

第一次作品：主成分分析實作

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作品目標：透過python將主成分概念視覺化表現出來

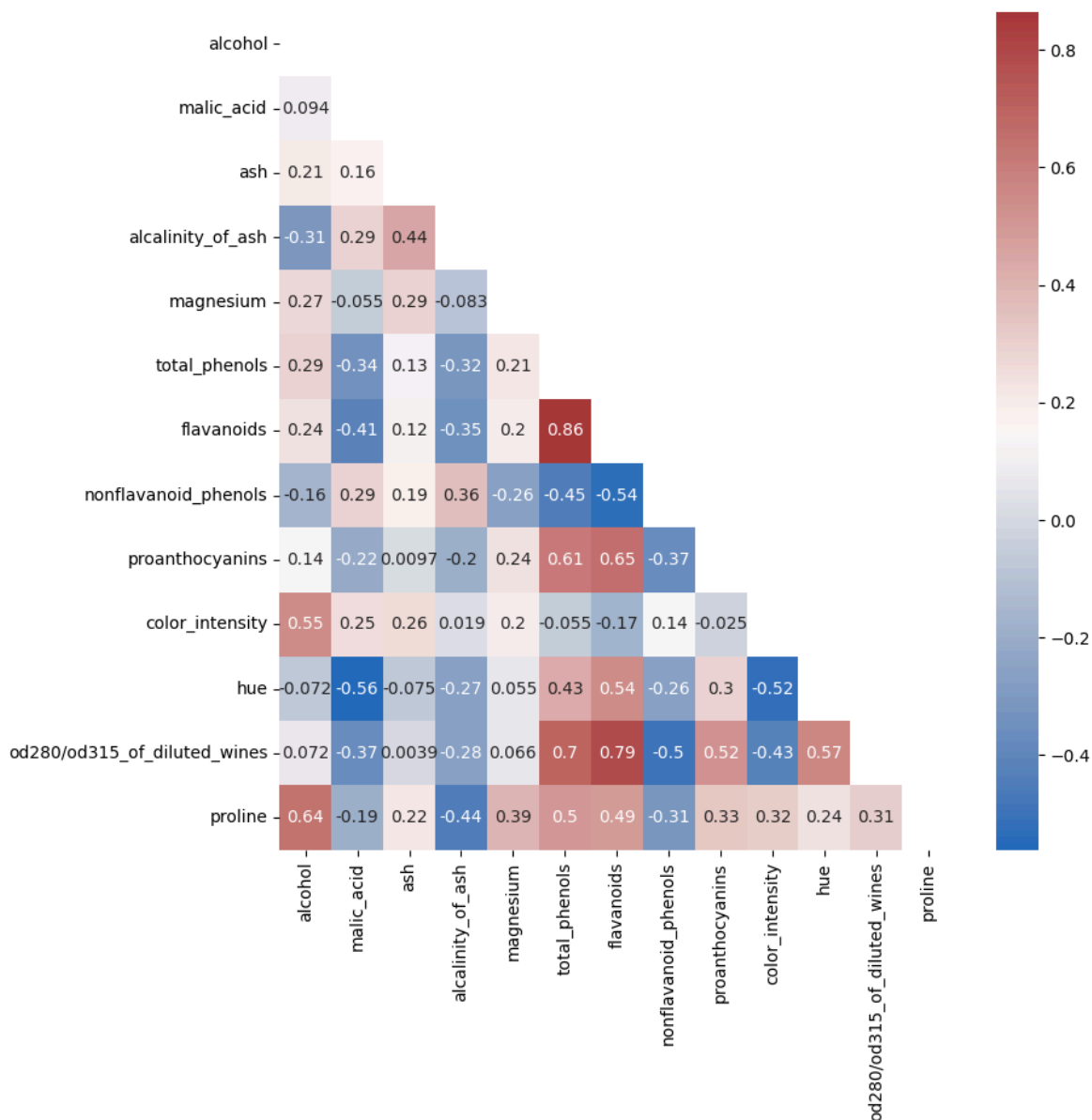
第 1 題：

有一組資料來自義大利某個地區三個紅酒製造商所產的紅酒，資料內容包括的 178 支紅酒的 13 種化學成分。利用這組資料回答下列問題：

(1) 繪製變數間的相關係數圖，以觀察變數間是否存在相關性。

- 在sklearn套件中下載紅酒資料
- 造出變數間的相關矩陣
- 由藍色到紅色依序表示相關程度由低到高

```
In [ ]: import pandas as pd
import numpy as np
import seaborn
import matplotlib.pyplot as plt
from sklearn.datasets import load_wine
# Load the wine dataset
X, y = load_wine(return_X_y=True, as_frame=True)
labels = X.columns
# Plot the correlation matrix
plt.figure(figsize = (9, 9))
R = X.corr()
mask = np.triu(np.ones_like(R, dtype=bool)) # diagonal mask
seaborn.heatmap(R, annot=True, mask = mask, cmap='vlag')
plt.show()
```



結論:

- 由圖形中可以看出，Flavanoids和Total_Phenols此兩變數最高度相關
- 相關係數矩陣為對稱矩陣，因此僅呈現下半部。

(2)繪製含每個化學成分變數盒鬚圖，分別畫為標準化與標準化。

- 資料未標準化之前為極度不平衡資料，可看出唯獨Proline 值特別大，因此需要做資料前處理
- 標準化後才不會受原始變數的數字大小所影響
- ratings為未標準化資料矩陣，ratings_為標準化資料矩陣

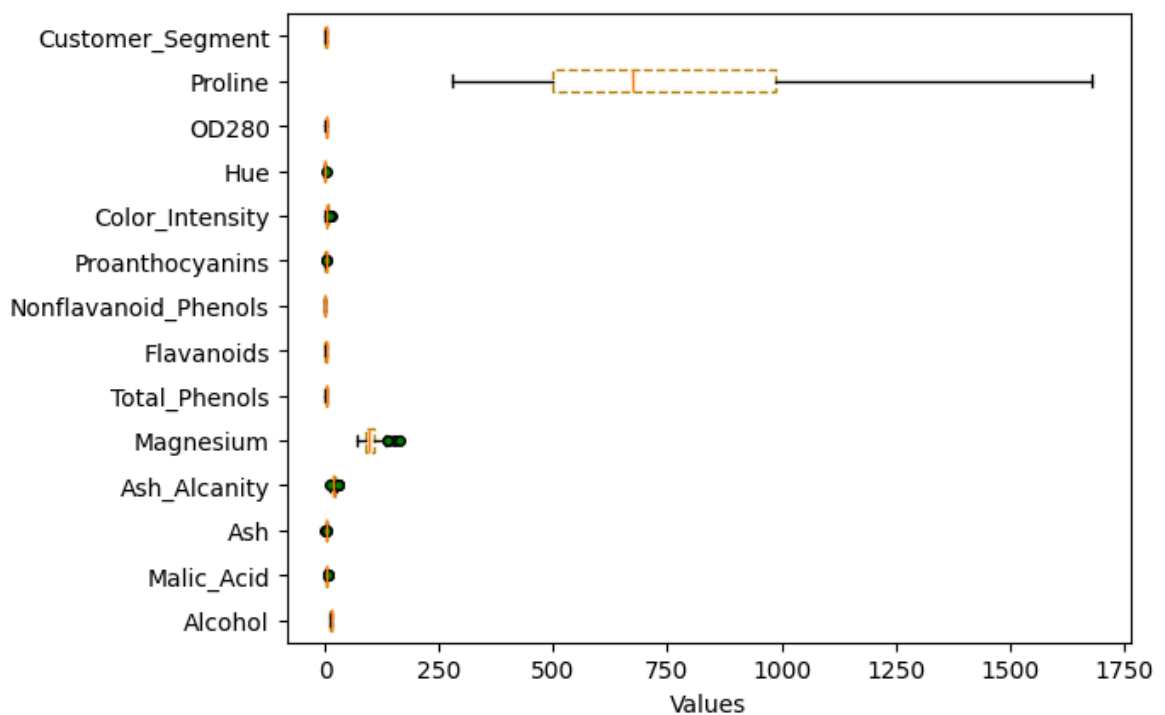
```
In [ ]: df = pd.read_excel('wine.xlsx')
ratings = np.array(df)
categories = df.columns
fig, ax = plt.subplots()
boxprops = dict(linestyle = '--', linewidth = 1, \
color = 'darkgoldenrod')
flierprops = dict(marker='o', markerfacecolor = 'green',
markersize = 4, linestyle = 'none')
```

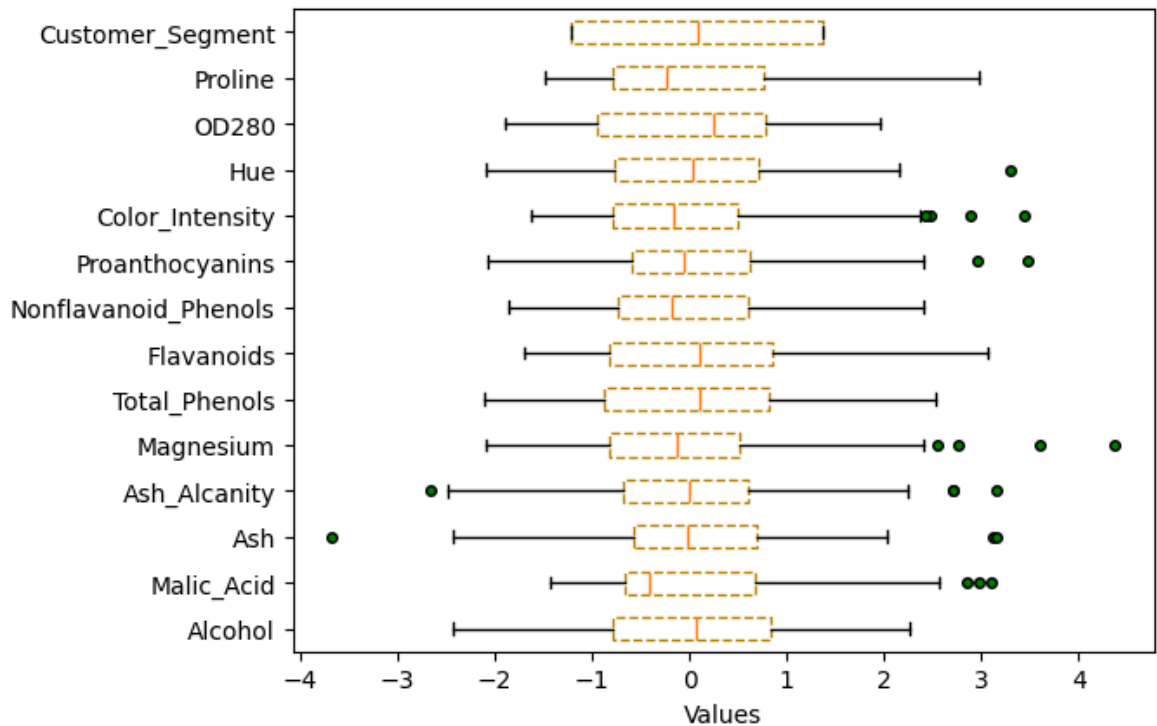
```

ax.boxplot(ratings, boxprops = boxprops, \
flierprops = flierprops, \
labels = categories, vert = False)
ax.set_xlabel('Values')
plt.show()

df = pd.read_excel('wine.xlsx')
ratings = np.array(df)
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(ratings)
ratings_ = scaler.transform(ratings)
categories = df.columns
fig, ax = plt.subplots()
boxprops = dict(linestyle = '--', linewidth = 1, \
color = 'darkgoldenrod')
flierprops = dict(marker='o', markerfacecolor = 'green',
markersize = 4, linestyle = 'none')
ax.boxplot(ratings_, boxprops = boxprops, \
flierprops = flierprops, \
labels = categories, vert = False)
ax.set_xlabel('Values')
plt.show()

```





(3) 進行主成分分析，繪製特徵值由大而小的分布與 scree plot。

- 利用numpy指令cov計算樣本共變異數矩陣 S_x
- 比較後發現 S_x 與 S_x -formula一致
- ratings_ is a 178 by 13 data matrix

```
In [ ]: import numpy as np
Sx = np.cov(ratings_.T, bias=False)
N = ratings_.shape[0]
mu_x = ratings_.mean(axis = 0)
Tmp = ratings_ - mu_x
Sx_formula = Tmp.T @ Tmp / (N - 1)
#print(Sx_formula)
```

接著進一步對共變異矩陣 S_x 進行特徵值與特徵向量分析，取得由大而小排列的特徵值及相對應特徵向量，最後再將特徵值與特徵向量合併回到原來的樣本共變異矩陣。

```
In [ ]: from numpy.linalg import eig
from numpy.linalg import inv
w, v = eig(Sx)
idx = np.argsort(-w) #sort eigenvalues in descending order
# idx = np.argsort(w)[::-1]
eigvals = w[idx]
eigvecs = v[:, idx]
Sigma_x = eigvecs @ np.diag(eigvals) @ eigvecs.T
```

將特徵分布印出觀察以下兩圖

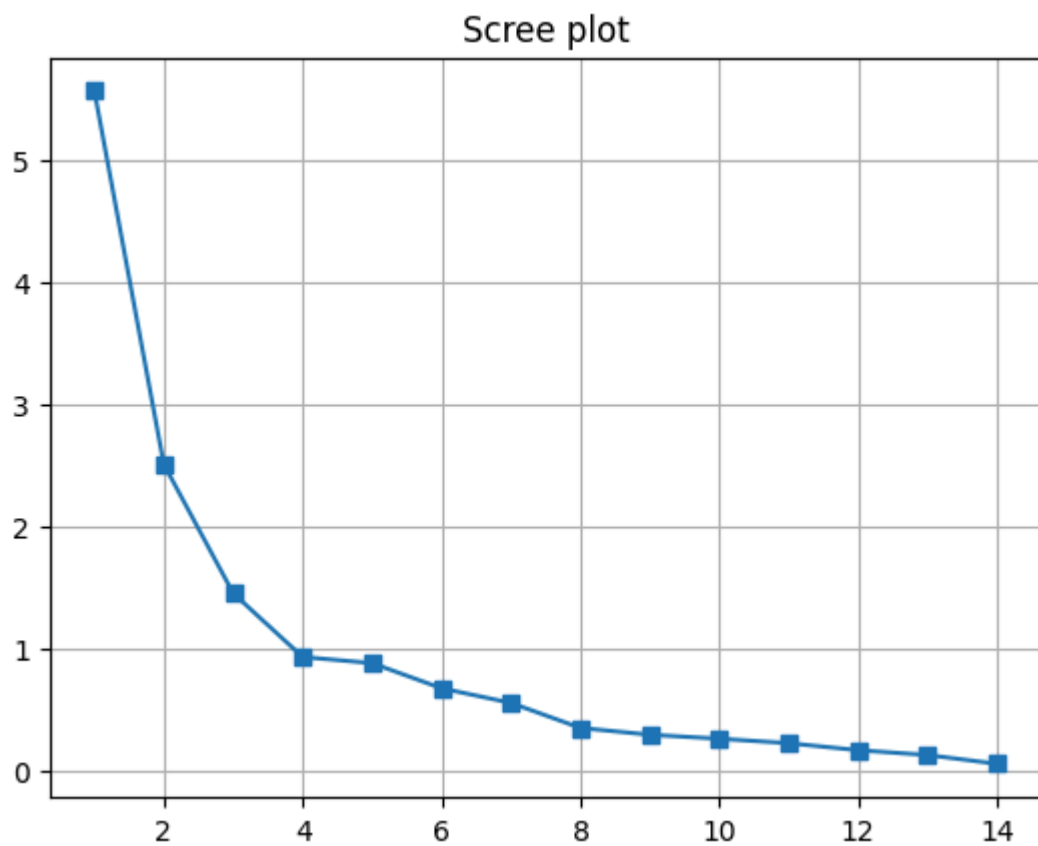
- Screen plot 主成分由大到小的分布
- Pareto plot 加入累積變異的比例

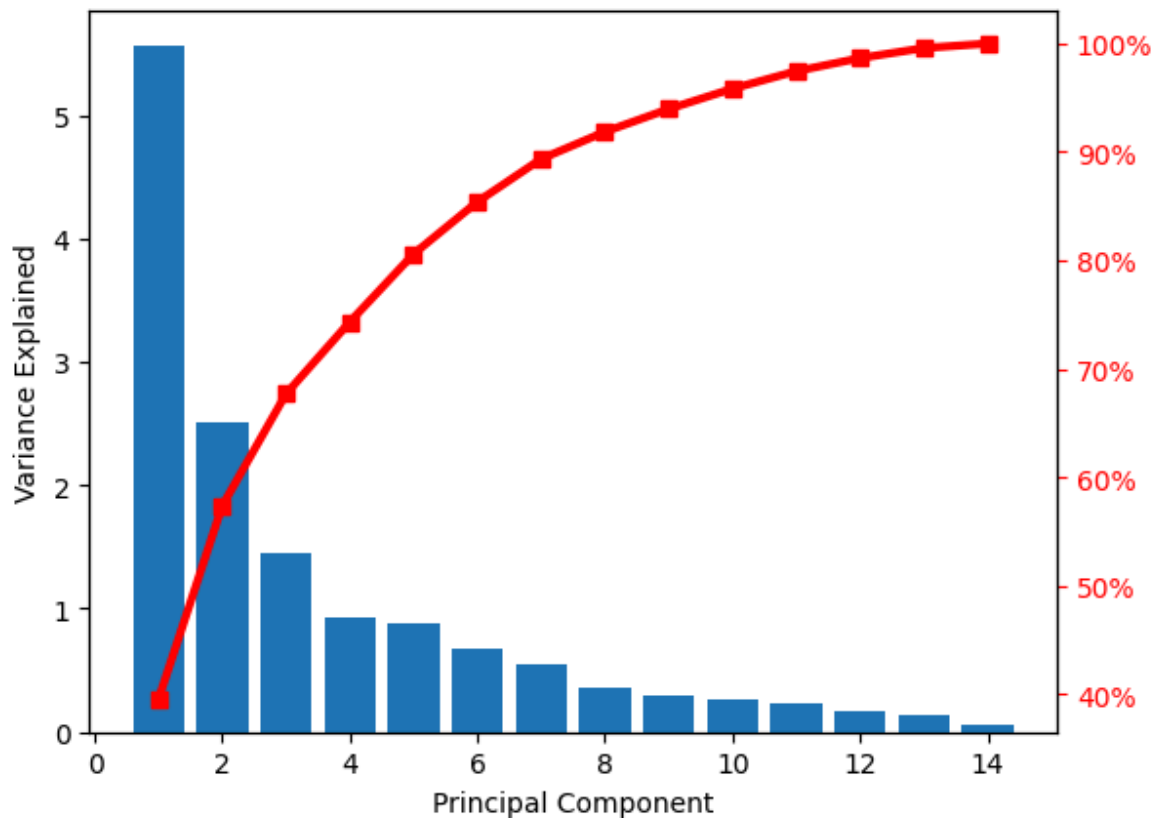
```
In [ ]: from matplotlib.ticker import PercentFormatter
plt.figure()
```

```

x = np.arange(1, 1+len(eigvals))
plt.plot(x, eigvals, marker='s')
plt.title('Scree plot')
plt.grid(True)
plt.show()
fig, ax = plt.subplots()
x = np.arange(1, 1+len(eigvals))
ax.bar(x, eigvals)
ax2 = ax.twinx()
ax2.plot(x, eigvals.cumsum()/eigvals.sum()*100, \
marker='s', color='red', lw=3)
ax2.tick_params(axis='y', colors='red')
ax2.yaxis.set_major_formatter(PercentFormatter())
ax.set_xlabel('Principal Component')
ax.set_ylabel('Variance Explained')
plt.show()

```



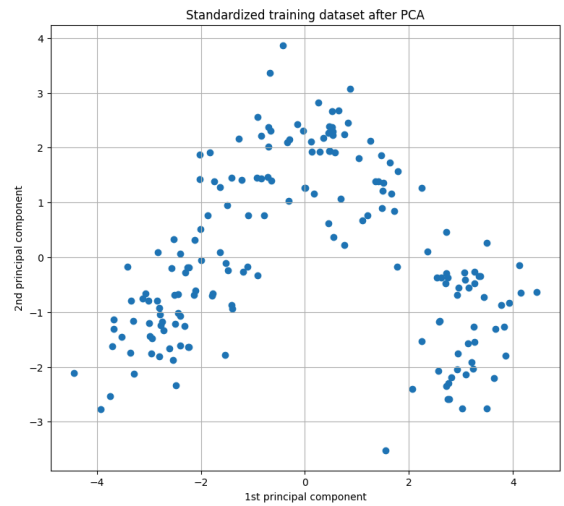
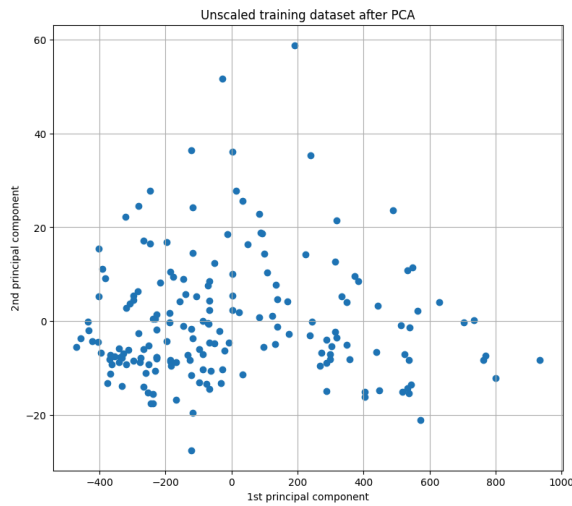


(4) 利用主成分分析取得前兩項成分，並繪製其散布圖

- 左圖為資料不做標準化，取前兩大主成分得到的散佈圖。
- 右圖為資料標準化後，取兩個主成分得到的散佈圖。

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler

# 對未標準化的資料做PCA
pca = PCA().fit(ratings)
Z = pca.transform(ratings)
# 對標準化的資料做PCA
scaler = StandardScaler()
scaler.fit(ratings_)
ratings_ = scaler.transform(ratings_)
pca = PCA().fit(ratings_)
Z1 = pca.transform(ratings_)
# 做圖
fig, ax = plt.subplots(1, 2, figsize = (20, 8))
ax[0].scatter(Z[:,0], Z[:,1])
ax[0].set_xlabel('1st principal component')
ax[0].set_ylabel('2nd principal component')
ax[0].set_title("Unscaled training dataset after PCA")
ax[0].grid(True)
ax[1].scatter(Z1[:,0], Z1[:,1])
ax[1].set_xlabel('1st principal component')
ax[1].set_ylabel('2nd principal component')
ax[1].grid(True)
ax[1].set_title("Standardized training dataset after PCA")
plt.show()
```



由右圖可以看出兩個主成分包含三個群組，並往下將此三組以顏色區隔

(5) 再依據每個資料的標籤，為每個在散布圖上的資料點依據標籤塗上顏色

- 左圖為資料不做標準化，得到標籤顏色分類的散佈圖。
- 右圖為資料標準化後，得到標籤顏色分類的散佈圖。

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler

# 對未標準化的資料做PCA
pca = PCA().fit(ratings)
Z = pca.transform(ratings)
# 對標準化的資料做PCA
scaler = StandardScaler()
scaler.fit(ratings_)
ratings_ = scaler.transform(ratings_)
pca = PCA().fit(ratings_)
Z1 = pca.transform(ratings_)
# 做圖
fig, (ax1, ax2) = plt.subplots(nrows=1, ncols=2, figsize=(10, 5))

target_classes = range(0, 3)
colors = ("blue", "red", "green")
markers = ("^", "s", "o")

for target_class, color, marker in zip(target_classes, colors, markers):
    ax1.scatter(
        x=Z[y == target_class, 0],
        y=Z[y == target_class, 1],
        color=color,
        label=f"class {target_class + 1}",
        alpha=0.5,
        marker=marker,
    )

    ax2.scatter(
        x=Z1[y == target_class, 0],
        y=Z1[y == target_class, 1],
        color=color,
```

```

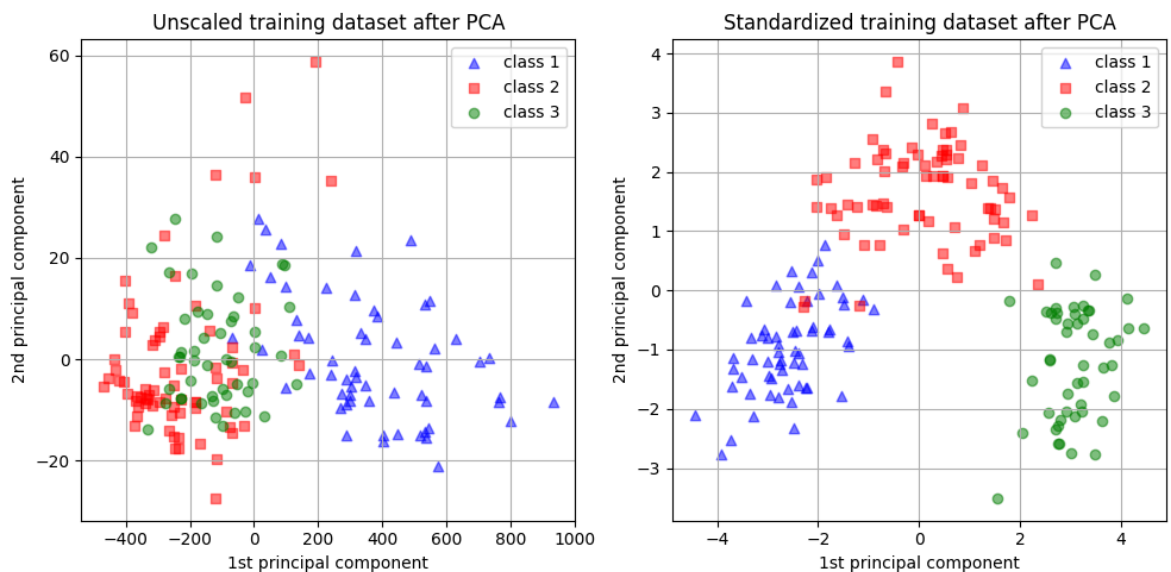
        label=f"class {target_class +1}",
        alpha=0.5,
        marker=marker,
    )

ax1.set_title("Unscaled training dataset after PCA")
ax2.set_title("Standardized training dataset after PCA")

for ax in (ax1, ax2):
    ax.set_xlabel("1st principal component")
    ax.set_ylabel("2nd principal component")
    ax.legend(loc="upper right")
    ax.grid()

_ = plt.tight_layout()

```



結論:

由比較圖可以看出資料是否做標準化相當重要，未做標準化主成分分析後並不能明確分群；

做完標準化之後，才能明顯區分來自不同酒莊的酒。

(6) 採取三個主成分，並繪製立體圖:

- 此圖為原始資料未做標準化得出的結果

```

In [ ]: import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.datasets import load_wine
from sklearn.decomposition import PCA

# Load the wine dataset
X, y = load_wine(return_X_y=True)

# unscale data Perform PCA
pca = PCA(n_components=3)
Z1 = pca.fit_transform(X)

```



```

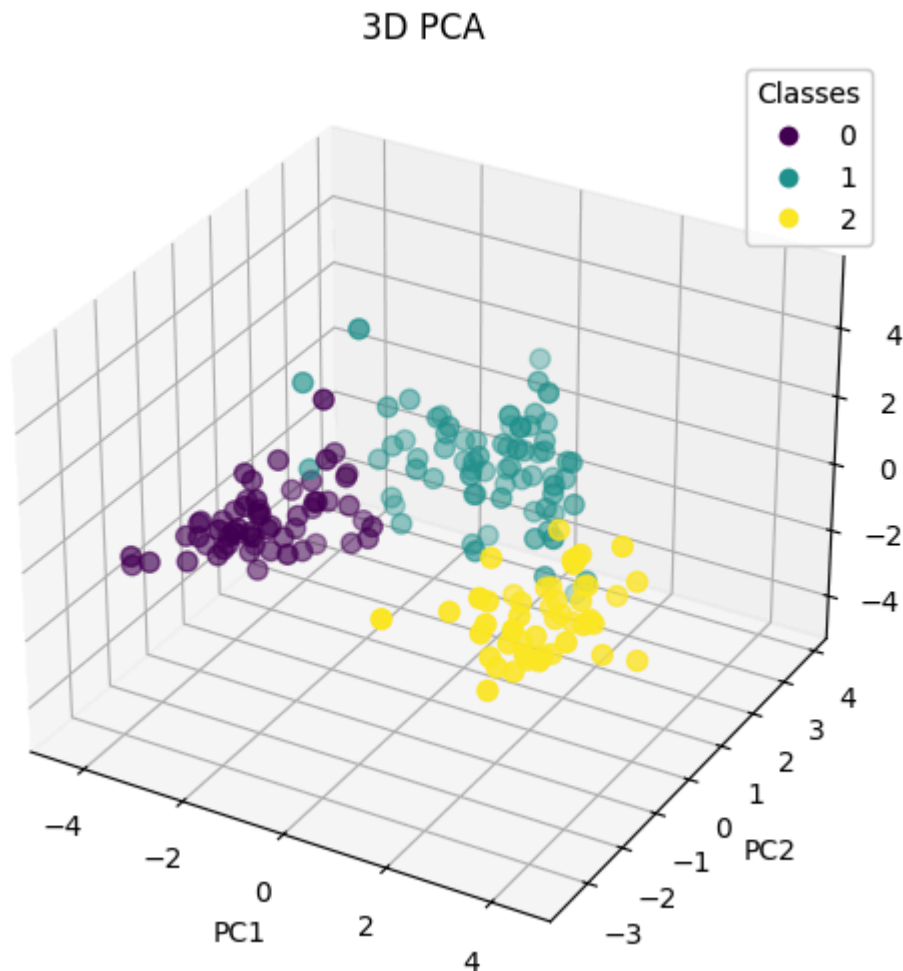
#scale data preform PCA
scaler = StandardScaler()
scaler.fit(ratings_)
ratings_ = scaler.transform(ratings_)
pca = PCA().fit(ratings_)
Z1 = pca.transform(ratings_)

# Plot 3D figure
fig = plt.figure(figsize=(8, 6))
ax = fig.add_subplot(111, projection='3d')

# Scatter plot
scatter = ax.scatter(Z1[:,0], Z1[:,1], Z1[:,2], c=y, cmap='viridis', s=50)
ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
ax.set_title('3D PCA')

# Legend
legend = ax.legend(*scatter.legend_elements(), title='Classes')
ax.add_artist(legend)
plt.show()

```



可以觀察到，第一個主成份的級距與另外兩座標軸相差極大，因此將資料標準化後再次觀察

```

In [ ]: import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

```

```

from sklearn.datasets import load_wine
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA

# Load the wine dataset
X, y = load_wine(return_X_y=True)

# Standardize the features
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)

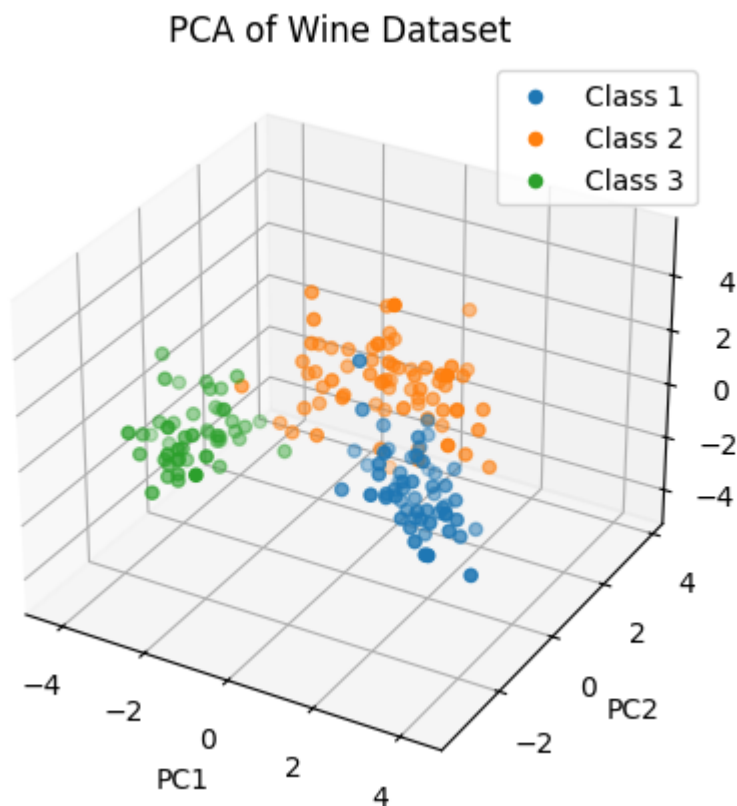
# Perform PCA
pca = PCA(n_components=3)
Z1 = pca.fit_transform(X_scaled)

# Create a 3D plot
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

# Plot each class separately
for i in np.unique(y):
    ax.scatter(Z1[y == i, 0], Z1[y == i, 1], Z1[y == i, 2], label=f'Class {i+1}')

ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
ax.set_title('PCA of Wine Dataset')
ax.legend()
plt.show()

```



做完資料標準化後，此時三個主成份級距接近，較能觀察出資料分群的概況，並嘗試轉化圖形角度，找出最適合看出分群概況的3D立體圖

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.datasets import load_wine
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA

# Load the wine dataset
X, y = load_wine(return_X_y=True)

# Standardize the features
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)

# Perform PCA
pca = PCA(n_components=3)
Z1 = pca.fit_transform(X_scaled)

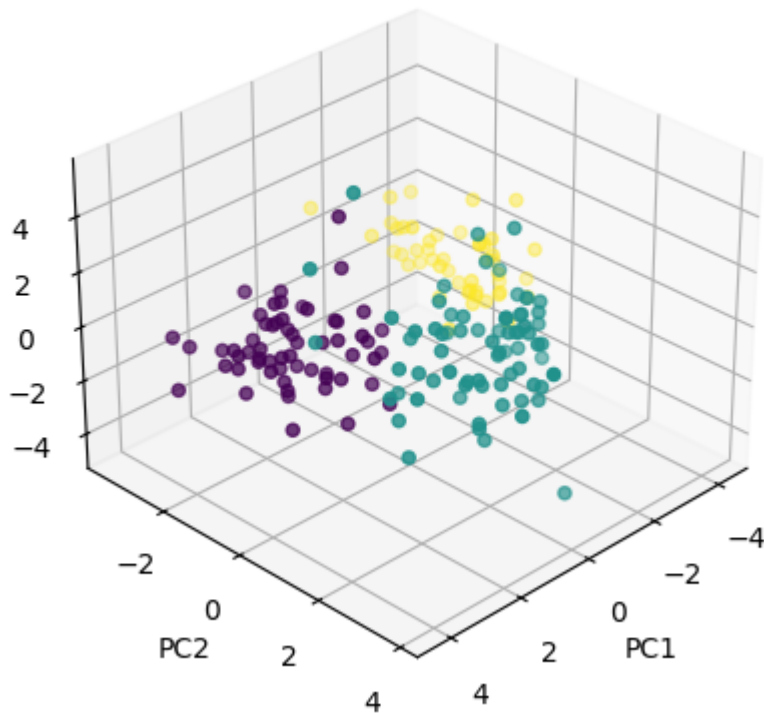
# Plot 3D scatter plot
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

# Scatter plot
ax.scatter(Z1[:, 0], Z1[:, 1], Z1[:, 2], c=y, cmap='viridis', marker='o')

# Set labels and title
ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
ax.set_title('PCA of Wine Dataset')

# Rotate the plot for better viewing angle
ax.view_init(elev=30, azimuth=45)
plt.show()
```

PCA of Wine Dataset



上圖的角度最能明確觀察到分群的狀況

(7) Z_1 與 Z_2 都是從原變數組合而成的新變數，可否從 Z_1 與 Z_2 的組成係數，看出原變數哪個比較重要？哪個比較不重要？若再與原變數間的相關係數圖對照，是否透露相同的訊息。

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
pca = PCA(n_components=1).fit(X) # 取第一個特徵向量
pca = PCA().fit(ratings_) # 進行主成分分析
#print(pca.explained_variance_ratio_) # 共變異矩陣特徵值佔比
# print(pca.explained_variance_) # 共變異矩陣的特徵值
# print(pca.components_) # 共變異矩陣的特徵向量
eigvals = pca.explained_variance_
#print(eigvals)
eigvecs = pca.components_.T # by column [v1 v2]
print(eigvecs)
```

```

[[-0.13632501 -0.48416087 -0.20740081 -0.08191848 -0.25089415 -0.13517139
  -0.09269887 -0.42154435 -0.45019071  0.31127983 -0.22154641 -0.26411262
  -0.05610645  0.09062605]
 [ 0.22267638 -0.22359095  0.08879606  0.46988824 -0.18860015 -0.59841948
  0.3743698  -0.08757556 -0.00602569 -0.32592413  0.06839251  0.1192121
  0.06675544 -0.02522531]
 [-0.00225793 -0.31585588  0.62610236 -0.24984122 -0.0935236  -0.10799983
  -0.16708856  0.17208034  0.26249446 -0.12452347 -0.49452428 -0.04502305
  -0.19201787 -0.00163582]
 [ 0.22429849  0.01161574  0.6119896  0.07199322  0.0465675  0.08811224
  -0.26872469 -0.41324857 -0.11863342  0.15716811  0.47461722 -0.06131271
  0.20007784 -0.09536107]
 [-0.12463016 -0.30055143  0.13098458 -0.16321412  0.77833048 -0.14483831
  0.32957951  0.14881189 -0.25253628  0.12773363  0.07119731  0.06116074
  0.05829909  0.02230075]
 [-0.35926404 -0.06711983  0.14650775  0.19098521 -0.14466563  0.14809748
  -0.03789829  0.36343884 -0.40637354 -0.30772263  0.29740957 -0.30087591
  -0.35952714 -0.25303779]
 [-0.39071171  0.00131345  0.15096275  0.14461667 -0.11200553  0.06247252
  -0.06773223  0.175405  -0.09091933 -0.14044  -0.03219187 -0.05001396
  0.59834288  0.60190917]
 [ 0.2670012  -0.0269887  0.16997551 -0.32801272 -0.43257916  0.25868639
  0.61111195  0.23075135 -0.15912282  0.24054263  0.12200984  0.04266558
  0.06403952  0.08223093]
 [-0.2790625  -0.04122256  0.14987959  0.46275771  0.0915882  0.46627764
  0.42292282 -0.3437392  0.26578679  0.10869629 -0.23292405 -0.09334264
  -0.11013538 -0.05864198]
 [ 0.08931829 -0.52978274 -0.1372663  0.07211248 -0.0462696  0.42525454
  -0.18613617  0.04069617 -0.07526459 -0.21704255  0.01972448  0.59795428
  0.15917751 -0.17882114]
 [-0.27682265  0.27790735  0.08532854 -0.43466618 -0.02986657 -0.01565089
  0.19204101 -0.48362564 -0.21241681 -0.50966073 -0.06140493  0.25774292
  -0.04923091 -0.02258256]
 [-0.35052618  0.16277625  0.16620436  0.15672341 -0.14419358 -0.21770365
  -0.0785098  0.06865116 -0.08426484  0.45570504  0.06646166  0.61109218
  -0.32941979  0.13509216]
 [-0.26951525 -0.36605886 -0.12668685 -0.2557949  -0.08440794 -0.0665655
  0.0542037  -0.11146671  0.54490539 -0.04620802  0.55130818 -0.07268036
  -0.17322892  0.21604362]
 [ 0.39366953 -0.00569041  0.00121795  0.12246373  0.15758395  0.20033864
  -0.05938234 -0.07179553 -0.16236882 -0.19899373  0.01444169  0.01575769
  -0.49224318  0.66904528]]

```

結論:

由上結果可以看出，透過觀察組成的係數，可以清楚理解原變數在建構 Z_1 Z_2 新變數時的重要性。係數的絕對值越大，則表示原變數的貢獻越大；相反的，如果組成係數趨近於零，則表示原始變數幾乎沒貢獻，在數據解釋中較不重要。而相關係數可以更直觀的理解變數之間的關係；因此，綜合考慮兩點才能更全面的理解數據。

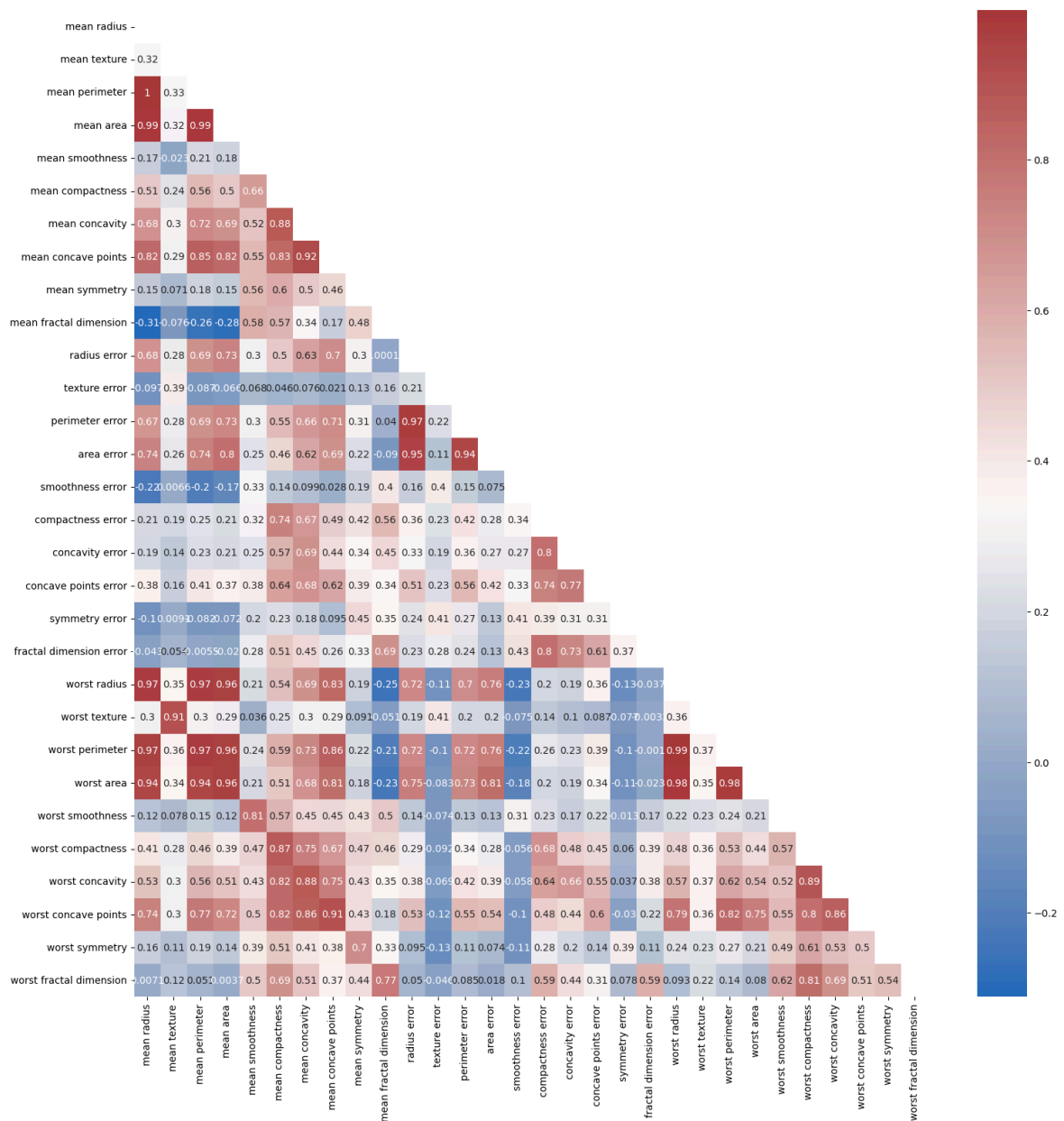
第 2 題：

有一組關於乳癌患者腫瘤的影像量測資料，資料內容包括30個變數，樣本數為 569 位患者，區分為兩個群組，分別是 Malignant (惡性腫瘤) 與 Benign (良性腫瘤)。利用這組資料回答下列問題：

(1) 繪製變數間的相關係數圖，以觀察變數間是否存在相關性。

- 在sklearn套件中下載breast_cancer資料
- 由下圖可知，方框越紅代表越高度相關

```
In [ ]: import pandas as pd
import numpy as np
import seaborn
import matplotlib.pyplot as plt
from sklearn.datasets import load_breast_cancer
# Load the breast cancer dataset
X, y = load_breast_cancer(return_X_y=True, as_frame=True)
labels = X.columns
# Plot the correlation matrix
plt.figure(figsize = (18, 18))
R = X.corr()
mask = np.triu(np.ones_like(R, dtype=bool)) # diagonal mask
seaborn.heatmap(R, annot=True, mask = mask, cmap='vlag')
plt.show()
```



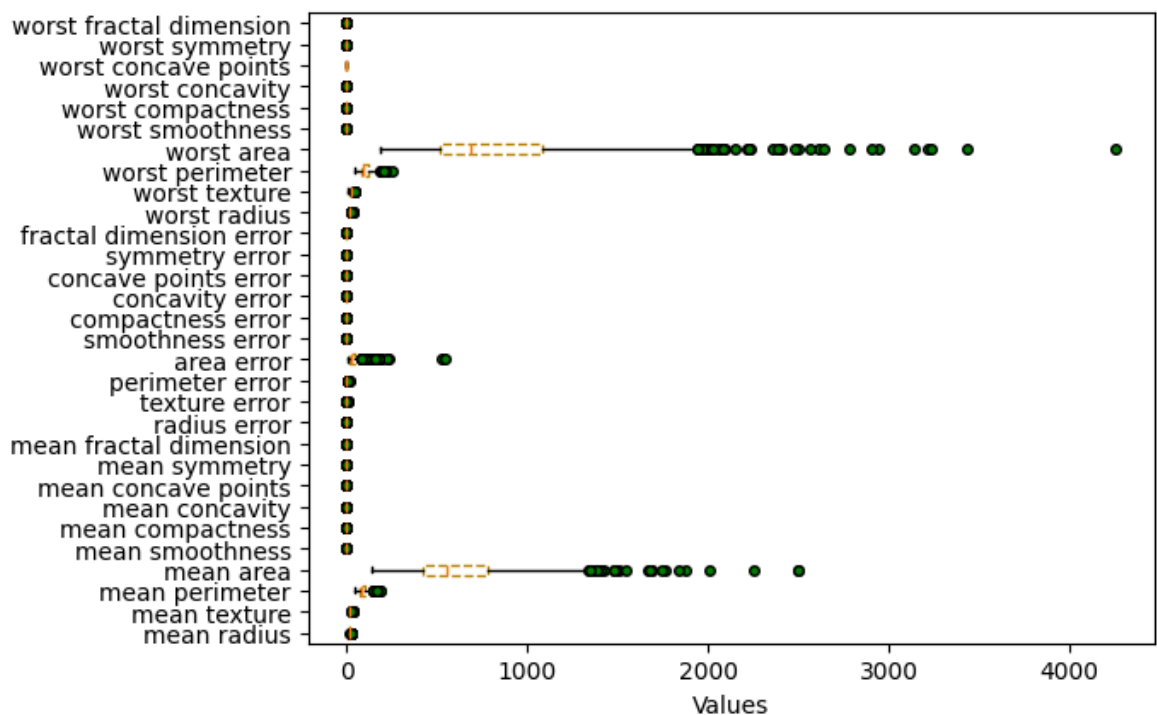
結論:

- 變數很多，故須將圖片放大才能清楚呈現變數之間的相關性
- 相關係數矩陣為對稱矩陣，因此僅呈現下半部。

(2)繪製含每個化學成分變數盒鬚圖，觀察每個變數的 scaling，分別畫為標準化與標準化。

- 下圖為未標準化的資料
- breast_cancer_data_array為未標準化資料矩陣

```
In [ ]: from sklearn.datasets import load_breast_cancer
import numpy as np
breast_cancer = load_breast_cancer(as_frame=True)
breast_cancer_data = breast_cancer.data
breast_cancer_target = breast_cancer.target
breast_cancer_data_array = np.array(breast_cancer_data)
breast_cancer_data_cate = breast_cancer_data.columns
fig, ax = plt.subplots()
boxprops = dict(linestyle = '--', linewidth = 1, \
color = 'darkgoldenrod')
flierprops = dict(marker='o', markerfacecolor = 'green', \
markersize = 4, linestyle = 'none')
ax.boxplot(breast_cancer_data_array
, boxprops = boxprops, \
flierprops = flierprops, \
labels = breast_cancer_data_cate
, vert = False)
ax.set_xlabel('Values')
plt.show()
```

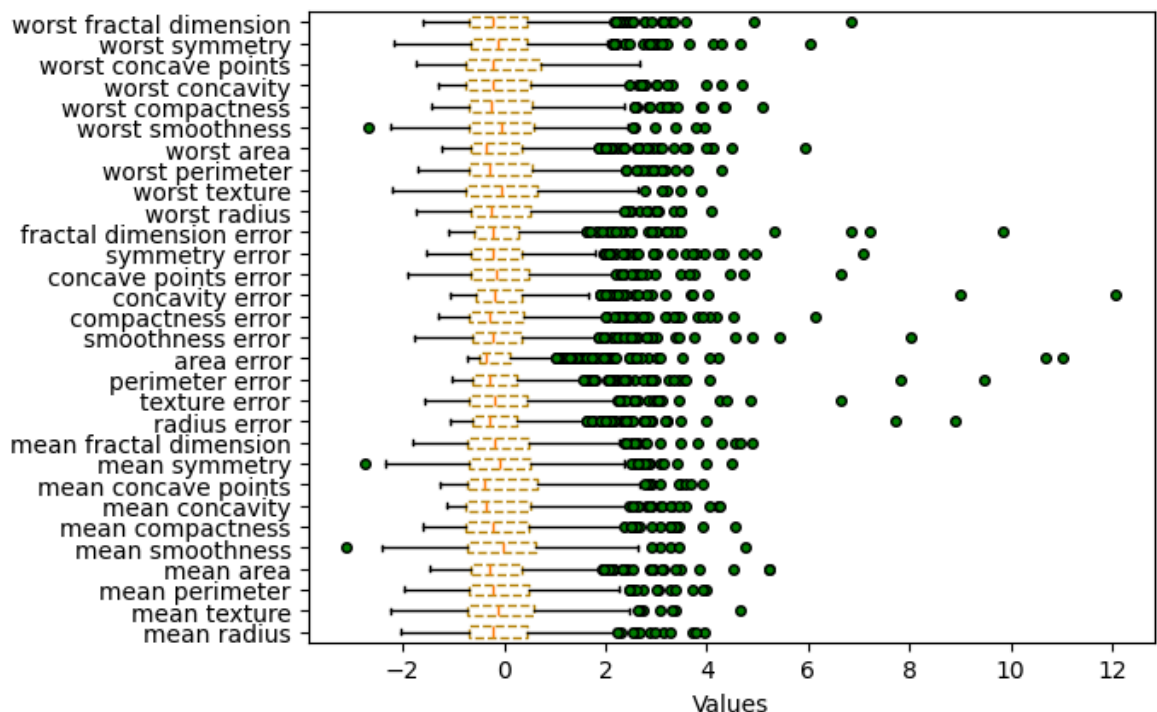


結論:

- 未標準化的資料，明顯發現需要標準化才能有相似的級距
- 可以觀察到 worst area 與mean area 這兩項變數的值特別不平衡

下圖為已標準化資料的盒鬚圖

```
In [ ]: from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(breast_cancer_data_array)
breast_cancer_data_array_ = scaler.transform(breast_cancer_data_array)
breast_cancer_data_cate = breast_cancer_data.columns
fig, ax = plt.subplots()
boxprops = dict(linestyle = '--', linewidth = 1, \
color = 'darkgoldenrod')
flierprops = dict(marker='o', markerfacecolor = 'green', \
markersize = 4, linestyle = 'none')
ax.boxplot(breast_cancer_data_array_, boxprops = boxprops, \
flierprops = flierprops, \
labels = breast_cancer_data_cate, vert = False)
ax.set_xlabel('Values')
plt.show()
```



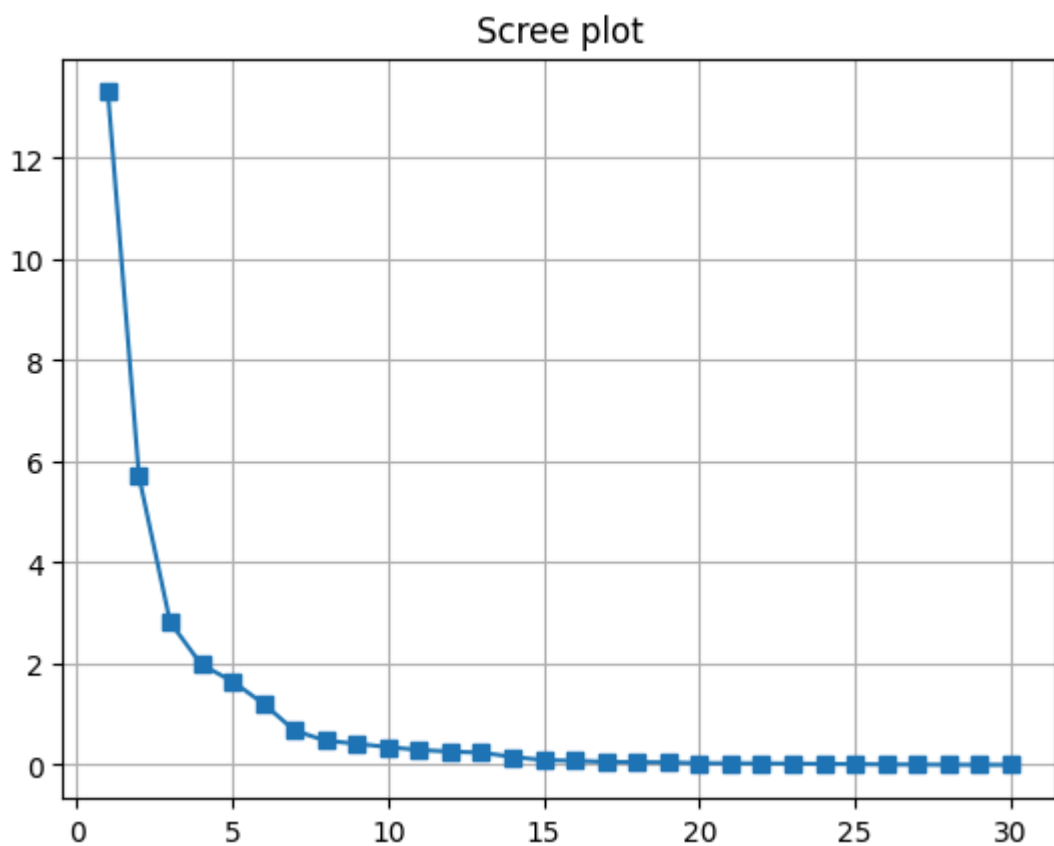
結論:在資料分析前都需要資料前處理，以確保不會有極端不平衡的狀況出現

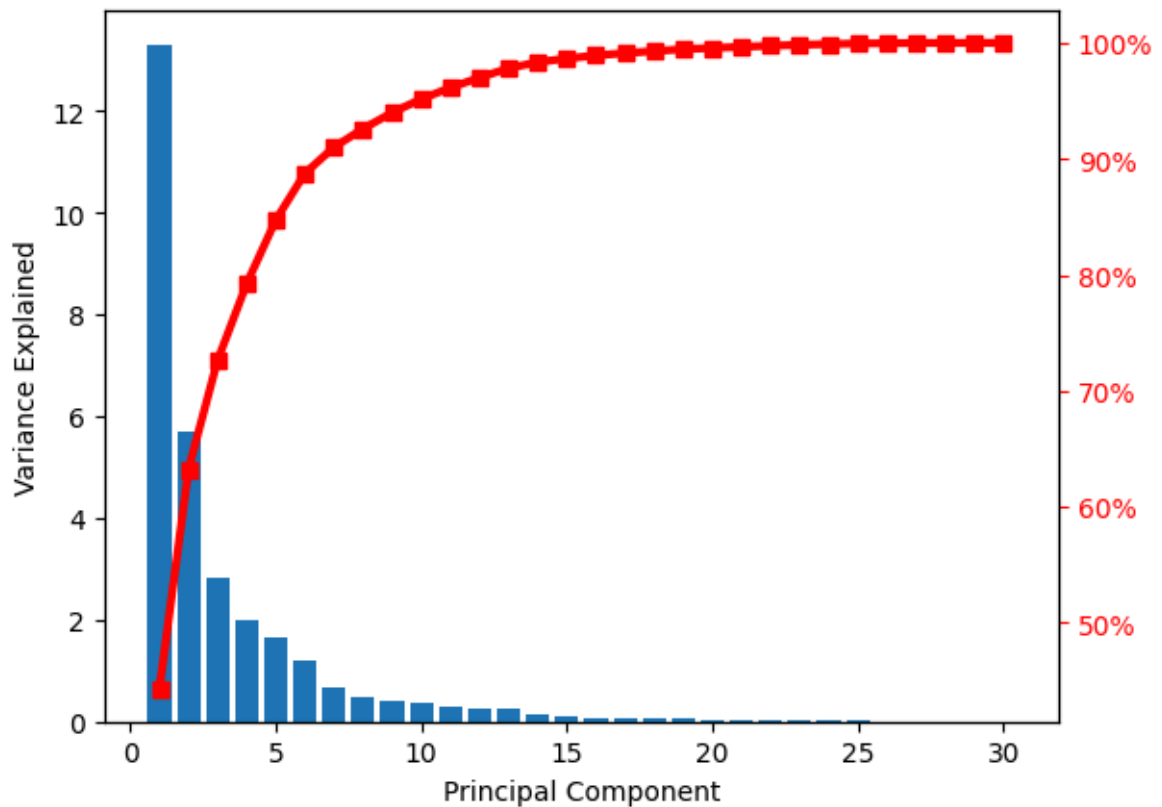
(3) 進行主成分分析，繪製特徵值由大而小的分布與 scree plot與累積百分比的 pareto plot。

```
In [ ]: import numpy as np
from numpy.linalg import eig
from numpy.linalg import inv
from matplotlib.ticker import PercentFormatter
Sx = np.cov(breast_cancer_data_array_.T, bias=False)
w, v = eig(Sx)
idx = np.argsort(-w) #sort eigenvalues in descending order
# idx = np.argsort(w)[::-1]
eigvals = w[idx]
eigvecs = v[:, idx]
```


#開始作主成分分析圖

```
plt.figure()
x = np.arange(1, 1+len(eigvals))
plt.plot(x, eigvals, marker='s')
plt.title('Scree plot')
plt.grid(True)
plt.show()
fig, ax = plt.subplots()
x = np.arange(1, 1+len(eigvals))
ax.bar(x, eigvals)
ax2 = ax.twinx()
ax2.plot(x, eigvals.cumsum()/eigvals.sum()*100, \
marker='s', color='red', lw=3)
ax2.tick_params(axis='y', colors='red')
ax2.yaxis.set_major_formatter(PercentFormatter())
ax.set_xlabel('Principal Component')
ax.set_ylabel('Variance Explained')
plt.show()
```





結論:

可以觀察到約採用五個主成分，其解釋變異量就高達85%，因此這是一筆適合用PCA維度縮減的資料檔。

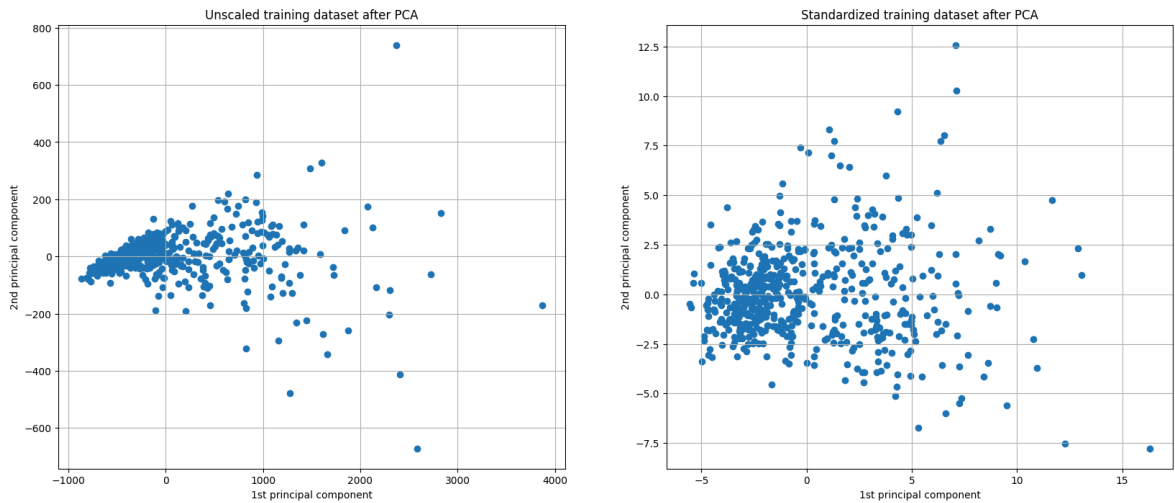
(4) 利用主成分分析取得前兩項成分，並繪製其散布圖

- 左圖為資料不做標準化，取前兩大主成分得到的散布圖。
- 右圖為資料標準化後，取兩個主成分得到的散布圖。

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler

# 對未標準化的資料做PCA
pca = PCA().fit(breast_cancer_data_array)
Z = pca.transform(breast_cancer_data_array)
# 對標準化的資料做PCA
scaler = StandardScaler()
scaler.fit(breast_cancer_data_array_)
ratings_ = scaler.transform(breast_cancer_data_array_)
pca = PCA().fit(breast_cancer_data_array_)
Z1 = pca.transform(breast_cancer_data_array_)
# 做圖
fig, ax = plt.subplots(1, 2, figsize = (20, 8))
ax[0].scatter(Z[:,0], Z[:,1])
ax[0].set_xlabel('1st principal component')
ax[0].set_ylabel('2nd principal component')
ax[0].set_title("Unscaled training dataset after PCA")
ax[0].grid(True)
ax[1].scatter(Z1[:,0], Z1[:,1])
```

```
ax[1].set_xlabel('1st principal component')
ax[1].set_ylabel('2nd principal component')
ax[1].grid(True)
ax[1].set_title("Standardized training dataset after PCA")
plt.show()
```



結論:

標準化後兩個主成分的級距較一致。

較第一題不太一樣的是，標準化後的資料進行主成分分析仍然觀察不太到點分群的狀況。

因次必須往下將CLASSES以不同顏色標出方可觀察。

(5) 再依據每個資料的標籤，為每個在散布圖上的資料點依據標籤塗上顏色

- 左圖為資料不做標準化，得到標籤顏色分類的散佈圖。
- 右圖為資料標準化後，得到標籤顏色分類的散佈圖。

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler

# 做圖
fig, (ax1, ax2) = plt.subplots(nrows=1, ncols=2, figsize=(10, 5))

target_classes = range(0, 3)
colors = ("blue", "red")
markers = ("^", "s")

for target_class, color, marker in zip(target_classes, colors, markers):
    ax1.scatter(
        x=Z[y == target_class, 0],
        y=Z[y == target_class, 1],
        color=color,
        label=f"class {target_class+1}",
        alpha=0.5,
        marker=marker,
    )

    ax2.scatter(
```

```

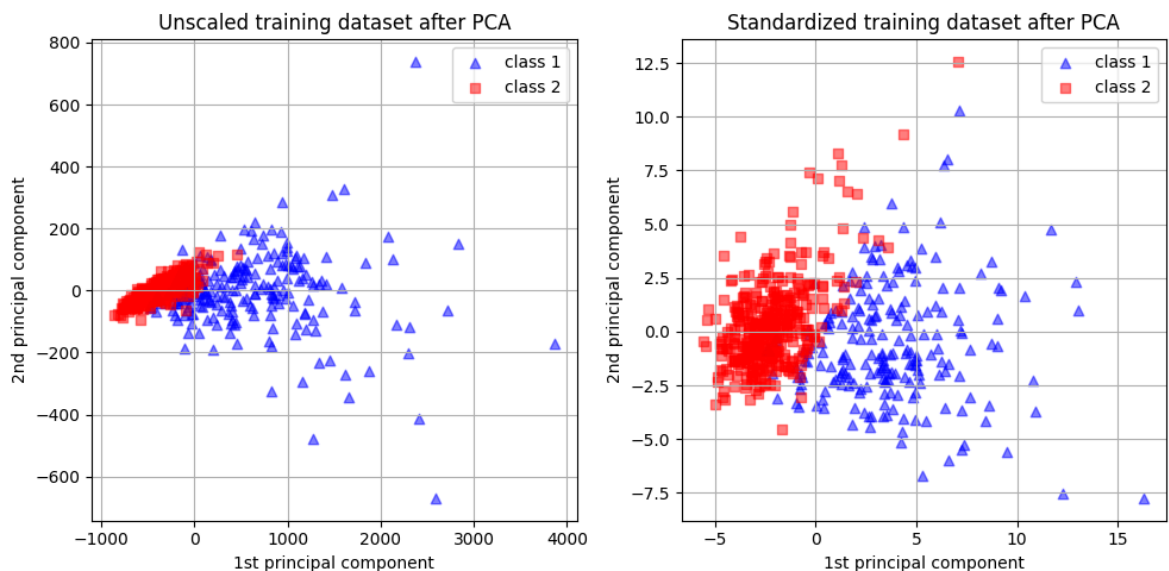
        x=Z1[y == target_class, 0],
        y=Z1[y == target_class, 1],
        color=color,
        label=f"class {target_class+1}",
        alpha=0.5,
        marker=marker,
    )

ax1.set_title("Unscaled training dataset after PCA")
ax2.set_title("Standardized training dataset after PCA")

for ax in (ax1, ax2):
    ax.set_xlabel("1st principal component")
    ax.set_ylabel("2nd principal component")
    ax.legend(loc="upper right")
    ax.grid()

_ = plt.tight_layout()

```



結論:

做完標準化後，兩個類別的資料分散較平均，兩個主成分的級距也較為相似。

而未做標準化的資料分配不平均，兩個主成分的級距也不相似

(6) 採取三個主成分，並繪製立體圖:

- 此圖為原始資料未做標準化得出的結果

```

In [ ]: import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.decomposition import PCA
from sklearn.datasets import load_breast_cancer
# Load the breast cancer dataset
X, y = load_breast_cancer(return_X_y=True, as_frame=True)
# unscale data Perform PCA
pca = PCA(n_components=3)
Z1 = pca.fit_transform(X)
# Plot 3D figure

```

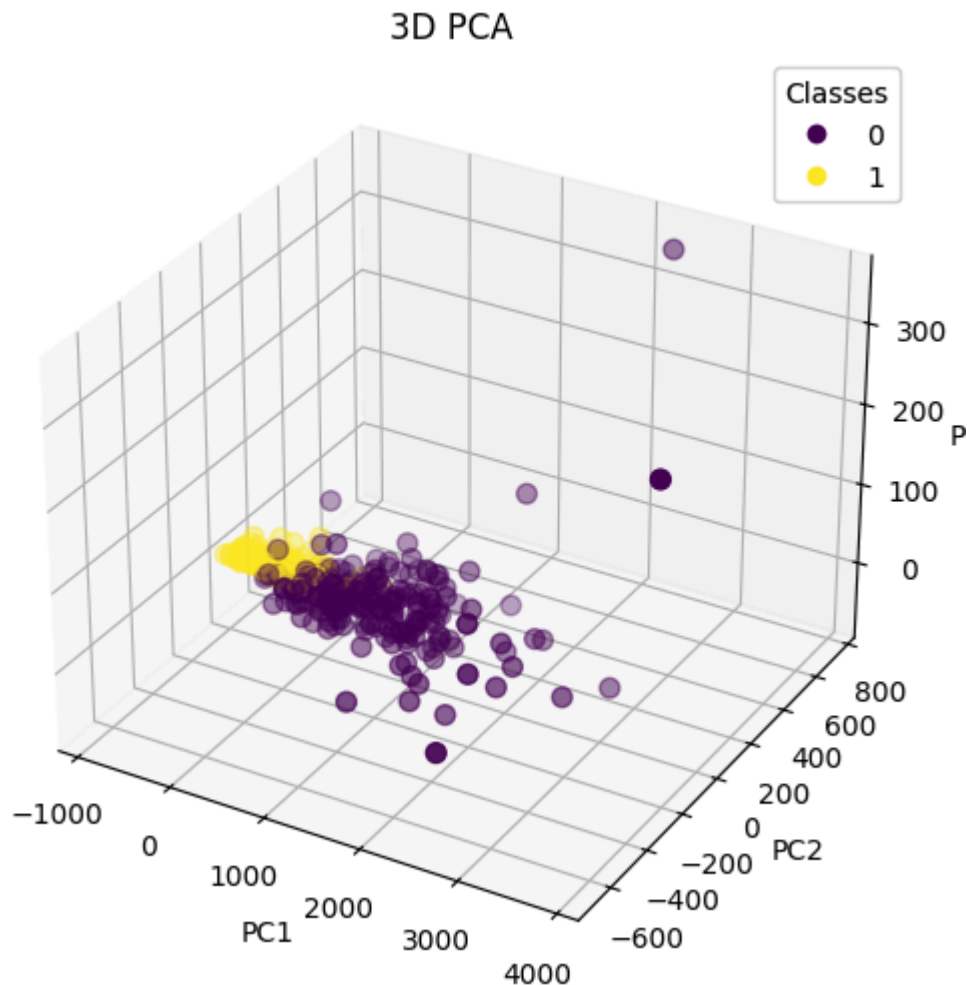
```

fig = plt.figure(figsize=(8, 6))
ax = fig.add_subplot(111, projection='3d')

# Scatter plot
scatter = ax.scatter(Z1[:,0], Z1[:,1], Z1[:,2], c=y, cmap='viridis', s=50)
ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
ax.set_title('3D PCA')

# Legend
legend = ax.legend(*scatter.legend_elements(), title='Classes')
ax.add_artist(legend)
plt.show()

```



發現三個主成分的級距都不一致，也不易觀察到分群的情況

- 標準化後得出的結果

```

In [ ]: import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.datasets import load_breast_cancer
# Load the breast cancer dataset
X, y = load_breast_cancer(return_X_y=True, as_frame=True)

```

```

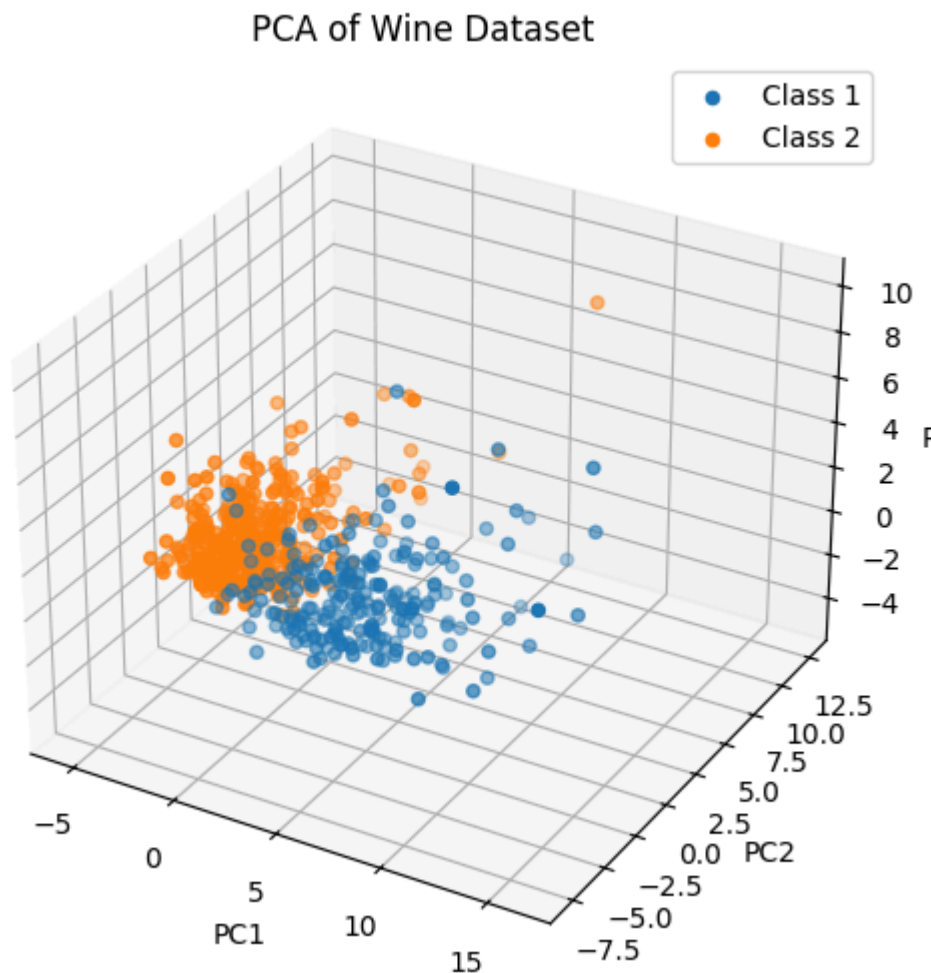
#scale data preform PCA
scaler = StandardScaler()
scaler.fit(breast_canser_data_array_)
ratings_ = scaler.transform(breast_canser_data_array_)
pca = PCA(n_components=3).fit(breast_canser_data_array_)
Z1 = pca.transform(breast_canser_data_array_)

# Create a 3D plot
fig = plt.figure(figsize=(8, 6))
ax = fig.add_subplot(111, projection='3d')

# Plot each class separately
for i in np.unique(y):
    ax.scatter(Z1[y == i, 0], Z1[y == i, 1], Z1[y == i, 2], label=f'Class {i+1}')

ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
ax.set_title('PCA of Wine Dataset')
ax.legend()
plt.show()

```



級距較一致，也較能區分兩個類別的資料點

- 轉換角度得出的結果

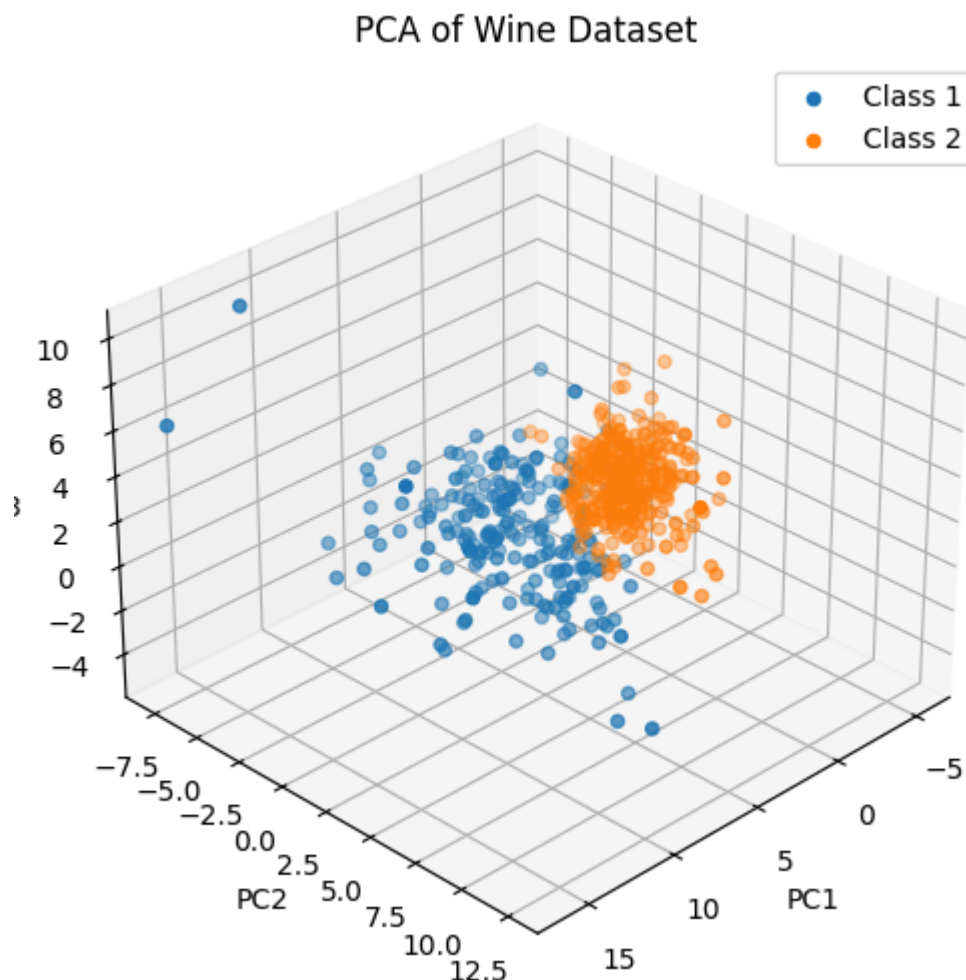
```
In [ ]: from sklearn.datasets import load_breast_cancer
# Load the breast cancer dataset
X, y = load_breast_cancer(return_X_y=True, as_frame=True)

#scale data preform PCA
scaler = StandardScaler()
scaler.fit(breast_cancer_data_array_)
ratings_ = scaler.transform(breast_cancer_data_array_)
pca = PCA(n_components=3).fit(breast_cancer_data_array_)
Z1 = pca.transform(breast_cancer_data_array_)

# Create a 3D plot
fig = plt.figure(figsize=(8, 6))
ax = fig.add_subplot(111, projection='3d')

# Plot each class separately
for i in np.unique(y):
    ax.scatter(Z1[y == i, 0], Z1[y == i, 1], Z1[y == i, 2], label=f'Class {i+1}')

ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
ax.set_title('PCA of Wine Dataset')
ax.legend()
ax.view_init(elev=30, azim=45)
plt.show()
```



結論:

因此未來在做主成分分析時，需要先將資料做標準化動作，然後觀察取幾個主成分最能滿足

維持原數據類別間的最大變異量，同時達到維度縮減的目的。

(7) Z_1 與 Z_2 都是從原變數組合而成的新變數，可否從 Z_1 與 Z_2 的組成係數，看出原變數哪個比較重要？哪個比較不重要？若再與原變數間的相關係數圖對照，是否透露相同的訊息。

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
pca = PCA(n_components=1).fit(X) # 取第一個特徵向量
pca = PCA().fit(breast_cancer_data_array_) # 進行主成分分析
#print(pca.explained_variance_ratio_) # 共變異矩陣特徵值佔比
# print(pca.explained_variance_) # 共變異矩陣的特徵值
# print(pca.components_) # 共變異矩陣的特徵向量
eigvals = pca.explained_variance_
#print(eigvals)
eigvecs = pca.components_.T # by column [v1 v2]
print(eigvecs)
```



```

[[ 2.18902444e-01 -2.33857132e-01 -8.53124284e-03 4.14089623e-02
 3.77863538e-02 1.87407904e-02 -1.24088340e-01 -7.45229622e-03
-2.23109764e-01 9.54864432e-02 4.14714866e-02 5.10674568e-02
 1.19672116e-02 5.95061348e-02 5.11187749e-02 -1.50583883e-01
 2.02924255e-01 1.46712338e-01 -2.25384659e-01 -4.96986642e-02
-6.85700057e-02 7.29289034e-02 -9.85526942e-02 1.82579441e-01
 1.92264989e-02 -1.29476396e-01 -1.31526670e-01 2.11194013e-01
 2.11460455e-01 -7.02414091e-01]
[ 1.03724578e-01 -5.97060883e-02 6.45499033e-02 -6.03050001e-01
-4.94688505e-02 -3.21788366e-02 1.13995382e-02 1.30674825e-01
 1.12699390e-01 2.40934066e-01 -3.02243402e-01 2.54896423e-01
 2.03461333e-01 -2.15600995e-02 1.07922421e-01 -1.57841960e-01
-3.87061187e-02 -4.11029851e-02 -2.97886446e-02 -2.44134993e-01
 4.48369467e-01 9.48006326e-02 -5.54997454e-04 -9.87867898e-02
-8.47459309e-02 -2.45566636e-02 -1.73573093e-02 -6.58114593e-05
-1.05339342e-02 -2.73661018e-04]
[ 2.27537293e-01 -2.15181361e-01 -9.31421972e-03 4.19830991e-02
 3.73746632e-02 1.73084449e-02 -1.14477057e-01 -1.86872582e-02
-2.23739213e-01 8.63856150e-02 1.67826374e-02 3.89261058e-02
 4.41095034e-02 4.85138123e-02 3.99029358e-02 -1.14453955e-01
 1.94821310e-01 1.58317455e-01 -2.39595276e-01 -1.76650122e-02
-6.97690429e-02 7.51604777e-02 -4.02447050e-02 1.16648876e-01
-2.70154137e-02 -1.25255946e-01 -1.15415423e-01 8.43382663e-02
 3.83826098e-01 6.89896968e-01]
[ 2.20994985e-01 -2.31076711e-01 2.86995259e-02 5.34337955e-02
 1.03312514e-02 -1.88774796e-03 -5.16534275e-02 3.46736038e-02
-1.95586014e-01 7.49564886e-02 1.10169643e-01 6.54375082e-02
 6.73757374e-02 1.08308292e-02 -1.39669069e-02 -1.32448032e-01
 2.55705763e-01 2.66168105e-01 2.73221894e-02 -9.01437617e-02
-1.84432785e-02 9.75657781e-02 7.77727342e-03 -6.98483369e-02
 2.10040780e-01 3.62727403e-01 4.66612477e-01 -2.72508323e-01
-4.22794920e-01 3.29473482e-02]
[ 1.42589694e-01 1.86113023e-01 -1.04291904e-01 1.59382765e-01
-3.65088528e-01 -2.86374497e-01 -1.40668993e-01 -2.88974575e-01
 6.42472194e-03 -6.92926813e-02 -1.37021842e-01 3.16727211e-01
 4.55736020e-02 4.45064860e-01 1.18143364e-01 -2.04613247e-01
 1.67929914e-01 -3.52226802e-01 1.64565843e-01 1.71009601e-02
-1.19491747e-01 6.38229479e-02 -2.06657211e-02 -6.86974224e-02
-2.89548850e-02 -3.70036864e-02 6.96899233e-02 1.47926883e-03
-3.43466700e-03 4.84745766e-03]
[ 2.39285354e-01 1.51891610e-01 -7.40915709e-02 3.17945811e-02
 1.17039713e-02 -1.41309489e-02 3.09184960e-02 -1.51396350e-01
-1.67841425e-01 1.29362000e-02 -3.08009633e-01 -1.04017044e-01
 2.29281304e-01 8.10105720e-03 -2.30899962e-01 1.70178367e-01
-2.03077075e-02 7.79413843e-03 -2.84222358e-01 4.88686329e-01
 1.92621396e-01 -9.80775567e-02 5.23603957e-02 1.04135518e-01
-3.96623231e-01 2.62808474e-01 9.77487054e-02 -5.46276696e-03
-4.10167739e-02 -4.46741863e-02]
[ 2.58400481e-01 6.01653628e-02 2.73383798e-03 1.91227535e-02
 8.63754118e-02 -9.34418089e-03 -1.07520443e-01 -7.28272853e-02
 4.05910064e-02 -1.35602298e-01 1.24190245e-01 6.56534798e-02
 3.87090806e-01 -1.89358699e-01 1.28283732e-01 2.69470206e-01
-1.59835337e-03 -2.69681105e-02 -2.26636013e-03 -3.33870858e-02
 5.57175335e-03 -1.85212003e-01 3.24870378e-01 -4.47410568e-02
 9.69773167e-02 -5.48876170e-01 3.64808397e-01 4.55386379e-02
-1.00147876e-02 -2.51386661e-02]
[ 2.60853758e-01 -3.47675005e-02 -2.55635406e-02 6.53359443e-02
-4.38610252e-02 -5.20499505e-02 -1.50482214e-01 -1.52322414e-01
-1.11971106e-01 8.05452775e-03 -7.24460264e-02 4.25892667e-02
 1.32138097e-01 -2.44794768e-01 2.17099194e-01 3.80464095e-01

```

3.45095087e-02 -8.28277367e-02 1.54972363e-01 -2.35407606e-01
-9.42381870e-03 -3.11852431e-01 -5.14087968e-02 -8.40276972e-02
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-4.20694931e-03 1.07726530e-03]
[1.38166959e-01 1.90348770e-01 -4.02399363e-02 6.71249840e-02
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2.56040084e-01 5.72069479e-01 1.63054081e-01 -2.88865504e-01
1.89933673e-01 3.07388563e-02 7.39617071e-02 -1.64661588e-01
-1.91737848e-01 1.73397790e-01 5.88111647e-02 2.60691555e-02
-8.69384844e-02 -1.84067326e-02 -5.12005770e-02 -1.93394733e-02
2.45836949e-02 -1.60440385e-02 -1.51648349e-02 1.43302642e-03
-7.56986244e-03 1.28037941e-03]
[6.43633464e-02 3.66575471e-01 -2.25740897e-02 4.85867649e-02
-4.44243602e-02 -1.19430668e-01 2.95760024e-01 -1.77121441e-01
-1.23740789e-01 8.11032072e-02 -3.80482687e-02 2.36358988e-01
1.06239082e-01 -3.77078865e-01 -5.17975705e-01 -4.07927860e-02
5.02252456e-02 8.78673570e-02 5.81570509e-02 -1.75637222e-01
-7.62718362e-02 2.87868885e-01 -8.46898562e-02 1.33260547e-01
2.07221864e-01 -9.74048386e-02 -1.01244946e-01 -6.31168651e-03
7.30143287e-03 4.75568480e-03]
[2.05978776e-01 -1.05552152e-01 2.68481387e-01 9.79412418e-02
-1.54456496e-01 -2.56032561e-02 3.12490037e-01 2.25399674e-02
2.49985002e-01 -4.95475941e-02 -2.53570194e-02 -1.66879153e-02
-6.81952298e-02 1.03474126e-02 1.10050711e-01 5.89057190e-02
-1.39396866e-01 -2.36216532e-01 -1.75883308e-01 -9.08005031e-02
8.63867747e-02 -1.50274681e-01 -2.64125317e-01 5.58701567e-01
1.74930429e-01 4.99770798e-02 2.12982901e-01 -1.92223890e-01
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結論:

由上結果可以看出，透過觀察組成的係數，可以清楚理解原變數在建構 Z_1 Z_2 新變數時的重要性。係數的絕對值越大，則表示原變數的貢獻越大；相反的，如果組成係數趨近於零，則表示原始變數幾乎沒貢獻，在數據解釋中較不重要。而相關係數可以更直觀的理解變數之間的關係；因此，綜合考慮兩點才能更全面的理解數據。