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

2019/09/30

Principal Component Analysis (PCA)

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

PCA es una técnica de reducción de dimensionalidad que se puede emplear para pre-procesamiento y visualización de datos. Se define como una transformación de un espacio vectorial 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
```

Análisis exploratorio

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

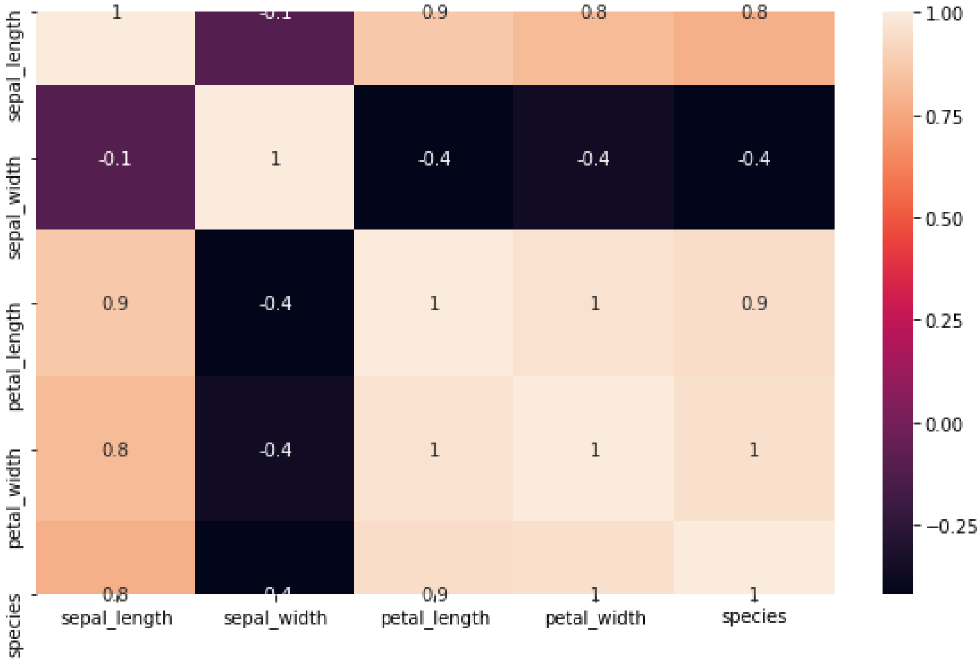
```
In [7]: df.drop('species', axis=1).head()
```

Out[7]:

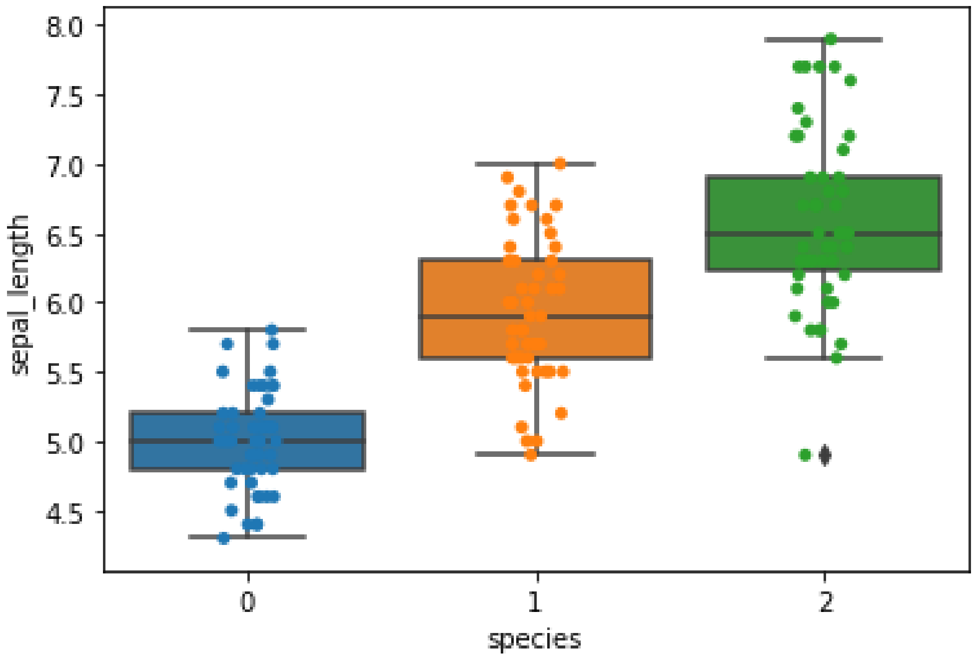
	sepal_length	sepal_width	petal_length	petal_width
0	5.1	3.5	1.4	0.2
1	4.9	3.0	1.4	0.2
2	4.7	3.2	1.3	0.2
3	4.6	3.1	1.5	0.2
4	5.0	3.6	1.4	0.2

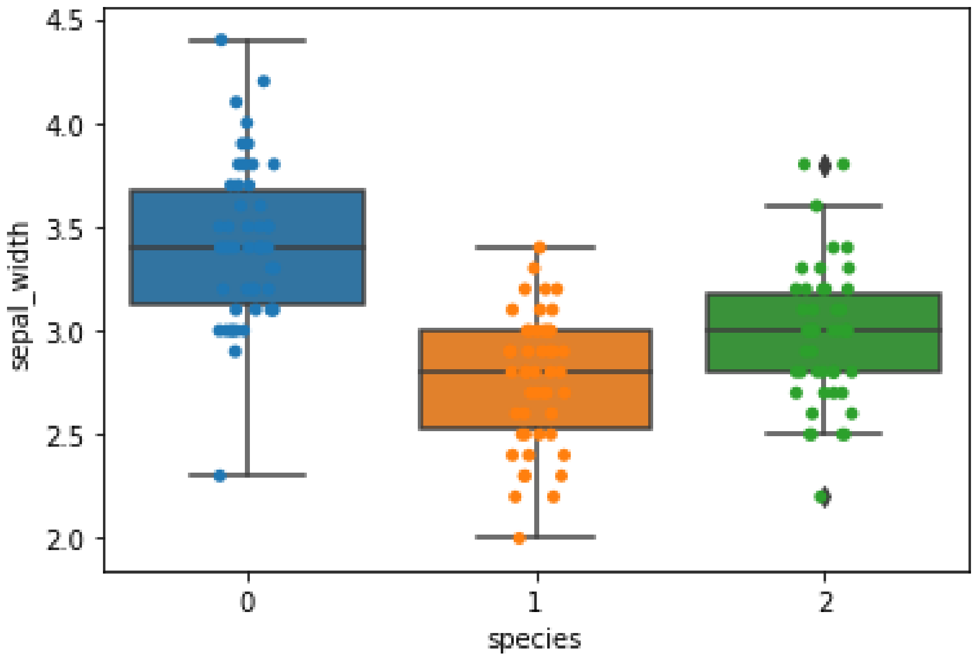
```
In [8]: corr = df.corr()
        plt.figure(figsize=(10, 6))
        sns.heatmap(corr, annot=True, fmt='.1g')
```

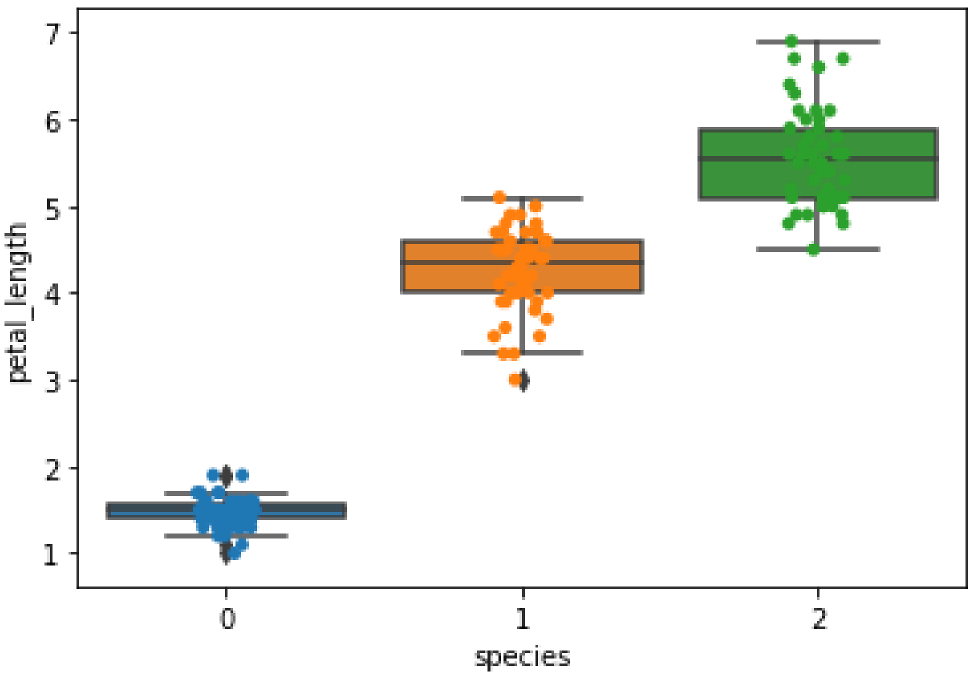
```
Out[8]: <matplotlib.axes._subplots.AxesSubplot at 0x7f6e30ed2a90>
```

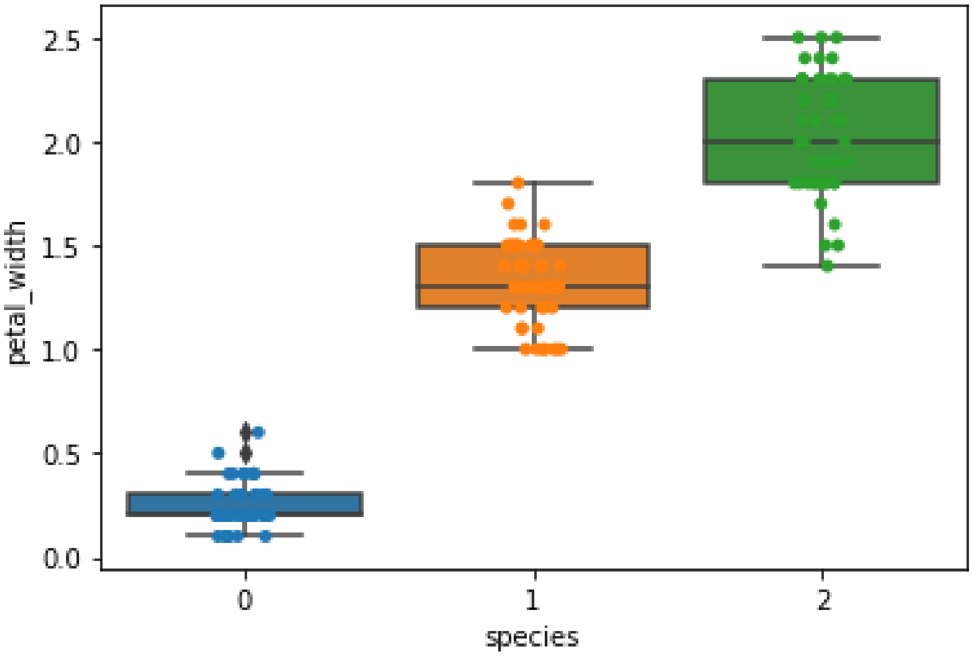


In [9]:
```
l=list(df.columns)
l[0:len(l)]
for i in range(0,len(l)-1):
    plt.figure()
    sns.boxplot(x='species' ,y=l[i], data=df)
    sns.stripplot(x='species' ,y=l[i], data=df)
```




4.5
4.0
3.5
3.0
2.5
2.0
sepal_width
0
1
2
species


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

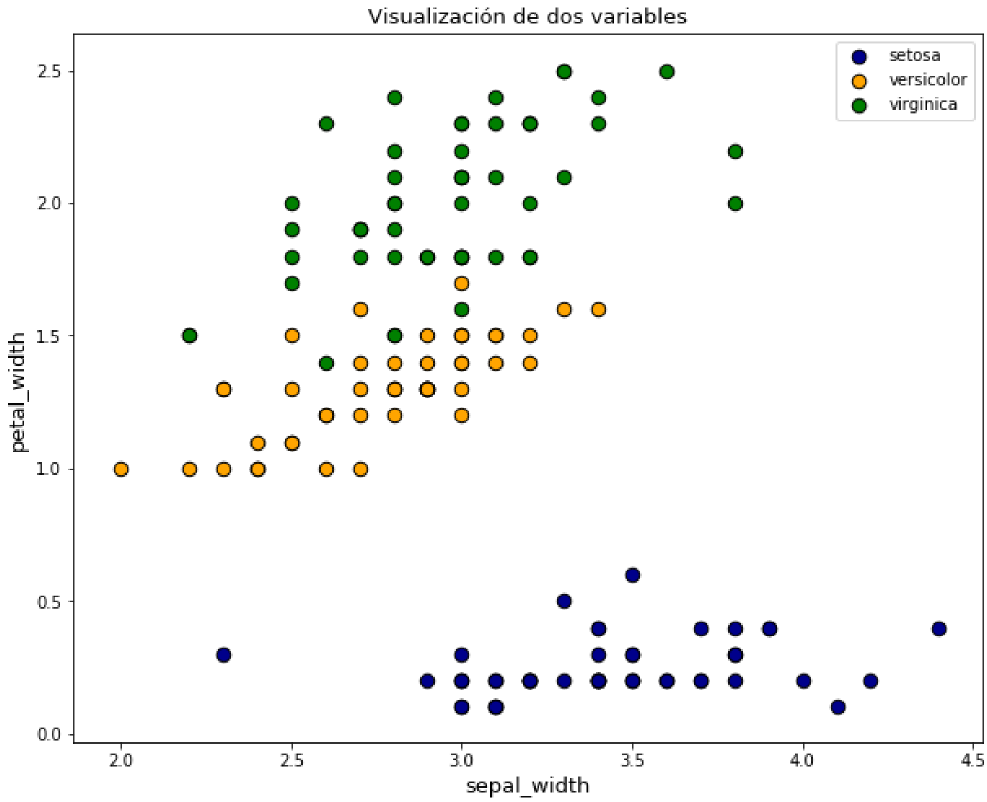


Plot de dos variables en 2d

- 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()
```



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))
```

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_
```

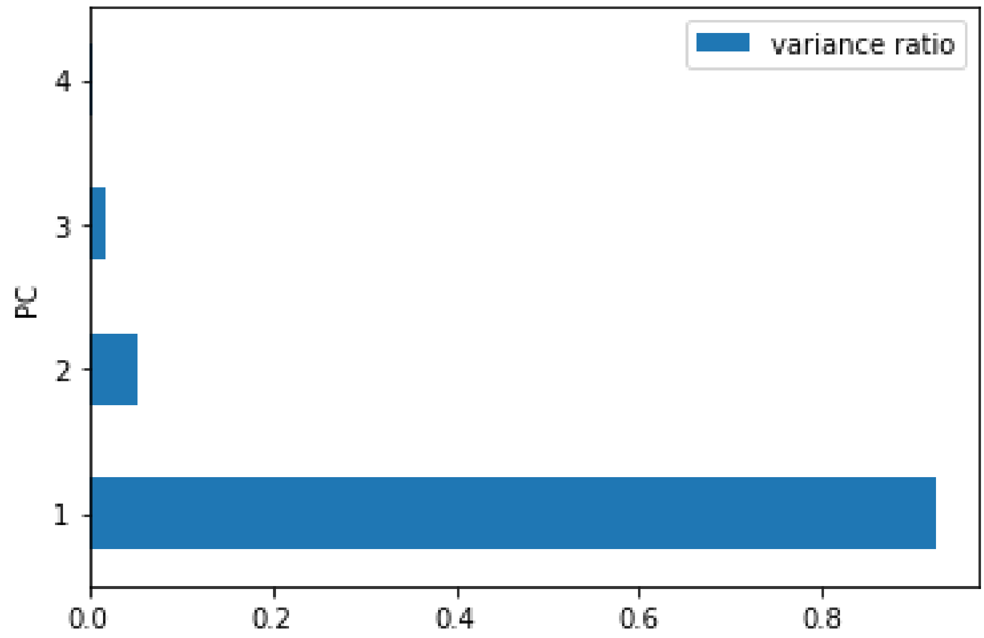
```
Out[14]: array([0.92461621, 0.05301557, 0.01718514, 0.00518309])
```

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

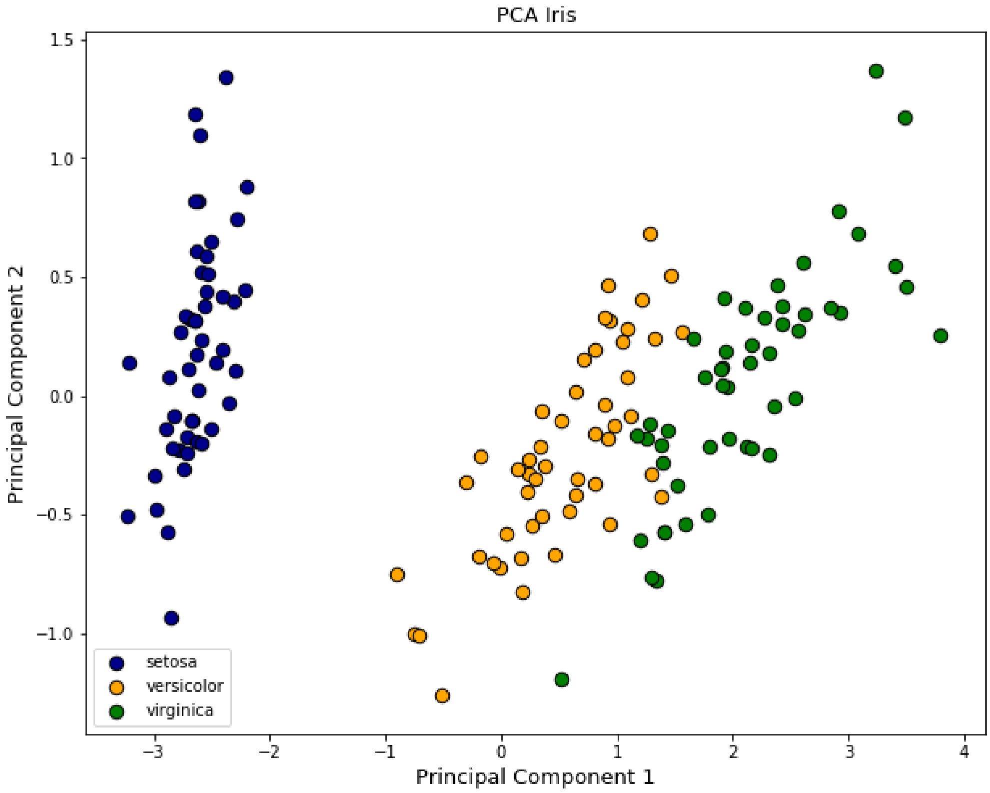
In [18]:
```
df_transn = pd.DataFrame(data=trans)
df_transn.head(10)
```

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

Dos componentes principales

In [19]:
```
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()
```

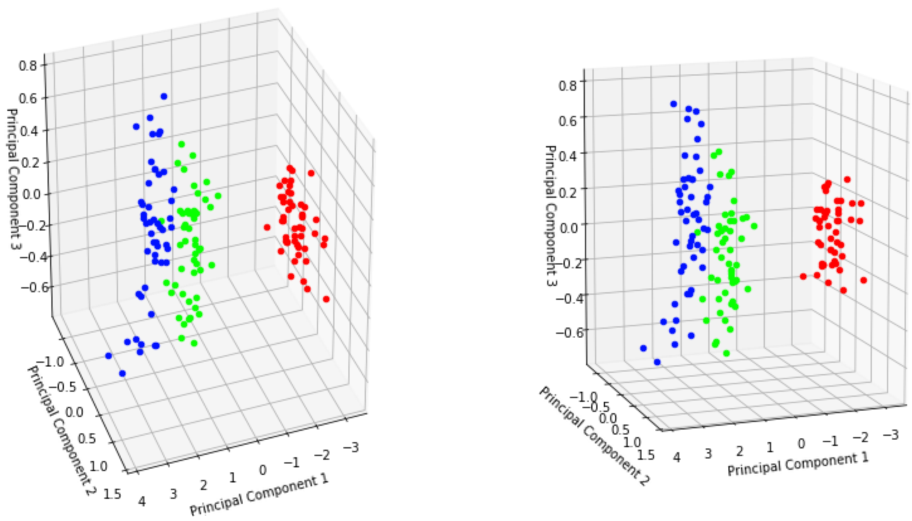


Tres componentes principales

- 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()
```



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]:

id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean
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

id	smoothness_mean	compactness_mean	concavity_mean
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

id	concave points_mean	symmetry_mean	…	texture_worst
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

id	perimeter_worst	area_worst	smoothness_worst	compactness_worst
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

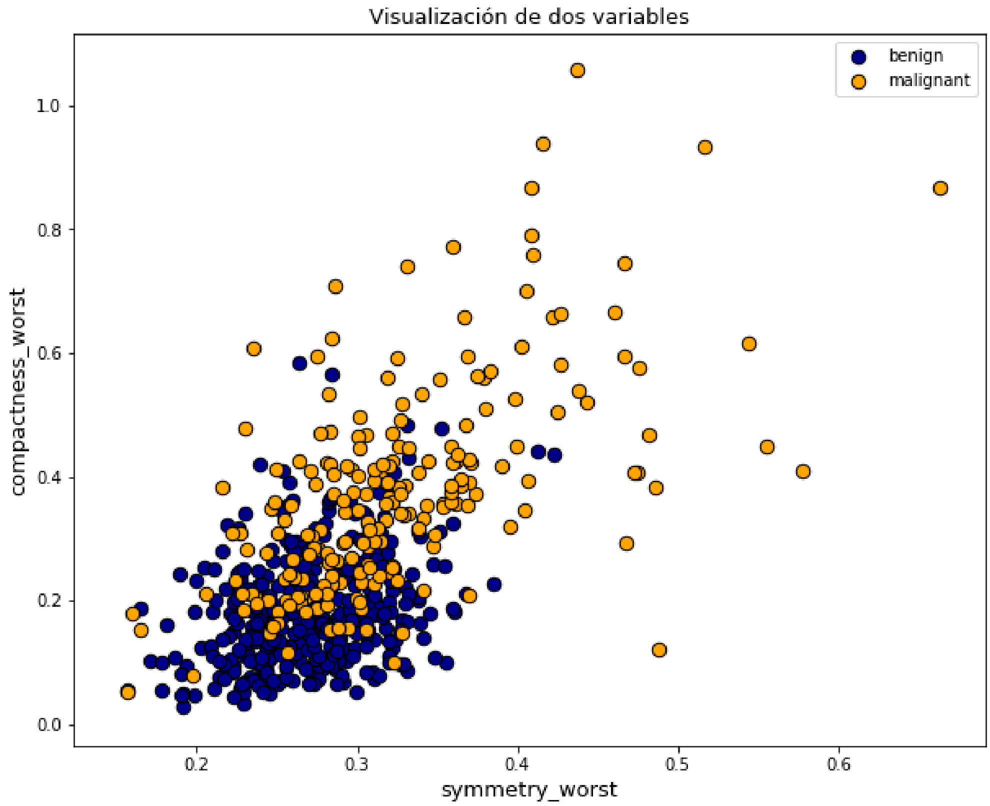
```
844981              106.20      739.3            0.1703             0.5401
84501001             97.65      711.4            0.1853             1.0580

           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]
```

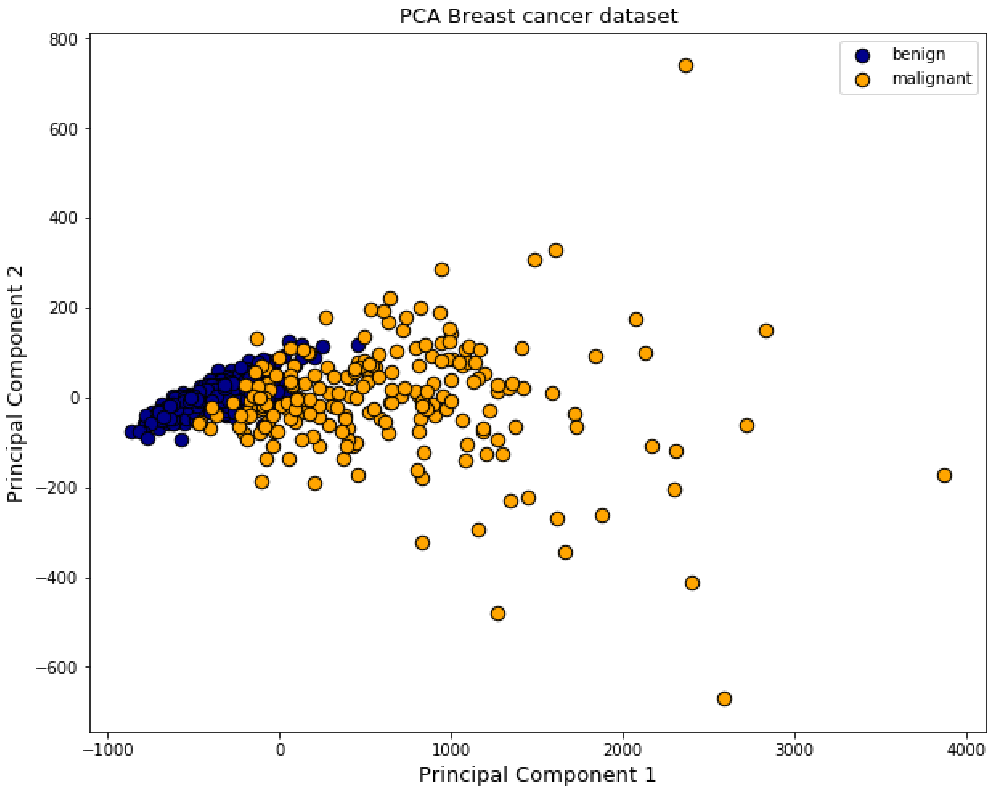
In [23]:
```
X_plot = np.concatenate(([df['symmetry_worst'].values], [df['compactness_worst'].values]
y = df['diagnosis'].values

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()
```



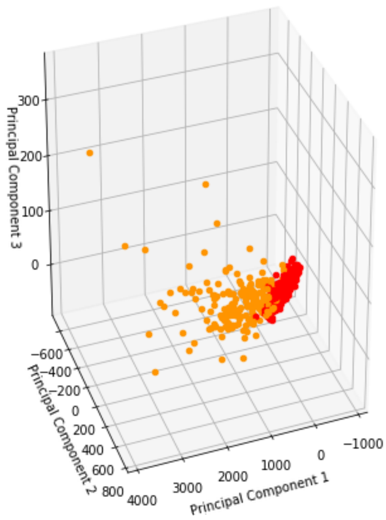

```
In [24]: pca = PCA(n_components=None)
         trans = pca.fit_transform(dfx)
```

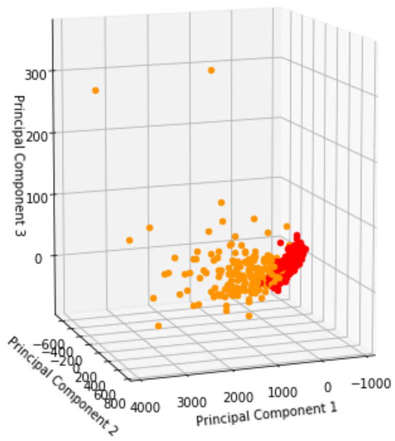
- Con PCA es más clara la separación de clases

```
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()
```





Visualizar dígitos

- El número de clases es mayor
- Se visualizan los pixeles de dígitos en 2 dimensiones

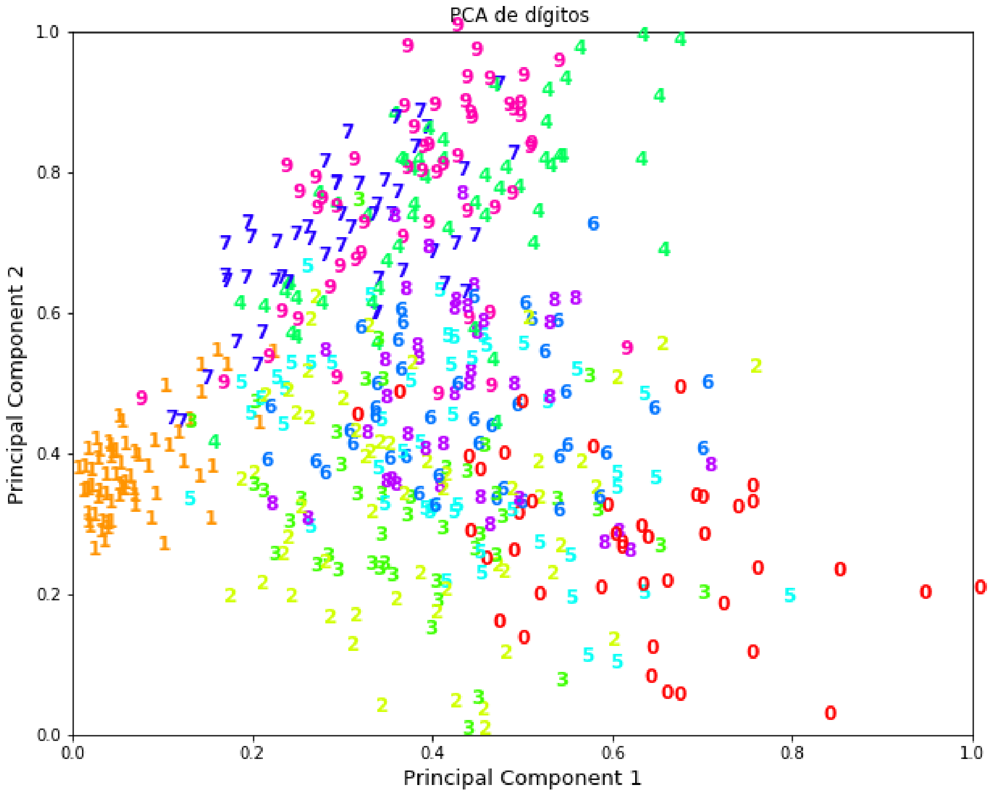
https://scikit-learn.org/stable/auto_examples/manifold/plot_lle_digits.html

```
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)
```

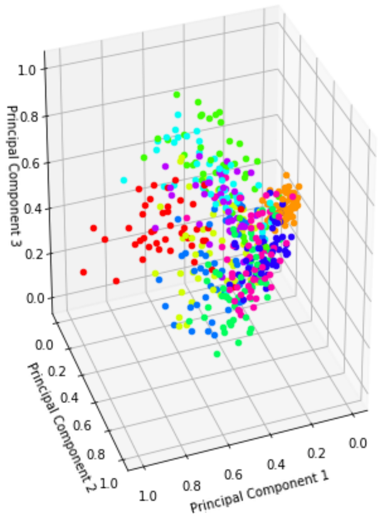
```
In [31]: x_min, x_max = np.min(X, 0), np.max(X, 0)
         X = (X - x_min) / (x_max - x_min)

         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()
```

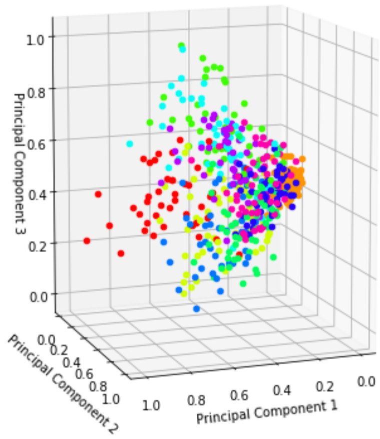


Tres componenetes principales

```
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)
```

```python
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