Análisis de Datos y Aprendizaje Máquina con Tensorflow 2.0: Clasificación

2019/09/30

Clasificación K-nearest neighbors y GridSearch (parameter tuning)

Objetivo: Comprender otro tipo de clasificación básica y el ajuste de hiperparámetros.

En la clasificación k-NN, se asigna el elemento a clasificar a la clase donde la mayoría de sus elementos de entrenamiento (vecinos) pertenecen. Si k = 1, entonces el objeto simplemente se asigna a la clase de ese vecino más cercano, si k = 3, se asigna a la clase donde la mayoría de los tres elementos pertenecen. Este tipo de clasificación es muy común y cuenta con muchas variantes.

https://scikit-learn.org/stable/modules/neighbors.html#unsupervised-nearest-neighbors
https://scikit-learn.org/stable/modules/grid_search.html

- Para ajustar el parámetro k con el menor error, así como otros parámetros (parameter tuning), se utiliza GridSearch de sklearn

```
In [1]: import sklearn
        import pandas as pd
        import seaborn as sns
        import matplotlib.pyplot as plt
```

Análisis exploratorio

Etiquetas de clase a valor numérico

- Diagnosis (M = malignant, B = benign)

```
In [2]: %matplotlib inline
        df = pd.read_csv("data-breast.csv",index_col=0)
        df.head(10)
```

```
Out[2]:          diagnosis  radius_mean  texture_mean  perimeter_mean  area_mean  \
        id
        842302           M        17.99         10.38          122.80     1001.0
        842517           M        20.57         17.77          132.90     1326.0
        84300903         M        19.69         21.25          130.00     1203.0
        84348301         M        11.42         20.38           77.58      386.1
        84358402         M        20.29         14.34          135.10     1297.0
```

```
843786          M       12.45         15.70           82.57      477.1
844359          M       18.25         19.98          119.60     1040.0
84458202        M       13.71         20.83           90.20      577.9
844981          M       13.00         21.82           87.50      519.8
84501001        M       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]
```

Análisis Exploratorio

- Verificar valores nulos

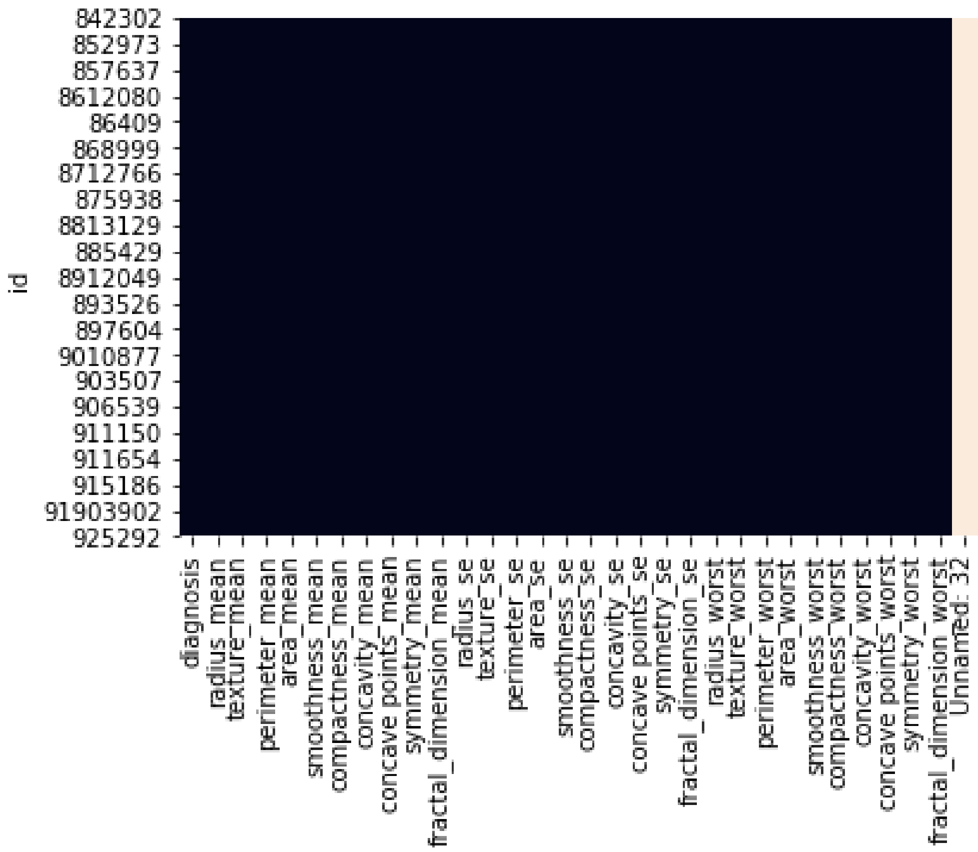
```
In [3]: df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 569 entries, 842302 to 92751
Data columns (total 32 columns):
diagnosis                  569 non-null object
radius_mean                569 non-null float64
texture_mean               569 non-null float64
perimeter_mean             569 non-null float64
area_mean                  569 non-null float64
smoothness_mean            569 non-null float64
compactness_mean           569 non-null float64
concavity_mean             569 non-null float64
concave points_mean        569 non-null float64
symmetry_mean              569 non-null float64
fractal_dimension_mean     569 non-null float64
radius_se                  569 non-null float64
texture_se                 569 non-null float64
perimeter_se               569 non-null float64
area_se                    569 non-null float64
smoothness_se              569 non-null float64
compactness_se             569 non-null float64
```

```
concavity_se               569 non-null float64
concave points_se          569 non-null float64
symmetry_se                569 non-null float64
fractal_dimension_se       569 non-null float64
radius_worst               569 non-null float64
texture_worst              569 non-null float64
perimeter_worst            569 non-null float64
area_worst                 569 non-null float64
smoothness_worst           569 non-null float64
compactness_worst          569 non-null float64
concavity_worst            569 non-null float64
concave points_worst       569 non-null float64
symmetry_worst             569 non-null float64
fractal_dimension_worst    569 non-null float64
Unnamed: 32                0 non-null float64
dtypes: float64(31), object(1)
memory usage: 146.7+ KB
```

```
In [4]: sns.heatmap(df.isnull(), cbar=False)
```

```
Out[4]: <matplotlib.axes._subplots.AxesSubplot at 0x7fb9e95cc1d0>
```



- Etiquetas a valor numérico

```
In [5]: df = df.replace({'B':0, 'M':1})
        df.head()
```

```
Out[5]:           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

                  smoothness_mean  compactness_mean  concavity_mean  \
        id
        842302            0.11840           0.27760          0.3001
        842517            0.08474           0.07864          0.0869
        84300903          0.10960           0.15990          0.1974
        84348301          0.14250           0.28390          0.2414
        84358402          0.10030           0.13280          0.1980

                  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

                  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

                  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

                  fractal_dimension_worst  Unnamed: 32
        id
```

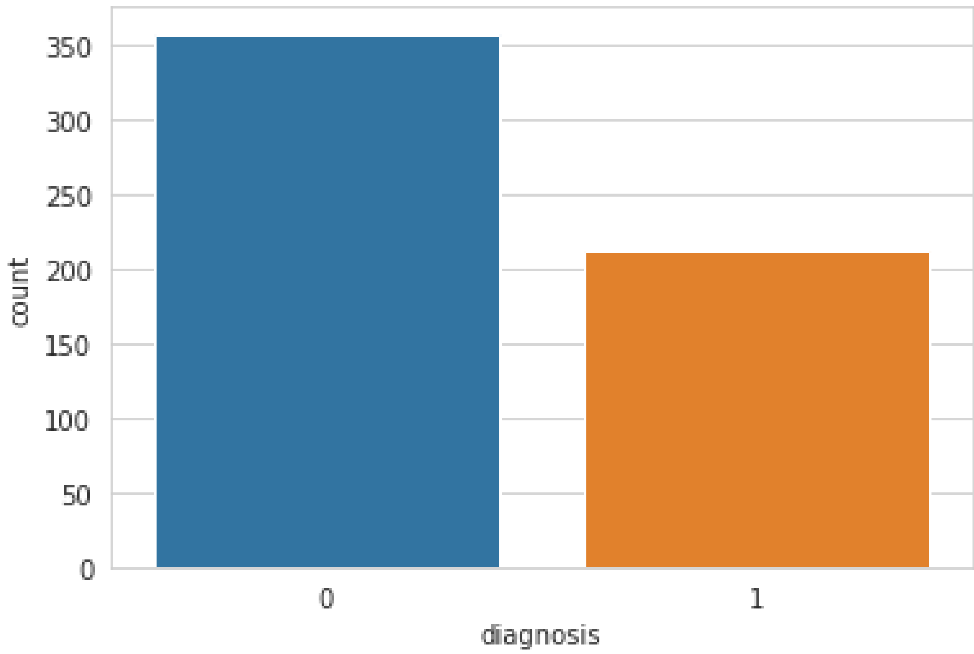
```
842302                  0.11890          NaN
842517                  0.08902          NaN
84300903                0.08758          NaN
84348301                0.17300          NaN
84358402                0.07678          NaN

[5 rows x 32 columns]
```

- Equilibrio de etiquetas

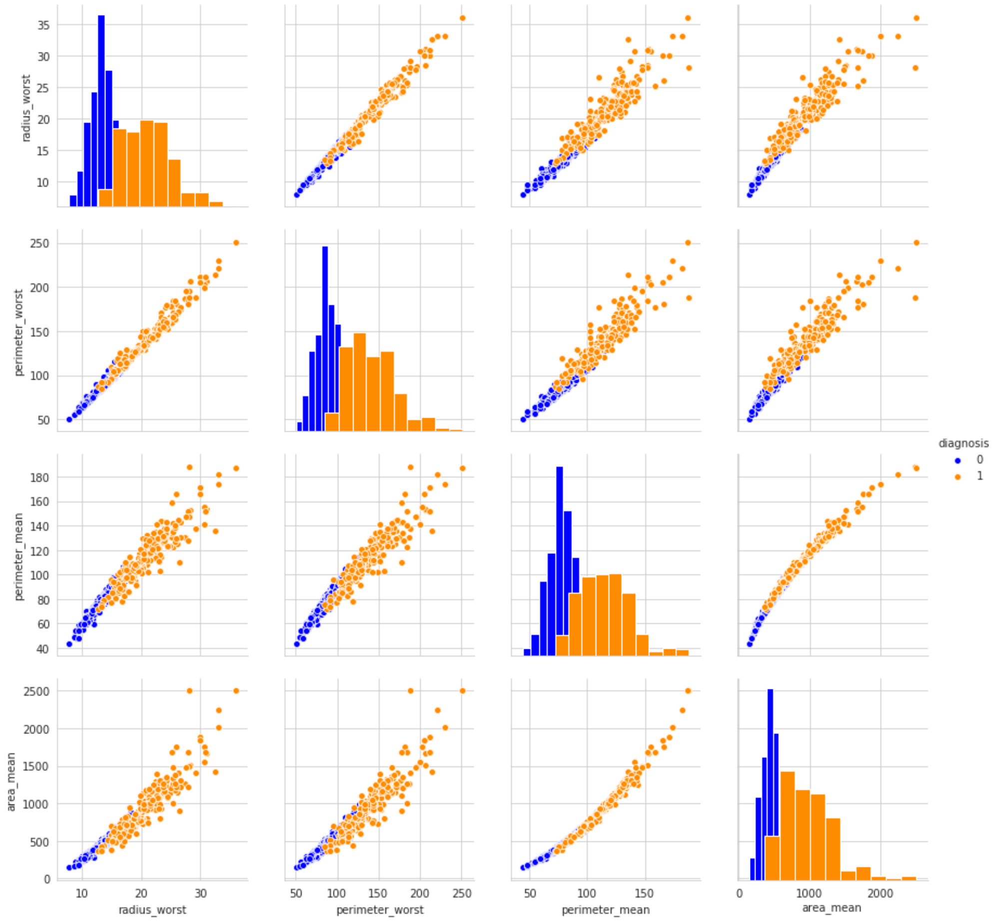
In [6]:
```
sns.set_style('whitegrid')
sns.countplot(x='diagnosis',data=df)
```

Out[6]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fb9e8dee090>
```



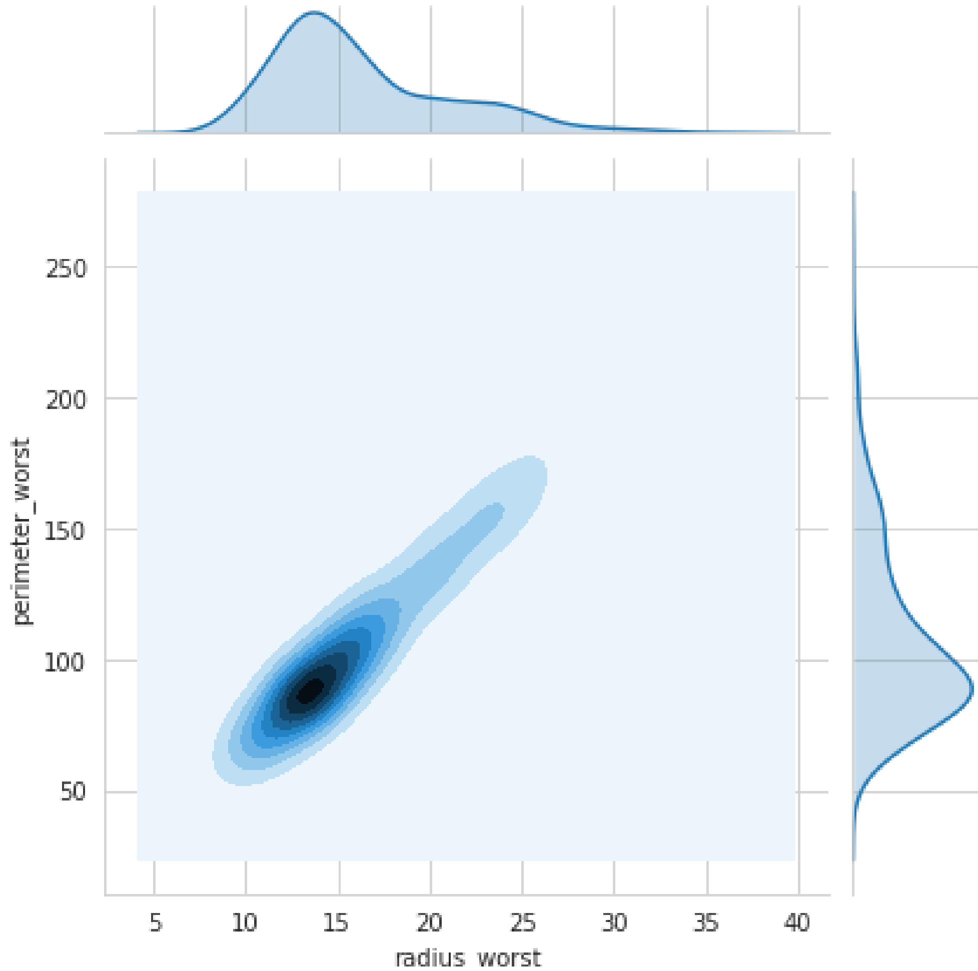
- Distribución de variable

In [7]:
```
sns.pairplot(df, vars=["radius_worst", "perimeter_worst", "perimeter_mean", "area_mean"],
             palette=sns.color_palette(['blue', 'darkorange']), hue='diagnosis', diag_kin
plt.show()
```



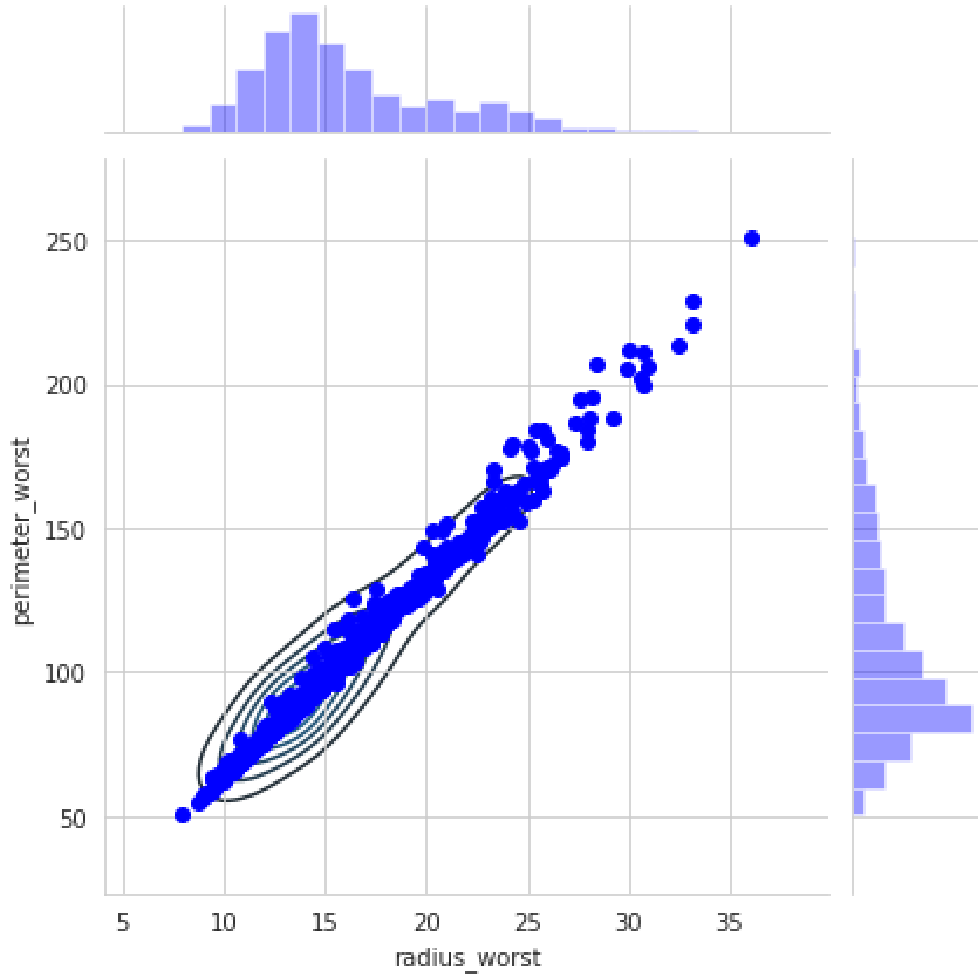

```
In [8]: sns.jointplot("radius_worst", "perimeter_worst", data=df, kind='kde')

Out[8]: <seaborn.axisgrid.JointGrid at 0x7fb9e7fa5a50>
```




```
In [9]: sns.jointplot("radius_worst", "perimeter_worst", data=df, color="b").plot_joint(sns.kdepl
```

```
Out[9]: <seaborn.axisgrid.JointGrid at 0x7fb9e5ff8110>
```




```
In [10]: from sklearn.neighbors import KNeighborsClassifier
         from sklearn.metrics import accuracy_score
         knn=KNeighborsClassifier()
```

```
In [11]: from sklearn.model_selection import train_test_split

         X = df.drop('diagnosis',axis=1)
         X = X.drop('Unnamed: 32',axis=1)
         y = df['diagnosis']
         # dividir datos
         train, test, train_labels, test_labels = train_test_split(X, y,
                                                    test_size = 0.3, random_state = 22)
```

Ajuste de parámetros de KNN con GridSearchCV

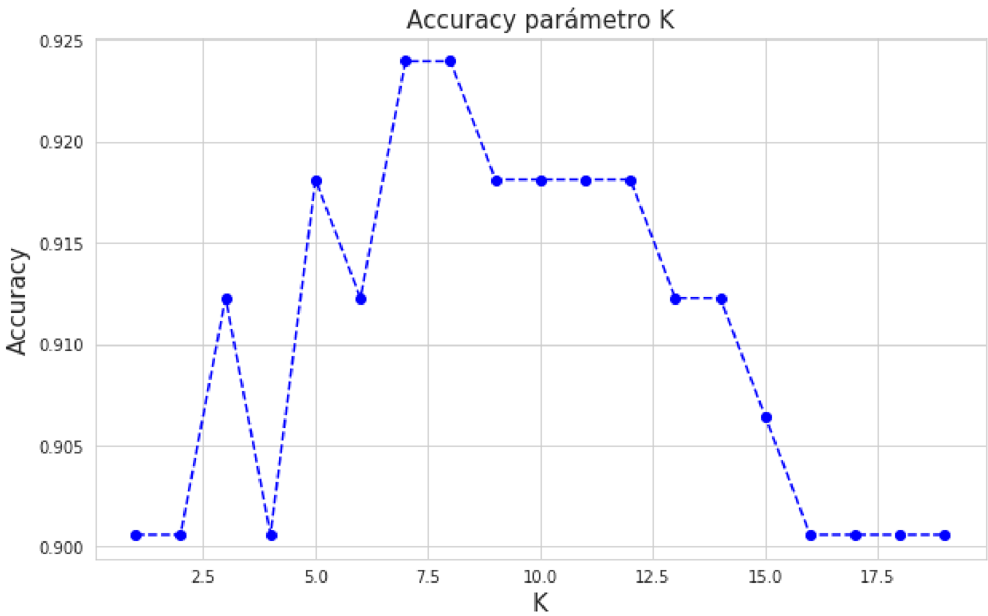
- GridSearchCV realiza una búsqueda por fuerza bruta sobre todos los posibles parámetros

- A diferencia del ejemplo de NaiveBayes, con grid search no se requiere 'for loop' para cada parámetro

In [12]:
```
acc = [] #guarda accuracy
for k in range(1,20):
    knn = KNeighborsClassifier(n_neighbors=k, metric='manhattan')
    knn.fit(train, train_labels)
    pred = knn.predict(test)
    acc.append(accuracy_score(test_labels, pred))
```

In [13]:
```
plt.figure(figsize=(10,6))
plt.plot(range(1,20),acc,color='blue', linestyle='--', marker='o')
plt.title('Accuracy parámetro K', fontsize=15)
plt.xlabel('K',fontsize=15)
plt.ylabel('Accuracy',fontsize=15)
```

Out[13]:
```
Text(0, 0.5, 'Accuracy')
```



- El ciclo indica que k=8 es el mejor parámetro con 'manhattan'

In [14]:
```
acc[7]
```

Out[14]:
```
0.9239766081871345
```

- Para evaluar los demás parámetros se importa GridSearchCV

In [15]:
```
from sklearn.model_selection import GridSearchCV
```

Se evalúan tres parámetros con GridSearchCV

- Además del parámetro 'k' se toma en cuenta 'weights' y 'metric'

In [16]:
```
train, test, train_labels, test_labels = train_test_split(X, y,
                                                        test_size = 0.15, random_state = 22)
```

In [17]:
```
import warnings
warnings.filterwarnings("ignore")
```

In [18]:
```
k_vecinos = list(range(1,20))
weight_options = ["uniform", "distance"]
metric_options = ["manhattan", 'minkowski']

param_grid = dict(n_neighbors = k_vecinos, weights = weight_options,
                  metric = metric_options)

knn = KNeighborsClassifier()

grid = GridSearchCV(knn, param_grid, scoring = 'accuracy',cv = 10)
grid.fit(train,train_labels)
```

Out[18]:
```
GridSearchCV(cv=10, error_score='raise-deprecating',
             estimator=KNeighborsClassifier(algorithm='auto', leaf_size=30,
                                            metric='minkowski',
                                            metric_params=None, n_jobs=None,
                                            n_neighbors=5, p=2,
                                            weights='uniform'),
             iid='warn', n_jobs=None,
             param_grid={'metric': ['manhattan', 'minkowski'],
                         'n_neighbors': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12,
                                         13, 14, 15, 16, 17, 18, 19],
                         'weights': ['uniform', 'distance']},
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='accuracy', verbose=0)
```

Los mejores parámetros

In [19]:
```
grid.best_score_
```

Out[19]:
```
0.94824016563147
```

In [20]:
```
grid.best_estimator_
```

Out[20]:
```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='manhattan',
                     metric_params=None, n_jobs=None, n_neighbors=7, p=2,
                     weights='uniform')
```

In [21]:
```
grid.best_params_
```

Out[21]:
```
{'metric': 'manhattan', 'n_neighbors': 7, 'weights': 'uniform'}
```

Evaluación de modelo

- Se obtienen las predicciones, informe de clasificación y matriz de confusión.
- Se crea modelo con los mejores parámetros
- Se obtienen las predicciones, informe de clasificación y matriz de confusión.

```
In [22]: predictions = grid.predict(test)
```

```
In [23]: grid.score(test, test_labels)
```

```
Out[23]: 0.9418604651162791
```

```
In [24]: from sklearn.metrics import classification_report,confusion_matrix
         print("Predicciones:\n")
         print(predictions)
         print("\nReporte de clasificación:\n")
         print(classification_report(predictions,test_labels))
```

```
Predicciones:

[0 1 1 1 0 0 0 0 0 0 0 0 1 0 0 0 1 1 0 0 1 1 1 0 1 0 1 0 0 0 0 1 0 1 0 1 1
 1 0 1 0 0 0 0 1 0 0 1 0 0 0 1 0 0 1 0 1 0 0 1 0 0 0 0 1 0 0 1 1 0 1 0 1 0
 0 1 0 0 1 0 1 0 1 0 0 1]

Reporte de clasificación:

              precision    recall  f1-score   support

           0       0.94      0.96      0.95        53
           1       0.94      0.91      0.92        33

    accuracy                           0.94        86
   macro avg       0.94      0.94      0.94        86
weighted avg       0.94      0.94      0.94        86
```

```
In [25]: print("Confusion matrix")
         conf_mat=confusion_matrix(predictions,test_labels)
         print(conf_mat)
```

```
Confusion matrix
[[51  2]
 [ 3 30]]
```

- Ajustando los parámetros se obtiene un modelo mas potente
- Probar los clasificadores aprendidos con un diferente dataset
- Experimentar con parámetros y GridSearch