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Лабораторная работа №4

# «Подготовка обучающей и тестовой выборки, кросс-валидация и подбор гиперпараметров на примере метода ближайших соседей»

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ПРОВЕРИЛ:

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**Цель лабораторной работы:** изучение сложных способов подготовки выборки и подбора гиперпараметров на примере метода ближайших соседей.

**Задание:**

1. Выберите набор данных (датасет) для решения задачи классификации или регрессии.
2. С использованием метода train_test_split разделите выборку на обучающую и тестовую.
3. Обучите модель ближайших соседей для произвольно заданного гиперпараметра K. Оцените качество модели с помощью подходящих для задачи метрик.
4. Постройте модель и оцените качество модели с использованием кросс-валидации.
5. Произведите подбор гиперпараметра K с использованием GridSearchCV и кросс-валидации.

## Выполнение работы

In [74]:
```
import numpy as np
import pandas as pd

from typing import Dict, Tuple
from scipy import stats
from sklearn.datasets import load_wine
from sklearn.model_selection import train_test_split, cross_val_score, cross_validate, GridSearchCV
from sklearn.neighbors import KNeighborsRegressor, KNeighborsClassifier
from sklearn.metrics import *

import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
sns.set(style="ticks")
```

In [75]:
```
wine = load_wine()
```

In [76]:
```
# Наименование признаков
wine.feature_names
```

Out[76]:
```
['alcohol',
 'malic_acid',
 'ash',
 'alcalinity_of_ash',
 'magnesium',
 'total_phenols',
 'flavanoids',
 'nonflavanoid_phenols',
 'proanthocyanins',
 'color_intensity',
 'hue',
 'od280/od315_of_diluted_wines',
 'proline']
```

In [77]:
```
# Размер датасета
wine.data.shape
```

Out[77]:
```
(178, 13)
```

Формирование DataFrame

In [78]:
```
wine_df = pd.DataFrame(data=np.c_[wine['data'], wine['target']],
                       columns=list(wine['feature_names']) + ['target'])
```

In [79]:
```
wine_df.describe()
```

Out[79]:

| | alcohol | malic_acid | ash | alcalinity_of_ash | magnesium | total_phenols | flavanoids | nonflavanoid_phenols | proanthocyanins | color_intensity | 1 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **count** | 178.000000 | 178.000000 | 178.000000 | 178.000000 | 178.000000 | 178.000000 | 178.000000 | 178.000000 | 178.000000 | 178.000000 | 1 |
| **mean** | 13.000618 | 2.336348 | 2.366517 | 19.494944 | 99.741573 | 2.295112 | 2.029270 | 0.361854 | 1.590899 | 5.058090 | |
| **std** | 0.811827 | 1.117146 | 0.274344 | 3.339564 | 14.282484 | 0.625851 | 0.998859 | 0.124453 | 0.572359 | 2.318286 | |
| **min** | 11.030000 | 0.740000 | 1.360000 | 10.600000 | 70.000000 | 0.980000 | 0.340000 | 0.130000 | 0.410000 | 1.280000 | |
| **25%** | 12.362500 | 1.602500 | 2.210000 | 17.200000 | 88.000000 | 1.742500 | 1.205000 | 0.270000 | 1.250000 | 3.220000 | |
| **50%** | 13.050000 | 1.865000 | 2.360000 | 19.500000 | 98.000000 | 2.355000 | 2.135000 | 0.340000 | 1.555000 | 4.690000 | |
| **75%** | 13.677500 | 3.082500 | 2.557500 | 21.500000 | 107.000000 | 2.800000 | 2.875000 | 0.437500 | 1.950000 | 6.200000 | |
| **max** | 14.830000 | 5.800000 | 3.230000 | 30.000000 | 162.000000 | 3.880000 | 5.080000 | 0.660000 | 3.580000 | 13.000000 | |

Разделение на обучающую и тестовую выборки

In [80]:
```
wine_X_train, wine_X_test, wine_Y_train, wine_Y_test = train_test_split(wine.data, wine.target,
                                                                        test_size=0.3, random_state=1)
```

In [81]:
```
# Размер обучающей выборки
wine_X_train.shape, wine_Y_train.shape
```

Out[81]:
```
((124, 13), (124,))
```

In [82]:
```
# Размер тестовой выборки
wine_X_test.shape, wine_Y_test.shape
```

Out[82]:
```
((54, 13), (54,))
```

In [83]:
```
# 3 ближайших соседа
cl1_1 = KNeighborsClassifier(n_neighbors=3)
cl1_1.fit(wine_X_train, wine_Y_train)

target1_1 = cl1_1.predict(wine_X_test)
len(target1_1), target1_1
```

Out[83]:
```
(54,
 array([0, 1, 2, 1, 0, 1, 2, 0, 2, 1, 0, 2, 1, 0, 2, 1, 1, 0, 1, 0, 0, 1,
        2, 0, 0, 2, 0, 0, 0, 1, 1, 1, 1, 0, 2, 1, 1, 2, 1, 0, 0, 1, 2, 0,
        0, 0, 0, 0, 0, 0, 1, 2, 2, 0]))
```

In [84]:
```
# 5 ближайших соседей
cl1_2 = KNeighborsClassifier(n_neighbors=5)
cl1_2.fit(wine_X_train, wine_Y_train)

target1_2 = cl1_2.predict(wine_X_test)
len(target1_2), target1_2
```

Out[84]:
```
(54,
 array([1, 1, 2, 2, 0, 1, 2, 0, 2, 1, 0, 2, 1, 0, 2, 1, 1, 0, 1, 0, 0, 1,
        2, 0, 0, 1, 0, 0, 0, 1, 1, 1, 1, 0, 2, 1, 1, 2, 1, 0, 0, 1, 2, 0,
        0, 0, 0, 0, 0, 0, 1, 2, 2, 0]))
```

Метрики качества классификации

In [85]:
```
# Accuracy
# wine_Y_test = эталон
# target = предсказанное значение классов

# 3 ближайших
accuracy_score(wine_Y_test, target1_1)
```

Out[85]:
```
0.7407407407407407
```

In [86]:
```
# 5 ближайших
accuracy_score(wine_Y_test, target1_2)
```

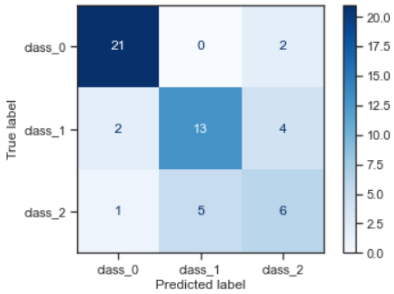
Out[86]:
```
0.7037037037037037
```

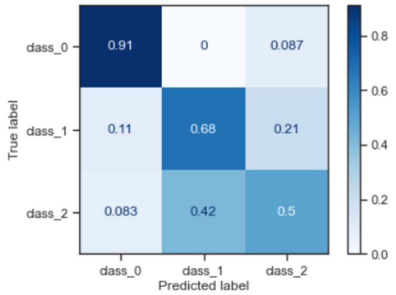
In [87]:
```
# Confusion Matrix
# Конвертация целевого признака в бинарный

def convert_target_to_binary(array:np.ndarray, target:int) -> np.ndarray:
    # Если целевой признак совпадает, то 1
    res = [1 if x==target else 0 for x in array]
    return res
bin_wine_Y_test = convert_target_to_binary(wine_Y_test, 2)
bin_target1_1 = convert_target_to_binary(target1_1, 2)
bin_target1_2 = convert_target_to_binary(target1_2, 2)

confusion_matrix(bin_wine_Y_test, bin_target1_1, labels=[0, 1])
```

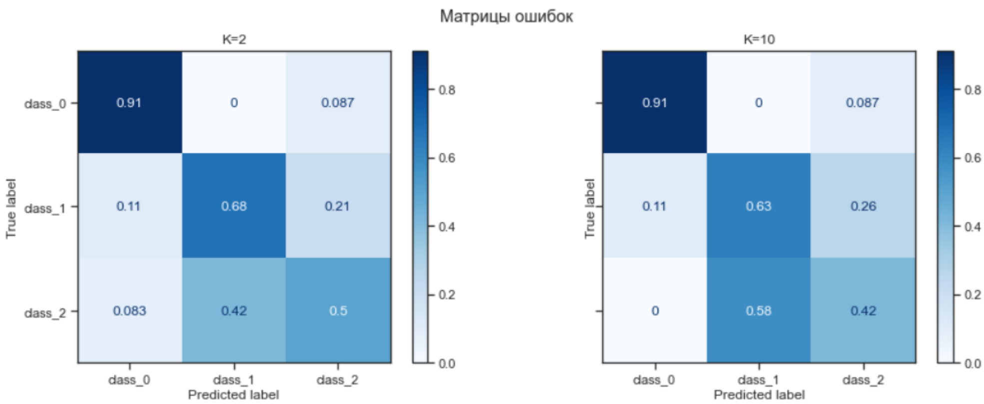
Out[87]:
```
array([[36,  6],
       [ 6,  6]], dtype=int64)
```

In [88]:
```
tn, fp, fn, tp = confusion_matrix(bin_wine_Y_test, bin_target1_1).ravel()
tn, fp, fn, tp
```

Out[88]:
```
(36, 6, 6, 6)
```

In [89]:
```
plot_confusion_matrix(cl1_1, wine_X_test, wine_Y_test,
                      display_labels=wine.target_names, cmap=plt.cm.Blues)
```
Out[89]:
```
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1a31610>
```



In [90]:
```
plot_confusion_matrix(cl1_1, wine_X_test, wine_Y_test,
                      display_labels=wine.target_names, cmap=plt.cm.Blues,
                      normalize='true')
```
Out[90]:
```
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1a59570>
```



In [91]:
```
fig, ax = plt.subplots(1, 2, sharex='col', sharey='row', figsize=(15,5))

plot_confusion_matrix(cl1_1, wine_X_test, wine_Y_test,
                      display_labels=wine.target_names,
                      cmap=plt.cm.Blues, normalize='true', ax=ax[0])

plot_confusion_matrix(cl1_2, wine_X_test, wine_Y_test,
                      display_labels=wine.target_names,
                      cmap=plt.cm.Blues, normalize='true', ax=ax[1])

fig.suptitle('Матрицы ошибок')
ax[0].title.set_text('K=2')
ax[1].title.set_text('K=10')
```



In [92]:
```
# Precision, recall, F-мера

# 3 ближайших
precision_score(bin_wine_Y_test, bin_target1_1), recall_score(bin_wine_Y_test, bin_target1_1)
```
Out[92]:
```
(0.5, 0.5)
```

In [93]:
```
# 5 ближайших
precision_score(bin_wine_Y_test, bin_target1_2), recall_score(bin_wine_Y_test, bin_target1_2)
```
Out[93]:
```
(0.4166666666666667, 0.4166666666666667)
```

In [94]:
```
precision_score(wine_Y_test, target1_1, average='micro')
```
Out[94]:
```
0.7407407407407407
```

In [95]:
```python
# Без учета веса класса
precision_score(wine_Y_test, target1_1, average='macro')
```
Out[95]: 0.6990740740740741

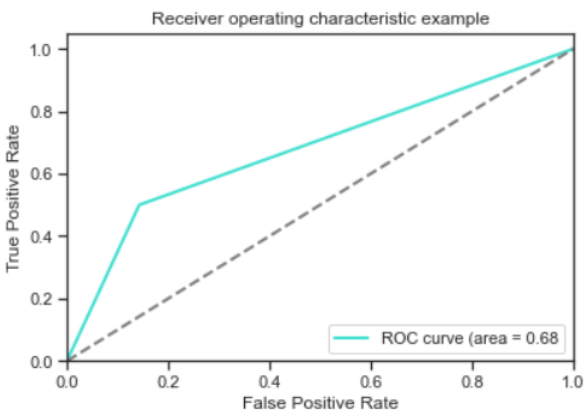
In [96]:
```python
# С учетом веса классов
precision_score(wine_Y_test, target1_1, average='weighted')
```
Out[96]: 0.7379115226337448

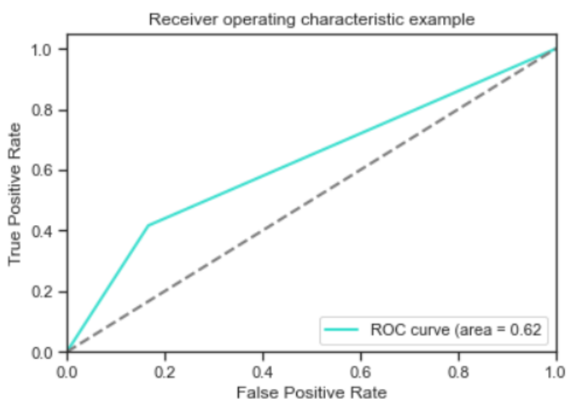
In [97]:
```python
classification_report(wine_Y_test, target1_1,
                      target_names=wine.target_names, output_dict=True)
```
Out[97]:
```
{'class_0': {'precision': 0.875,
  'recall': 0.9130434782608695,
  'f1-score': 0.8936170212765957,
  'support': 23},
 'class_1': {'precision': 0.7222222222222222,
  'recall': 0.6842105263157895,
  'f1-score': 0.7027027027027027,
  'support': 19},
 'class_2': {'precision': 0.5, 'recall': 0.5, 'f1-score': 0.5, 'support': 12},
 'accuracy': 0.7407407407407407,
 'macro avg': {'precision': 0.6990740740740741,
  'recall': 0.6990846681922197,
  'f1-score': 0.6987732413264328,
  'support': 54},
 'weighted avg': {'precision': 0.7379115226337448,
  'recall': 0.7407407407407407,
  'f1-score': 0.7389730155687603,
  'support': 54}}
```

ROC-кривая и ROC AUC

In [98]:
```python
fpr, tpr, thresholds = roc_curve(bin_wine_Y_test, bin_target1_1,
                                 pos_label=1)
fpr, tpr, thresholds
```
Out[98]:
```
(array([0.        , 0.14285714, 1.        ]),
 array([0. , 0.5, 1. ]),
 array([2, 1, 0]))
```

In [125]:
```python
def draw_roc_curve(y_true, y_score, pos_label, average):
    fpr, tpr, thresholds = roc_curve(y_true, y_score,
                                     pos_label=pos_label)
    roc_auc_value = roc_auc_score(y_true, y_score, average=average)

    plt.figure()
    lw = 2
    plt.plot(fpr, tpr, color='turquoise',
             lw=lw, label='ROC curve (area = %0.2f' % roc_auc_value)
    plt.plot([0, 1], [0, 1], color='grey', lw=lw, linestyle='--')
    plt.xlim([0.0, 1.0])
    plt.ylim([0.0, 1.05])
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')
    plt.title('Receiver operating characteristic example')
    plt.legend(loc='lower right')
    plt.show()

# 3 ближайших
draw_roc_curve(bin_wine_Y_test, bin_target1_1, pos_label=1, average='micro')

# 5 ближайших
draw_roc_curve(bin_wine_Y_test, bin_target1_2, pos_label=1, average='micro')
```




Исходя из полученных метрик качества классификации, можно судить о среднем качестве классификации.

Разбиение выборки на k частей с помощью кросс-валидации. Стратегия кросс-валидации определяется автоматически (cross_val_score).

In [100]:
```
wine_cross = cross_val_score(KNeighborsClassifier(n_neighbors=2),
                             wine.data, wine.target, cv=11)
wine_cross
```

Out[100]:
```
array([0.58823529, 0.64705882, 0.6875    , 0.5625    , 0.5625    ,
       0.625     , 0.8125    , 0.6875    , 0.8125    , 0.75      ,
       0.75      ])
```

In [101]:
```
np.mean(wine_cross)
```

Out[101]:
```
0.68048128342246
```

In [102]:
```
wining = {'precision': 'precision_weighted',
          'recall': 'recall_weighted',
          'f1': 'f1_weighted'}

wine_cross = cross_validate(KNeighborsClassifier(n_neighbors=2),
                            wine.data, wine.target, scoring=wining,
                            cv=3, return_train_score=True)
wine_cross
```

Out[102]:
```
{'fit_time': array([0.00100255, 0.00050139, 0.00050163]),
 'score_time': array([0.00651455, 0.00601339, 0.00601387]),
 'test_precision': array([0.48984127, 0.62317561, 0.70585516]),
 'train_precision': array([0.91000807, 0.8877454 , 0.85825075]),
 'test_recall': array([0.56666667, 0.6440678 , 0.72881356]),
 'train_recall': array([0.89830508, 0.87394958, 0.83193277]),
 'test_f1': array([0.51069094, 0.6198816 , 0.6798559 ]),
 'train_f1': array([0.89415947, 0.8703245 , 0.8181316 ])}
```

Нахождение наилучшего гиперпараметра K с использованием GridSearchCV и кросс-валидации

In [103]:
```
n_range = np.array(range(5, 30, 1))
tuned_parameters = [{'n_neighbors': n_range}]
tuned_parameters
```

Out[103]:
```
[{'n_neighbors': array([ 5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21,
         22, 23, 24, 25, 26, 27, 28, 29])}]
```

In [104]:
```
%%time
clf_gs = GridSearchCV(KNeighborsClassifier(), tuned_parameters,
                      cv=5, scoring='accuracy')
clf_gs.fit(wine_X_train, wine_Y_train)
```

```
Wall time: 605 ms
```

Out[104]:
```
GridSearchCV(cv=5, error_score=nan,
             estimator=KNeighborsClassifier(algorithm='auto', leaf_size=30,
                                            metric='minkowski',
                                            metric_params=None, n_jobs=None,
                                            n_neighbors=5, p=2,
                                            weights='uniform'),
             iid='deprecated', n_jobs=None,
             param_grid=[{'n_neighbors': array([ 5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21,
       22, 23, 24, 25, 26, 27, 28, 29])}],
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='accuracy', verbose=0)
```

In [105]:
```
clf_gs.cv_results_
```

Out[105]:
```
{'mean_fit_time': array([0.00060105, 0.00070167, 0.00110264, 0.00100374, 0.00070162,
        0.00090179, 0.00100331, 0.00080175, 0.00060048, 0.00059934,
        0.00080385, 0.00050073, 0.00060158, 0.00050139, 0.00060096,
        0.0005003 , 0.00120263, 0.00360789, 0.00110283, 0.0019032 ,
        0.0006012 , 0.00060024, 0.00200419, 0.00050144, 0.00049877]),
 'std_fit_time': array([2.00510280e-04, 2.45477094e-04, 2.00057562e-04, 6.33204593e-04,
        2.45613048e-04, 5.84434964e-04, 6.35954867e-04, 2.45340545e-04,
        1.97347260e-04, 2.01643006e-04, 4.04373868e-04, 4.86280395e-07,
        2.00605477e-04, 3.37174788e-07, 1.99961740e-04, 1.73636832e-06,
        5.10856311e-04, 3.72841647e-03, 4.90582888e-04, 1.83205304e-03,
        2.00557822e-04, 2.01647077e-04, 2.76327783e-03, 3.50402318e-07,
        4.77551878e-06]),
 'mean_score_time': array([0.00200458, 0.00952134, 0.00440965, 0.00460882, 0.00220475,
        0.00240555, 0.00240407, 0.00260611, 0.00210381, 0.00200453,
        0.00200257, 0.00190687, 0.00200438, 0.00220475, 0.00200481,
        0.0030066 , 0.00440979, 0.0034102 , 0.00430913, 0.00320711,
        0.00260568, 0.00751648, 0.00320783, 0.00260663, 0.00220509]),
 'std_score_time': array([0.00031681, 0.01453806, 0.00260213, 0.00496464, 0.0004005 ,
        0.00058461, 0.0005853 , 0.00097204, 0.00020111, 0.00031741,
        0.0003172 , 0.000378  , 0.00063396, 0.00051116, 0.00063403,
        0.00100243, 0.00171867, 0.00111435, 0.00333295, 0.00136722,
```

```
        0.00124381, 0.01027917, 0.00081394, 0.00124365, 0.00040045]),
 'param_n_neighbors': masked_array(data=[5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19,
                    20, 21, 22, 23, 24, 25, 26, 27, 28, 29],
              mask=[False, False, False, False, False, False, False, False,
                    False, False, False, False, False, False, False, False,
                    False, False, False, False, False, False, False, False,
                    False],
        fill_value='?',
             dtype=object),
 'params': [{'n_neighbors': 5},
  {'n_neighbors': 6},
  {'n_neighbors': 7},
  {'n_neighbors': 8},
  {'n_neighbors': 9},
  {'n_neighbors': 10},
  {'n_neighbors': 11},
  {'n_neighbors': 12},
  {'n_neighbors': 13},
  {'n_neighbors': 14},
  {'n_neighbors': 15},
  {'n_neighbors': 16},
  {'n_neighbors': 17},
  {'n_neighbors': 18},
  {'n_neighbors': 19},
  {'n_neighbors': 20},
  {'n_neighbors': 21},
  {'n_neighbors': 22},
  {'n_neighbors': 23},
  {'n_neighbors': 24},
  {'n_neighbors': 25},
  {'n_neighbors': 26},
  {'n_neighbors': 27},
  {'n_neighbors': 28},
  {'n_neighbors': 29}],
 'split0_test_score': array([0.64, 0.64, 0.6 , 0.6 , 0.64, 0.64, 0.64, 0.64, 0.64, 0.6 , 0.6 ,
        0.76, 0.76, 0.72, 0.68, 0.76, 0.76, 0.76, 0.72, 0.72, 0.76, 0.76,
        0.76, 0.76, 0.76]),
 'split1_test_score': array([0.72, 0.8 , 0.72, 0.8 , 0.76, 0.64, 0.68, 0.76, 0.72, 0.72, 0.76,
        0.8 , 0.8 , 0.8 , 0.8 , 0.8 , 0.8 , 0.84, 0.8 , 0.76, 0.8 , 0.84,
        0.8 , 0.76, 0.8 ]),
 'split2_test_score': array([0.76, 0.8 , 0.76, 0.72, 0.76, 0.76, 0.76, 0.84, 0.8 , 0.84, 0.8 ,
        0.68, 0.68, 0.68, 0.76, 0.72, 0.72, 0.72, 0.72, 0.72, 0.72, 0.72,
        0.72, 0.72, 0.72]),
     'split3_test_score': array([0.68, 0.76, 0.72, 0.76, 0.72, 0.76, 0.72, 0.72, 0.72, 0.64, 0.64,
         0.64, 0.64, 0.64, 0.64, 0.64, 0.64, 0.68, 0.64, 0.64, 0.64, 0.64,
         0.64, 0.64, 0.64]),
     'split4_test_score': array([0.58333333, 0.625     , 0.54166667, 0.5       , 0.58333333,
         0.58333333, 0.58333333, 0.54166667, 0.66666667, 0.625     ,
         0.66666667, 0.70833333, 0.75      , 0.79166667, 0.75      ,
         0.75      , 0.75      , 0.75      , 0.75      , 0.75      ,
         0.66666667, 0.70833333, 0.625     , 0.70833333, 0.625     ]),
     'mean_test_score': array([0.67666667, 0.725     , 0.66833333, 0.676     , 0.69266667,
         0.67666667, 0.67666667, 0.70033333, 0.70933333, 0.685     ,
         0.69333333, 0.71766667, 0.726     , 0.72633333, 0.726     ,
         0.734     , 0.734     , 0.75      , 0.726     , 0.718     ,
         0.71733333, 0.73366667, 0.709     , 0.71766667, 0.709     ]),
     'std_test_score': array([0.06146363, 0.0770714 , 0.08301272, 0.1105622 , 0.07006029,
         0.07111806, 0.06146363, 0.10224372, 0.05491003, 0.08729261,
         0.07495184, 0.05676071, 0.05782733, 0.0621861 , 0.05782733,
         0.05351635, 0.05351635, 0.05291503, 0.052     , 0.04214262,
         0.05866667, 0.06573009, 0.06755738, 0.04406561, 0.06755738]),
     'rank_test_score': array([21,  9, 25, 24, 19, 22, 22, 17, 14, 20, 18, 11,  6,  5,  6,  2,  2,
          1,  6, 10, 13,  4, 15, 11, 15], dtype=int32)}
```

In [106]:
```
# Лучшая модель
clf_gs.best_estimator_
```

Out[106]:
```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                     metric_params=None, n_jobs=None, n_neighbors=22, p=2,
                     weights='uniform')
```

In [107]:
```
# Лучшее значение метрики
clf_gs.best_score_
```

Out[107]:
```
0.7500000000000001
```

In [108]:
```
# Лучшее значение параметров
clf_gs.best_params_
```

Out[108]:
```
{'n_neighbors': 22}
```

Как видно, лучшее найденное значение гиперпараметра K = 22. При этом K наилучшее значение метрики = 0,75.