Clustering completo con Python

Importar el dataset

In [13]:
```
import pandas as pd
import numpy as np
```

In [14]:
```
df = pd.read_csv("../../Data-Sets/datasets/wine/winequality-red.csv" , sep=";")
df2 = pd.read_csv("../../Data-Sets/datasets/wine/winequality-white.csv" , sep=";")
df.shape, df2.shape
```

Out[14]:
```
((1599, 12), (4898, 12))
```

In [15]:
```
df.head()
```

Out[15]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	q
0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4	
1	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.8	
2	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.8	
3	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.9980	3.16	0.58	9.8	
4	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4	

In [16]:
```
df2.head()
```

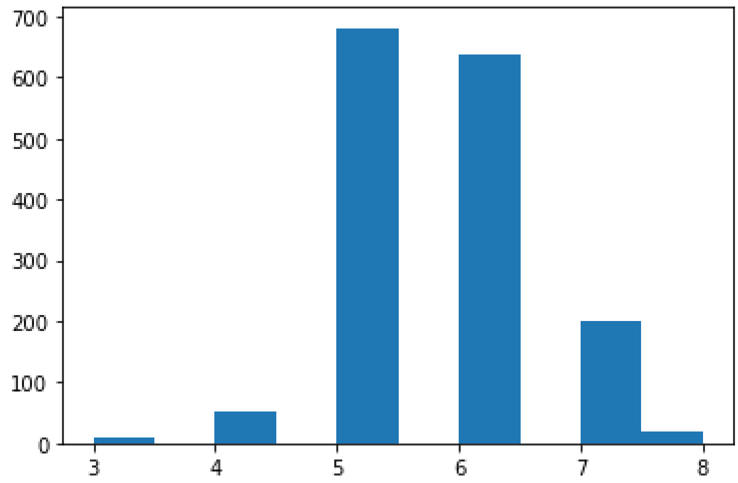
Out[16]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	q
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	

In [17]:
```
import matplotlib.pyplot as plt
```

In [18]:
```
plt.hist(df["quality"])
```

Out[18]:
```
(array([ 10.,   0.,  53.,   0., 681.,   0., 638.,   0., 199.,  18.]),
 array([3. , 3.5, 4. , 4.5, 5. , 5.5, 6. , 6.5, 7. , 7.5, 8. ]),
 <BarContainer object of 10 artists>)
```



In [20]:

```
df.groupby ("quality").mean()
```

Out[20]:

quality	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH
3	8.360000	0.884500	0.171000	2.635000	0.122500	11.000000	24.900000	0.997464	3.398000
4	7.779245	0.693962	0.174151	2.694340	0.090679	12.264151	36.245283	0.996542	3.381509
5	8.167254	0.577041	0.243686	2.528855	0.092736	16.983847	56.513950	0.997104	3.304949
6	8.347179	0.497484	0.273824	2.477194	0.084956	15.711599	40.869906	0.996615	3.318072
7	8.872362	0.403920	0.375176	2.720603	0.076588	14.045226	35.020101	0.996104	3.290754
8	8.566667	0.423333	0.391111	2.577778	0.068444	13.277778	33.444444	0.995212	3.267222

Como vemos en la tabla de promedios, la volatilidad del ácido y los cloros influyen negativamente en la calidad del vino. Los sulfatos influyes positivamente al igual que el ácido cítrico. 2- , 2+ y el reso neutras. La idea es ver la influencia de las variables en el resultado final.

Normalización de los datos

In [22]:

```
df_norm = (df-df.min())/(df.max()-df.min())
df_norm.head()
```

Out[22]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates
0	0.247788	0.397260	0.00	0.068493	0.106845	0.140845	0.098940	0.567548	0.606299	0.137725
1	0.283186	0.520548	0.00	0.116438	0.143573	0.338028	0.215548	0.494126	0.362205	0.209581
2	0.283186	0.438356	0.04	0.095890	0.133556	0.197183	0.169611	0.508811	0.409449	0.191617
3	0.584071	0.109589	0.56	0.068493	0.105175	0.225352	0.190813	0.582232	0.330709	0.149701
4	0.247788	0.397260	0.00	0.068493	0.106845	0.140845	0.098940	0.567548	0.606299	0.137725

Todos los valores oscilarán entre cero y uno mediante la normalización.

Clustering jerárquico con scikit-learn

In [24]:
```
from sklearn.cluster import AgglomerativeClustering
```

In [25]:
```
clus = AgglomerativeClustering(n_clusters=6, linkage="ward").fit(df_norm)
```

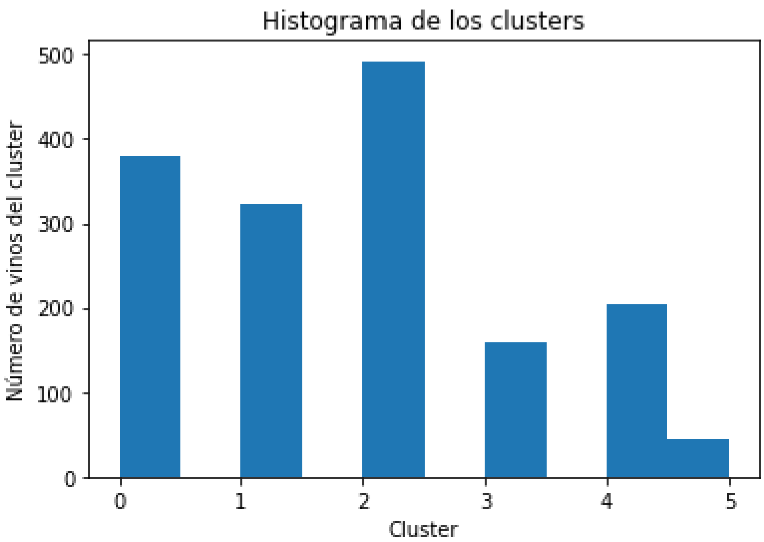
In [27]:
```
clus.labels_
```

Out[27]:
```
array([2, 2, 2, ..., 4, 4, 0], dtype=int64)
```

In [44]:
```
md_h = pd.Series(clus.labels_)
```

In [45]:
```
plt.hist(md_h)
plt.title("Histograma de los clusters")
plt.xlabel("Cluster")
plt.ylabel("Número de vinos del cluster")
```

Out[45]:
```
Text(0, 0.5, 'Número de vinos del cluster')
```



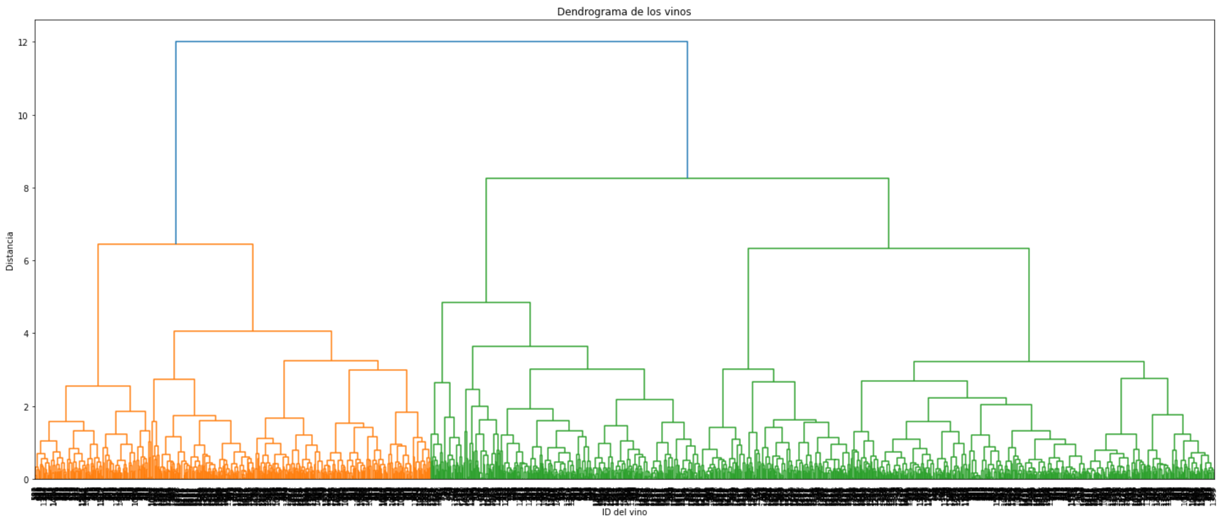
In [30]:
```
clus.children_
```

Out[30]:
```
array([[   0,    4],
       [ 135,  140],
       [ 750,  751],
       ...,
       [3179, 3191],
       [3192, 3193],
       [3194, 3195]], dtype=int64)
```

In [31]:
```
from scipy.cluster.hierarchy import dendrogram, linkage
```

In [32]:
```
Z = linkage(df_norm, "ward")
```

In [34]:
```
plt.figure(figsize=(25,10))
plt.title("Dendrograma de los vinos")
plt.xlabel("ID del vino")
plt.ylabel("Distancia")
dendrogram(Z, leaf_rotation=90., leaf_font_size=9.)
plt.show()
```



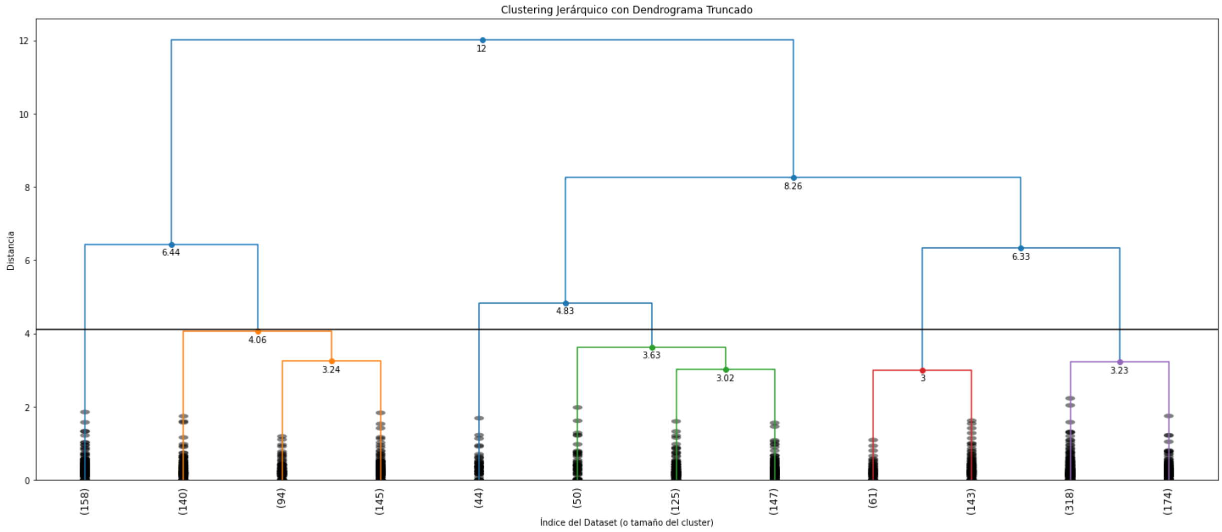
In [35]:
```
def dendrogram_tuned(*args, **kwargs):
    max_d=kwargs.pop("max_d", None)
    if max_d and 'color_threshold' not in kwargs:
        kwargs['color_threshold'] = max_d
    annotate_above = kwargs.pop('annotate_above', 0)

    ddata = dendrogram(*args, **kwargs)

    if not kwargs.get('no_plot', False):
        plt.title("Clustering Jerárquico con Dendrograma Truncado")
        plt.xlabel("Índice del Dataset (o tamaño del cluster)")
        plt.ylabel("Distancia")
        for i, d, c in zip(ddata['icoord'], ddata['dcoord'], ddata['color_list']):
            x = 0.5 * sum(i[1:3])
            y = d[1]
            if y>annotate_above:
                plt.plot(x,y, 'o', c=c)
                plt.annotate('%.3g'%y, (x,y), xytext=(0,-5),
                             textcoords="offset points", va="top", ha="center")
    if max_d:
        plt.axhline(y=max_d, c='k')

    return ddata
```

In [38]:
```
plt.figure(figsize=(25,10))
dendrogram_tuned(Z, truncate_mode='lastp', p=12,
                 leaf_rotation=90., leaf_font_size=12., show_contracted=True,
                 annotate_above=3, max_d = 4.1)
plt.show()
```



K-means

In [69]:
```
from sklearn.cluster import KMeans
from sklearn import datasets
```

In [70]:
```
model = KMeans(n_clusters=6)
model.fit(df_norm)
```

Out[70]:
```
KMeans(n_clusters=6)
```

In [71]:
```
md_k = pd.Series(model.labels_)
```

In [72]:
```
df_norm["clust_h"]=md_h
df_norm["clust_k"]=md_k
```

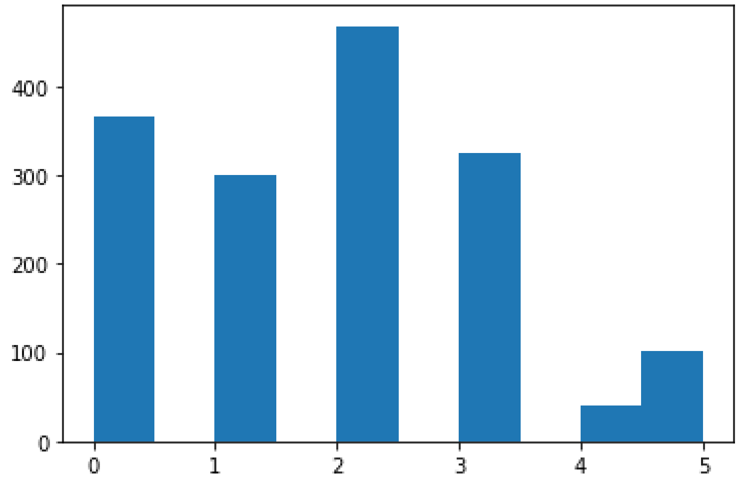
In [73]:
```
df_norm.head()
```

Out[73]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates
0	0.247788	0.397260	0.00	0.068493	0.106845	0.140845	0.098940	0.567548	0.606299	0.137725
1	0.283186	0.520548	0.00	0.116438	0.143573	0.338028	0.215548	0.494126	0.362205	0.209581
2	0.283186	0.438356	0.04	0.095890	0.133556	0.197183	0.169611	0.508811	0.409449	0.191617
3	0.584071	0.109589	0.56	0.068493	0.105175	0.225352	0.190813	0.582232	0.330709	0.149701
4	0.247788	0.397260	0.00	0.068493	0.106845	0.140845	0.098940	0.567548	0.606299	0.137725

In [74]:
```
plt.hist(md_k)
```

Out[74]:
```
(array([365.,   0., 300.,   0., 468.,   0., 325.,   0.,  40., 101.]),
 array([0. , 0.5, 1. , 1.5, 2. , 2.5, 3. , 3.5, 4. , 4.5, 5. ]),
 <BarContainer object of 10 artists>)
```



In [63]:

```
model.cluster_centers_
```

Out[63]:

```
array([[3.75027276e-01, 2.82107337e-01, 2.83013699e-01, 1.04531807e-01,
        1.11976582e-01, 1.95755354e-01, 1.09347016e-01, 4.84175165e-01,
        4.61115306e-01, 2.07628578e-01, 3.94836670e-01, 5.67123288e-01,
        3.61369863e+00, 2.00000000e+00],
       [3.07182800e-01, 2.84845365e-01, 2.92975460e-01, 1.49445332e-01,
        1.26954945e-01, 3.46496155e-01, 2.83205792e-01, 5.36028306e-01,
        4.36138351e-01, 1.75636457e-01, 2.05128205e-01, 4.52147239e-01,
        1.07975460e+00, 3.99693252e+00],
       [2.64368687e-01, 3.60762371e-01, 1.07387580e-01, 9.12264234e-02,
        1.23735848e-01, 1.44418976e-01, 1.01527682e-01, 4.88513554e-01,
        4.89571566e-01, 1.52713844e-01, 2.26102235e-01, 4.52676660e-01,
        2.00214133e+00, 1.01927195e+00],
       [3.61150442e-01, 1.64486301e-01, 4.15266667e-01, 1.05365297e-01,
        1.07779633e-01, 1.83309859e-01, 9.98586572e-02, 4.27513461e-01,
        4.26272966e-01, 2.28822355e-01, 4.59743590e-01, 6.76000000e-01,
        1.66666667e-02, 3.04333333e+00],
       [3.44469027e-01, 3.02054795e-01, 4.27750000e-01, 8.40753425e-02,
        4.28213689e-01, 2.51760563e-01, 2.08392226e-01, 5.10682819e-01,
        2.83464567e-01, 4.95359281e-01, 2.17307692e-01, 4.70000000e-01,
        4.70000000e+00, 5.00000000e+00],
       [4.33014983e-01, 2.07073105e-01, 4.22178218e-01, 1.48853926e-01,
        1.18299476e-01, 1.79054525e-01, 1.06007067e-01, 5.50115584e-01,
        4.03211975e-01, 2.11655896e-01, 3.41203351e-01, 5.50495050e-01,
        1.68316832e-01, 4.44089210e-16]])
```

In [64]:

```
model.inertia_
```

Out[64]:

```
458.263238598056
```

Interpretación final

In [127…

```
df_norm.groupby("clust_k").mean()
```

Out[127…

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	su
clust_k										
0	0.375027	0.282107	0.283014	0.104532	0.111977	0.195755	0.109347	0.484175	0.461115	(
1	0.361150	0.164486	0.415267	0.105365	0.107780	0.183310	0.099859	0.427513	0.426273	(

clust_k	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	su
2	0.264447	0.360679	0.107500	0.091163	0.123661	0.144171	0.101386	0.488431	0.489670	(
3	0.307202	0.284731	0.293385	0.149715	0.127073	0.347476	0.283968	0.536293	0.435833	(
4	0.344469	0.302055	0.427750	0.084075	0.428214	0.251761	0.208392	0.510683	0.283465	(
5	0.433015	0.207073	0.422178	0.148854	0.118299	0.179055	0.106007	0.550116	0.403212	(

In [80]:

```
df_norm.head()
```

Out[80]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates
0	0.247788	0.397260	0.00	0.068493	0.106845	0.140845	0.098940	0.567548	0.606299	0.137725
1	0.283186	0.520548	0.00	0.116438	0.143573	0.338028	0.215548	0.494126	0.362205	0.209581
2	0.283186	0.438356	0.04	0.095890	0.133556	0.197183	0.169611	0.508811	0.409449	0.191617
3	0.584071	0.109589	0.56	0.068493	0.105175	0.225352	0.190813	0.582232	0.330709	0.149701
4	0.247788	0.397260	0.00	0.068493	0.106845	0.140845	0.098940	0.567548	0.606299	0.137725

In [77]:

```
from scipy.cluster.hierarchy import fcluster
```

In [110…

```
X = df_norm.columns.values.tolist()[13:]
X1 = df_norm[X]
```

In [123…

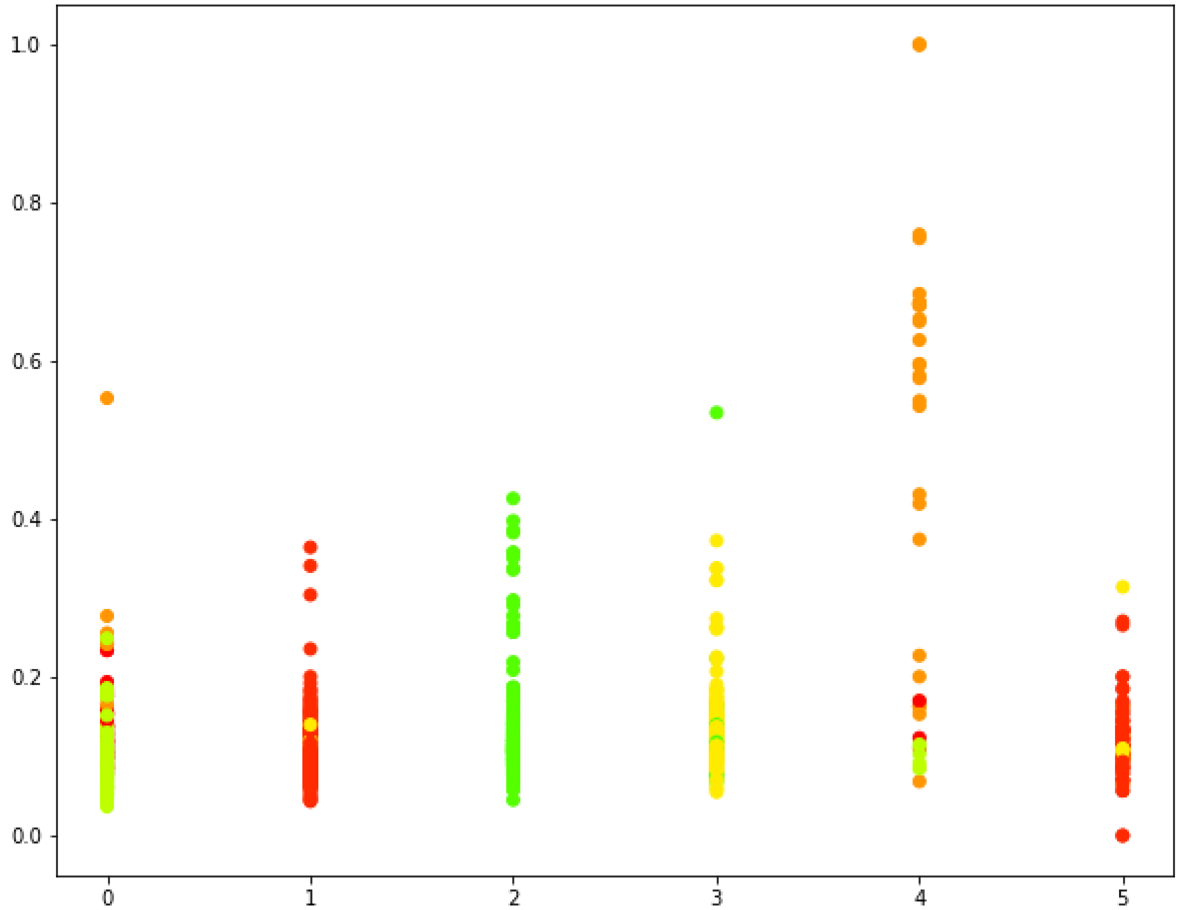
```
df_norm["clust_k"]
```

Out[123…

```
0       2
1       2
2       2
3       0
4       2
       ..
1594    0
1595    0
1596    0
1597    0
1598    1
Name: clust_k, Length: 1599, dtype: int32
```

In [125…

```
max_d=4.2
clusters = fcluster(Z, max_d, criterion="distance")
plt.figure(figsize=(10,8))
plt.scatter(df_norm["clust_k"], df_norm["chlorides"], c= clusters, cmap="prism")
plt.show()
```



No se puede hacer una representación gráfica con más de una variable, pues requerimos 12 dimensiones para ver la nube de dispersión. Sólo se podría hacer seleccionadndo alguna columna contra otra columna.