practice2_code

October 27, 2023

1 Práctica 2: PCA - Red Wine

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Fecha: 27 Oct 23

De la base de datos red wine de kaggle, se hará un análisis PCA. El objetivo es poder observar si es posible reducir la dimensionalidad de los datos y poder clasificarlos en base a la calidad del vino.

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

from mpl_toolkits.mplot3d import Axes3D
import plotly.graph_objs as go
import plotly.express as px
```

2 Parte 1: Data

2.1 Lectura de Datos

Se observan 12 columnas y 1599 filas, donde la columna de calidad es la variable objetivo. Las variables son las siguientes: - fixed acidity: acidez fija - volatile acidity: acidez volátil - citric acid: ácido cítrico - residual sugar: azúcar residual - chlorides: cloruros - free sulfur dioxide: dióxido de azufre libre - total sulfur dioxide: dióxido de azufre total - density: densidad - pH: pH - sulphates: sulfatos - alcohol: alcohol - quality: calidad (puntuación entre 3 y 8)

[ ]:
```
# read data from numpy
red_wine = pd.read_csv("data/winequality-red.csv")
red_wine
```

[ ]:
```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0               7.4             0.700         0.00             1.9      0.076
1               7.8             0.880         0.00             2.6      0.098
2               7.8             0.760         0.04             2.3      0.092
3              11.2             0.280         0.56             1.9      0.075
```

```
4               7.4             0.700         0.00              1.9       0.076
…             …               …          …             …         …
1594            6.2             0.600         0.08              2.0       0.090
1595            5.9             0.550         0.10              2.2       0.062
1596            6.3             0.510         0.13              2.3       0.076
1597            5.9             0.645         0.12              2.0       0.075
1598            6.0             0.310         0.47              3.6       0.067

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
0                    11.0                  34.0  0.99780  3.51       0.56
1                    25.0                  67.0  0.99680  3.20       0.68
2                    15.0                  54.0  0.99700  3.26       0.65
3                    17.0                  60.0  0.99800  3.16       0.58
4                    11.0                  34.0  0.99780  3.51       0.56
…                   …                   …      …    …        …
1594                 32.0                  44.0  0.99490  3.45       0.58
1595                 39.0                  51.0  0.99512  3.52       0.76
1596                 29.0                  40.0  0.99574  3.42       0.75
1597                 32.0                  44.0  0.99547  3.57       0.71
1598                 18.0                  42.0  0.99549  3.39       0.66

      alcohol  quality
0         9.4        5
1         9.8        5
2         9.8        5
3         9.8        6
4         9.4        5
…       …      …
1594     10.5        5
1595     11.2        6
1596     11.0        6
1597     10.2        5
1598     11.0        6

[1599 rows x 12 columns]
```

[ ]:
```python
# drop 'quality'
quality_by_wine = red_wine['quality'].copy()
quality_by_wine = 'quality_' + quality_by_wine.astype(str)
red_wine = red_wine.drop('quality', axis='columns')
```

2.2 Preparando los Datos

Para hacer un análisis PCA, primero se estandariza la data para que tenga media 0 y desviación estándar 1. Esto se hace para que las variables tengan el mismo peso en el análisis.

```
[ ]: # get numpy array
X = red_wine.copy().to_numpy()
X.shape
```

```
[ ]: (1599, 11)
```

```
[ ]: # scale array
Xstand = X - np.mean(X, axis=0)
Xstand = np.divide(Xstand, np.std(Xstand, ddof=1, axis=0))
```

Revizamos que la media y la desviación estándar sean 0 y 1 respectivamente.

```
[ ]: # look if the data is centered
print(f"data is centered: {np.all(np.isclose(Xstand.mean(axis=0), 0))}")

# look if the data is centered
print(f"data is scaled: {np.all(np.isclose(Xstand.std(axis=0, ddof=1), 1))}")
```

```
data is centered: True
data is scaled: True
```

Obtenemos la matriz de covarianza usando el sesgo de Besel:

$$\frac{1}{n-1}X^TX$$

```
[ ]: # variance-covariance matrix
m_size = Xstand.shape[0]
S = (1 / (m_size - 1)) * (Xstand.T @ Xstand)
```

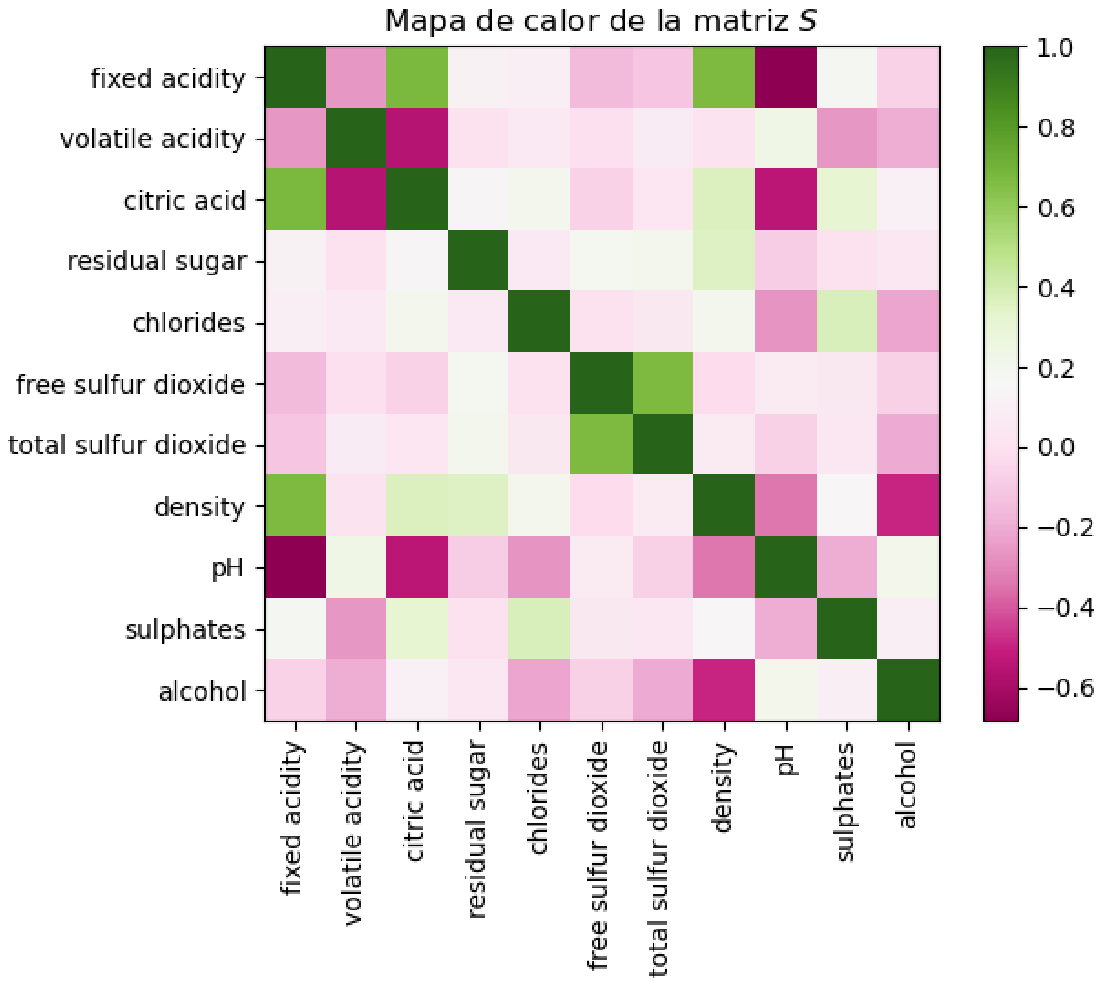
```
Intel MKL WARNING: Support of Intel(R) Streaming SIMD Extensions 4.2 (Intel(R)
SSE4.2) enabled only processors has been deprecated. Intel oneAPI Math Kernel
Library 2025.0 will require Intel(R) Advanced Vector Extensions (Intel(R) AVX)
instructions.
```

2.3 Mapa de Calor

Se observa una fuerte correlación entre `free sulfure dioxide` y `total sulfure dioxide`, por lo que es muy probable que están correlacionadas, por lo que seguramente una componente principal tendrá muy poca varianza explciada gracias a la colinealidad de estas dos variables. De igual forma vemos la fuerte relación entre `volatile acidity` y `citric acid`.

```
[ ]: # create a heatmap
plt.imshow(S, cmap='PiYG', interpolation='nearest')
plt.colorbar()
# add ticks
plt.xticks(range(len(red_wine.columns)), red_wine.columns, rotation=90)
plt.yticks(range(len(red_wine.columns)), red_wine.columns, rotation=0)
# add title
plt.title("Mapa de calor de la matriz $S$")
```

```
# Display the plot or save it to a file
plt.show()
```



3 Parte 2: PCA

3.1 Cálculo de eigenvectores de $S = A^T A$

[ ]:
```
# get eigenvectors
eigvalues, eigvectors = np.linalg.eig(S)
```

3.2 Proyección Datos

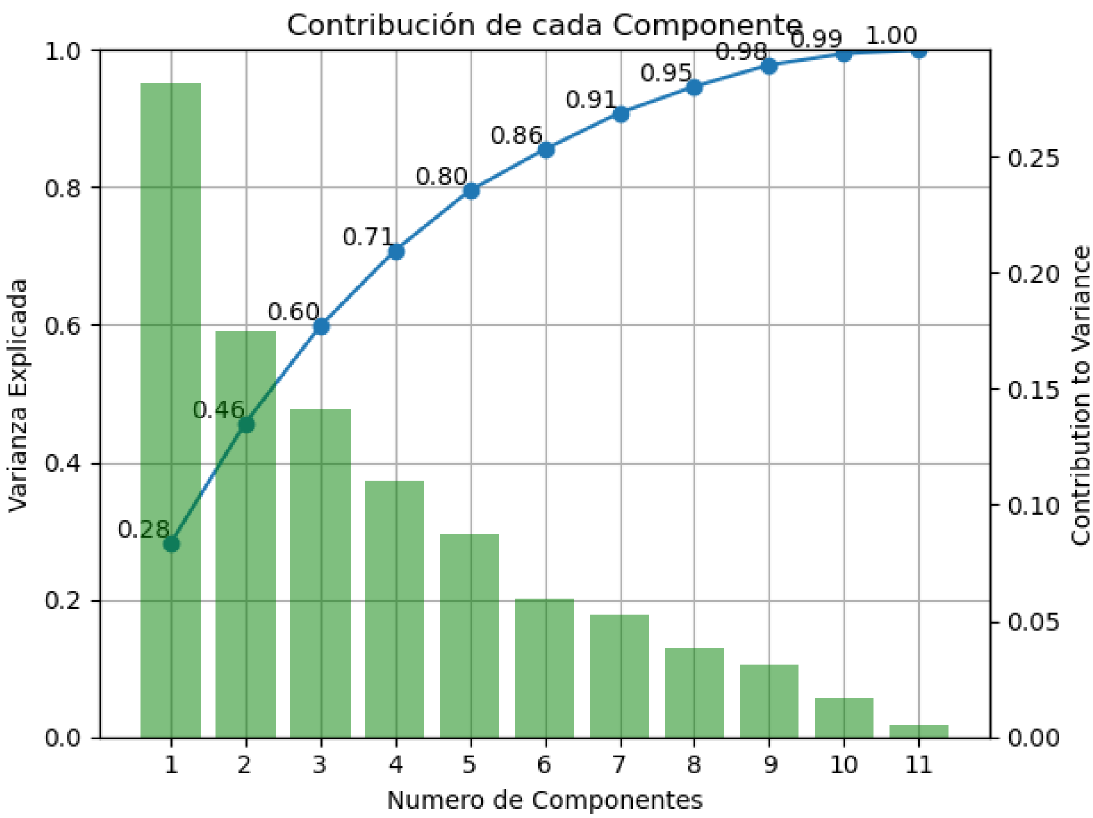
[ ]:
```
# proyect data
Xstand_proy = Xstand @ eigvectors
```

4 Parte 3: Varianza Acumulada

Observamos que la varianza explicada para las variables 1 y 2 es moderadamente buena, pues con solo dos variables se logra explicar casi el 50% de la varianza de 12 variables. Por lo que podemos decir que estas variables son las que más explican la varianza de los datos. De todos modos, observamos como se ve con 3 componentes, las cuales ya explican el 60% de la varianza total.

[ ]:
```python
import numpy as np
import matplotlib.pyplot as plt

# Assuming eigvalues is a numpy array containing the eigenvalues
# Sort the eigenvalues in descending order
eigvalues.sort()
eigvalues = eigvalues[::-1]

# Calculate the cumulative explained variance
cumulative_variance = eigvalues.cumsum() / eigvalues.sum()

# Create a figure and axis for the cumulative variance explained graph
fig, ax = plt.subplots()

# Plot the cumulative explained variance
ax.plot(np.arange(1, eigvalues.size + 1), cumulative_variance, '-o')

# Set better formatting for the tick labels
ax.set_xticks(np.arange(1, eigvalues.size + 1))
ax.set_xticklabels(np.arange(1, eigvalues.size + 1))
ax.set_xlabel("Numero de Componentes")
ax.set_ylabel("Varianza Explicada")
ax.grid(True)

# Annotate data points with y-values
for i, var in enumerate(cumulative_variance):
    ax.text(i + 1, var, f'{var:.2f}', ha='right', va='bottom')

# set limits
ax.set_ylim(0, 1)

# Create a bar chart for individual contributions
individual_contributions = eigvalues / eigvalues.sum()
x = np.arange(1, eigvalues.size + 1)
ax2 = ax.twinx()  # Create a secondary y-axis
ax2.bar(x, individual_contributions, align='center', alpha=0.5, color='g',␣
 ↪label='Contribución Individual')
ax2.set_ylabel("Contribution to Variance")

# Show the plot
```

```
plt.title("Contribución de cada Componente")
plt.tight_layout()
plt.show()
```



5 Parte 4: Contribución

La primera componente podría explicar el tradeoff entre acidez y alcanilidad, mientras que la segunda componente podría explicar el tradeoff entre alcohol y carbonatado.

[ ]:
```
# look eigenvectors
df_eig = pd.DataFrame(
    eigvectors,
    columns=['PC' + str(i+1) for i in range(eigvalues.size)],
    index=red_wine.columns
)
df_eig
```

[ ]:
```
                        PC1       PC2       PC3       PC4       PC5  \
fixed acidity      0.489314 -0.110503 -0.123302 -0.229617 -0.082614
volatile acidity  -0.238584  0.274930 -0.449963  0.078960  0.218735
```

citric acid	0.463632	-0.151791	0.238247	-0.079418	-0.058573
residual sugar	0.146107	0.272080	0.101283	-0.372793	0.732144
chlorides	0.212247	0.148052	-0.092614	0.666195	0.246501
free sulfur dioxide	-0.036158	0.513567	0.428793	-0.043538	-0.159152
total sulfur dioxide	0.023575	0.569487	0.322415	-0.034577	-0.222465
density	0.395353	0.233575	-0.338871	-0.174500	0.157077
pH	-0.438520	0.006711	0.057697	-0.003788	0.267530
sulphates	0.242921	-0.037554	0.279786	0.550872	0.225962
alcohol	-0.113232	-0.386181	0.471673	-0.122181	0.350681

	PC6	PC7	PC8	PC9	PC10 \
fixed acidity	-0.639691	-0.249523	0.194021	-0.177595	-0.350227
volatile acidity	-0.002389	0.365925	-0.129110	-0.078775	-0.533735
citric acid	0.070910	0.621677	-0.381450	-0.377516	0.105497
residual sugar	-0.184030	0.092872	0.007523	0.299845	0.290663
chlorides	-0.053065	-0.217671	0.111339	-0.357009	0.370413
free sulfur dioxide	0.051421	0.248483	0.635405	-0.204781	-0.116596
total sulfur dioxide	-0.068702	-0.370750	-0.592116	0.019036	-0.093662
density	0.567332	-0.239990	0.020719	-0.239223	-0.170481
pH	-0.340711	-0.010970	-0.167746	-0.561391	-0.025138
sulphates	-0.069555	0.112320	-0.058367	0.374604	-0.447469
alcohol	0.314526	-0.303015	0.037603	-0.217626	-0.327651

	PC11
fixed acidity	0.101479
volatile acidity	0.411449
citric acid	0.069593
residual sugar	0.049156
chlorides	0.304339
free sulfur dioxide	-0.014000
total sulfur dioxide	0.136308
density	-0.391152
pH	-0.522116
sulphates	-0.381263
alcohol	0.361645

Vemos que en la primera componente, la `fixed acidity` es la variable que más aporta información. Por otro lado, la que más aporta en la segunda componente es `total sulfur dioxide`. Esto nos indica que estas dos variables son las que más variación aportan al modelo.

[ ]:
```
# for each component, get the index with highest value
list_max_contr = []
for name, pc in df_eig.T.iterrows():
    # get maximum contributor
    pc = pc.sort_values(key=np.abs, ascending=False) # sort by abs value
    max_value = pc[0]
    max_contrib_var = pc.index[0]
```

```
    # save
    list_max_contr.append((name, max_contrib_var, max_value))

# to dataframe
pd.DataFrame(list_max_contr, columns=['PC', 'variable', 'contribution']).
 ↪set_index('PC')
```

[ ]:

```
                  variable  contribution
PC
PC1          fixed acidity      0.489314
PC2   total sulfur dioxide      0.569487
PC3                alcohol      0.471673
PC4              chlorides      0.666195
PC5         residual sugar      0.732144
PC6          fixed acidity     -0.639691
PC7            citric acid      0.621677
PC8    free sulfur dioxide      0.635405
PC9                     pH     -0.561391
PC10      volatile acidity     -0.533735
PC11                    pH     -0.522116
```

Pareciera que la variable `fixed acidity` es la que tiene mayor correlación con las demás variables, por lo que es la que más contribuye a la varianza de los datos.

[ ]:

```
# look S matrix
pd.DataFrame(
    S,
    columns=red_wine.columns,
    index=red_wine.columns
)
```

[ ]:

```
                      fixed acidity  volatile acidity  citric acid  \
fixed acidity              1.000000         -0.256131     0.671703
volatile acidity          -0.256131          1.000000    -0.552496
citric acid                0.671703         -0.552496     1.000000
residual sugar             0.114777          0.001918     0.143577
chlorides                  0.093705          0.061298     0.203823
free sulfur dioxide       -0.153794         -0.010504    -0.060978
total sulfur dioxide      -0.113181          0.076470     0.035533
density                    0.668047          0.022026     0.364947
pH                        -0.682978          0.234937    -0.541904
sulphates                  0.183006         -0.260987     0.312770
alcohol                   -0.061668         -0.202288     0.109903

                      residual sugar  chlorides  free sulfur dioxide  \
fixed acidity               0.114777   0.093705            -0.153794
volatile acidity            0.001918   0.061298            -0.010504
citric acid                 0.143577   0.203823            -0.060978
```

```
residual sugar              1.000000   0.055610             0.187049
chlorides                   0.055610   1.000000             0.005562
free sulfur dioxide         0.187049   0.005562             1.000000
total sulfur dioxide        0.203028   0.047400             0.667666
density                     0.355283   0.200632            -0.021946
pH                         -0.085652  -0.265026             0.070377
sulphates                   0.005527   0.371260             0.051658
alcohol                     0.042075  -0.221141            -0.069408

                      total sulfur dioxide   density        pH  sulphates  \
fixed acidity                    -0.113181  0.668047 -0.682978   0.183006
volatile acidity                  0.076470  0.022026  0.234937  -0.260987
citric acid                       0.035533  0.364947 -0.541904   0.312770
residual sugar                    0.203028  0.355283 -0.085652   0.005527
chlorides                         0.047400  0.200632 -0.265026   0.371260
free sulfur dioxide               0.667666 -0.021946  0.070377   0.051658
total sulfur dioxide              1.000000  0.071269 -0.066495   0.042947
density                           0.071269  1.000000 -0.341699   0.148506
pH                               -0.066495 -0.341699  1.000000  -0.196648
sulphates                         0.042947  0.148506 -0.196648   1.000000
alcohol                          -0.205654 -0.496180  0.205633   0.093595

                       alcohol
fixed acidity        -0.061668
volatile acidity     -0.202288
citric acid           0.109903
residual sugar        0.042075
chlorides            -0.221141
free sulfur dioxide  -0.069408
total sulfur dioxide -0.205654
density              -0.496180
pH                    0.205633
sulphates             0.093595
alcohol               1.000000
```

6 Parte 5: Biplot

6.1 3D

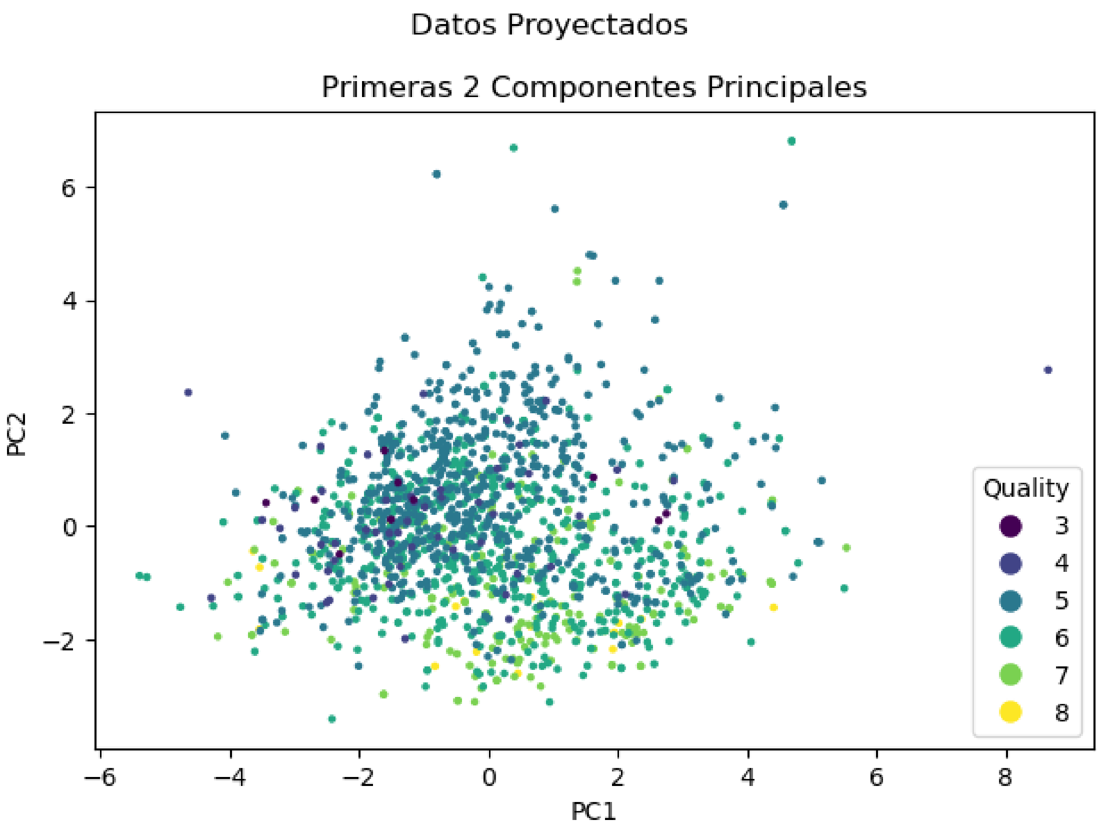
Graficando tanto las primeras 2 componentes principales como las 3 primas componentes principales, se puede observar que las componentes principales no son capaces de separar del todo las clases de vino por calidad. Si bien se ve un poco de orden creciente de arriba hacia abajo, la separación no es evidente.

[ ]:
```python
# Create a DataFrame with your data
df = pd.DataFrame(Xstand_proy[:, :3], columns=["PC1", "PC2", "PC3"])
```

```python
df["quality"] = pd.Categorical(quality_by_wine, categories=quality_by_wine.
    ↪sort_values().unique(), ordered=True)
df = df.sort_values('quality', ascending=False)

# Create an interactive 3D scatter plot with the "Viridis" color scale
fig = px.scatter_3d(df, x="PC1", y="PC2", z="PC3", color="quality",␣
    ↪title="Primeras 3 Componentes Principales", color_discrete_sequence=px.
    ↪colors.sequential.Viridis_r)

# Add a legend
fig.update_traces(marker=dict(size=3), selector=dict(mode='markers'),␣
    ↪showlegend=True)

# Show the plot
fig.show()
```

6.2 2D

[ ]:
```python
# Scatter plot of the first two vectors
scatter = plt.scatter(df['PC1'], df['PC2'], c=df['quality'].cat.codes,␣
    ↪cmap='viridis', s=5)

# Add labels
plt.xlabel('PC1')
plt.ylabel('PC2')

# Create a legend
quality_values = df['quality'].sort_values().cat.codes.unique()
legend_elements = [plt.Line2D([0], [0], marker='o', color='w',␣
    ↪markerfacecolor=scatter.cmap(scatter.norm(quality_values[i])),
                              markersize=10, label=quality_values[i]+3) for i␣
    ↪in range(len(quality_values))]
plt.legend(handles=legend_elements, title='Quality')

# Show the plot
plt.suptitle("Datos Proyectados")
plt.title("Primeras 2 Componentes Principales")
plt.tight_layout()
plt.show()
```



7 Referencias

- Analisis Numerico, Erick Palacios, 2022