PortafolioImplementacion-M5-TC3007C

December 2, 2022

[ ]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from scipy.stats import anderson, probplot, multivariate_normal, chi2
from pingouin import multivariate_normality
%matplotlib inline
```

[ ]:
```
url = "https://raw.githubusercontent.com/crisb-7/Mercurio/main/mercurio.csv"

columnNames = ["ID", "Lago", "Alcalinidad", "pH", "Calcio", "Clorofila",␣
 ↪"Mercurio",
               "N_Peces", "MinMercurio", "MaxMercurio", "Estimacion", "Edad"]

df = pd.read_csv(url, names = columnNames, header = 0)
```

[ ]:
```
df.head()
```

[ ]:

	ID	Lago	Alcalinidad	pH	Calcio	Clorofila	Mercurio	N_Peces	\
0	1	Alligator	5.9	6.1	3.0	0.7	1.23	5	
1	2	Annie	3.5	5.1	1.9	3.2	1.33	7	
2	3	Apopka	116.0	9.1	44.1	128.3	0.04	6	
3	4	Blue Cypress	39.4	6.9	16.4	3.5	0.44	12	
4	5	Brick	2.5	4.6	2.9	1.8	1.20	12	

	MinMercurio	MaxMercurio	Estimacion	Edad
0	0.85	1.43	1.53	1
1	0.92	1.90	1.33	0
2	0.04	0.06	0.04	0
3	0.13	0.84	0.44	0
4	0.69	1.50	1.33	1

[ ]:
```
df = df.drop(columns = "ID")
columnNames.remove("ID")
```

[ ]:
```
df.describe()
```

[ ]:

	Alcalinidad	pH	Calcio	Clorofila	Mercurio	N_Peces
count	53.000000	53.000000	53.000000	53.000000	53.000000	53.000000
mean	37.530189	6.590566	22.201887	23.116981	0.527170	13.056604
std	38.203527	1.288449	24.932574	30.816321	0.341036	8.560677
min	1.200000	3.600000	1.100000	0.700000	0.040000	4.000000
25%	6.600000	5.800000	3.300000	4.600000	0.270000	10.000000
50%	19.600000	6.800000	12.600000	12.800000	0.480000	12.000000
75%	66.500000	7.400000	35.600000	24.700000	0.770000	12.000000
max	128.000000	9.100000	90.700000	152.400000	1.330000	44.000000

	MinMercurio	MaxMercurio	Estimacion	Edad
count	53.000000	53.000000	53.000000	53.000000
mean	0.279811	0.874528	0.513208	0.811321
std	0.226406	0.522047	0.338729	0.394998
min	0.040000	0.060000	0.040000	0.000000
25%	0.090000	0.480000	0.250000	1.000000
50%	0.250000	0.840000	0.450000	1.000000
75%	0.330000	1.330000	0.700000	1.000000
max	0.920000	2.040000	1.530000	1.000000

1 Análisis de Normalidad

[ ]:
```
numericVars =list(df.describe().columns)
numericVars
```

[ ]:
```
['Alcalinidad',
 'pH',
 'Calcio',
 'Clorofila',
 'Mercurio',
 'N_Peces',
 'MinMercurio',
 'MaxMercurio',
 'Estimacion',
 'Edad']
```

Prueba de normalidad univariada de cada variable

[ ]:
```
# Anderson() SciPy
# If the returned statistic is larger than these critical values then for the␣
 ↪corresponding significance level,
# the null hypothesis that the data come from the chosen distribution can be␣
 ↪rejected.
# The returned statistic is referred to as 'A2' in the references.
```

[ ]:
```
aN = [] # Anderson Normal - Boolean
aS = [] # Anderson Statistic
```

```
aC = [] # Anderson Critical Values
aL = [] # Anderson Significance Levels

for var in numericVars:

  ds = df[var]
  nt = anderson(ds, dist="norm")

  aS.append(nt.statistic)
  aC.append(nt.critical_values)
  aL.append(nt.significance_level)

  if nt.statistic < nt.critical_values[2]:
    aN.append(True)
  else:
    aN.append(False)

univar_normal = pd.DataFrame({"Variable":numericVars, "Normal":aN, "Statistic":
 ↪aS, "Crit":aC, "Significance":aL})
univar_normal.head(10)
```

[ ]:

	Variable	Normal	Statistic	Crit	\
0	Alcalinidad	False	3.672490	[0.54, 0.615, 0.738, 0.861, 1.024]	
1	pH	True	0.349555	[0.54, 0.615, 0.738, 0.861, 1.024]	
2	Calcio	False	4.050986	[0.54, 0.615, 0.738, 0.861, 1.024]	
3	Clorofila	False	5.428596	[0.54, 0.615, 0.738, 0.861, 1.024]	
4	Mercurio	False	0.925285	[0.54, 0.615, 0.738, 0.861, 1.024]	
5	N_Peces	False	8.694305	[0.54, 0.615, 0.738, 0.861, 1.024]	
6	MinMercurio	False	1.977048	[0.54, 0.615, 0.738, 0.861, 1.024]	
7	MaxMercurio	True	0.658470	[0.54, 0.615, 0.738, 0.861, 1.024]	
8	Estimacion	False	1.046948	[0.54, 0.615, 0.738, 0.861, 1.024]	
9	Edad	False	14.334971	[0.54, 0.615, 0.738, 0.861, 1.024]	

	Significance
0	[15.0, 10.0, 5.0, 2.5, 1.0]
1	[15.0, 10.0, 5.0, 2.5, 1.0]
2	[15.0, 10.0, 5.0, 2.5, 1.0]
3	[15.0, 10.0, 5.0, 2.5, 1.0]
4	[15.0, 10.0, 5.0, 2.5, 1.0]
5	[15.0, 10.0, 5.0, 2.5, 1.0]
6	[15.0, 10.0, 5.0, 2.5, 1.0]
7	[15.0, 10.0, 5.0, 2.5, 1.0]
8	[15.0, 10.0, 5.0, 2.5, 1.0]
9	[15.0, 10.0, 5.0, 2.5, 1.0]

[ ]:
```
print("Hay", univar_normal.Normal.sum(), "variable(s) Anderson normale(s)")
```

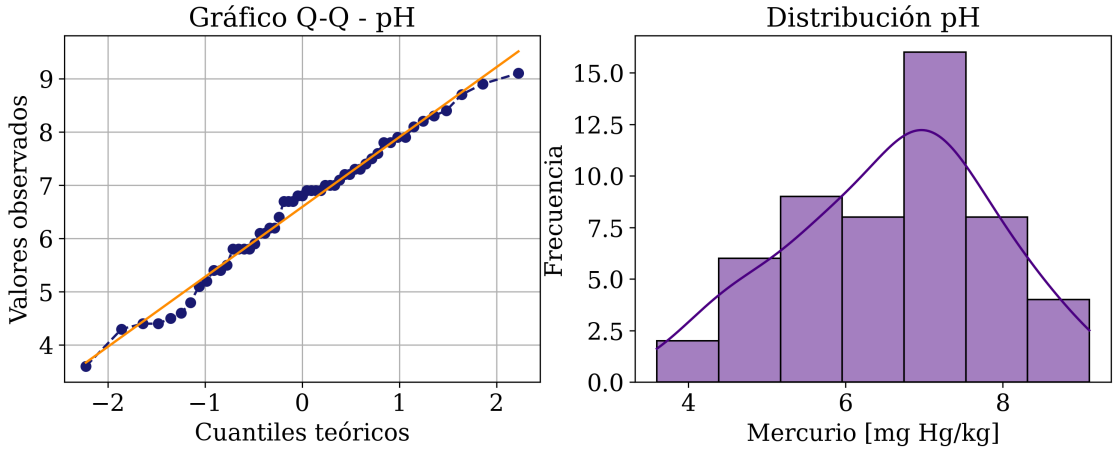
```
Hay 2 variable(s) Anderson normale(s)
```

Variable normal de acuerdo con la prueba de Anderson-Darling

[ ]:
```
univar_normal.loc[aN]
```

[ ]:
```
       Variable  Normal  Statistic                                    Crit  \
1            pH    True   0.349555  [0.54, 0.615, 0.738, 0.861, 1.024]
7  MaxMercurio    True   0.658470  [0.54, 0.615, 0.738, 0.861, 1.024]

                  Significance
1  [15.0, 10.0, 5.0, 2.5, 1.0]
7  [15.0, 10.0, 5.0, 2.5, 1.0]
```

[ ]:
```
plt.rcParams['figure.dpi'] = 300
plt.rcParams['font.family'] = 'serif'
plt.rcParams['font.size'] = 15
# plt.rcParams["text.usetex"] = True
plt.rcParams["axes.titlesize"] = 17

# plt.rcParams.update({"figure.dpi": 180, "font.family": "serif", "text.usetex":
  ↪ True, "font.size": 14, "axes.titlesize": 16,})

fig, axes = plt.subplots(1,2, figsize=(12,4))

probplot(df.pH, plot = axes[0])
axes[0].get_lines()[0].set_marker('o')
axes[0].get_lines()[0].set_linestyle('--')
axes[0].get_lines()[0].set_color('midnightblue')
axes[0].get_lines()[1].set_color('darkorange')
axes[0].set_title("Gráfico Q-Q - pH")
axes[0].set_xlabel("Cuantiles teóricos")
axes[0].set_ylabel("Valores observados")
axes[0].grid()

sns.histplot(data = df, x = "pH", kde = True, color="indigo", ax = axes[1])
axes[1].set_title("Distribución pH")
axes[1].set_xlabel("Mercurio [mg Hg/kg]")
axes[1].set_ylabel("Frecuencia")
plt.show()
```



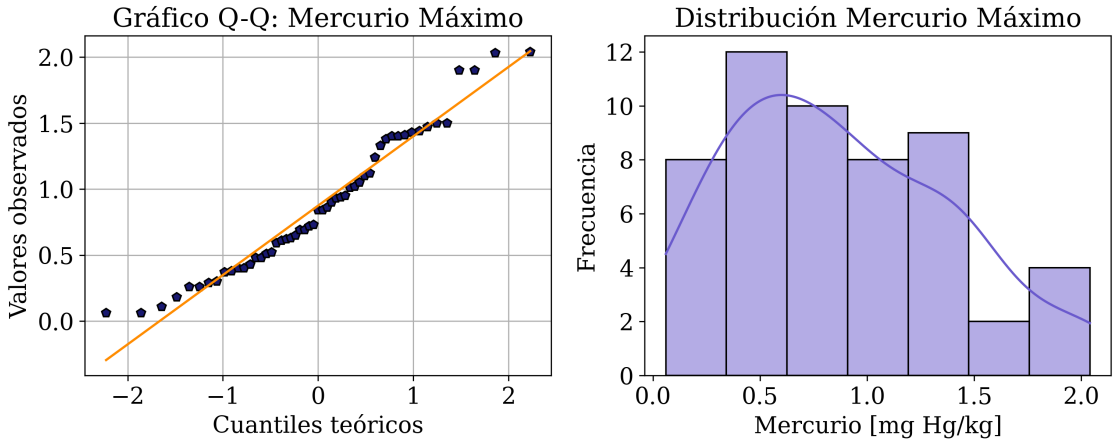
[ ]:
```
df.MaxMercurio.skew()
```

[ ]: 0.4920966176197896

[ ]:
```
df.MaxMercurio.kurtosis()
```

[ ]: -0.5149449394161021

[ ]:
```
fig, axes = plt.subplots(1,2, figsize=(12,4))
probplot(df.MaxMercurio, plot = axes[0])
axes[0].get_lines()[0].set_marker('p')
axes[0].get_lines()[0].set_markeredgecolor("k")
# axes[0].get_lines()[0].set_linestyle('-')
axes[0].get_lines()[0].set_color('midnightblue')
axes[0].get_lines()[1].set_color('darkorange')
axes[0].set_title("Gráfico Q-Q: Mercurio Máximo")
axes[0].set_xlabel("Cuantiles teóricos")
axes[0].set_ylabel("Valores observados")
axes[0].grid()

sns.histplot(data = df, x = "MaxMercurio", kde = True, color="slateblue", ax =␣
↪axes[1])
axes[1].set_title("Distribución Mercurio Máximo")
axes[1].set_xlabel("Mercurio [mg Hg/kg]")
axes[1].set_ylabel("Frecuencia")
plt.show()
```



[ ]:
```
multivariate_normality(df[["pH", "MaxMercurio"]], alpha=0.05)
```

[ ]:
```
HZResults(hz=0.7695729297184755, pval=0.10247634232414388, normal=True)
```

Prueba de normalidad multivariada de todas las combinaciones

[ ]:
```
numericVars
```

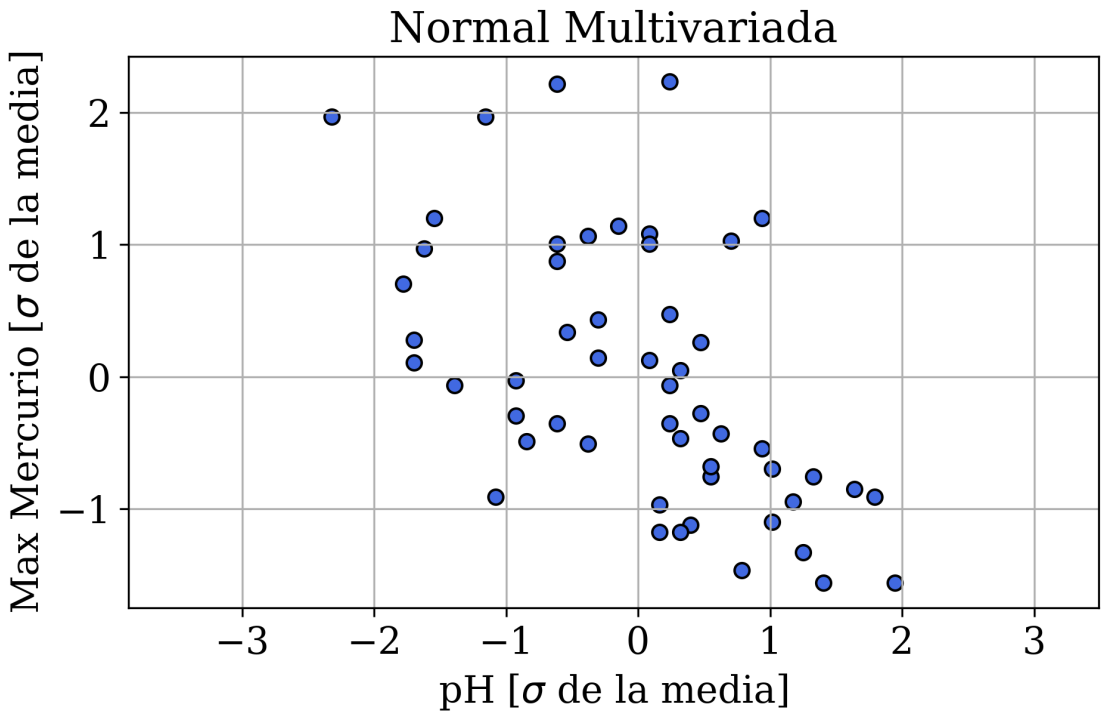
[ ]:
```
['Alcalinidad',
 'pH',
 'Calcio',
 'Clorofila',
 'Mercurio',
 'N_Peces',
 'MinMercurio',
 'MaxMercurio',
 'Estimacion',
 'Edad']
```

[ ]:
```
from itertools import combinations

nn = len(numericVars)
c = 0

for i in range(2, nn):
  comb = combinations(numericVars, i)
  for j in comb:
    cols = list(j)
    # print(cols)
    data = df[cols]
    lol = multivariate_normality(data, alpha=0.05)
    if lol.normal:
```

```
      c += 1
      print(list(data.columns))

print("Hay", c, "normal(es) multivariada(s)")
```

```
['pH', 'MaxMercurio']
Hay 1 normal(es) multivariada(s)
```

[ ]:
```
X1 = (df.pH - df.pH.mean())/df.pH.std()
X2 = (df.MaxMercurio - df.MaxMercurio.mean())/df.MaxMercurio.std()

plt.scatter(X1, X2, color = "royalblue", edgecolor="k")

fig = plt.gcf()
fig.set_size_inches(7, 4)

plt.title("Normal Multivariada")
plt.ylabel(r"Max Mercurio [$\sigma$ de la media]")
plt.xlabel(r"pH [$\sigma$ de la media]")
plt.grid()
plt.axis("equal")
plt.show()
```



[ ]:
```
S = np.cov(X1, X2)
S
```

[ ]:
```
array([[ 1.        , -0.55181523],
       [-0.55181523,  1.        ]])
```

[ ]:
```
rho = -S[0,1]/(np.sqrt(S[0,0])*np.sqrt(S[1,1]))
rho
```

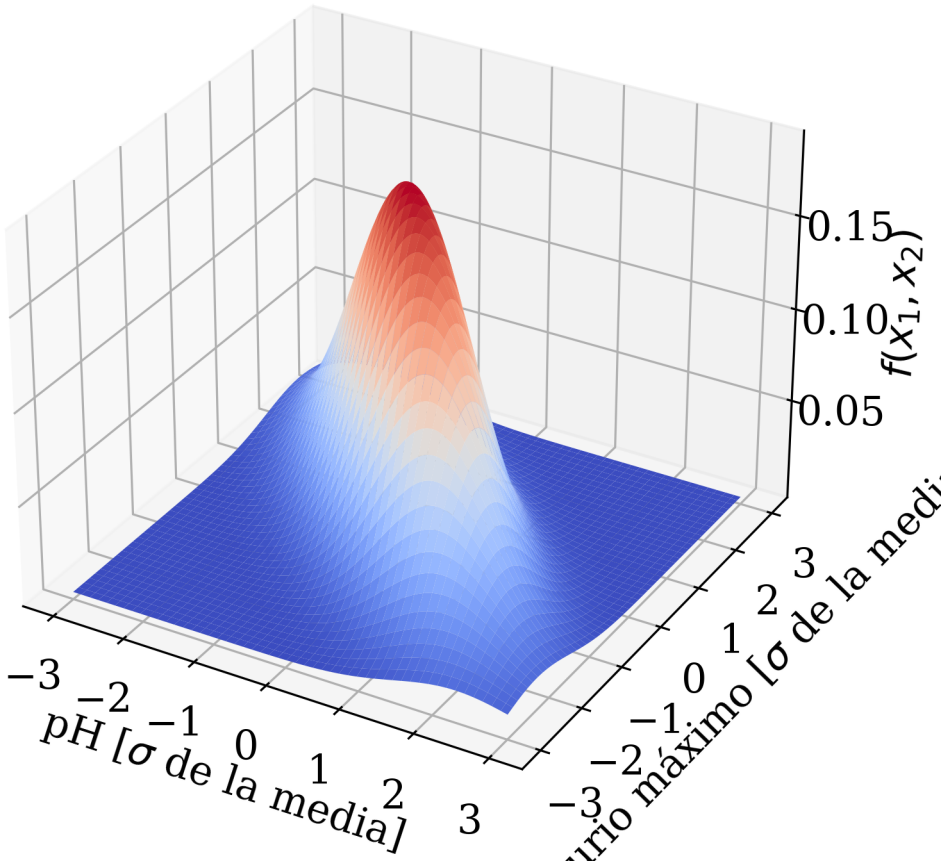
[ ]:
```
0.5518152316870063
```

[ ]:
```
lol = np.ones(len(df))*(-0.05)
```

[ ]:
```
x = np.linspace(-3,3, 200)
y = np.linspace(-3,3, 200)


rv = np.random.multivariate_normal([X1.mean(), X2.mean()], S, size = 250)

X, Y = np.meshgrid(x,y)
f = (1/(2*np.pi*np.sqrt(1-rho**2)))*np.exp( -( 1/(2*(1-rho**2)) ) * (X**2 +␣
 ↪Y**2) - 2*rho*X*Y )
```

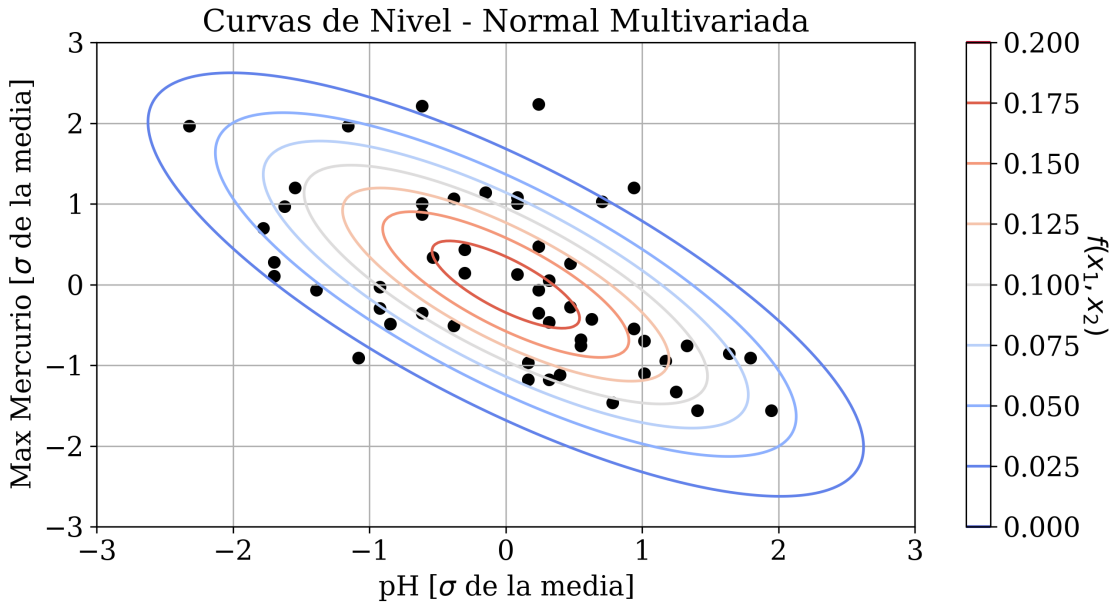
[ ]:
```
# from mpl_toolkits.mplot3d import axes3d

fig = plt.figure(figsize=(12,6))

ax = fig.add_subplot(projection="3d")
ax.plot_surface(X, Y, f, cmap="coolwarm")

# ax.scatter(X1, X2, zs=-0.2, color="k")

ax.set_title("Normal Multivariada: pH y Mercurio máximo")
ax.set_xlabel(r"pH [$\sigma$ de la media]")
ax.set_ylabel(r"Mercurio máximo [$\sigma$ de la media]")
ax.set_zlabel(r"$f(x_1, x_2)$")
plt.show()
```

Normal Multivariada: pH y Mercurio máximo



[ ]:
```
plt.contour(X, Y, f, 8, cmap='coolwarm', linestyles="solid")

fig = plt.gcf()
fig.set_size_inches(9, 5)

ax.set_figure
cbar = plt.colorbar()
cbar.ax.get_yaxis().labelpad = 15
cbar.ax.set_ylabel(r"$f(x_1, x_2)$", rotation=270)

plt.scatter(X1, X2, color = "k")

plt.title("Curvas de Nivel - Normal Multivariada")
ax.set_xlabel(r"pH [$\sigma$ de la media]")
ax.set_ylabel(r"Mercurio máximo [$\sigma$ de la media]")
plt.ylabel(r"Max Mercurio [$\sigma$ de la media]")
```

```
plt.xlabel(r"pH [$\sigma$ de la media]")
plt.grid()
plt.tight_layout()

plt.show()
```

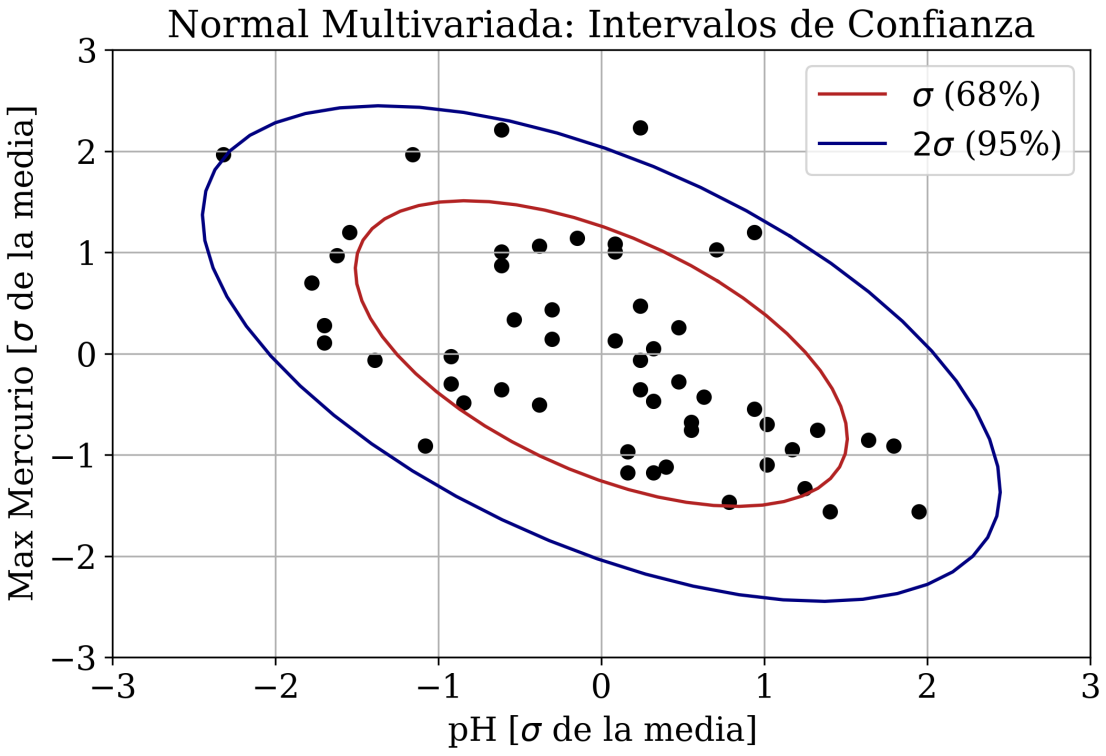


[ ]:
```
Md = pd.DataFrame(np.array([X1, X2]).T)
lam, v = np.linalg.eig(S)
```

[ ]:
```
# Chi_2^2 (alpha 0.05) = 5.99 - 95% confidence

def get_confidence_interval(alpha):
  gl = 2
  significance = 1 - alpha
  ci = chi2.ppf(significance, gl)
  print(ci)
  theta = np.linspace(0, 2*np.pi, len(X1));
  ab = np.sqrt(ci*lam[None,:])
  return (ab * v) @ np.array([np.sin(theta), np.cos(theta)])

ellipsis68 = get_confidence_interval(0.32)
ellipsis95 = get_confidence_interval(0.05)
```

```
2.278868566376729
5.991464547107979
```

[ ]:
```
# plt.scatter(Md[0], Md[1], color = "blue")
plt.scatter(X1, X2, color = "k", edgecolor="k")

fig = plt.gcf()
fig.set_size_inches(8, 5)

plt.plot(ellipsis68[0,:], ellipsis68[1,:], color = "firebrick",␣
 ↪label=r"$\sigma$ (68%)")
plt.plot(ellipsis95[0,:], ellipsis95[1,:], color = "navy", label=r"$2\sigma$␣
 ↪(95%)")

plt.title("Normal Multivariada: Intervalos de Confianza")
plt.xlabel(r"pH [$\sigma$ de la media]")
plt.ylabel(r"Max Mercurio [$\sigma$ de la media]")
plt.xlim([-3, 3])
plt.ylim([-3,3])
plt.legend()
plt.grid()
plt.show()
```



2 Análisis de Componentes Principales

[ ]:
```
cols = df.corr(numeric_only=True).columns
dfs = df[cols]
```

[ ]:
```
from sklearn.preprocessing import MinMaxScaler, StandardScaler
```

[ ]:
```
# scaler = MinMaxScaler()
scaler = StandardScaler()
dfs = scaler.fit_transform(dfs)
dfs = pd.DataFrame(dfs, columns = cols)
```

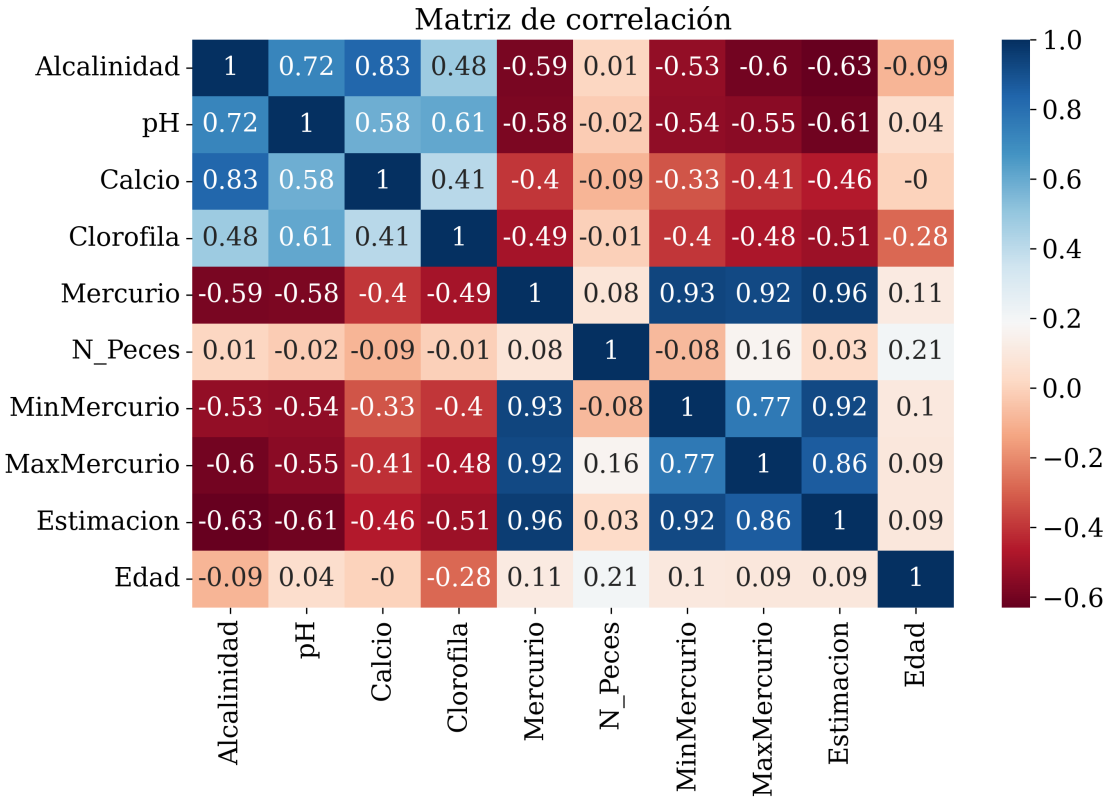
[ ]:
```
dfs.head()
```

[ ]:

	Alcalinidad	pH	Calcio	Clorofila	Mercurio	N_Peces	MinMercurio	MaxMercurio	Estimacion	Edad
0	-0.835862	-0.384385	-0.777523	-0.734400	2.080592	-0.950124	2.542537	1.074209	3.030510	0.482243
1	-0.899285	-1.167939	-0.822064	-0.652498	2.376623	-0.714262	2.854675	1.983127	2.434418	-2.073644
2	2.073650	1.966277	0.886698	3.445888	-1.442171	-0.832193	-1.069346	-1.575190	-1.410376	-2.073644
3	0.049412	0.242458	-0.234930	-0.642669	-0.258049	-0.124606	-0.668026	-0.066773	-0.218192	-2.073644
4	-0.925711	-1.559716	-0.781572	-0.698363	1.991783	-0.124606	1.829079	1.209580	2.434418	0.482243

[ ]:
```
R = dfs.corr()
lam, v = np.linalg.eig(R)
```

[ ]:
```
# PCA on similar correlation variables and compare them???
fig, ax = plt.subplots(figsize=(10, 6))
sns.heatmap(R.round(decimals=2), cmap="RdBu", annot=True, ax = ax)
plt.title("Matriz de correlación")
plt.show()
```



Eigenvalores

[ ]:
```
pd.DataFrame(lam).head()
```

[ ]:
```
          0
0  5.361226
1  1.254261
2  1.216681
3  0.909433
4  0.591417
```

Eigenvectores

[ ]:
```
pd.DataFrame(v).head()
```

[ ]:
```
          0         1         2         3         4         5         6  \
0 -0.350659 -0.216916 -0.347291 -0.009131  0.340505  0.075475  0.338235
1 -0.337004 -0.219409 -0.236097  0.017242 -0.393960  0.731210  0.086296
2 -0.281683 -0.262507 -0.511378 -0.146950  0.362059 -0.313423 -0.343122
3 -0.283342  0.101951 -0.263961  0.432676 -0.630934 -0.441122 -0.134352
4  0.398308 -0.121042 -0.299664  0.080630 -0.030469  0.074369  0.013778
```

```
          7         8         9
0 -0.686230 -0.022398  0.042840
1  0.287692  0.044453  0.013636
2  0.455688  0.026347 -0.115083
3 -0.190070 -0.039824 -0.063331
4  0.016748 -0.848276  0.062433
```

Varianza explicada

[ ]:
```
var_expl = (lam/lam.sum())*100
pd.DataFrame(var_expl).round(decimals=4).head()
```

[ ]:
```
         0
0  53.6123
1  12.5426
2  12.1668
3   9.0943
4   5.9142
```

[ ]:
```
np.cumsum(var_expl)
```

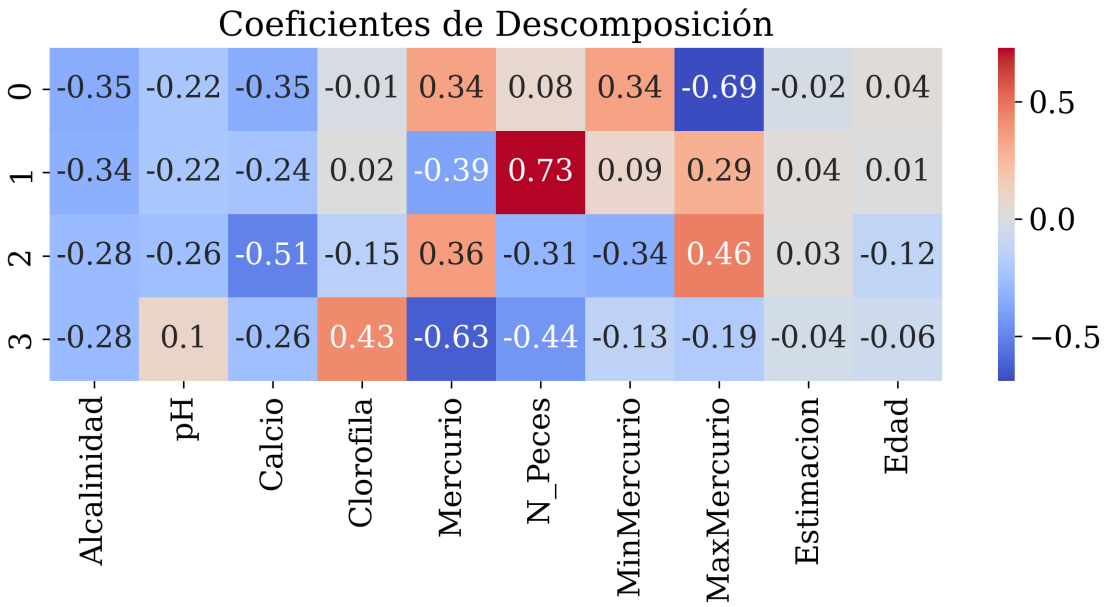
[ ]:
```
array([ 53.61226408,  66.15487501,  78.32168878,  87.41601552,
        93.33018911,  96.36166322,  98.42902665,  99.29723991,
        99.48360976, 100.        ])
```

[ ]:
```
df.head()
```

[ ]:
```
           Lago  Alcalinidad   pH  Calcio  Clorofila  Mercurio  N_Peces  \
0     Alligator          5.9  6.1     3.0        0.7      1.23        5
1         Annie          3.5  5.1     1.9        3.2      1.33        7
2        Apopka        116.0  9.1    44.1      128.3      0.04        6
3  Blue Cypress         39.4  6.9    16.4        3.5      0.44       12
4         Brick          2.5  4.6     2.9        1.8      1.20       12

   MinMercurio  MaxMercurio  Estimacion  Edad
0         0.85         1.43        1.53     1
1         0.92         1.90        1.33     0
2         0.04         0.06        0.04     0
3         0.13         0.84        0.44     0
4         0.69         1.50        1.33     1
```

[ ]:
```
coeffs = pd.DataFrame(v, columns = cols).loc[0:4, :]
coeffs = coeffs.round(decimals=2)#.abs()
# coeffs = (coeffs > 0.69/2).astype(int)

if coeffs.min().min() > 0:
  colormap = "Purples"
else:
```

```
  colormap = "coolwarm"

# fig, ax = plt.subplots(figsize=(10,6))
fig, ax = plt.subplots(figsize=(10,3))
sns.heatmap(coeffs.loc[0:3, :], cmap=colormap, annot=True, ax = ax)
plt.title("Coeficientes de Descomposición")
# plt.title("Eigenvectores de S")
plt.show()
```



[ ]:
```
df.head()
```

[ ]:

	Lago	Alcalinidad	pH	Calcio	Clorofila	Mercurio	N_Peces	\
0	Alligator	5.9	6.1	3.0	0.7	1.23	5	
1	Annie	3.5	5.1	1.9	3.2	1.33	7	
2	Apopka	116.0	9.1	44.1	128.3	0.04	6	
3	Blue Cypress	39.4	6.9	16.4	3.5	0.44	12	
4	Brick	2.5	4.6	2.9	1.8	1.20	12	

	MinMercurio	MaxMercurio	Estimacion	Edad
0	0.85	1.43	1.53	1
1	0.92	1.90	1.33	0
2	0.04	0.06	0.04	0
3	0.13	0.84	0.44	0
4	0.69	1.50	1.33	1

[ ]:
```
# n = 5 #len(df)
# pcs = 3
# pc_evol = np.zeros((pcs, n, len(dfs.columns)))
# for pc in range(pcs):
#   for datapoint in range(n):
#     PC = coeffs.loc[pc, :]
#     data = df[cols].loc[datapoint]
#     pc_evol[pc, datapoint,:] = np.cumsum(PC*data)

# plt.plot(pc_evol[0].T, color="r", marker="o", linestyle="--")
# plt.plot(pc_evol[1].T, color="b", marker="*", linestyle="-.")
# plt.plot(pc_evol[2].T, color="g", marker="p", linestyle="--")
# plt.show()
```

PCA1 - Variacion del nivel de alcalinidad, ph y calcio en funcion del nivel de mercurio y nivel minimo de mercurio en el lago regulado por el nivel maximo de mercurio

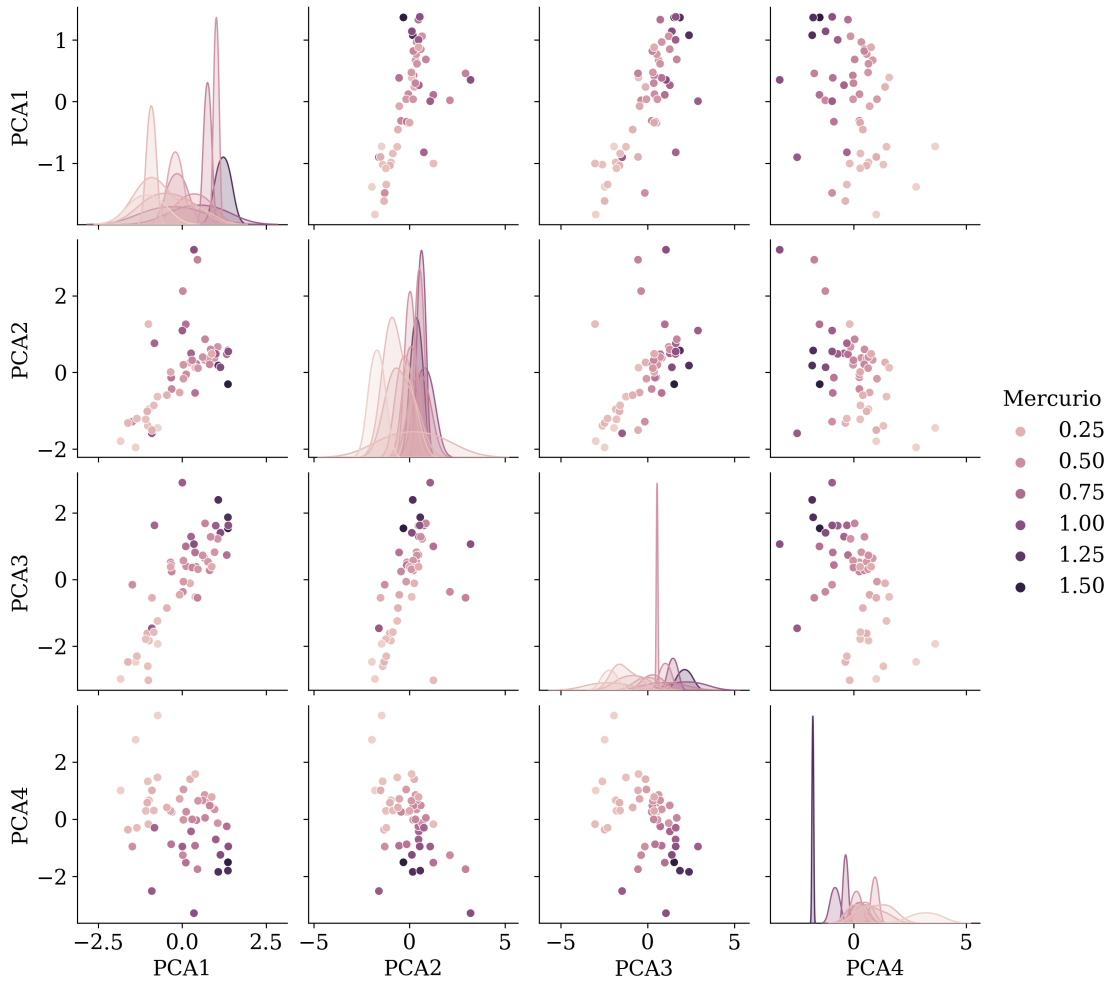
[ ]:
```
M = np.array(dfs[cols])
```

[ ]:
```
PCA = (v @ M.T)

pca_columns = ["PCA1", "PCA2", "PCA3", "PCA4", "PCA5", "PCA6", "PCA7", "PCA8",␣
 ↪"PCA9", "PCA10"]

PCA = pd.DataFrame(PCA.T, columns = pca_columns)
PCA.head()
```

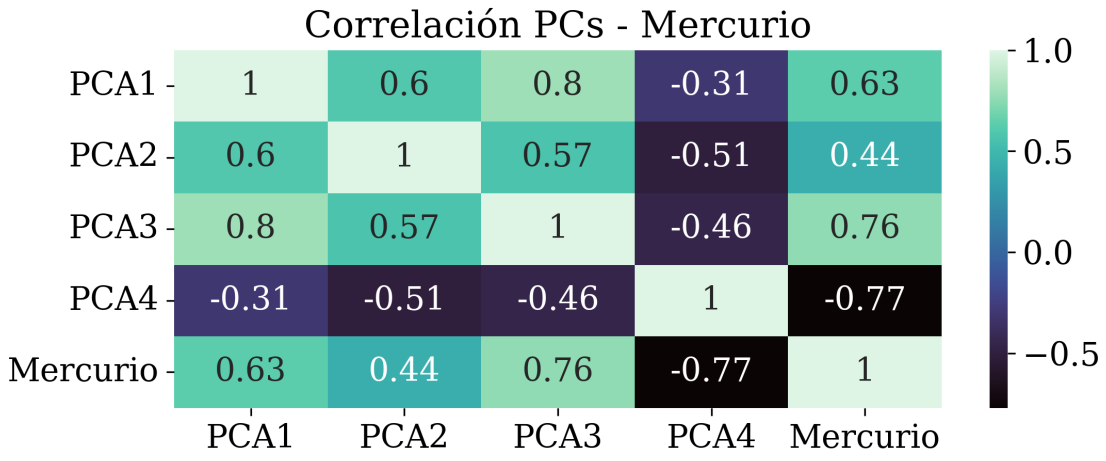
[ ]:

	PCA1	PCA2	PCA3	PCA4	PCA5	PCA6	PCA7	PCA8	PCA9	PCA10
0	1.365559	-0.307733	1.534418	-1.505468	-2.734255	0.629991	2.632404	-1.486107	0.604568	-0.547665
1	1.076792	0.180404	2.387485	-1.840094	-2.270600	1.271905	1.296590	-2.483843	2.595180	-0.322780
2	-1.384938	-1.956949	-2.470802	2.777381	1.607941	0.805398	-1.852539	1.073979	1.821683	-1.675864
3	-0.343811	-0.129749	0.514318	0.254899	0.052811	-0.870858	-1.323597	-0.100963	1.515232	0.355154
4	1.364295	0.571494	1.864928	-1.797432	-2.061472	1.150706	1.991394	-0.874413	0.356363	0.104145

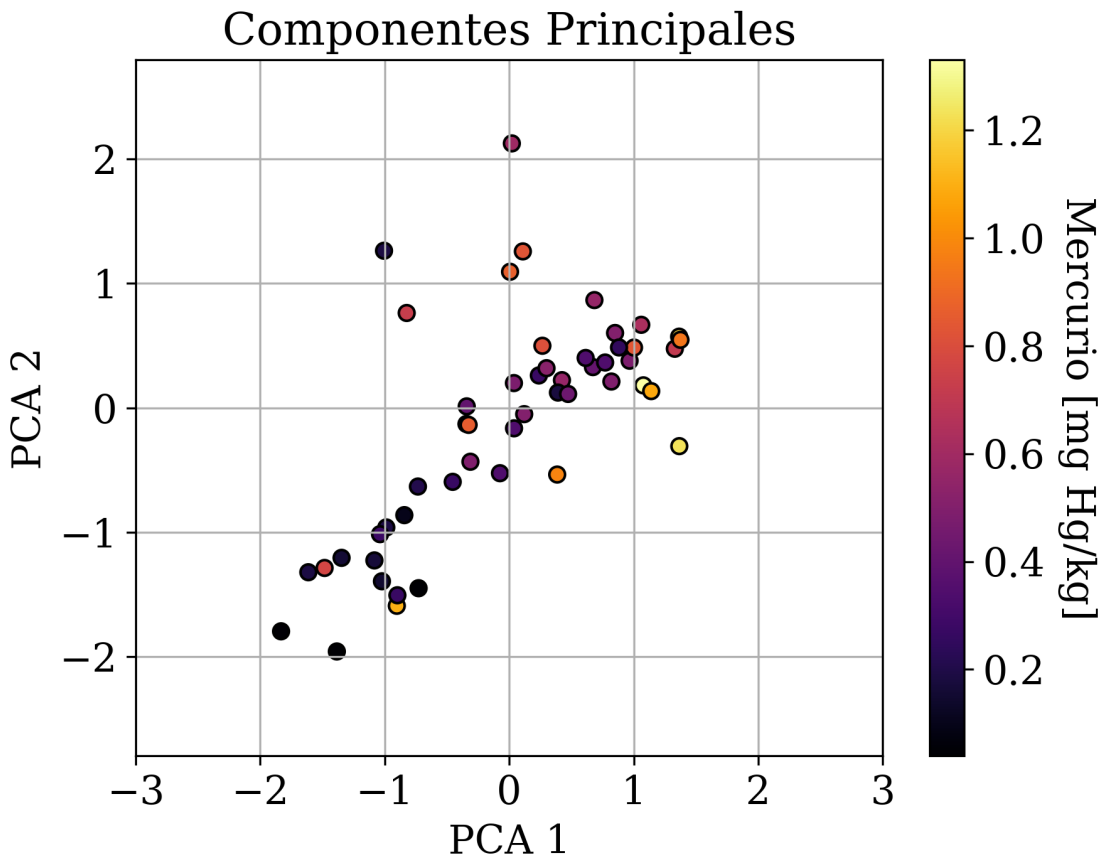
[ ]:
```
dummy = PCA.loc[:,PCA.columns[0:4]]
dummy["Mercurio"] = df.Estimacion

sns.pairplot(data=dummy, hue="Mercurio")
plt.show()
```



[ ]:
```
dummy = PCA.loc[:,PCA.columns[0:4]]
dummy["Mercurio"] = df.Estimacion
colormap = "mako"
fig, ax = plt.subplots(figsize=(8,3))
sns.heatmap(dummy.corr(), cmap=colormap, annot=True, ax = ax)
plt.title("Correlación PCs - Mercurio")
plt.show()
```



[ ]:
```
plt.scatter(PCA.PCA1, PCA.PCA2, c=df.Mercurio, cmap="inferno", edgecolor="k")

# plt.colorbar()
ax.set_figure
cbar = plt.colorbar()
cbar.ax.get_yaxis().labelpad = 20
cbar.ax.set_ylabel("Mercurio [mg Hg/kg]", rotation=270)

plt.title("Componentes Principales")
plt.xlabel("PCA 1")
plt.ylabel("PCA 2")
plt.grid()
plt.axis("equal")
plt.xlim([-3, 3])
plt.ylim([-3, 3])

plt.show()
```


Componentes Principales
PCA 2
PCA 1
Mercurio [mg Hg/kg]
2
1
0
−1
−2
−3
−2
−1
0
1
2
3
1.2
1.0
0.8
0.6
0.4
0.2