Análisis de Datos y Aprendizaje Máquina con Tensorflow 2.0: Clustering y reducción de dimensionalidad

2019/09/30

1 Principal Component Analysis (PCA)

Objetivo: Comprender el uso de PCA y aplicarlo a un dataset.

- Documentación: https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html

PCA es una técnica de reducción de dimensionalidad que se puede emplear para preprocesamiento y visualización de datos. Se define como una transformación de un espacio de alta dimensionalidad a un espacio de menor dimensionalidad. Los datos se proyectan en la dirección de máxima varianza, también se buscan las direcciónes donde el error de reconstrucción de los datos es menor.

Si se asume que se tiene una matriz de datos $X \in^{n\times d}$ donde $x_i \in \mathbb{R}^d$

La matriz de covarianza de X es $C \in \mathbb{R}^{d\times d}$ y se define por

$$C = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)(x_i - \mu)^T$$

donde $\mu \in \mathbb{R}^d$ es la media

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Singular value decomposition (SVD) descompone la matriz A en eigenvectores y una matriz diagonal de valores singulares $\Sigma \in \mathbb{R}^{n\times d}$, donde cada valor singular está asociado a un eigenvector. En otra forma de mostrar PCA, se descompone la matriz $\frac{1}{n}X^TX$ que es la matriz de covarianza de los datos centrados, donde μ es nulo:

$$A = U\Sigma V^T$$

donde $U \in \mathbb{R}^{n\times n}$ y $V \in \mathbb{R}^{d\times d}$

Si se toman los datos X^TX, se puede mostrar que $A^TA = V\Sigma^2V^T$, donde las columnas de V contienen los eigenvectores de X^TX. Los datos transformados a una menor dimensión se obtienen por $N = XP$ donde la matriz $P \in \mathbb{R}^{d\times f}$ contiene $f < d$ eigenvectores de V.

In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
```

1.1 Análisis exploratorio

1.1.1 Etiquetas de clase a valor numérico

- Número de variables y etiquetas
- Valores caracter a numérico

In [2]:
```
df = pd.read_csv('iris.csv')
df.head(10)
```

Out[2]:

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa
5	5.4	3.9	1.7	0.4	setosa
6	4.6	3.4	1.4	0.3	setosa
7	5.0	3.4	1.5	0.2	setosa
8	4.4	2.9	1.4	0.2	setosa
9	4.9	3.1	1.5	0.1	setosa

In [3]:
```
df.tail(10)
```

Out[3]:

	sepal_length	sepal_width	petal_length	petal_width	species
140	6.7	3.1	5.6	2.4	virginica
141	6.9	3.1	5.1	2.3	virginica
142	5.8	2.7	5.1	1.9	virginica
143	6.8	3.2	5.9	2.3	virginica
144	6.7	3.3	5.7	2.5	virginica
145	6.7	3.0	5.2	2.3	virginica
146	6.3	2.5	5.0	1.9	virginica
147	6.5	3.0	5.2	2.0	virginica
148	6.2	3.4	5.4	2.3	virginica
149	5.9	3.0	5.1	1.8	virginica

In [4]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 150 entries, 0 to 149
Data columns (total 5 columns):
sepal_length    150 non-null float64
sepal_width     150 non-null float64
petal_length    150 non-null float64
petal_width     150 non-null float64
```

```
species          150 non-null object
dtypes: float64(4), object(1)
memory usage: 6.0+ KB
```

```
In [5]: df = df.replace({'setosa':0, 'versicolor':1, 'virginica' :2})
```

```
In [6]: df.head(10)
```

Out[6]:

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	0
1	4.9	3.0	1.4	0.2	0
2	4.7	3.2	1.3	0.2	0
3	4.6	3.1	1.5	0.2	0
4	5.0	3.6	1.4	0.2	0
5	5.4	3.9	1.7	0.4	0
6	4.6	3.4	1.4	0.3	0
7	5.0	3.4	1.5	0.2	0
8	4.4	2.9	1.4	0.2	0
9	4.9	3.1	1.5	0.1	0

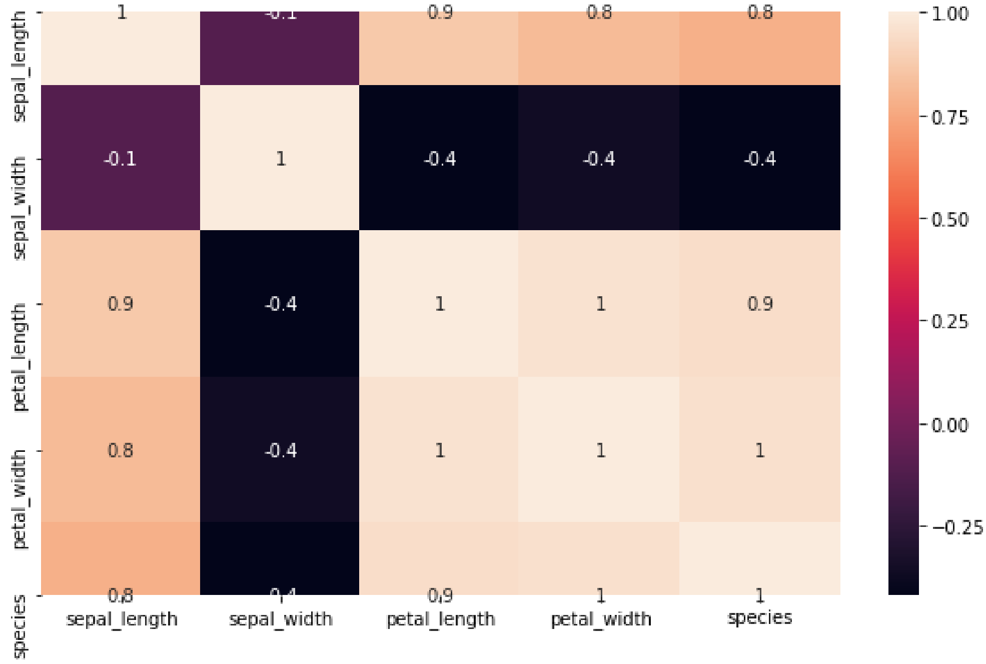
```
In [7]: df.drop('species', axis=1).head()
```

Out[7]:

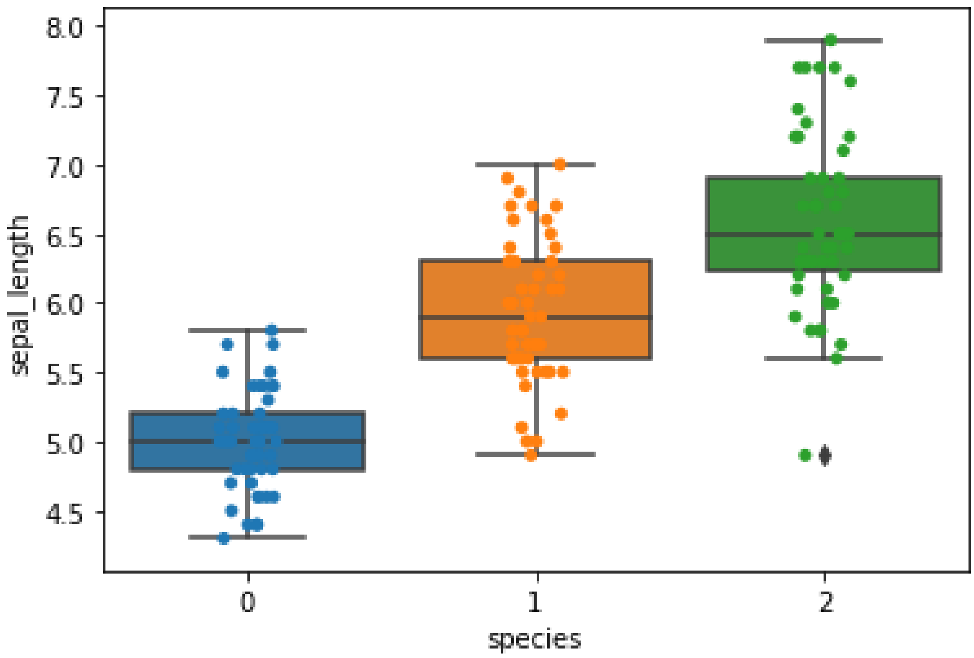
	sepal_length	sepal_width	petal_length	petal_width
0	5.1	3.5	1.4	0.2
1	4.9	3.0	1.4	0.2
2	4.7	3.2	1.3	0.2
3	4.6	3.1	1.5	0.2
4	5.0	3.6	1.4	0.2

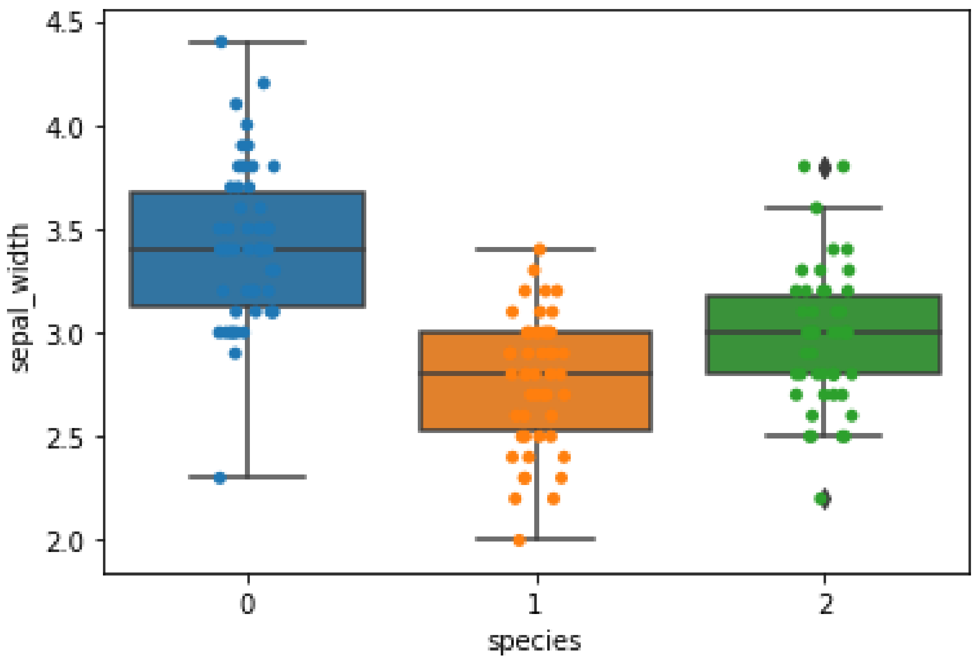
```
In [8]: corr = df.corr()
        plt.figure(figsize=(10, 6))
        sns.heatmap(corr, annot=True, fmt='.1g')
```

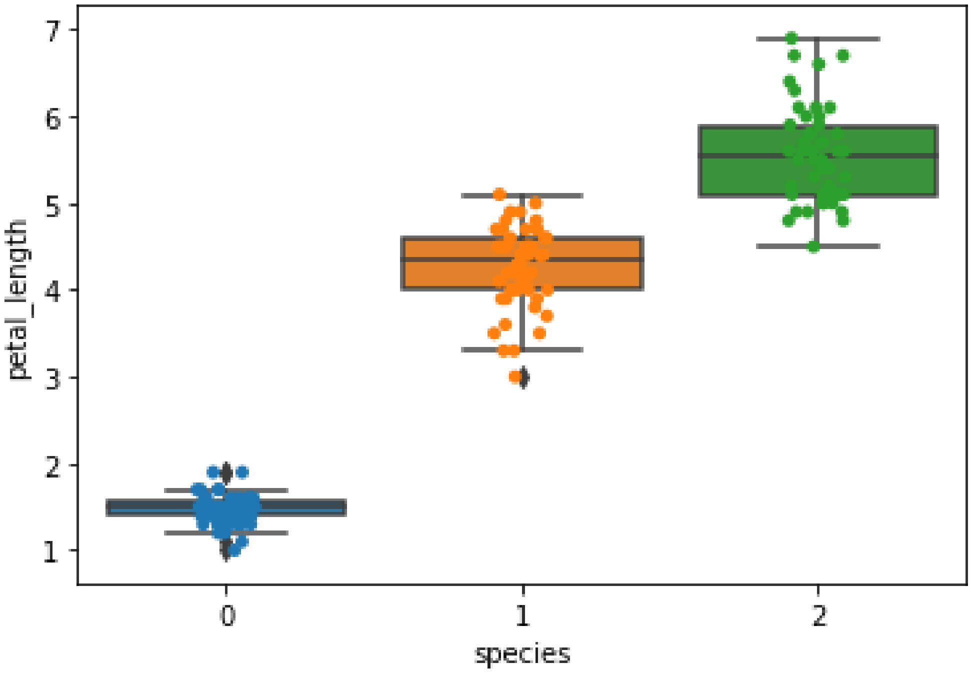
```
Out[8]: <matplotlib.axes._subplots.AxesSubplot at 0x7f6e30ed2a90>
```



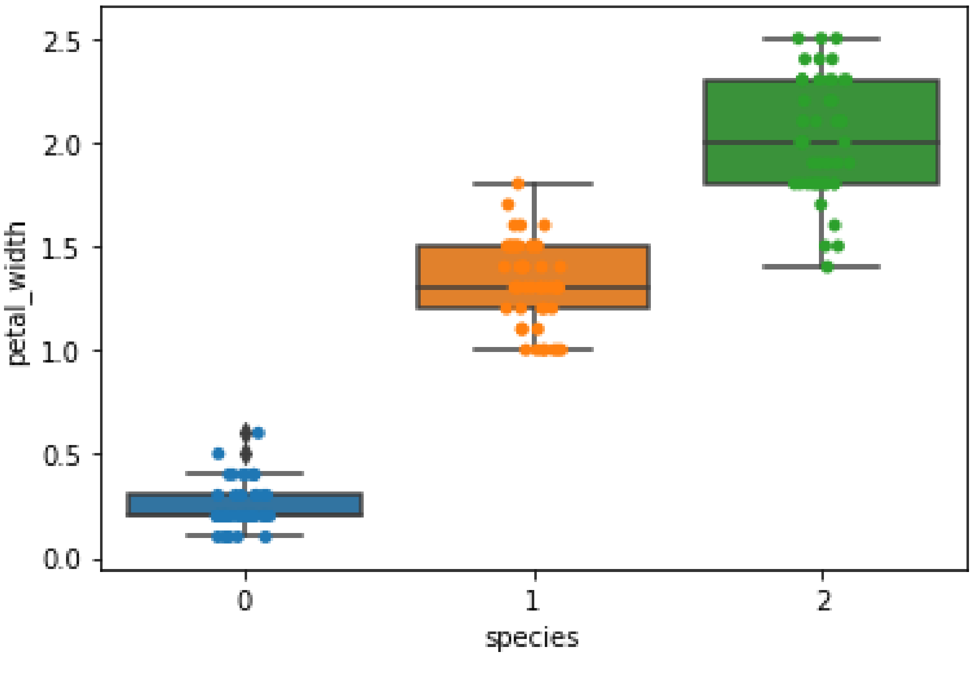

```
In [9]: l=list(df.columns)
        l[0:len(l)]
        for i in range(0,len(l)-1):
            plt.figure()
            sns.boxplot(x='species' ,y=l[i], data=df)
            sns.stripplot(x='species' ,y=l[i], data=df)
```


sepal_length
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
0
1
2
species


sepal_width
4.5
4.0
3.5
3.0
2.5
2.0
0
1
2
species



7
6
5
4
3
2
1
petal_length
0
1
2
species



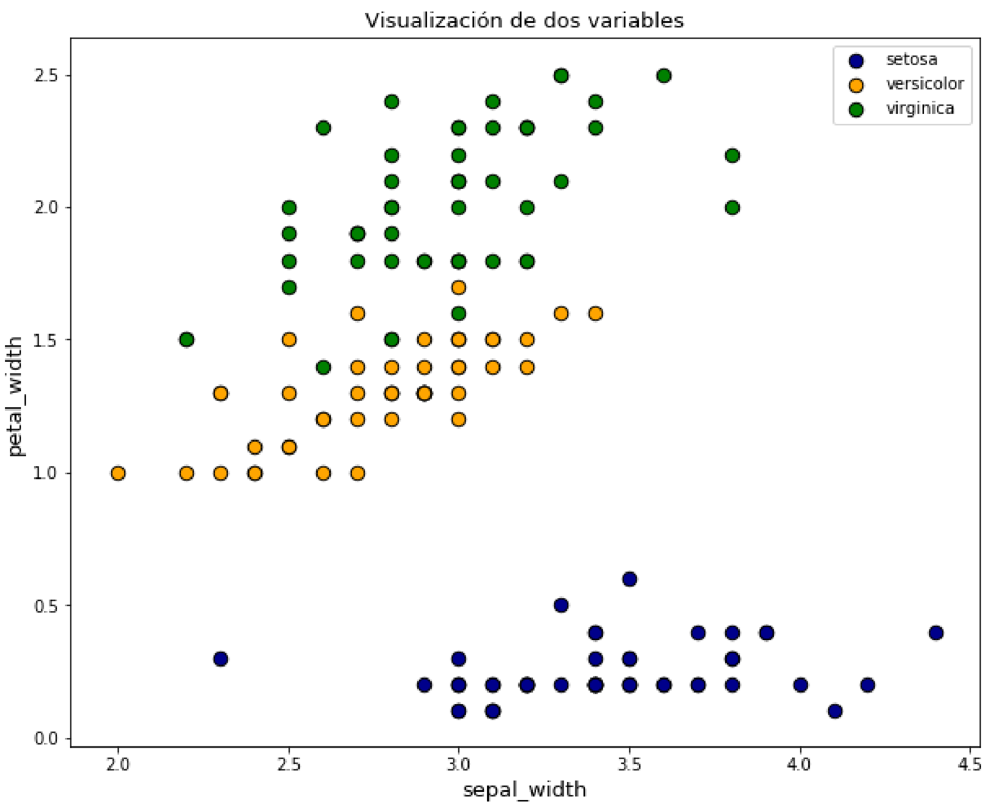
2.5
2.0
1.5
1.0
0.5
0.0
petal_width
0
1
2
species

1.2 Plot de dos variables en 2d

- Se puede conseguir una mejor visualización con pca

```
In [10]: target_ids = np.unique(df.values[:,-1])
         X_plot = np.concatenate(([df['sepal_width'].values], [df['petal_width'].values]), axis=0
         y = df['species'].values
```

```
In [11]: plt.figure(figsize=(10,8))
         colors = ['darkblue','orange','green']
         target_names = ['setosa', 'versicolor', 'virginica']


         for i, c, label in zip(target_ids, colors, target_names):
             plt.scatter(X_plot[0,i == y], X_plot[1,i == y], c = c,  edgecolors='black', s=285,la
         plt.legend()
         plt.title("Visualización de dos variables",fontsize=13)
         plt.xlabel("sepal_width",fontsize=13)
         plt.ylabel("petal_width",fontsize=13)
         plt.show()
```



1.3 PCA de sklearn

- Se pueden indicar el número de dimensiones con n_components

In [12]:
```
from sklearn.decomposition import PCA
```

In [13]:
```
pca = PCA(n_components=None)
dfx_pcan = pca.fit(df.drop('species', axis=1))
```

1.3.1 Varianza de cada PC

- Escalando los datos con 'StandardScaler' se obtiene un mejor resultado, en este caso se visualizará la varianza sin previamente escalar

In [14]:
```
dfx_pcan.explained_variance_ratio_
```

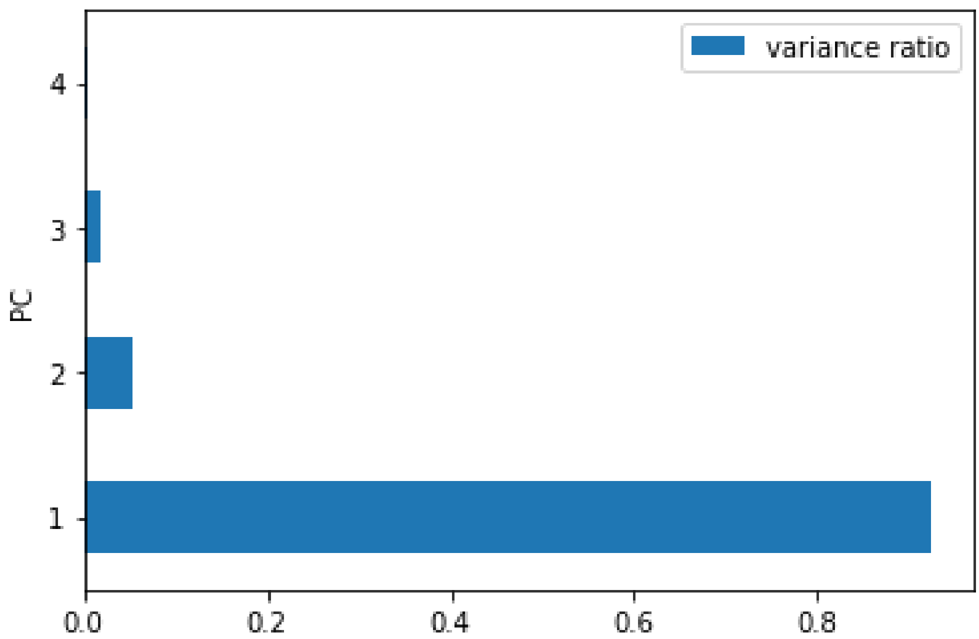
Out[14]:
```
array([0.92461621, 0.05301557, 0.01718514, 0.00518309])
```

In [15]:
```
p_df = pd.DataFrame({'PC':np.arange(1,5), 'variance ratio':dfx_pcan.explained_variance_r
p_df
```

Out[15]:

	PC	variance ratio
0	1	0.924616
1	2	0.053016
2	3	0.017185
3	4	0.005183

In [16]:
```
ax = p_df.plot.barh('PC')
```



In [17]:
```python
trans = pca.transform(df.drop('species', axis=1))
```

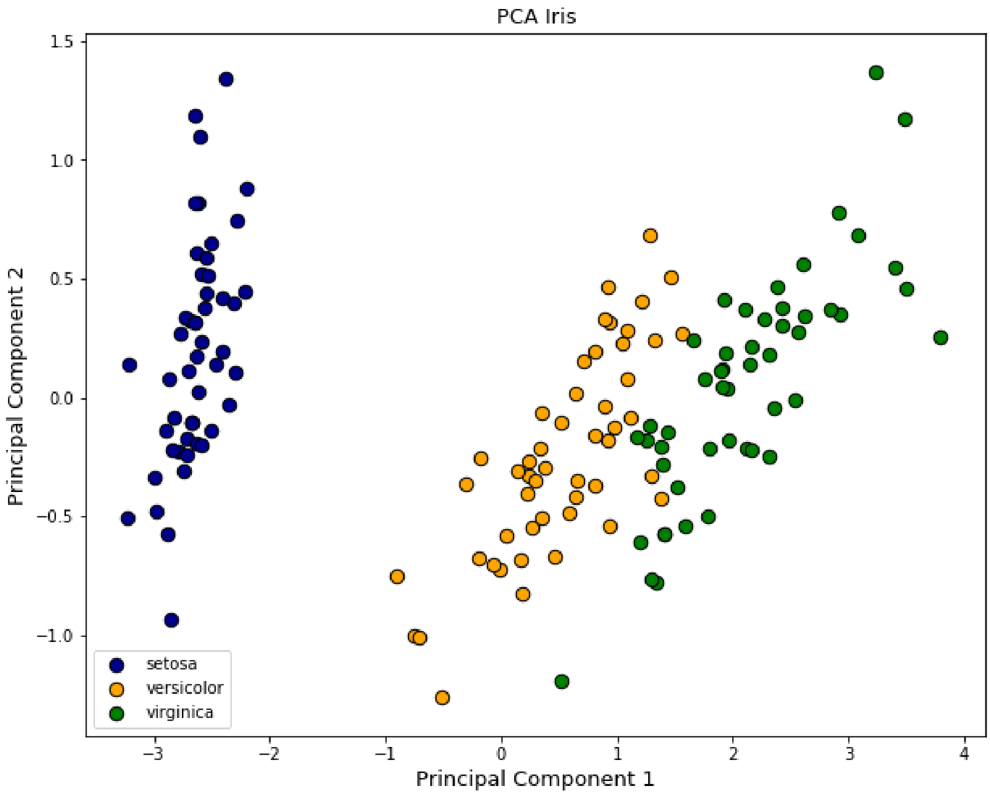
In [18]:
```python
df_transn = pd.DataFrame(data=trans)
df_transn.head(10)
```

Out[18]:

	0	1	2	3
0	-2.684207	0.326607	-0.021512	0.001006
1	-2.715391	-0.169557	-0.203521	0.099602
2	-2.889820	-0.137346	0.024709	0.019305
3	-2.746437	-0.311124	0.037672	-0.075955
4	-2.728593	0.333925	0.096230	-0.063129
5	-2.279897	0.747783	0.174326	-0.027147
6	-2.820891	-0.082105	0.264251	-0.050100
7	-2.626482	0.170405	-0.015802	-0.046282
8	-2.887959	-0.570798	0.027335	-0.026615
9	-2.673845	-0.106692	-0.191533	-0.055891

1.4 Dos componentes principales

In [19]:
```python
target_ids = np.unique(y)
plt.figure(figsize=(10,8))

for i, c, label in zip(target_ids, colors, target_names):
    plt.scatter(trans[i == y,0], trans[i == y,1], c = c,  edgecolors='black', s=285,labe
plt.legend()
plt.title('PCA Iris',fontsize=13)
plt.xlabel("Principal Component 1",fontsize=13)

plt.ylabel("Principal Component 2",fontsize=13)


plt.show()
```

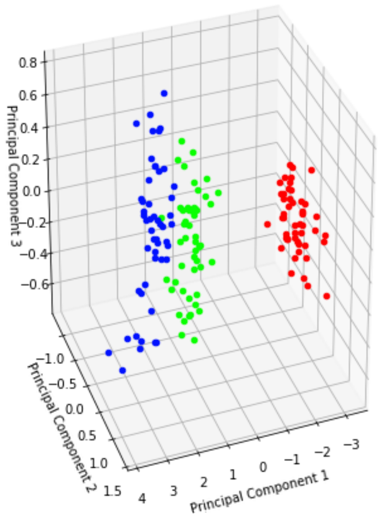


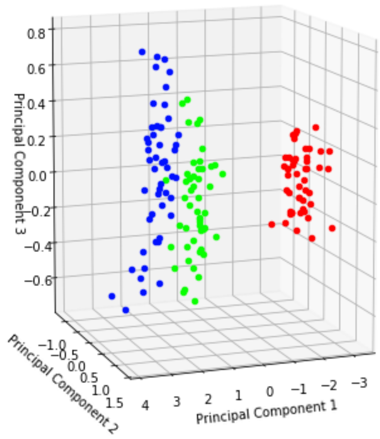
1.5 Tres componentes principales

- Con 'Axes3D' se puede visualizar en 3d

```
In [20]: from mpl_toolkits.mplot3d import Axes3D

         fig = plt.figure(figsize=(14,8))
         ax = fig.add_subplot(1, 2, 1, projection="3d")
         for i in range(trans.shape[0]):
             ax.scatter(trans[i, 0], trans[i, 1], trans[i, 2],color=plt.cm.hsv(y[i] / 3.),marker=
         ax.view_init(30, 70)
         ax.set_xlabel("Principal Component 1")
         ax.set_ylabel("Principal Component 2")
         ax.set_zlabel("Principal Component 3")

         ax = fig.add_subplot(1, 2, 2, projection="3d")
         for i in range(trans.shape[0]):
             ax.scatter(trans[i, 0], trans[i, 1], trans[i, 2],color=plt.cm.hsv(y[i] / 3.),marker=
         ax.view_init(10, 70)
         ax.set_xlabel("Principal Component 1")
```

```
ax.set_ylabel("Principal Component 2")
ax.set_zlabel("Principal Component 3")
plt.show()
```





2

2.1 PCA de Breast Cancer

- Visualizar el dataset de los clasificadores anteriores

In [21]:
```
df = pd.read_csv("data-breast.csv",index_col=0)
df = df.replace({'B':0, 'M':1})
df.head()
df.head(10)
```

Out[21]:
```
          diagnosis  radius_mean  texture_mean  perimeter_mean  area_mean  \
id
842302            1        17.99         10.38          122.80     1001.0
842517            1        20.57         17.77          132.90     1326.0
84300903          1        19.69         21.25          130.00     1203.0
84348301          1        11.42         20.38           77.58      386.1
84358402          1        20.29         14.34          135.10     1297.0
843786            1        12.45         15.70           82.57      477.1
844359            1        18.25         19.98          119.60     1040.0
84458202          1        13.71         20.83           90.20      577.9
844981            1        13.00         21.82           87.50      519.8
84501001          1        12.46         24.04           83.97      475.9
```

```
          smoothness_mean  compactness_mean  concavity_mean  \
id
842302            0.11840           0.27760         0.30010
842517            0.08474           0.07864         0.08690
84300903          0.10960           0.15990         0.19740
84348301          0.14250           0.28390         0.24140
84358402          0.10030           0.13280         0.19800
843786            0.12780           0.17000         0.15780
844359            0.09463           0.10900         0.11270
84458202          0.11890           0.16450         0.09366
844981            0.12730           0.19320         0.18590
84501001          0.11860           0.23960         0.22730

          concave points_mean  symmetry_mean  ...  texture_worst  \
id                                            ...
842302                0.14710         0.2419  ...          17.33
842517                0.07017         0.1812  ...          23.41
84300903              0.12790         0.2069  ...          25.53
84348301              0.10520         0.2597  ...          26.50
84358402              0.10430         0.1809  ...          16.67
843786                0.08089         0.2087  ...          23.75
844359                0.07400         0.1794  ...          27.66
84458202              0.05985         0.2196  ...          28.14
844981                0.09353         0.2350  ...          30.73
84501001              0.08543         0.2030  ...          40.68

          perimeter_worst  area_worst  smoothness_worst  compactness_worst  \
id
842302             184.60      2019.0            0.1622             0.6656
842517             158.80      1956.0            0.1238             0.1866
84300903           152.50      1709.0            0.1444             0.4245
84348301            98.87       567.7            0.2098             0.8663
84358402           152.20      1575.0            0.1374             0.2050
843786             103.40       741.6            0.1791             0.5249
844359             153.20      1606.0            0.1442             0.2576
84458202           110.60       897.0            0.1654             0.3682
844981             106.20       739.3            0.1703             0.5401
84501001            97.65       711.4            0.1853             1.0580

          concavity_worst  concave points_worst  symmetry_worst  \
id
842302             0.7119                0.2654          0.4601
842517             0.2416                0.1860          0.2750
84300903           0.4504                0.2430          0.3613
84348301           0.6869                0.2575          0.6638
84358402           0.4000                0.1625          0.2364
843786             0.5355                0.1741          0.3985
844359             0.3784                0.1932          0.3063
84458202           0.2678                0.1556          0.3196
```

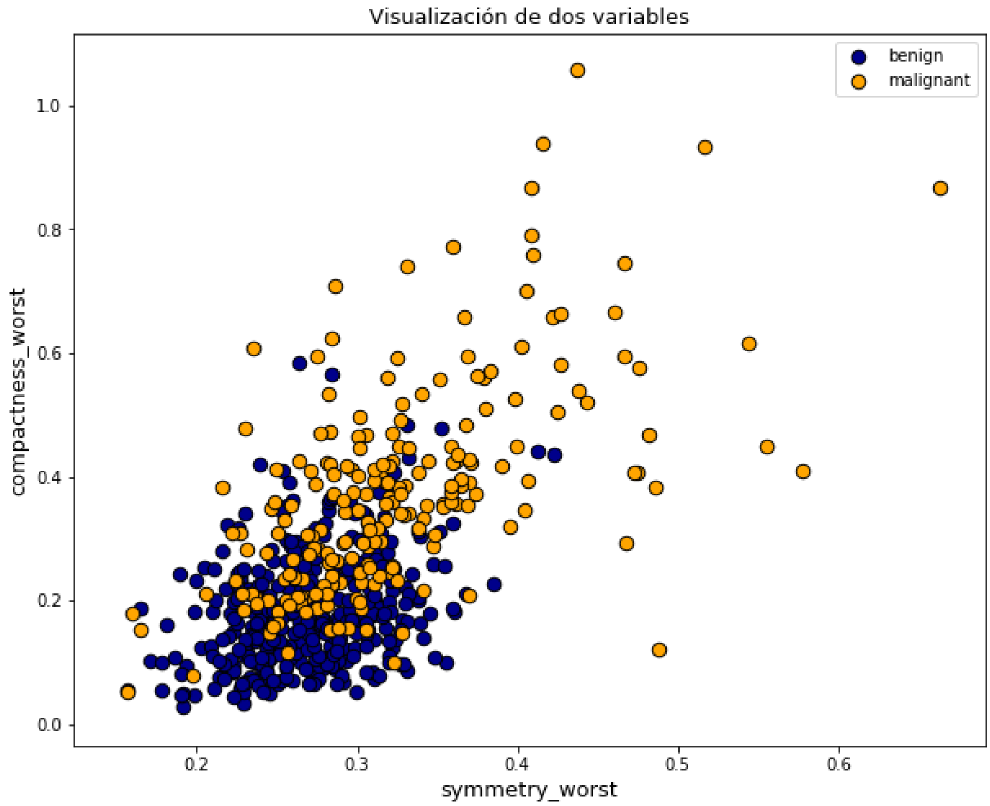
```
844981              0.5390               0.2060          0.4378
84501001            1.1050               0.2210          0.4366

          fractal_dimension_worst  Unnamed: 32
id
842302                    0.11890          NaN
842517                    0.08902          NaN
84300903                  0.08758          NaN
84348301                  0.17300          NaN
84358402                  0.07678          NaN
843786                    0.12440          NaN
844359                    0.08368          NaN
84458202                  0.11510          NaN
844981                    0.10720          NaN
84501001                  0.20750          NaN

[10 rows x 32 columns]
```

```
In [22]: y = df['diagnosis']
         X = df.drop(['diagnosis','Unnamed: 32'],axis=1)
         dfx = pd.DataFrame(data=X,columns=df.columns[1:31])
         dfx.tail()
```

```
Out[22]:         radius_mean  texture_mean  perimeter_mean  area_mean  smoothness_mean  \
         id
         926424        21.56         22.39          142.00     1479.0          0.11100
         926682        20.13         28.25          131.20     1261.0          0.09780
         926954        16.60         28.08          108.30      858.1          0.08455
         927241        20.60         29.33          140.10     1265.0          0.11780
         92751          7.76         24.54           47.92      181.0          0.05263

                 compactness_mean  concavity_mean  concave points_mean  symmetry_mean  \
         id
         926424           0.11590         0.24390              0.13890         0.1726
         926682           0.10340         0.14400              0.09791         0.1752
         926954           0.10230         0.09251              0.05302         0.1590
         927241           0.27700         0.35140              0.15200         0.2397
         92751            0.04362         0.00000              0.00000         0.1587

                 fractal_dimension_mean  ...  radius_worst  texture_worst  \
         id                              ...
         926424                 0.05623  ...        25.450          26.40
         926682                 0.05533  ...        23.690          38.25
         926954                 0.05648  ...        18.980          34.12
         927241                 0.07016  ...        25.740          39.42
         92751                  0.05884  ...         9.456          30.37

                 perimeter_worst  area_worst  smoothness_worst  compactness_worst  \
         id
         926424           166.10      2027.0           0.14100            0.21130
```

```
926682          155.00      1731.0           0.11660            0.19220
926954          126.70      1124.0           0.11390            0.30940
927241          184.60      1821.0           0.16500            0.86810
92751            59.16       268.6           0.08996            0.06444

        concavity_worst  concave points_worst  symmetry_worst  \
id
926424           0.4107                0.2216          0.2060
926682           0.3215                0.1628          0.2572
926954           0.3403                0.1418          0.2218
927241           0.9387                0.2650          0.4087
92751            0.0000                0.0000          0.2871

        fractal_dimension_worst
id
926424                  0.07115
926682                  0.06637
926954                  0.07820
927241                  0.12400
92751                   0.07039

[5 rows x 30 columns]
```

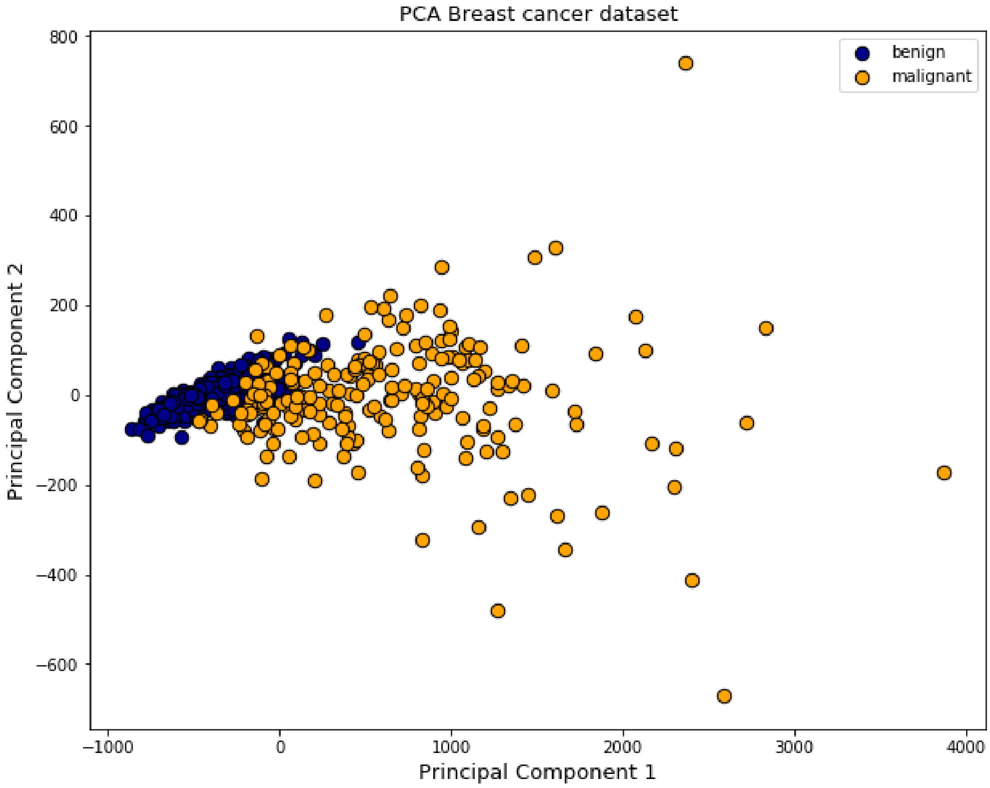
In [23]:
```
X_plot = np.concatenate(([df['symmetry_worst'].values], [df['compactness_worst'].values]
y = df['diagnosis'].values

plt.figure(figsize=(10,8))
colors = ['darkblue','orange']
target_names = ['benign', 'malignant']

for i, c, label in zip(target_ids, colors, target_names):
    plt.scatter(X_plot[0,i == y], X_plot[1,i == y], c = c,  edgecolors='black', s=285,la
plt.legend()
plt.title("Visualización de dos variables",fontsize=13)
plt.xlabel("symmetry_worst",fontsize=13)
plt.ylabel("compactness_worst",fontsize=13)
plt.show()
```



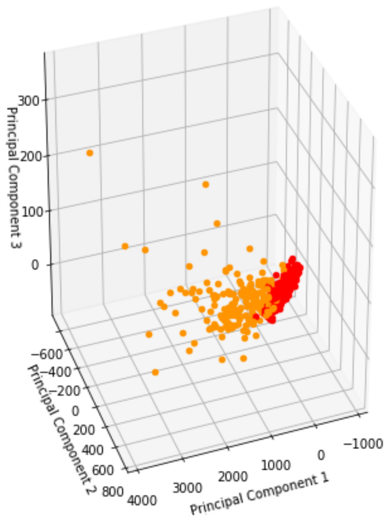

```
In [24]: pca = PCA(n_components=None)
         trans = pca.fit_transform(dfx)
```

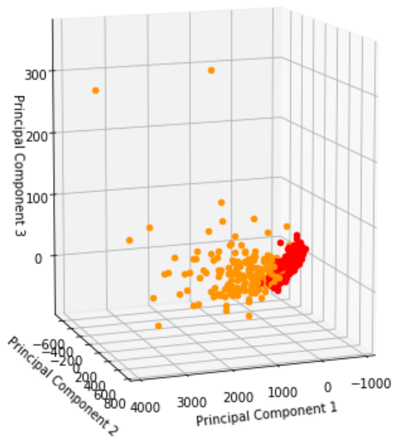
- Con PCA es más clara la separación de clases

```
In [25]: plt.figure(figsize=(10,8))
         colors = ['darkblue','orange']
         target_names = ['benign', 'malignant']

         for i, c, label in zip(target_ids, colors, target_names):
             plt.scatter(trans[i == y,0], trans[i == y,1], c = c,  edgecolors='black', s=285,labe
         plt.legend()
         plt.title("PCA Breast cancer dataset",fontsize=13)
         plt.xlabel("Principal Component 1",fontsize=13)
         plt.ylabel("Principal Component 2",fontsize=13)
         plt.show()
```



In [26]:
```
fig = plt.figure(figsize=(14,8))
ax = fig.add_subplot(1, 2, 1, projection="3d")
for i in range(trans.shape[0]):
    ax.scatter(trans[i, 0],trans[i, 1], trans[i, 2],color=plt.cm.hsv(y[i] / 10.),marker=
ax.view_init(30, 70)
ax.set_xlabel("Principal Component 1")
ax.set_ylabel("Principal Component 2")
ax.set_zlabel("Principal Component 3")

ax = fig.add_subplot(1, 2, 2, projection="3d")
for i in range(trans.shape[0]):
    ax.scatter(trans[i, 0], trans[i, 1], trans[i, 2],color=plt.cm.hsv(y[i] / 10.),marker
ax.view_init(10, 70)
ax.set_xlabel("Principal Component 1")
ax.set_ylabel("Principal Component 2")
ax.set_zlabel("Principal Component 3")
plt.show()
```





3 Visualizar dígitos

Referencia: https://scikit-learn.org/stable/auto_examples/manifold/plot_lle_digits.html - El número de clases es mayor - Se visualizan los pixeles de dígitos en 2 dimensiones

In [27]:
```
from tensorflow import keras

mnist = keras.datasets.mnist

(x_train, y_train), (x_test, y_test) = mnist.load_data()

X = x_test.reshape(x_test.shape[0], -1)
y = y_test
```

In [28]:
```
print(X.shape)
print(y.shape)
```

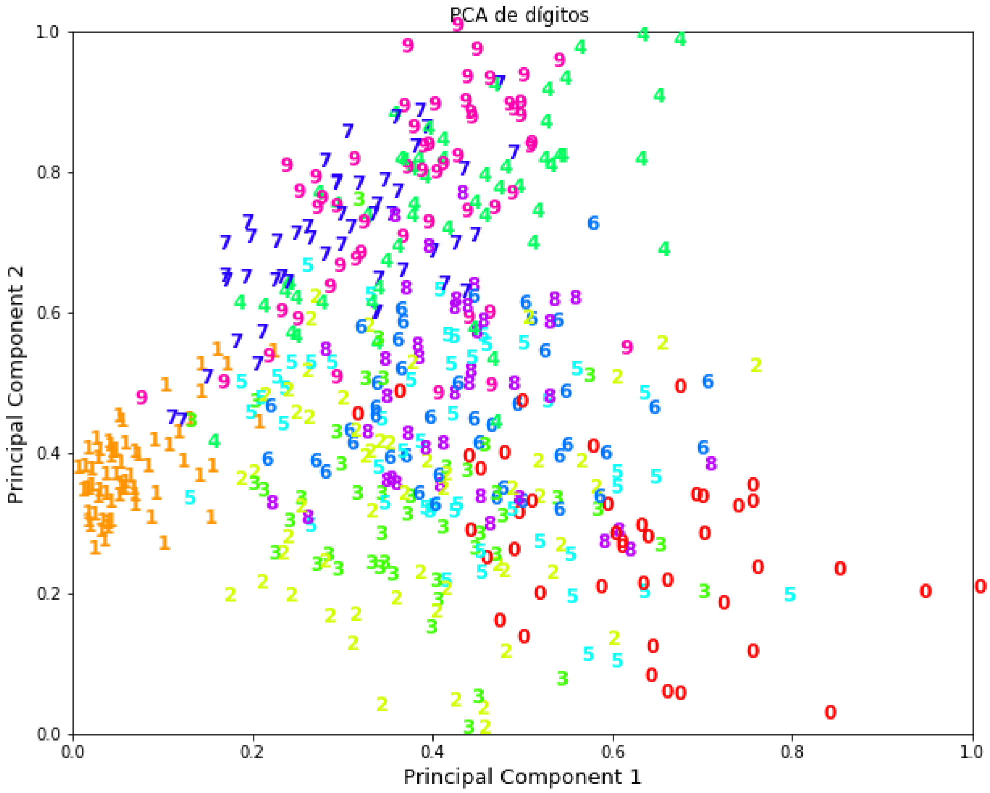
```
(10000, 784)
(10000,)
```

- Solo algunos elementos

In [29]:
```
X = X[:500, :]
y = y[:500]
```

In [30]:
```
X = PCA(n_components=3).fit_transform(X)
```

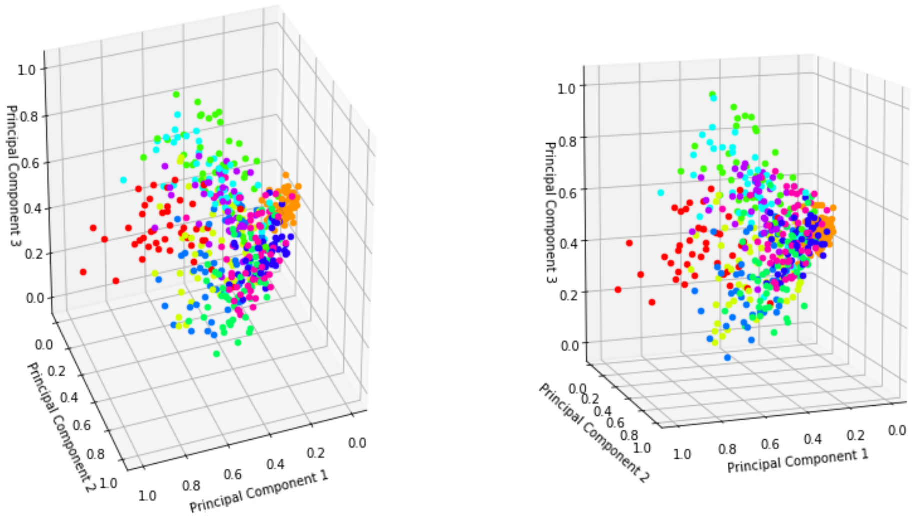
```
In [31]: x_min, x_max = np.min(X, 0), np.max(X, 0)
         X = (X - x_min) / (x_max - x_min)

         plt.figure(figsize=(10,8))
         for i in range(X.shape[0]):
             plt.text(X[i, 0], X[i, 1], str(y[i]), color=plt.cm.hsv(y[i] / 10.),
                      fontdict={'weight': 'bold', 'size': 12})

         plt.title("PCA de dígitos ")
         plt.xlabel("Principal Component 1",fontsize=13)
         plt.ylabel("Principal Component 2",fontsize=13)
         plt.show()
```



3.1 Tres componenetes principales

```
In [32]: fig = plt.figure(figsize=(14,8))
         ax = fig.add_subplot(1, 2, 1, projection="3d")
         for i in range(X.shape[0]):
             ax.scatter(X[i, 0], X[i, 1], X[i, 2],color=plt.cm.hsv(y[i] / 10.),marker='o')
         ax.view_init(30, 70)
```

```
ax.set_xlabel("Principal Component 1")
ax.set_ylabel("Principal Component 2")
ax.set_zlabel("Principal Component 3")

ax = fig.add_subplot(1, 2, 2, projection="3d")
for i in range(X.shape[0]):
    ax.scatter(X[i, 0], X[i, 1], X[i, 2],color=plt.cm.hsv(y[i] / 10.),marker='o')
ax.view_init(10, 70)
ax.set_xlabel("Principal Component 1")
ax.set_ylabel("Principal Component 2")
ax.set_zlabel("Principal Component 3")
plt.show()
```



- Se obtiene una visualización de datos de alta dimensión
- Probar PCA con diferentes datasets, después aplicar clasificación