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

2019/09/30

1 K-means

Objetivo: Entender el concepto de clustering y aplicarlo en un dataset.

• Documentación: https://scikit-learn.org/stable/modules/clustering.html#k-means

K-means es un método de agrupamiento, cada observación pertenece al grupo donde la distancia a la media es menor, el objetivo es asignar un conjunto de n observaciones a k grupos, esto también es conocido como aprendizaje no supervisado.

Inicialización

- elegir k posiciones aleatorias
- asignar los centroides $C = \{c_1, \ldots, c_k\}$ a esas posiciones

• Iteraración

- asignar cada x_i al cluster que tenga la distancia mínima

$$\min_{c_k \in C} ||x_i - c_k||^2 \tag{1}$$

- actualizar centroides, moviando el centroide a la media de los puntos del cluster, donde n_k es el número de elementos en el cluster k:

$$c_k = \frac{1}{n_k} \sum_{i=1}^{n_k} x_i \tag{2}$$

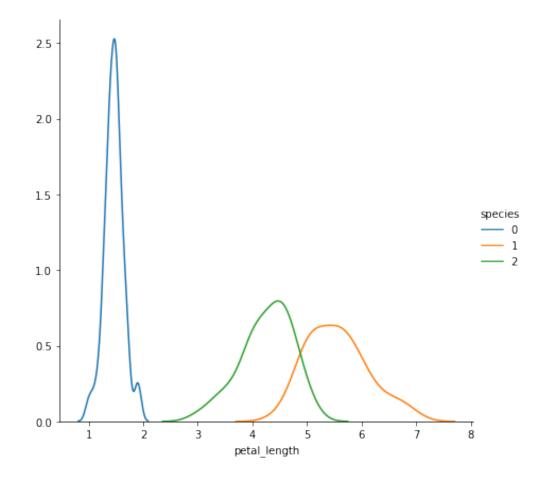
hasta que exista convergencia

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

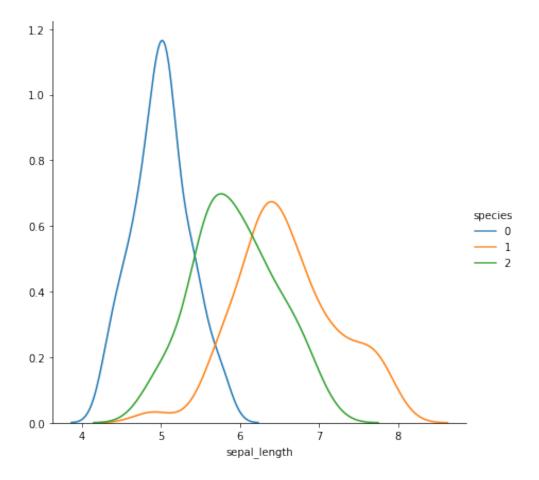
```
In [2]: df = pd.read_csv('iris.csv')
        df.head(10)
Out[2]:
           sepal_length sepal_width petal_length petal_width species
        0
                    5.1
                                 3.5
                                               1.4
                                                            0.2 setosa
                    4.9
                                 3.0
                                              1.4
                                                            0.2 setosa
        1
        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
                                                           0.2 setosa
                    5.0
                                3.4
                                              1.5
        8
                    4.4
                                 2.9
                                              1.4
                                                           0.2 setosa
        9
                    4.9
                                 3.1
                                              1.5
                                                           0.1 setosa
In [3]: 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
                150 non-null float64
petal_length
                150 non-null float64
petal_width
species
                150 non-null object
dtypes: float64(4), object(1)
memory usage: 6.0+ KB
In [4]: df = df.replace({'setosa':0, 'virginica':1, 'versicolor':2})
        df.tail()
Out[4]:
             sepal_length sepal_width petal_length petal_width species
        145
                      6.7
                                   3.0
                                                5.2
                                                              2.3
        146
                      6.3
                                   2.5
                                                 5.0
                                                              1.9
                                                                         1
                                                 5.2
                                                              2.0
        147
                      6.5
                                   3.0
                                                                         1
        148
                      6.2
                                   3.4
                                                 5.4
                                                              2.3
                                                                         1
        149
                      5.9
                                   3.0
                                                5.1
                                                              1.8
                                                                         1
In [5]: 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
                150 non-null int64
species
dtypes: float64(4), int64(1)
memory usage: 6.0 KB
```

1.1 Viisualizar separación de clases por variables

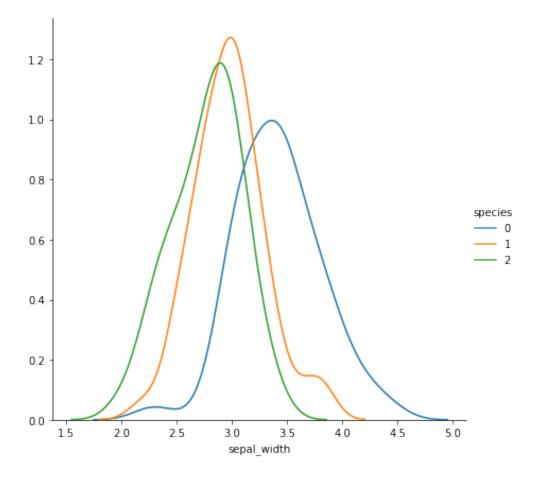
Out[6]: <seaborn.axisgrid.FacetGrid at 0x7fc4db7c9b10>



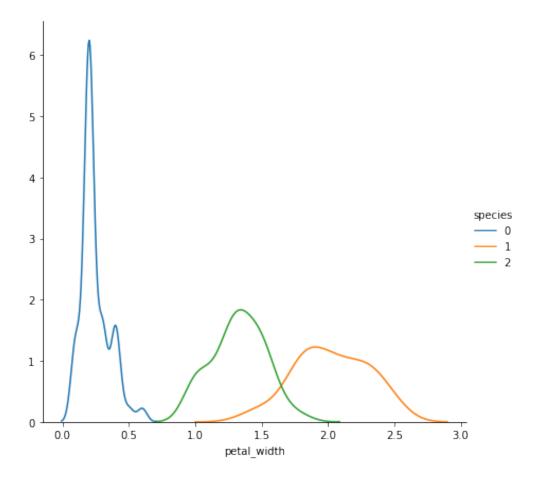
Out[7]: <seaborn.axisgrid.FacetGrid at 0x7fc4db4c2290>



Out[8]: <seaborn.axisgrid.FacetGrid at 0x7fc4db398250>



Out[9]: <seaborn.axisgrid.FacetGrid at 0x7fc4db36ecd0>



1.2 K Means

• Se asigna el parámetro 'K' que indica el número de clusters. También se puede asignar el número de iteraciones

```
, 3.07368421, 5.74210526, 2.07105263],
Out[13]: array([[6.85
      [5.006
          , 3.418 , 1.464
                   , 0.244
      [5.9016129 , 2.7483871 , 4.39354839 , 1.43387097]])
In [14]: print(kmeans.labels_)
0 2]
In [15]: df['species'].values
2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
      1.2.1 Adaptar para 'kmeans.labels_'
In [16]: labels = df.replace(\{0:1, 1:0\})
   labels.species.values
2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
      Comportamiento de etiquetas 'K-means'
 • Se obtienen las predicciones, informe de clasificación y matriz de confusión.
In [17]: from sklearn.metrics import classification_report,confusion_matrix
   print("Predicciones:\n")
   print(kmeans.labels )
   print("\nReporte de clasificación:\n")
   print(classification_report(kmeans.labels_,labels.species.values))
Predicciones:
```

Reporte de clasificación:

```
precision recall f1-score
                                           support
                 0.72
          0
                         0.95
                                   0.82
                                               38
                                    1.00
          1
                          1.00
                                               50
          2
                 0.96
                           0.77
                                    0.86
                                               62
                                    0.89
                                              150
   accuracy
                 0.89
                           0.91
                                    0.89
                                              150
  macro avg
weighted avg
                 0.91
                           0.89
                                    0.89
                                              150
```

1.4 Utilizando PCA para visualizar la clasificación de K-means

```
In [19]: from sklearn.decomposition import PCA
    pca = PCA(n_components=2).fit(df.drop('species',axis=1))
    y = kmeans.labels_
    X_pca = pca.transform(df.drop('species',axis=1))
    clus_cent=kmeans.cluster_centers_
    cent = pca.transform(clus_cent)
```

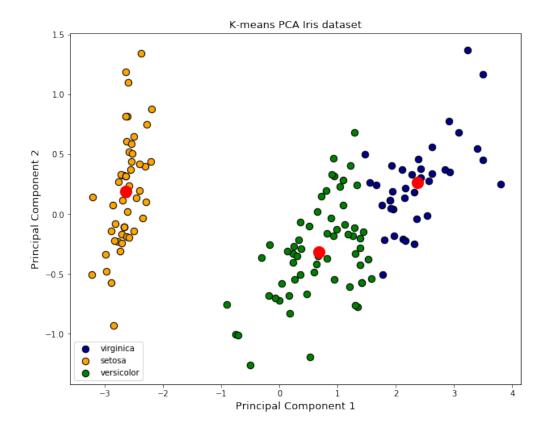
1.5 Ploteando centroides

```
In [20]: plt.figure(figsize=(10,6))
    target_ids = np.unique(df.values[:,-1])
    colors = ['darkblue', 'orange', 'green']
    target_names = ['virginica', 'setosa', 'versicolor']

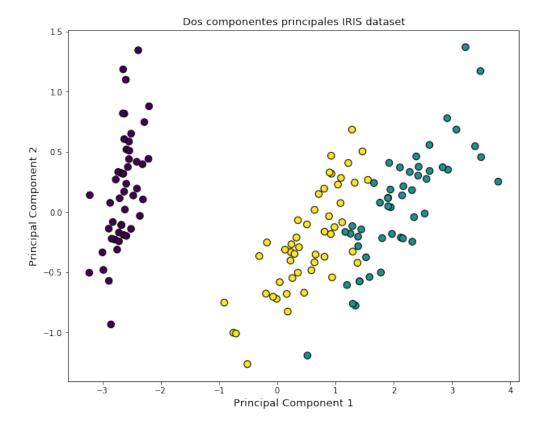
plt.figure(figsize=(10,8))
    for i, c, label in zip(target_ids, colors, target_names):
        plt.scatter(X_pca[i == y,0], X_pca[i == y,1], c = c, edgecolors='black', s=285,labe plt.legend()
    plt.scatter(cent[:,0], cent[:,1], s=200, color = 'red')
    plt.title("K-means PCA Iris dataset",fontsize=13)
```

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

<Figure size 720x432 with 0 Axes>



2 Etiquetas originales



2.1 K-means con dataset de los ejercicios de clasificación

- Visualizar dataset de clasificación
- Se crean dos grupos para tratar de separar de manera no-supervisada y visualizar el comportamiento del algoritmo
- Se escalan los datos con 'StandardScaler'

```
In [22]: from sklearn.preprocessing import StandardScaler
         scaler = StandardScaler()
In [23]: df = pd.read_csv("data-breast.csv",index_col=0)
         df = df.replace({'B':0, 'M':1})
         df.head()
         df.head(10)
Out[23]:
                   diagnosis radius_mean texture_mean perimeter_mean area_mean \
         id
         842302
                                     17.99
                                                   10.38
                                                                  122.80
                                                                              1001.0
                           1
                                    20.57
         842517
                           1
                                                   17.77
                                                                  132.90
                                                                              1326.0
         84300903
                                    19.69
                                                   21.25
                                                                  130.00
                                                                              1203.0
                           1
         84348301
                                    11.42
                                                   20.38
                                                                   77.58
                                                                              386.1
```

```
84358402
                           20.29
                                          14.34
                                                          135.10
                                                                     1297.0
                  1
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
                                          21.82
                                                          87.50
844981
                  1
                            13.00
                                                                      519.8
84501001
                  1
                            12.46
                                          24.04
                                                          83.97
                                                                      475.9
          smoothness_mean compactness_mean concavity_mean \
id
842302
                                     0.27760
                                                     0.30010
                  0.11840
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
                                               . . .
                                       0.1812 ...
842517
                      0.07017
                                                             23.41
                                       0.2069
                                                             25.53
84300903
                      0.12790
84348301
                      0.10520
                                       0.2597
                                                             26.50
                                               . . .
                                       0.1809
84358402
                      0.10430
                                               . . .
                                                            16.67
843786
                      0.08089
                                       0.2087
                                                             23.75
                                               . . .
                                                             27.66
844359
                      0.07400
                                       0.1794
84458202
                      0.05985
                                       0.2196
                                                             28.14
                                               . . .
844981
                      0.09353
                                       0.2350
                                                             30.73
                                               . . .
                                                             40.68
84501001
                      0.08543
                                       0.2030 ...
          perimeter_worst area_worst smoothness_worst compactness_worst \
id
842302
                   184.60
                                2019.0
                                                  0.1622
                                                                      0.6656
                                                                      0.1866
842517
                   158.80
                                1956.0
                                                  0.1238
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
                                1606.0
                                                  0.1442
844359
                   153.20
                                                                      0.2576
                                 897.0
                                                                      0.3682
84458202
                   110.60
                                                  0.1654
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
```

```
0.1860
         842517
                            0.2416
                                                                    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
                                                   0.2210
                                                                    0.4366
                             1.1050
                   {\tt fractal\_dimension\_worst}
                                             Unnamed: 32
         id
         842302
                                    0.11890
                                                      NaN
         842517
                                    0.08902
                                                      NaN
                                                      NaN
         84300903
                                    0.08758
         84348301
                                                      NaN
                                    0.17300
         84358402
                                    0.07678
                                                      NaN
         843786
                                    0.12440
                                                      NaN
         844359
                                                      NaN
                                    0.08368
         84458202
                                                      NaN
                                    0.11510
         844981
                                    0.10720
                                                      NaN
         84501001
                                    0.20750
                                                      NaN
         [10 rows x 32 columns]
In [24]: y_true = df['diagnosis']
         X = df.drop(['diagnosis','Unnamed: 32'],axis=1)
         X = scaler.fit_transform(X)
         dfx = pd.DataFrame(data=X,columns=df.columns[1:31])
         dfx.tail()
Out [24]:
              radius_mean texture_mean perimeter_mean area_mean smoothness_mean
         564
                 2.110995
                                0.721473
                                                2.060786
                                                            2.343856
                                                                            1.041842
         565
                 1.704854
                                2.085134
                                                1.615931
                                                            1.723842
                                                                             0.102458
         566
                 0.702284
                                2.045574
                                                0.672676
                                                            0.577953
                                                                            -0.840484
         567
                 1.838341
                                2.336457
                                                1.982524
                                                            1.735218
                                                                             1.525767
         568
                -1.808401
                                1.221792
                                               -1.814389 -1.347789
                                                                            -3.112085
              compactness_mean concavity_mean concave points_mean symmetry_mean
         564
                      0.219060
                                       1.947285
                                                             2.320965
                                                                           -0.312589
         565
                     -0.017833
                                       0.693043
                                                             1.263669
                                                                           -0.217664
         566
                     -0.038680
                                       0.046588
                                                                           -0.809117
                                                             0.105777
         567
                      3.272144
                                       3.296944
                                                             2.658866
                                                                            2.137194
         568
                     -1.150752
                                      -1.114873
                                                            -1.261820
                                                                           -0.820070
              fractal_dimension_mean
                                       ... radius_worst texture_worst
         564
                           -0.931027
                                                1.901185
                                                                0.117700
                                       . . .
         565
                            -1.058611
                                                1.536720
                                                                2.047399
                                      . . .
         566
                            -0.895587
                                                0.561361
                                                                1.374854
                                      . . .
```

```
567
                         1.043695 ...
                                                        2.237926
                                          1.961239
        568
                        -0.561032 ...
                                          -1.410893
                                                        0.764190
            perimeter_worst area_worst smoothness_worst compactness_worst \
                                              0.378365
                                                               -0.273318
        564
                   1.752563
                              2.015301
        565
                   1.421940
                              1.494959
                                             -0.691230
                                                               -0.394820
        566
                   0.579001
                              0.427906
                                             -0.809587
                                                                0.350735
        567
                   2.303601
                             1.653171
                                              1.430427
                                                                3.904848
                            -1.075813
        568
                  -1.432735
                                             -1.859019
                                                               -1.207552
            concavity_worst concave points_worst symmetry_worst
        564
                   0.664512
                                       1.629151
                                                     -1.360158
        565
                   0.236573
                                                     -0.531855
                                       0.733827
        566
                   0.326767
                                       0.414069
                                                     -1.104549
        567
                   3.197605
                                       2.289985
                                                     1.919083
        568
                                                     -0.048138
                  -1.305831
                                      -1.745063
            fractal_dimension_worst
        564
                         -0.709091
        565
                         -0.973978
        566
                         -0.318409
        567
                          2.219635
        568
                         -0.751207
        [5 rows x 30 columns]
In [25]: kmeans = KMeans(n_clusters=2,max_iter=300,n_init=20, random_state=110)
        kmeans.fit(dfx)
        y = kmeans.labels
        pca = PCA(n_components=2).fit(dfx)
        clus_cent_breast=kmeans.cluster_centers_
        cent = pca.transform(clus cent breast)
In [26]: pca = PCA(n components=2)
        X pca = pca.fit transform(dfx)
In [27]: df['diagnosis'].values
1, 1, 0, 1, 0, 0, 0, 0, 1, 1, 0, 1, 1, 0, 0, 0, 0, 1, 0, 1, 1,
              0, 0, 0, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 0, 0, 1, 1, 0, 1, 1, 1,
              0, 0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 1, 1, 0, 0, 0, 0, 1, 0, 0, 1, 0,
              0, 0, 0, 0, 0, 0, 1, 1, 1, 0, 1, 1, 0, 0, 0, 1, 1, 0, 1, 0, 1,
              1, 0, 1, 1, 0, 0, 1, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0,
              0, 0, 1, 0, 0, 0, 1, 1, 0, 1, 0, 0, 1, 1, 0, 0, 1, 1, 0, 0, 0,
              0, 1, 0, 0, 1, 1, 1, 0, 1, 0, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 1, 1,
              1, 1, 0, 1, 1, 1, 0, 1, 0, 1, 0, 0, 1, 0, 1, 1, 1, 1, 0, 0, 1, 1,
              0, 0, 0, 1, 0, 0, 0, 0, 1, 1, 0, 0, 1, 0, 0, 1, 1, 0, 1, 0, 0,
              0, 0, 1, 0, 0, 0, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
```

2.2 Comportamiento de etiquetas 'K-means'

Predicciones:

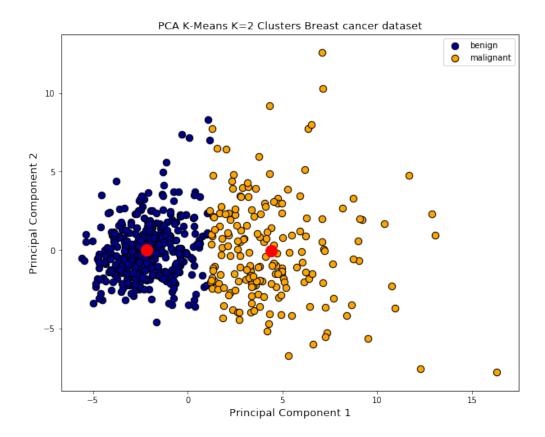
0 0 0 0 0 0 0 1 1 1 1 1 1 0]

Reporte de clasificación:

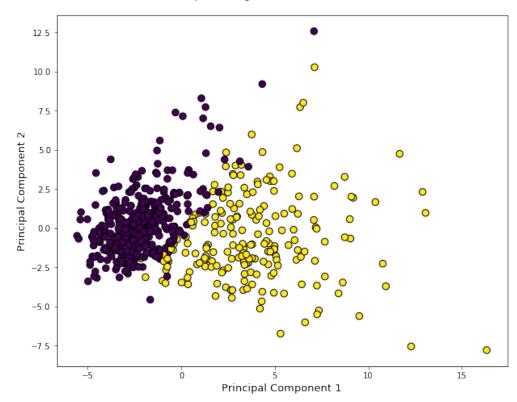
support	f1-score	recall	precision	
380	0.93	0.90	0.96	0
189	0.87	0.93	0.83	1
569	0.91			accuracy
569	0.90	0.91	0.89	macro avg

weighted avg 0.92 0.91 0.91 569

2.3 K-means con PCA



2.4 Etiquetas originales



$2.5 ext{ K} = 3$

• Ahora se crean 3 clases

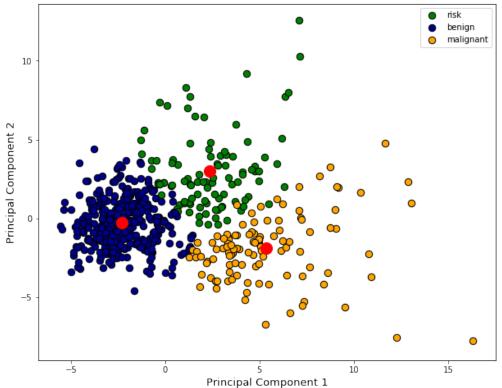
```
In [32]: kmeans = KMeans(n_clusters=3,max_iter=300,n_init=20, random_state=1221)
    kmeans.fit(dfx)
    y = kmeans.labels_
    pca = PCA(n_components=2).fit(dfx)
    clus_cent_breast=kmeans.cluster_centers_
    cent = pca.transform(clus_cent_breast)

In [33]: pca = PCA(n_components=2)
    X_pca = pca.fit_transform(dfx)

In [34]: target_ids = np.unique(y)
    plt.figure(figsize=(10,8))
    colors = ['green', 'darkblue', 'orange']
    target_names = ['risk', 'benign', 'malignant']
    for i, c, label in zip(target_ids, colors, target_names):
        plt.scatter(X_pca[i == y,0], X_pca[i == y,1], c = c, edgecolors='black', s=285,labely)
```

```
plt.legend()
plt.scatter(cent[:,0], cent[:,1], s=200, color = 'red')
plt.title('PCA K-Means K=3 Clusters Breast cancer dataset',fontsize=13)
plt.xlabel("Principal Component 1",fontsize=13)
plt.ylabel("Principal Component 2",fontsize=13)
plt.show()
```





- Probar K-means con un diferente dataset
- Crear diferentes clusters