (4 in this_
↳case).
dof = 4
alpha = 0.95 #Confidence level for the threshold (95% quantile)

#Calculate the threshold value (square root because we compute Euclidean-like_
↳distances).
threshold_maha = np.sqrt(chi2.ppf(alpha, dof))

#Flag observations as outliers if their Mahalanobis distance exceeds the_
↳threshold.
df['Outlier_Mahalanobis'] = df['Mahalanobis_dist'] > threshold_maha

#Print the number of outliers detected using the Mahalanobis method.
print("Mahalanobis method detected outliers(Without PCA):",_
↳df['Outlier_Mahalanobis'].sum())

```

Mahalanobis method detected outliers(Without PCA): 9

4.3.1 Using the PCA applied dataset

```

[9]: cov_matrix = np.cov(principaldf[['PC1', 'PC2']].values.T)
    cov_inv = np.linalg.inv(cov_matrix)

    #Compute Mahalanobis distances for all observations.
    m_dist = []

    #Calculate the mean of the features to center the data.
    mean_df = principaldf[['PC1', 'PC2']].mean().values

```

```

#Iterate through each row (observation) in the DataFrame.
for i, row in principaldf[['PC1','PC2']].iterrows():
    #Calculate the difference between the observation and the mean.
    diff = row.values - mean_df

    #Compute the Mahalanobis distance for the observation.
    md = np.sqrt(np.dot(np.dot(diff.T, cov_inv), diff))

    m_dist.append(md)

#Add the Mahalanobis distances to the DataFrame.
principaldf['Mahalanobis_dist'] = m_dist

#Determine the threshold from the chi-square distribution.
#dof: degrees of freedom, which is equal to the number of features (2 in this
    ↪case).
dof = 2
alpha = 0.95 #Confidence level for the threshold (95% quantile)

#Calculate the threshold value (square root because we compute Euclidean-like
    ↪distances).
threshold_maha = np.sqrt(chi2.ppf(alpha, dof))

#Flag observations as outliers if their Mahalanobis distance exceeds the
    ↪threshold.
principaldf['Outlier_Mahalanobis'] = principaldf['Mahalanobis_dist'] >
    ↪threshold_maha

#Print the number of outliers detected using the Mahalanobis method.
print("Mahalanobis method detected outliers(after applying PCA):",
    ↪principaldf['Outlier_Mahalanobis'].sum())

```

Mahalanobis method detected outliers(after applying PCA): 6

4.4 Visualizing

```

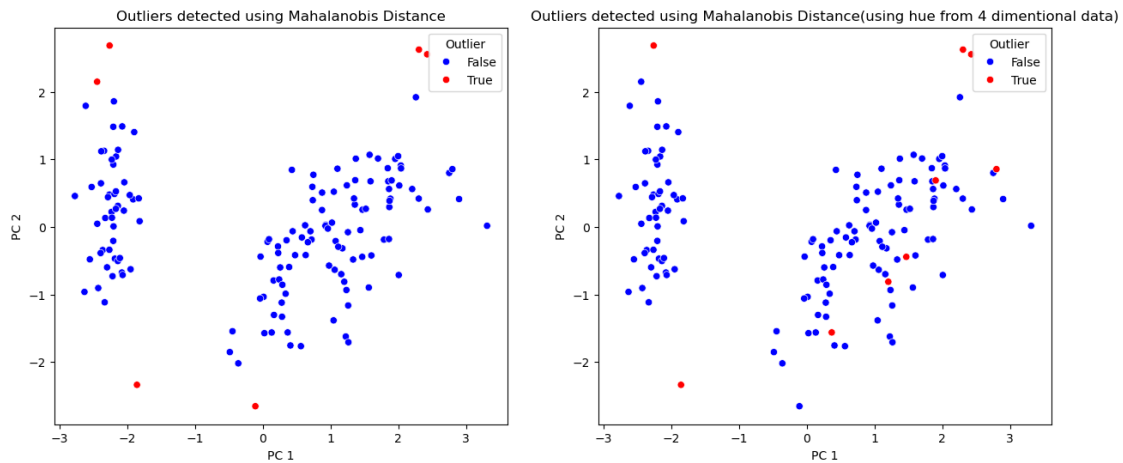
[10]: plt.figure(figsize=(15,6))
plt.subplot(1,2,1)
sns.
    ↪scatterplot(x='PC1',y='PC2',data=principaldf,hue='Outlier_Mahalanobis',palette={False:
    ↪'blue',True:'red'})
plt.title("Outliers detected using Mahalanobis Distance")
plt.xlabel("PC 1")
plt.ylabel("PC 2")
plt.legend(title='Outlier')
plt.subplot(1,2,2)

```

```

sns.
    ↳scatterplot(x='PC1',y='PC2',data=principaldf,hue=df['Outlier_Mahalanobis'],palette={False:
    ↳'blue',True:'red'})
plt.title("Outliers detected using Mahalanobis Distance(using hue from 4_
    ↳dimensional data)")
plt.xlabel("PC 1")
plt.ylabel("PC 2")
plt.legend(title='Outlier')
plt.show()

```



4.4.1 Inference:

- Using Mahalanobis Distance for outlier detection on the 4 features without PCA we have got 9 outliers and after applying PCA we got 6 outliers
- Data points of different index are identified as outliers before and after applying PCA.