# practice2_raw

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## 1 Práctica 2: PCA - Red Wine

**Román Alberto Vélez Jiménez**

CU: 165462

De la base de datos red wine de kaggle, se hará un análisis PCA.

[ ]:
```python
# 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

[ ]:
```python
# 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

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

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

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

[ ]:
```python
# 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))}")
```

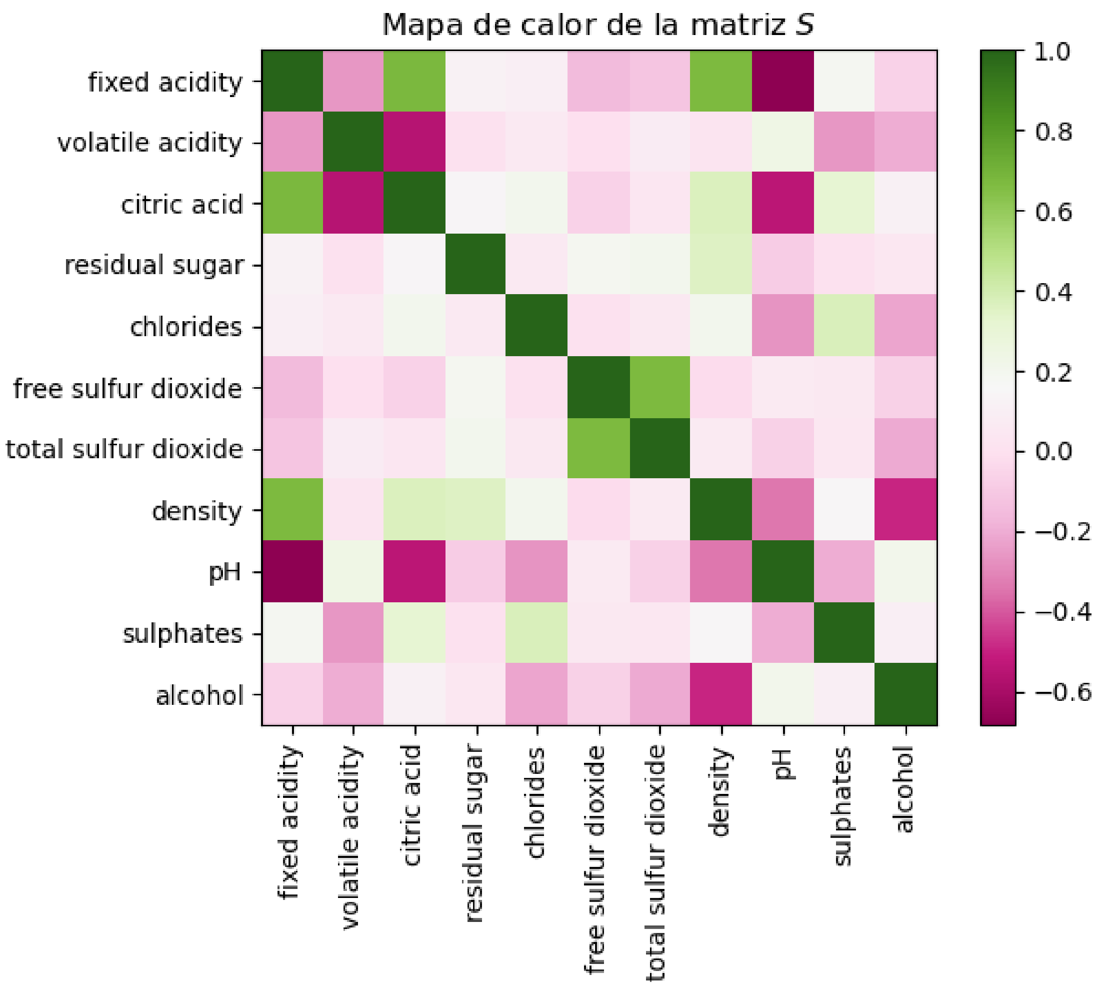
```
data is centered: True
data is scaled: True
```

[ ]:
```
# 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

[ ]:
```
# 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 $S = A^T A$

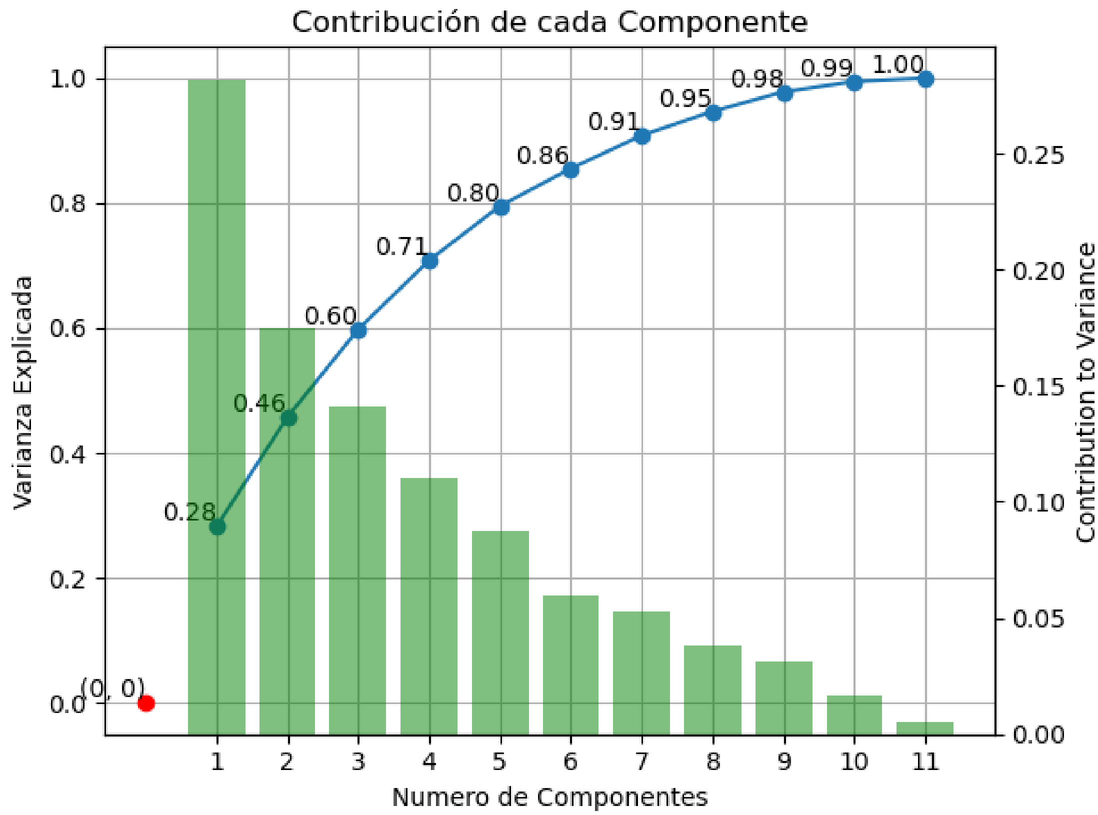
[ ]:
```
# get eigenvectors
eigvalues, eigvectors = np.linalg.eig(S)
```

## 3.2 Proyección Datos

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

# 4 Parte 3: Varianza Acumulada

[ ]:
```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')

# Add a point at (0,0) and label it on the cumulative variance explained graph
ax.plot(0, 0, 'ro')  # Red dot at (0,0)
ax.text(0, 0, "(0, 0)", ha='right', va='bottom')

# 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

Doubt: does the PC is the column of eigenvecs or the rows?

[ ]:
```
# 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
```

[ ]:
```python
# 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
```

[ ]:
```python
# 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

[ ]:
```python
# Create a DataFrame with your data
from turtle import title


df = pd.DataFrame(Xstand_proy[:, :3], columns=["PC1", "PC2", "PC3"])
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()
```

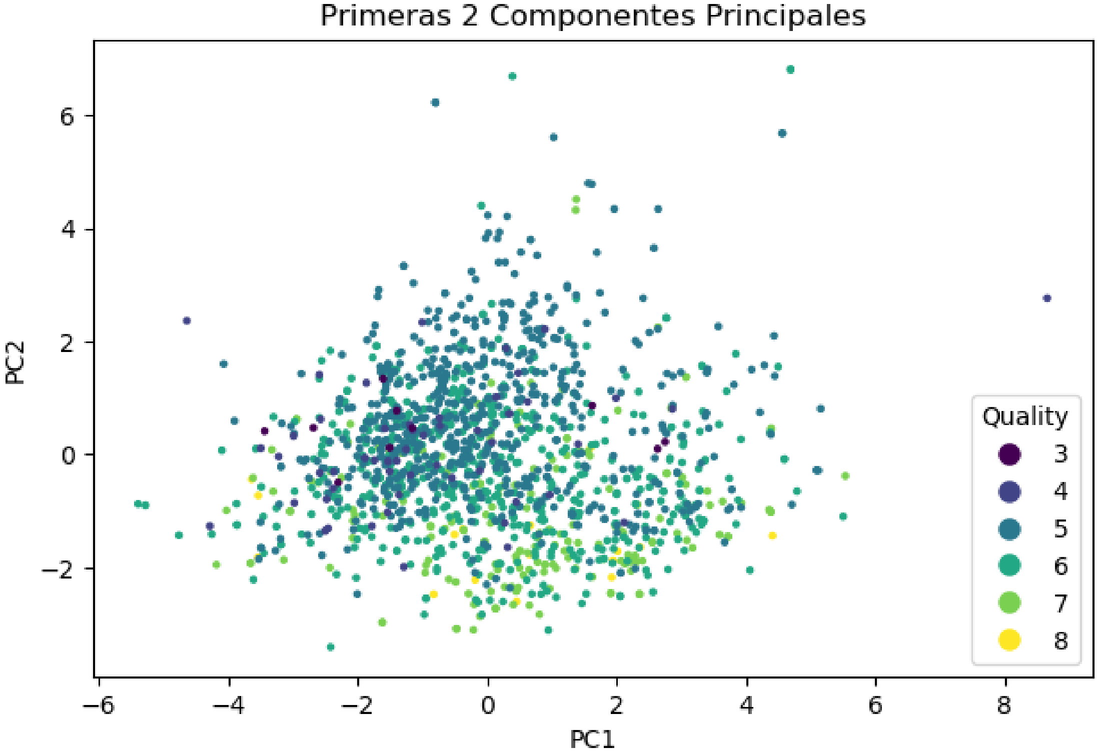
### 6.2 2D

[ ]:
```
df['quality'].cat.codes.unique()
```

[ ]: array([2, 3, 4, 1, 5, 0], dtype=int8)

[ ]:
```
# 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()
```

Datos Proyectados




[ ]:

[ ]:

[ ]:

[ ]: