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высшего образования

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Курс «Технологии машинного обучения»

Отчет по лабораторной работе №3

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

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

Задание:

- Выберите набор данных (датасет) для решения задачи классификации или регрессии.
- С использованием метода train_test_split разделите выборку на обучающую и тестовую.
- Обучите модель ближайших соседей для произвольно заданного гиперпараметра K. Оцените качество модели с помощью подходящих для задачи метрик.
- Произведите подбор гиперпараметра K с использованием GridSearchCV и/или RandomizedSearchCV и кросс-валидации, оцените качество оптимальной модели. Желательно использование нескольких стратегий кросс-валидации.
- Сравните метрики качества исходной и оптимальной моделей.

Набор данных: Wine recognition dataset

Текст программы и экранные формы с примерами выполнения программы (ячейки ноутбука):

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In [1]:

```
import numpy as np
import pandas as pd
import seaborn as sns
from sklearn.datasets import *
from IPython.display import Image
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsRegressor, KNeighborsClassifier
from sklearn.model_selection import cross_val_score, cross_validate
from sklearn.model_selection import KFold, RepeatedKFold, LeaveOneOut, LeavePOut, Shuffle
Split, StratifiedKFold
from sklearn.metrics import accuracy_score, balanced_accuracy_score
from sklearn.metrics import precision_score, recall_score, f1_score, classification_repor
t
from sklearn.metrics import confusion_matrix
from sklearn.metrics import mean_absolute_error, mean_squared_error, mean_squared_log_err
or, median_absolute_error, r2_score
from sklearn.metrics import roc_curve, roc_auc_score
from sklearn.model_selection import GridSearchCV, RandomizedSearchCV
from sklearn.model_selection import learning_curve, validation_curve
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
sns.set(style="ticks")
```

In [1]:

```
#data = pd.read_csv('archive/heart.csv')
#def make_dataframe(ds_function):
    #ds = ds_function()
    #df = pd.DataFrame(data= np.c_[ds['data'], ds['target']],
                     #columns= list(ds['feature_names']) + ['target'])
    #return df

#data = make_dataframe(load_iris)
```

In [2]:

```
wine = load_wine()
```

Разделение выборки на обучающую и тестовую

In [3]:

```
wine_X_train, wine_X_test, wine_y_train, wine_y_test = train_test_split(
    wine.data, wine.target, test_size=0.5, random_state=1)
```

In [95]:

```
# Размер обучающей выборки
wine_X_train.shape, wine_y_train.shape
```

Out[95]:

```
((89, 13), (89,))
```

In [96]:

```
# Размер тестовой выборки
wine_X_test.shape, wine_y_test.shape
```

Out[96]:

```
((89, 13), (89,))
```

((89, 13), (89,))

In [97]:

```
np.unique(wine_y_train)
```

Out[97]:

```
array([0, 1, 2])
```

In [98]:

```
np.unique(wine_y_test)
```

Out[98]:

```
array([0, 1, 2])
```

Обучение модели k ближайших соседей

In [8]:

```
# 2 ближайших соседа
cl1_1 = KNeighborsClassifier(n_neighbors=2)
cl1_1.fit(wine_X_train, wine_y_train)
target1_1 = cl1_1.predict(wine_X_test)
len(target1_1), target1_1
```

Out[8]:

```
(89,
 array([0, 1, 2, 1, 0, 1, 2, 0, 1, 1, 0, 1, 1, 0, 2, 1, 1, 1, 1, 0, 0, 1,
        1, 0, 0, 1, 0, 0, 0, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 0, 0, 1, 1, 0,
        0, 1, 0, 0, 0, 0, 1, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1, 0, 1, 1, 2, 0,
        1, 0, 1, 1, 1, 0, 1, 0, 1, 1, 2, 2, 0, 1, 0, 0, 1, 0, 1, 1, 1, 0,
        1]))
```

In [9]:

```
# 10 ближайших соседей
cl1_2 = KNeighborsClassifier(n_neighbors=10)
cl1_2.fit(wine_X_train, wine_y_train)
target1_2 = cl1_2.predict(wine_X_test)
len(target1_2), target1_2
```

Out[9]:

```
(89,
 array([1, 1, 2, 1, 0, 1, 1, 0, 1, 1, 0, 1, 1, 0, 1, 1, 1, 0, 1, 0, 0, 1,
        2, 0, 2, 1, 0, 0, 0, 2, 1, 2, 1, 0, 2, 1, 1, 1, 1, 0, 0, 1, 1, 2,
        0, 2, 2, 0, 0, 0, 1, 1, 1, 0, 1, 0, 0, 1, 1, 1, 1, 0, 2, 2, 1, 0,
        1, 0, 1, 2, 1, 1, 1, 2, 1, 1, 2, 1, 0, 2, 1, 0, 1, 0, 1, 1, 1, 0,
        1]))
```

Метрики качества регрессии

1) Accuracy

In [10]:

```
# 2 ближайших соседа
accuracy_score(wine_y_test, target1_1)
```

Out[10]:

```
0.6404494382022472
```

In [11]:

```
# 10 ближайших соседей
```

```
accuracy_score(wine_y_test, target1_2)
```

Out[11]:

```
0.6629213483146067
```

In [111]:

```
# Конвертация целевого признака в бинарный
def convert_target_to_binary(array:np.ndarray, target:int) -> np.ndarray:
    # Если целевой признак совпадает с указанным, то 1 иначе 0
    res = [1 if x==target else 0 for x in array]
    return res
```

In [112]:

```
# Если целевой признак ==2,
# то будем считать этот случай 1 в бинарном признаке
bin_wine_y_train = convert_target_to_binary(wine_y_train, 2)
list(zip(wine_y_train, bin_wine_y_train))[:10]
```

Out[112]:

```
[(1, 0),
 (1, 0),
 (0, 0),
 (1, 0),
 (1, 0),
 (1, 0),
 (2, 1),
 (1, 0),
 (1, 0),
 (1, 0)]
```

In [113]:

```
bin_wine_y_test = convert_target_to_binary(wine_y_test, 2)
list(zip(wine_y_test, bin_wine_y_test))[:10]
```

Out[113]:

```
[(2, 1),
 (1, 0),
 (0, 0),
 (1, 0),
 (0, 0),
 (2, 1),
 (1, 0),
 (0, 0),
 (2, 1),
 (1, 0)]
```

In [114]:

```
# Конвертация предсказанных признаков
bin_target1_1 = convert_target_to_binary(target1_1, 2)
bin_target1_2 = convert_target_to_binary(target1_2, 2)
```

In [115]:

```
balanced_accuracy_score(bin_wine_y_test, bin_target1_1)
```

Out[115]:

```
0.5156037991858887
```

In [116]:

```
balanced_accuracy_score(bin_wine_y_test, bin_target1_2)
```

Out[116]:

```
0.5390094979647219
```

2) Матрица ошибок или Confusion Matrix

In [117]:

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

Out[117]:

```
array([[63,  4],
       [20,  2]], dtype=int64)
```

In [118]:

```
tn, fp, fn, tp = confusion_matrix(bin_wine_y_test, bin_target1_1).ravel()
tn, fp, fn, tp
```

Out[118]:

```
(63, 4, 20, 2)
```

In [120]:

```
# Пример для небинарной классификации
confusion_matrix(wine_y_test, target1_1, labels=[0, 1, 2])
```

Out[120]:

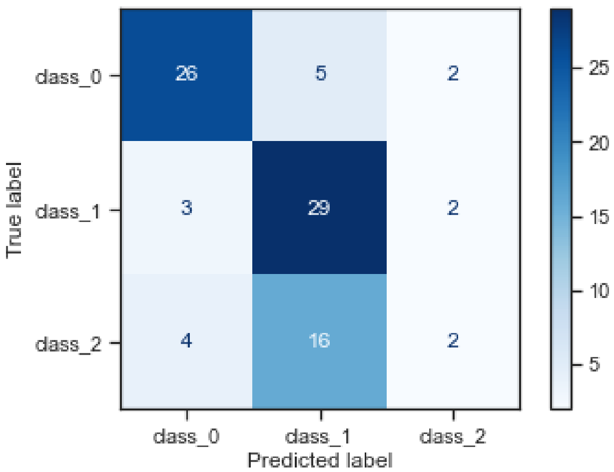
```
array([[26,  5,  2],
       [ 3, 29,  2],
       [ 4, 16,  2]], dtype=int64)
```

In [12]:

```
from sklearn.metrics import confusion_matrix
from sklearn.metrics import plot_confusion_matrix
plot_confusion_matrix(cl1_1, wine_X_test, wine_y_test,
                      display_labels=wine.target_names, cmap=plt.cm.Blues)
```

Out[12]:

```
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1e888199d90>
```

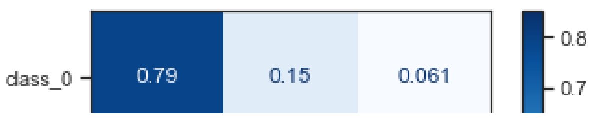


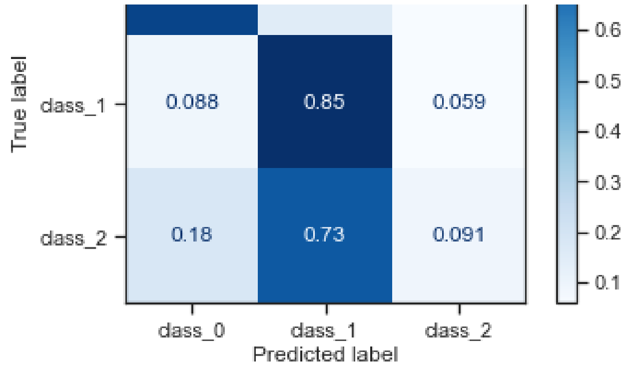
In [13]:

```
plot_confusion_matrix(cl1_1, wine_X_test, wine_y_test,
                      display_labels=wine.target_names,
                      cmap=plt.cm.Blues, normalize='true')
```

Out[13]:

```
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1e8886b80a0>
```



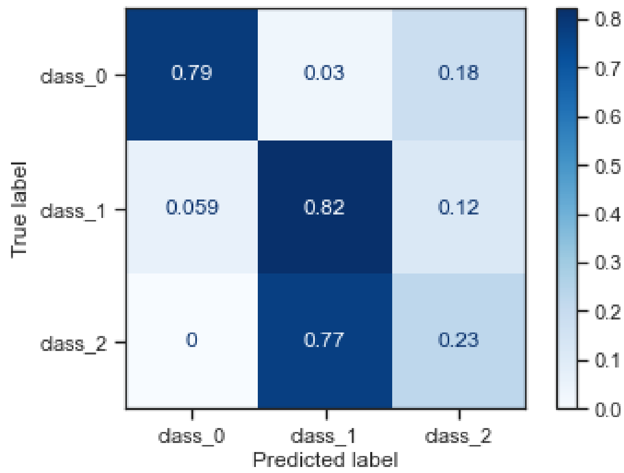


In [14]:

```
plot_confusion_matrix(cl1_2, wine_X_test, wine_y_test,
                      display_labels=wine.target_names,
                      cmap=plt.cm.Blues, normalize='true')
```

Out[14]:

```
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1e888621b80>
```



3) Precision, recall и F-мера

In [128]:

```
# Для 2 ближайших соседей
precision_score(bin_wine_y_test, bin_target1_1), recall_score(bin_wine_y_test, bin_target1_1)
```

Out[128]:

```
(0.3333333333333333, 0.09090909090909091)
```

In [129]:

```
# Для 10 ближайших соседей
precision_score(bin_wine_y_test, bin_target1_2), recall_score(bin_wine_y_test, bin_target1_2)
```

Out[129]:

```
(0.3333333333333333, 0.22727272727272727)
```

In [131]:

```
# Параметры TP, TN, FP, FN считаются как сумма по всем классам
precision_score(wine_y_test, target1_1, average='micro')
```

Out[131]:

```
0.6404494382022472
```

In [132]:

```
# Параметры TP, TN, FP, FN считаются отдельно для каждого класса
# и берется среднее значение, дисбаланс классов не учитывается.
precision_score(wine_y_test, target1_1, average='macro')
```

Out[132]:

```
0.567070707070707
```

In [133]:

```
# Параметры TP, TN, FP, FN считаются отдельно для каждого класса
# и берется средневзвешенное значение, дисбаланс классов учитывается
# в виде веса классов (вес - количество истинных значений каждого класса).
precision_score(wine_y_test, target1_1, average='weighted')
```

Out[133]:

```
0.5961048689138577
```

F-мера

In [134]:

```
f1_score(bin_wine_y_test, bin_target1_2)
```

Out[134]:

```
0.27027027027027023
```

In [135]:

```
f1_score(wine_y_test, target1_1, average='micro')
```

Out[135]:

```
0.6404494382022472
```

In [136]:

```
f1_score(wine_y_test, target1_1, average='macro')
```

Out[136]:

```
0.5404040404040403
```

In [137]:

```
f1_score(wine_y_test, target1_1, average='weighted')
```

Out[137]:

```
0.5912252541466024
```

In [138]:

```
# Значения точности, полноты и F-меры для всех классов выборки
classification_report(wine_y_test, target1_1,
                      target_names=wine.target_names, output_dict=True)
```

Out[138]:

```
{'class_0': {'precision': 0.7878787878787878,
  'recall': 0.7878787878787878,
  'f1-score': 0.7878787878787878,
  'support': 33},
 'class_1': {'precision': 0.58,
  'recall': 0.8529411764705882,
  'f1-score': 0.6904761904761905,
  'support': 34},
 'class_2': {'precision': 0.3333333333333333,
  'recall': 0.09090909090909091,
  'f1-score': 0.14285714285714288,
  'support': 22},
```

```
 'accuracy': 0.6404494382022472,
 'macro avg': {'precision': 0.5670707070707070707,
  'recall': 0.5772430184194889,
  'f1-score': 0.5404040404040403,
  'support': 89},
 'weighted avg': {'precision': 0.5961048689138577,
  'recall': 0.6404494382022472,
  'f1-score': 0.5912252541466024,
  'support': 89}}
```

4) ROC-кривая и ROC AUC

In [139]:

```
# Обучим модели на задаче бинарной классифкации,
# чтобы получить вероятности классов

# 2 ближайших соседа
bin_cl1_1 = KNeighborsClassifier(n_neighbors=2)
bin_cl1_1.fit(wine_X_train, bin_wine_y_train)
# предскажем метки классов
bin_cl1_1.predict(wine_X_test)
```

Out[139]:

```
array([0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0])
```

In [140]:

```
# Классы возвращаются в следующем порядке
bin_cl1_1.classes_
```

Out[140]:

```
array([0, 1])
```

In [141]:

```
# предскажем вероятности классов
proba_target1_1 = bin_cl1_1.predict_proba(wine_X_test)
len(proba_target1_1), proba_target1_1
```

Out[141]:

```
(89,
 array([[1. , 0. ],
        [1. , 0. ],
        [0. , 1. ],
        [1. , 0. ],
        [1. , 0. ],
        [1. , 0. ],
        [0. , 1. ],
        [1. , 0. ],
        [0.5, 0.5],
        [1. , 0. ],
        [1. , 0. ],
        [0.5, 0.5],
        [1. , 0. ],
        [1. , 0. ],
        [0. , 1. ],
        [1. , 0. ],
        [1. , 0. ],
        [0.5, 0.5],
        [1. , 0. ],
        [1. , 0. ],
        [1. , 0. ],
        [1. , 0. ],
        [0.5, 0.5],
```

```
       [1. , 0. ],
       [0.5, 0.5],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [0.5, 0.5],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [0. , 1. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [0.5, 0.5],
       [1. , 0. ],
       [0.5, 0.5],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [0. , 1. ],
       [0. , 1. ],
       [1. , 0. ],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ],
       [0.5, 0.5],
       [0.5, 0.5],
       [1. , 0. ],
       [1. , 0. ],
       [1. , 0. ]]))
```

In [142]:

```
# вероятность единичного (истинного) класса
true_proba_target1_1 = proba_target1_1[:,1]
```

```
true_proba_target1_1
```

Out[142]:

```
array([0. , 0. , 1. , 0. , 0. , 0. , 1. , 0. , 0.5, 0. , 0. , 0.5, 0. ,
       0. , 1. , 0. , 0. , 0.5, 0. , 0. , 0. , 0. , 0.5, 0. , 0.5, 0.5,
       0. , 0. , 0. , 0. , 0. , 0. , 0. , 0. , 0.5, 0. , 0. , 0.5, 0. ,
       0. , 0. , 0.5, 0.5, 0. , 0. , 0.5, 0. , 0. , 0. , 0. , 0. , 0.5,
       0.5, 0. , 0.5, 0. , 0.5, 0. , 0.5, 0. , 0. , 0. , 0.5, 0. , 1. ,
       0. , 0. , 0. , 0. , 0.5, 0.5, 0. , 0.5, 0.5, 0. , 0. , 1. , 1. ,
       0. , 0.5, 0. , 0. , 0. , 0. , 0.5, 0.5, 0. , 0. , 0. ])
```

In [144]:

```
fpr, tpr, thresholds = roc_curve(bin_wine_y_test, true_proba_target1_1,
                                 pos_label=1)
fpr, tpr, thresholds
```

Out[144]:

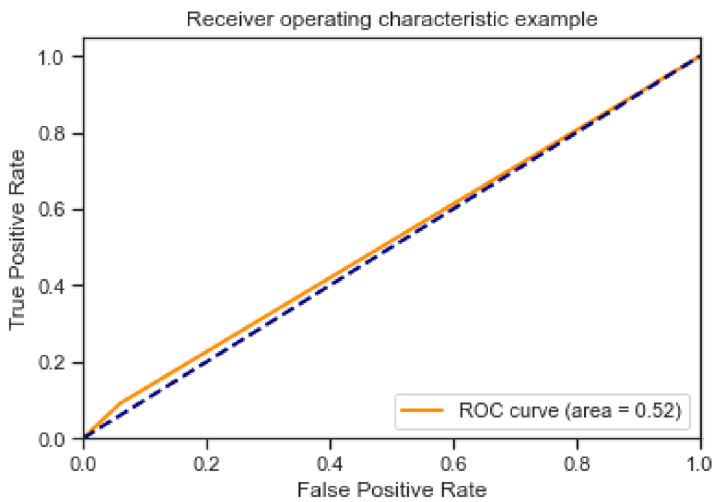
```
(array([0.        , 0.05970149, 0.23880597, 1.        ]),
 array([0.        , 0.09090909, 0.63636364, 1.        ]),
 array([2. , 1. , 0.5, 0. ]))
```

In [145]:

```
# Отрисовка ROC-кривой
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='darkorange',
             lw=lw, label='ROC curve (area = %0.2f)' % roc_auc_value)
    plt.plot([0, 1], [0, 1], color='navy', 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()
```

In [146]:

```
# Для 2 ближайших соседей
draw_roc_curve(bin_wine_y_test, bin_target1_1, pos_label=1, average='micro')
```



In [148]:

```
# Для 10 ближайших соседей
bin_cl1_2 = KNeighborsClassifier(n_neighbors=10)
bin_cl1_2.fit(wine_X_train, bin_wine_y_train)
```

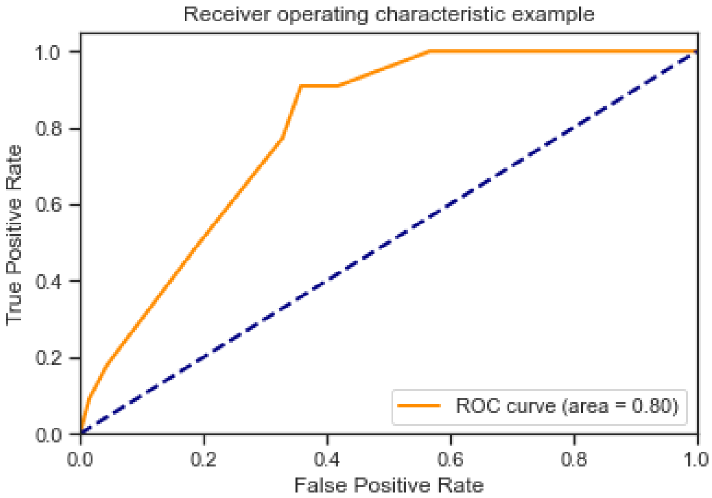
```
proba_target2_1 = bin_cl1_2.predict_proba(wine_X_test)
true_proba_target2_1 = proba_target2_1[:,1]
roc_curve_k10_res = roc_curve(bin_wine_y_test, true_proba_target2_1, pos_label=1)
roc_curve_k10_res
```

Out[148]:

```
(array([0.        , 0.01492537, 0.04477612, 0.19402985, 0.32835821,
        0.35820896, 0.41791045, 0.56716418, 1.        ]),
 array([0.        , 0.09090909, 0.18181818, 0.5       , 0.77272727,
        0.90909091, 0.90909091, 1.        , 1.        ]),
 array([1.7, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1, 0. ]))
```

In [149]:

```
draw_roc_curve(bin_wine_y_test, true_proba_target2_1, pos_label=1, average='micro')
```



Подбор гиперпараметра K с использованием GridSearchCV

In [24]:

```
from sklearn.model_selection import GridSearchCV
```

In [152]:

```
n_range = np.array(range(5, 55, 5))
tuned_parameters = [{'n_neighbors': n_range}]
tuned_parameters
```

Out[152]:

```
[{'n_neighbors': array([ 5, 10, 15, 20, 25, 30, 35, 40, 45, 50])}]
```

In [156]:

```
%%time
clf_gs = GridSearchCV(KNeighborsClassifier(), tuned_parameters, cv=5, scoring='accuracy'
)
clf_gs.fit(wine_X_train, wine_y_train)
```

```
Wall time: 100 ms
```

Out[156]:

```
GridSearchCV(cv=5, estimator=KNeighborsClassifier(),
             param_grid=[{'n_neighbors': array([ 5, 10, 15, 20, 25, 30, 35, 40, 45, 50])}
],
             scoring='accuracy')
```

In [157]:

```
clf_gs.cv_results_
```

Out[157]:

```
{'mean_fit_time': array([0.00020146, 0.        , 0.        , 0.        , 0.        ,
       0.        , 0.        , 0.0031333 , 0.        , 0.        ]),
 'std_fit_time': array([0.00040293, 0.        , 0.        , 0.        , 0.        ,
       0.        , 0.        , 0.00626659, 0.        , 0.        ]),
 'mean_score_time': array([0.        , 0.00312614, 0.        , 0.00312381, 0.00313234,
       0.00110168, 0.        , 0.        , 0.        , 0.0031251 ]),
 'std_score_time': array([0.        , 0.00625229, 0.        , 0.00624762, 0.00626469,
       0.00220337, 0.        , 0.        , 0.        , 0.00625019]),
 'param_n_neighbors': masked_array(data=[5, 10, 15, 20, 25, 30, 35, 40, 45, 50],
             mask=[False, False, False, False, False, False, False, False,
                   False, False],
       fill_value='?',
            dtype=object),
 'params': [{'n_neighbors': 5},
  {'n_neighbors': 10},
  {'n_neighbors': 15},
  {'n_neighbors': 20},
  {'n_neighbors': 25},
  {'n_neighbors': 30},
  {'n_neighbors': 35},
  {'n_neighbors': 40},
  {'n_neighbors': 45},
  {'n_neighbors': 50}],
 'split0_test_score': array([0.77777778, 0.77777778, 0.83333333, 0.72222222, 0.77777778,
       0.72222222, 0.72222222, 0.72222222, 0.77777778, 0.77777778]),
 'split1_test_score': array([0.72222222, 0.66666667, 0.72222222, 0.66666667, 0.77777778,
       0.77777778, 0.77777778, 0.77777778, 0.72222222, 0.72222222]),
 'split2_test_score': array([0.66666667, 0.72222222, 0.61111111, 0.72222222, 0.72222222,
       0.66666667, 0.72222222, 0.66666667, 0.66666667, 0.61111111]),
 'split3_test_score': array([0.83333333, 0.77777778, 0.72222222, 0.72222222, 0.77777778,
       0.77777778, 0.61111111, 0.66666667, 0.72222222, 0.72222222]),
 'split4_test_score': array([0.47058824, 0.47058824, 0.70588235, 0.70588235, 0.52941176,
       0.52941176, 0.64705882, 0.58823529, 0.58823529, 0.64705882]),
 'mean_test_score': array([0.69411765, 0.68300654, 0.71895425, 0.70784314, 0.71699346,
       0.69477124, 0.69607843, 0.68431373, 0.69542484, 0.69607843]),
 'std_test_score': array([0.12481093, 0.11392065, 0.07057613, 0.0215389 , 0.09622726,
       0.09237678, 0.05943761, 0.06328742, 0.06408563, 0.05943761]),
 'rank_test_score': array([ 8, 10,  1,  3,  2,  7,  4,  9,  6,  4])}
```

In [158]:

```
#Лучшая модель:
clf_gs.best_estimator_
```

Out[158]:

```
KNeighborsClassifier(n_neighbors=15)
```

In [159]:

```
#Лучшее значение параметров:
clf_gs.best_params_
```

Out[159]:

```
{'n_neighbors': 15}
```

In [160]:

```
#Лучшее значение метрики:
clf_gs.best_score_
```

Out[160]:

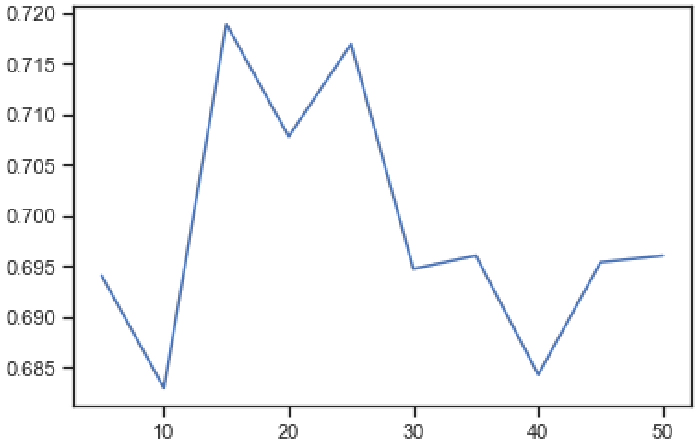
```
0.7189542483660132
```

In [162]:

```
# Изменение качества на тестовой выборке в зависимости К соседей:
plt.plot(n_range, clf_gs.cv_results_['mean_test_score'])
```

Out[162]:

```
[<matplotlib.lines.Line2D at 0x1dbda57b430>]
```



Подбор гиперпараметра K с использованием кросс-валидации и решетчатого поиска

In [6]:

```
from sklearn.model_selection import cross_val_score
```

In [7]:

```
from sklearn.model_selection import validation_curve
from sklearn.model_selection import learning_curve
from sklearn.linear_model import Ridge
from sklearn.svm import SVC
```

In [17]:

```
# Формирование обучающей и тестовой выборки
wine = load_wine()
wine_X_train, wine_X_test, wine_y_train, wine_y_test = train_test_split(
    wine.data, wine.target, test_size=0.5, random_state=1)
```

In [18]:

```
# Первичное обучение модели и оценка качества
cl1_1 = KNeighborsClassifier(n_neighbors=50)
cl1_1.fit(wine_X_train, wine_y_train)
target1_0 = cl1_1.predict(wine_X_train)
target1_1 = cl1_1.predict(wine_X_test)
accuracy_score(wine_y_train, target1_0), accuracy_score(wine_y_test, target1_1)
```

Out[18]:

```
(0.6741573033707865, 0.7191011235955056)
```

In [19]:

```
#Оценка качества модели с использованием кросс-валидации
scores = cross_val_score(KNeighborsClassifier(n_neighbors=50),
                         wine.data, wine.target,
                         cv=LeaveOneOut())
scores, np.mean(scores)
```

Out[19]:

```
(array([1., 1., 1., 1., 0., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
        1., 1., 0., 0., 0., 1., 1., 0., 0., 1., 1., 1., 1., 1., 1., 1., 1.,
        1., 1., 1., 1., 1., 0., 0., 1., 1., 0., 1., 1., 1., 1., 1., 1., 1.,
        1., 1., 1., 1., 1., 1., 1., 1., 1., 0., 1., 0., 1., 1., 0., 1., 1.,
        0., 0., 0., 1., 1., 0., 0., 1., 1., 1., 0., 1., 1., 0., 0., 1., 1.,
        1., 1., 0., 0., 0., 1., 1., 1., 1., 1., 0., 0., 1., 0., 1., 0., 0.,
        1., 1., 0., 1., 1., 1., 1., 0., 0., 1., 0., 1., 1., 1., 1., 1., 1.,
        0., 0., 1., 1., 1., 1., 1., 1., 1., 1., 0., 1., 0., 1., 1., 1., 1.,
        1., 0., 1., 1., 1., 1., 0., 0., 0., 1., 0., 1., 1., 0., 0., 0., 0.,
        1., 1., 1., 0., 0., 1., 1., 0., 1., 1., 1., 1., 0., 1., 1., 1., 1.,
```

```
        0., 0., 1., 1., 1., 1., 0., 1.]),
 0.7078651685393258)
```

In [20]:

```
#Подбор гиперпараметров на основе решетчатого поиска и кросс-валидации
n_range = np.array(range(5,55,5))
tuned_parameters = [{'n_neighbors': n_range}]
tuned_parameters
```

Out[20]:

```
[{'n_neighbors': array([ 5, 10, 15, 20, 25, 30, 35, 40, 45, 50])}]
```

In [21]:

```
%%time
clf_gs = GridSearchCV(KNeighborsClassifier(), tuned_parameters, cv=LeaveOneOut(), scorin
g='accuracy')
clf_gs.fit(wine.data, wine.target)
```

```
Wall time: 2.49 s
```

Out[21]:

```
GridSearchCV(cv=LeaveOneOut(), estimator=KNeighborsClassifier(),
             param_grid=[{'n_neighbors': array([ 5, 10, 15, 20, 25, 30, 35, 40, 45, 50])}
],
             scoring='accuracy')
```

In [22]:

```
clf_gs.best_params_
```

Out[22]:

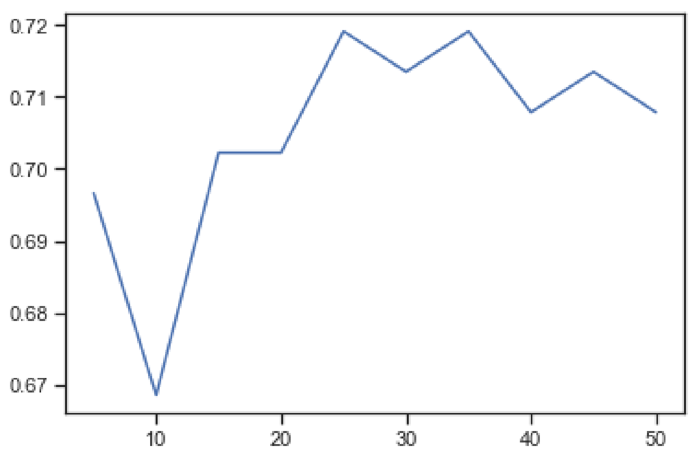
```
{'n_neighbors': 25}
```

In [23]:

```
plt.plot(n_range, clf_gs.cv_results_['mean_test_score'])
```

Out[23]:

```
[<matplotlib.lines.Line2D at 0x1a6e8cf7970>]
```



In [24]:

```
#Обучение модели и оценка качества с учетом подобранных гиперпараметров
clf_gs.best_estimator_.fit(wine_X_train, wine_y_train)
target2_0 = clf_gs.best_estimator_.predict(wine_X_train)
target2_1 = clf_gs.best_estimator_.predict(wine_X_test)
```

In [25]:

```
# Новое качество модели
accuracy_score(wine_y_train, target2_0), accuracy_score(wine_y_test, target2_1)
```

Out[25]:

```
(0.7078651685393258, 0.7303370786516854)
```

In [26]:

```
# Качество модели до подбора гиперпараметров
accuracy_score(wine_y_train, target1_0), accuracy_score(wine_y_test, target1_1)
```

Out[26]:

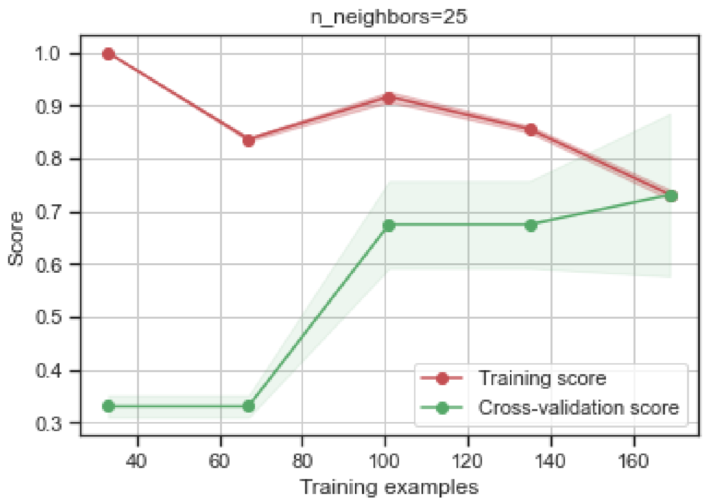
```
(0.6741573033707865, 0.7191011235955056)
```

In [31]:

```
# Построение кривых обучения и валидации
plot_learning_curve(clf_gs.best_estimator_, 'n_neighbors=25',
                    wine.data, wine.target, cv=20, train_sizes=np.linspace(.2, 1.0, 5))
```

Out[31]:

```
<module 'matplotlib.pyplot' from 'C:\\ProgramData\\Anaconda3\\lib\\site-packages\\matplot
lib\\pyplot.py'>
```



In [32]:

```
n_range2 = np.array(range(5,125,5))
```

In [33]:

```
plot_validation_curve(clf_gs.best_estimator_, 'knn',
                      wine.data, wine.target,
                      param_name='n_neighbors', param_range=n_range2,
                      cv=20, scoring="accuracy")
```

Out[33]:

```
<module 'matplotlib.pyplot' from 'C:\\ProgramData\\Anaconda3\\lib\\site-packages\\matplot
lib\\pyplot.py'>
```

n_neighbors

Построение кривой обучения

In [27]:

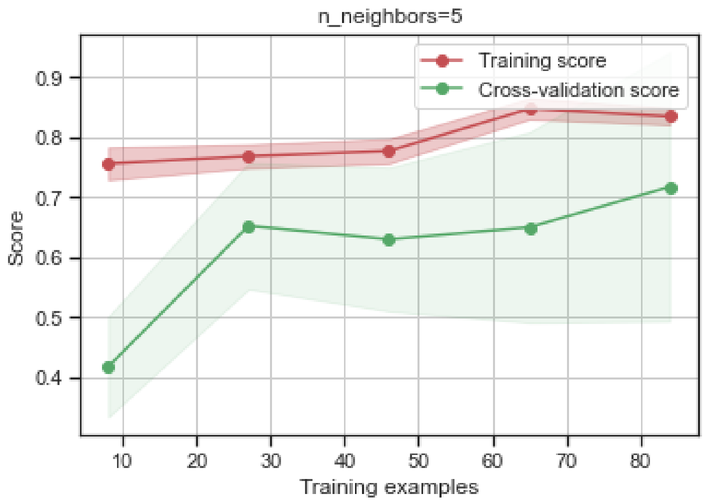
```
def plot_learning_curve(estimator, title, X, y, axes=None, ylim=None, cv=None,
                        n_jobs=None, train_sizes=np.linspace(.1, 1.0, 5)):
    plt.figure()
    plt.title(title)
    if ylim is not None:
        plt.ylim(*ylim)
    plt.xlabel("Training examples")
    plt.ylabel("Score")
    train_sizes, train_scores, test_scores = learning_curve(
        estimator, X, y, cv=cv, n_jobs=n_jobs,train_sizes=train_sizes)
    train_scores_mean = np.mean(train_scores, axis = 1)
    train_scores_std = np.std(train_scores, axis = 1)
    test_scores_mean = np.mean(test_scores, axis = 1)
    test_scores_std = np.std(test_scores, axis = 1)
    plt.grid()
    plt.fill_between(train_sizes,train_scores_mean - train_scores_std,
                     train_scores_mean + train_scores_std, alpha=0.3, color="r")
    plt.fill_between(train_sizes,test_scores_mean - test_scores_std,
                     test_scores_mean + test_scores_std, alpha=0.1, color="g")
    plt.plot(train_sizes,train_scores_mean, 'o-', color="r",
            label="Training score")
    plt.plot(train_sizes,test_scores_mean, 'o-', color="g",
            label="Cross-validation score")
    plt.legend(loc="best")
    return plt
```

In [176]:

```
plot_learning_curve(KNeighborsClassifier(n_neighbors=5),'n_neighbors=5',
                   wine_X_train, wine_y_train, cv=20)
```

Out[176]:

```
<module 'matplotlib.pyplot' from 'C:\\ProgramData\\Anaconda3\\lib\\site-packages\\matplot
lib\\pyplot.py'>
```



Построение кривой валидации

In [28]:

```
def plot_validation_curve(estimator, title, X, y,
                          param_name, param_range, cv, scoring="accuracy"):
    train_scores, test_scores = validation_curve(estimator, X, y,
                          param_name=param_name, param_range=param_range, cv=cv,
                                                 scoring=scoring, n_jobs=1)
```

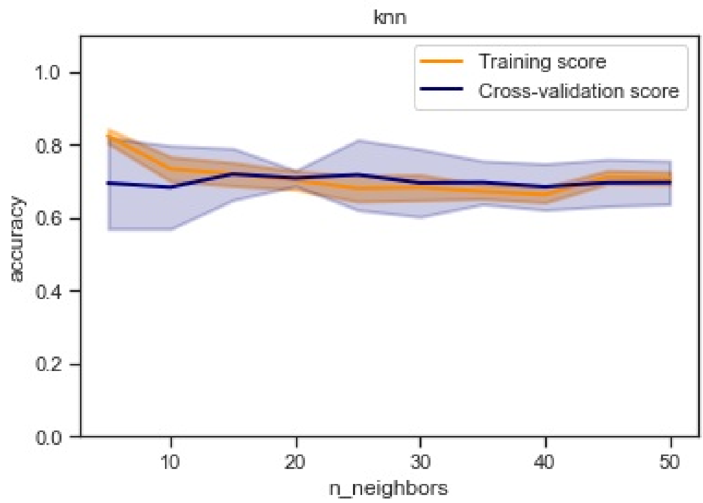
```
    train_scores_mean = np.mean(train_scores, axis = 1)
    train_scores_std = np.std(train_scores, axis = 1)
    test_scores_mean = np.mean(test_scores, axis = 1)
    test_scores_std = np.std(test_scores, axis = 1)
    plt.title(title)
    plt.xlabel(param_name)
    plt.ylabel(str(scoring))
    plt.ylim(0.0, 1.1)
    lw = 2
    plt.plot(param_range,train_scores_mean, label= "Training score", color="darkorange",
            lw=lw)
    plt.fill_between(param_range,train_scores_mean - train_scores_std,
                    train_scores_mean + train_scores_std, alpha=0.4, color="darkorange",
            lw=lw)
    plt.plot(param_range,test_scores_mean, label= "Cross-validation score", color="navy"
,
            lw=lw)
    plt.fill_between(param_range,test_scores_mean - test_scores_std,
                    test_scores_mean + test_scores_std, alpha=0.2, color="navy",
            lw=lw)
    plt.legend(loc="best")
    return plt
```

In [183]:

```
plot_validation_curve(KNeighborsClassifier(), 'knn',
                     wine_X_train,wine_y_train,
                     param_name='n_neighbors', param_range = n_range,
                     cv=5, scoring = "accuracy")
```

Out[183]:

```
<module 'matplotlib.pyplot' from 'C:\\ProgramData\\Anaconda3\\lib\\site-packages\\matplot
lib\\pyplot.py'>
```



In [ ]: