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Факультет «Информатика и управление»

Кафедра ИУ5. Курс «Технологии машинного обучения»

Отчет по лабораторной работе №4: «Подготовка обучающей и тестовой выборки, кросс-валидация и подбор гиперпараметров на примере метода ближайших соседей»

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Подпись и дата:

Проверил:

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In [1]:
```
import numpy as np
import pandas as pd
pd.set_option('display.max.rows', 1000)
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
sns.set(style='ticks')
```

Подготовка датасета

In [2]:
```
# Red Wine Quality
# Simple and clean practice dataset for regression or classification modelling
data = pd.read_csv('data/winequality-red.csv')
data.shape
```

Out[2]:
```
(1599, 12)
```

In [3]:
```
data.isnull().sum()
```

Out[3]:
```
fixed acidity           0
volatile acidity        0
citric acid             0
residual sugar          0
chlorides               0
free sulfur dioxide     0
total sulfur dioxide    0
density                 0
pH                      0
sulphates               0
alcohol                 0
quality                 0
dtype: int64
```

In [4]:
```
data.dtypes
```

Out[4]:
```
fixed acidity           float64
volatile acidity        float64
citric acid             float64
residual sugar          float64
chlorides               float64
free sulfur dioxide     float64
total sulfur dioxide    float64
density                 float64
pH                      float64
sulphates               float64
alcohol                 float64
quality                   int64
dtype: object
```

In [5]:
```
# пропусков нет, разделим на обучающую и тестовую выборку
from sklearn.model_selection import train_test_split
```

In [6]:
```
# перед этим разделим исходный датасет на 2: один содержит независимые параметры, другой — зависимый (quality)
X, y = data[data.columns[range(11)]], data[data.columns[[11]]]
```

In [7]:
```
X.dtypes
```

Out[7]:
```
fixed acidity           float64
volatile acidity        float64
citric acid             float64
residual sugar          float64
chlorides               float64
free sulfur dioxide     float64
total sulfur dioxide    float64
density                 float64
pH                      float64
sulphates               float64
alcohol                 float64
dtype: object
```

In [8]:
```
y.dtypes
```

Out[8]:
```
quality    int64
dtype: object
```

In [9]:
```
test_size = 0.2
state = 42
xTrain, xTest, yTrain, yTest = train_test_split(X, y, test_size=test_size, random_state=state)
len(xTrain), len(xTest), len(yTrain), len(yTest)
```

Out[9]:
```
(1279, 320, 1279, 320)
```

Обучение модели на произвольном гиперпараметре K

In [10]:
```
# quality имеет целочисленные значения от 0 до 10 включительно (на самом деле 6). Используем Classifier
from sklearn.neighbors import KNeighborsClassifier
print('Кол-во классов:', len(data['quality'].unique()))
```

```
Кол-во классов: 6
```

In [11]:
```
# обучим модель для произвольно заданного гиперпараметра K
K_value = 3
KNeighborsClassifierObj = KNeighborsClassifier(n_neighbors=K_value)
KNeighborsClassifierObj.fit(xTrain, yTrain.values.ravel())
```

Out[11]:
```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                     metric_params=None, n_jobs=None, n_neighbors=3, p=2,
                     weights='uniform')
```

In [12]:
```
yPredictedTest = KNeighborsClassifierObj.predict(xTest)
yPredictedTest
```

Out[12]:
```
array([6, 5, 6, 5, 6, 5, 5, 5, 6, 6, 8, 5, 6, 6, 6, 7, 6, 5, 7, 5, 4, 5,
       5, 5, 5, 5, 7, 5, 5, 6, 5, 5, 5, 6, 5, 5, 6, 6, 6, 5, 6, 5, 6, 5,
       6, 6, 6, 6, 5, 4, 5, 5, 5, 7, 4, 6, 6, 7, 6, 5, 5, 8, 6, 5, 6, 6,
       7, 5, 5, 5, 5, 5, 6, 5, 6, 5, 5, 5, 5, 5, 5, 7, 5, 5, 6, 5, 5, 6,
       6, 4, 5, 5, 5, 6, 5, 6, 5, 4, 5, 5, 5, 5, 6, 7, 6, 6, 6, 6, 5, 5,
       6, 5, 7, 5, 6, 6, 5, 5, 5, 7, 5, 6, 7, 5, 5, 6, 6, 6, 5, 6, 6, 6,
       5, 7, 4, 5, 6, 6, 4, 6, 5, 5, 7, 6, 6, 5, 6, 7, 5, 5, 6, 6, 5, 5,
       6, 6, 5, 4, 6, 5, 7, 5, 5, 5, 6, 6, 6, 5, 5, 5, 6, 5, 7, 6, 5, 5,
       4, 4, 5, 7, 6, 5, 5, 6, 5, 5, 6, 6, 7, 6, 6, 6, 6, 7, 4, 5, 6, 5,
       3, 6, 5, 5, 5, 6, 7, 6, 5, 5, 4, 5, 7, 5, 6, 7, 6, 5, 5, 6, 5, 5,
       6, 5, 6, 6, 6, 6, 5, 6, 5, 5, 5, 5, 7, 4, 5, 6, 5, 6, 5, 5, 7, 5,
       5, 5, 6, 7, 5, 5, 7, 5, 6, 5, 5, 6, 6, 5, 6, 6, 8, 6, 6, 6, 4, 7,
       6, 6, 5, 5, 6, 6, 6, 4, 6, 6, 5, 5, 6, 7, 5, 6, 5, 6, 5, 5, 5, 6,
       5, 5, 6, 6, 5, 6, 5, 6, 5, 5, 5, 6, 5, 5, 5, 5, 6, 7, 5, 5, 6, 4,
       6, 7, 5, 5, 5, 5, 6, 6, 5, 5, 5, 6])
```

In [13]:
```
yPredictedTrain = KNeighborsClassifierObj.predict(xTrain)
yPredictedTrain
```

Out[13]:
```
array([6, 5, 6, ..., 5, 6, 7])
```

In [14]:
```
yTest['quality'].values
```

Out[14]:
```
array([6, 5, 6, 5, 6, 5, 5, 5, 5, 6, 7, 3, 5, 5, 6, 7, 5, 7, 8, 5, 5, 6,
       5, 6, 6, 6, 7, 6, 5, 6, 5, 5, 6, 5, 6, 5, 7, 5, 4, 6, 5, 5, 7, 5,
       5, 6, 7, 6, 5, 6, 5, 5, 5, 7, 6, 6, 6, 5, 5, 5, 5, 7, 5, 6, 6, 5,
       6, 5, 6, 5, 6, 4, 6, 6, 6, 5, 8, 5, 6, 6, 5, 6, 5, 6, 6, 7, 5, 6,
       7, 4, 7, 6, 5, 5, 5, 6, 5, 6, 5, 6, 5, 5, 5, 7, 6, 7, 6, 5, 6, 5,
       8, 5, 6, 5, 6, 7, 6, 6, 5, 6, 6, 6, 6, 6, 6, 6, 7, 6, 5, 5, 6, 5,
       5, 5, 6, 5, 5, 5, 5, 6, 7, 6, 8, 5, 5, 5, 6, 6, 6, 5, 6, 7, 6, 5,
       6, 5, 5, 6, 6, 6, 7, 5, 7, 5, 5, 5, 6, 6, 5, 5, 6, 5, 7, 6, 7, 6,
       6, 5, 5, 6, 4, 6, 5, 7, 5, 5, 4, 5, 7, 6, 5, 6, 6, 7, 6, 5, 5, 6,
       5, 7, 5, 6, 6, 5, 7, 5, 5, 5, 6, 7, 7, 5, 5, 6, 6, 7, 6, 5, 6, 6,
       6, 6, 6, 7, 4, 5, 5, 7, 5, 5, 5, 5, 6, 6, 5, 7, 5, 6, 6, 6, 5, 4,
       6, 7, 6, 7, 5, 6, 6, 5, 5, 6, 5, 6, 4, 5, 6, 6, 5, 6, 6, 5, 5, 6,
       7, 7, 6, 5, 6, 6, 5, 6, 5, 6, 5, 5, 5, 6, 6, 6, 7, 5, 5, 6, 5, 7,
       5, 6, 4, 6, 6, 8, 6, 5, 5, 6, 5, 7, 6, 6, 5, 5, 7, 6, 6, 5, 6, 6,
       5, 7, 6, 6, 6, 6, 5, 6, 5, 5, 6, 4])
```

In [15]:
```
# оценим качество модели классификации
from sklearn.metrics import accuracy_score, confusion_matrix, precision_score, f1_score

print('Accuracy (train): {} %'.format(accuracy_score(yTrain, yPredictedTrain) * 100))
print('Accuracy (test): {} %'.format(accuracy_score(yTest, yPredictedTest) * 100))
```

```
Accuracy (train): 74.12040656763097 %
Accuracy (test): 45.3125 %
```

In [16]:
```
print('Матрица ошибок: столбцы — предсказанное значение, строки — истинное значение')
print('Train\n', confusion_matrix(yTrain, yPredictedTrain))
print('Test\n', confusion_matrix(yTest, yPredictedTest))
```

```
Матрица ошибок: столбцы — предсказанное значение, строки — истинное значение
Train
 [[  8   0   1   0   0   0]
 [  3  15  16   8   1   0]
 [  0  14 464  70   3   0]
 [  1  12 109 366  17   1]
 [  1   5  27  30  93   1]
 [  0   1   4   4   2   2]]
Test
 [[ 0  0  1  0  0  0]
 [ 0  1  2  7  0  0]
 [ 1  4 81 40  3  1]
 [ 0 11 57 51 13  0]
 [ 0  0 10 18 12  2]
 [ 0  0  1  2  2  0]]
```

In [17]:
```
print('Train\n', precision_score(yTrain, yPredictedTrain, average='weighted'))
print('Test\n', precision_score(yTest, yPredictedTest, average='weighted'))
```

```
Train
 0.7433691543962138
Test
 0.44922551014719003
```

In [18]:
```
print('Train\n', f1_score(yTrain, yPredictedTrain, average='weighted'))
print('Test\n', f1_score(yTest, yPredictedTest, average='weighted'))
```

```
Train
 0.7377685441292957
Test
 0.4478315057283142
```

качество оставляет желать лучшего

Оценим качество с использованием *кросс-валидации*

In [19]:
```
from sklearn.model_selection import cross_val_score, cross_validate
# автоматически выбирается стратегия
scores = cross_val_score(KNeighborsClassifierObj, X, y.values.ravel(), cv=3)  # 3 фолда
scores  # accuracy by default
```

Out[19]:
```
array([0.4635514 , 0.42401501, 0.38229755])
```

In [20]:
```
np.mean(scores)
```

Out[20]:
```
0.4232879876796997
```

In [21]:
```
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, X, y.values.ravel(), scoring=scoring, cv=3, return_train_sco
re=True)
scores
```

```
/Users/artyom.andreev/Study/.venv/lib/python3.7/site-packages/sklearn/metrics/classification.py:1143: Undefi
nedMetricWarning: Precision is ill-defined and being set to 0.0 in labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
/Users/artyom.andreev/Study/.venv/lib/python3.7/site-packages/sklearn/metrics/classification.py:1143: Undefi
nedMetricWarning: F-score is ill-defined and being set to 0.0 in labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
/Users/artyom.andreev/Study/.venv/lib/python3.7/site-packages/sklearn/metrics/classification.py:1143: Undefi
nedMetricWarning: Precision is ill-defined and being set to 0.0 in labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
/Users/artyom.andreev/Study/.venv/lib/python3.7/site-packages/sklearn/metrics/classification.py:1143: Undefi
nedMetricWarning: F-score is ill-defined and being set to 0.0 in labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
```

Out[21]:
```
{'fit_time': array([0.00234604, 0.00160694, 0.00212288]),
 'score_time': array([0.05179119, 0.04728293, 0.04403687]),
 'test_precision': array([0.45371836, 0.41355857, 0.38212618]),
 'train_precision': array([0.75838617, 0.73362752, 0.76695829]),
 'test_recall': array([0.4635514 , 0.42401501, 0.38229755]),
 'train_recall': array([0.75657895, 0.74202627, 0.76872659]),
 'test_f1': array([0.44416531, 0.41751315, 0.37968412]),
 'train_f1': array([0.75435552, 0.73580897, 0.76481946])}
```

In [22]:
```
# Попробуем различные стратегии кросс-валидации
```

In [23]:
```
# 1) K-fold
from sklearn.model_selection import KFold
scores = cross_val_score(KNeighborsClassifierObj, X, y.values.ravel(), cv=KFold(n_splits=12))
scores
```

Out[23]:
```
array([0.57462687, 0.51492537, 0.41791045, 0.47368421, 0.45112782,
       0.56390977, 0.36090226, 0.27819549, 0.38345865, 0.31578947,
       0.36842105, 0.4962406 ])
```

In [24]:
```
np.mean(scores)
```

Out[24]:
```
0.4332660008229529
```

In [25]:
```
import warnings
warnings.filterwarnings("ignore")
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, X, y.values.ravel(), scoring=scoring, cv=KFold(n_splits=12),
return_train_score=True)
scores
```

Out[25]:
```
{'fit_time': array([0.00311399, 0.00163817, 0.00166607, 0.0016489 , 0.00195003,
        0.00162411, 0.00163603, 0.00163603, 0.00167012, 0.00169396,
        0.00176001, 0.00165486]),
 'score_time': array([0.01807165, 0.01277804, 0.01297998, 0.02003312, 0.01504779,
        0.01295805, 0.01273513, 0.01311803, 0.01537585, 0.01284575,
        0.01283503, 0.01267815]),
 'test_precision': array([0.54795758, 0.45864117, 0.44446117, 0.46288116, 0.46474052,
        0.57842938, 0.36485284, 0.33095317, 0.43917689, 0.30308986,
        0.36386895, 0.51856484]),
 'train_precision': array([0.75888839, 0.74756499, 0.75879577, 0.74220849, 0.74908284,
        0.74108407, 0.76002248, 0.75521553, 0.7492982 , 0.75575271,
        0.75141529, 0.75360119]),
 'test_recall': array([0.57462687, 0.51492537, 0.41791045, 0.47368421, 0.45112782,
        0.56390977, 0.36090226, 0.27819549, 0.38345865, 0.31578947,
        0.36842105, 0.4962406 ]),
 'train_recall': array([0.75972696, 0.74880546, 0.76109215, 0.74829468, 0.75102319,
        0.74351978, 0.7633015 , 0.75579809, 0.75102319, 0.75716235,
        0.75306958, 0.75648022]),
 'test_f1': array([0.56085392, 0.47780696, 0.42727506, 0.46691705, 0.45773251,
        0.56945078, 0.34749188, 0.28744032, 0.39043245, 0.3060682 ,
        0.36398584, 0.50176834]),
 'train_f1': array([0.75614053, 0.74510228, 0.75676104, 0.74282655, 0.74680767,
        0.73865275, 0.75896004, 0.75132209, 0.74709044, 0.75328954,
        0.74868941, 0.7516    ])}
```

In [26]:
```
# 2) ShuffleSplit
from sklearn.model_selection import ShuffleSplit
scores = cross_val_score(KNeighborsClassifierObj, X, y.values.ravel(), cv=ShuffleSplit(n_splits=12, test_size
=0.2))
scores
```

Out[26]:
```
array([0.48125 , 0.484375, 0.496875, 0.50625 , 0.5375  , 0.496875,
       0.475   , 0.5375  , 0.5     , 0.490625, 0.5125  , 0.45625 ])
```

In [27]:
```
np.mean(scores)
```

Out[27]:
```
0.4979166666666666
```

In [28]:
```
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, X, y.values.ravel(), scoring=scoring, cv=ShuffleSplit(n_splits=12, test_size=0.2), return_train_score=True)
scores
```

Out[28]:
```
{'fit_time': array([0.00483608, 0.00173998, 0.00169802, 0.00152802, 0.00154281,
        0.00161099, 0.00154805, 0.00161314, 0.00155735, 0.00182295,
        0.00151014, 0.00193   ]),
 'score_time': array([0.03395581, 0.02847791, 0.02867103, 0.02507496, 0.025419  ,
        0.02515411, 0.02548289, 0.02572799, 0.02603269, 0.02527618,
        0.02530003, 0.03058004]),
 'test_precision': array([0.50027396, 0.48993412, 0.53625678, 0.46816591, 0.50789372,
        0.48495138, 0.53453958, 0.49157191, 0.51932948, 0.48270354,
        0.50674642, 0.44517754]),
 'train_precision': array([0.73477805, 0.73502993, 0.74046874, 0.73166586, 0.75345453,
        0.75179927, 0.73666561, 0.74540789, 0.7364081 , 0.72409601,
        0.74274148, 0.74512196]),
 'test_recall': array([0.5     , 0.496875, 0.528125, 0.471875, 0.503125, 0.49375 ,
        0.5375  , 0.503125, 0.525   , 0.503125, 0.496875, 0.459375]),
 'train_recall': array([0.7404222 , 0.73807662, 0.73338546, 0.7365129 , 0.74902267,
        0.74980453, 0.73416732, 0.74354965, 0.73729476, 0.73025801,
        0.73885848, 0.74745895]),
 'test_f1': array([0.49572049, 0.49330035, 0.53013501, 0.45797217, 0.50152362,
        0.48859339, 0.52915093, 0.49484982, 0.5179659 , 0.48987322,
        0.49705098, 0.44602371]),
 'train_f1': array([0.73440278, 0.73419772, 0.73000969, 0.73164122, 0.74789842,
        0.74779044, 0.73053053, 0.74067687, 0.73429997, 0.72509098,
        0.73595374, 0.74346027])}
```

In [29]:
```
# 3) RepeatedKFold
from sklearn.model_selection import RepeatedKFold
scores = cross_val_score(KNeighborsClassifierObj, X, y.values.ravel(), cv=RepeatedKFold(n_splits=12, n_repeat
s=2))
scores
```

Out[29]:
```
array([0.53731343, 0.59701493, 0.49253731, 0.44360902, 0.52631579,
       0.48120301, 0.56390977, 0.47368421, 0.5037594 , 0.60902256,
       0.44360902, 0.51879699, 0.53731343, 0.52985075, 0.50746269,
       0.5112782 , 0.53383459, 0.42857143, 0.45864662, 0.52631579,
       0.56390977, 0.4887218 , 0.56390977, 0.53383459])
```

In [30]:
```
np.mean(scores)
```

Out[30]:
```
0.5156010361725208
```

In [31]:
```
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, X, y.values.ravel(), scoring=scoring, cv=RepeatedKFold(n_spl
its=12, n_repeats=2), return_train_score=True)
scores
```

Out[31]:

```
{'fit_time': array([0.00366402, 0.00231385, 0.00170398, 0.00156426, 0.00163507,
       0.00149918, 0.001719  , 0.00172305, 0.00169086, 0.00154781,
       0.00151396, 0.00155997, 0.00153923, 0.00152588, 0.00154114,
       0.00168681, 0.00154996, 0.00152397, 0.001652  , 0.00163102,
       0.00165892, 0.0015099 , 0.00158596, 0.00158691]),
 'score_time': array([0.01764894, 0.01748037, 0.0125711 , 0.01268482, 0.01247811,
       0.01261473, 0.01392102, 0.01424384, 0.01279306, 0.01244807,
       0.01275396, 0.01259232, 0.01287484, 0.01264906, 0.01368499,
       0.01262212, 0.01244903, 0.01229215, 0.01441789, 0.01256704,
       0.01260018, 0.01313305, 0.01411104, 0.01246119]),
 'test_precision': array([0.59021476, 0.50674804, 0.50396235, 0.4761139 , 0.47961535,
       0.53571468, 0.5376912 , 0.44268718, 0.5683527 , 0.53032048,
       0.55129544, 0.50481781, 0.48771708, 0.50925415, 0.53971808,
       0.53585591, 0.51904771, 0.48257422, 0.50786582, 0.48876679,
       0.47982167, 0.49292162, 0.57956108, 0.57213148]),
 'train_precision': array([0.75393492, 0.7452139 , 0.75226825, 0.74596184, 0.74561895,
       0.76135916, 0.74583512, 0.74690259, 0.74933892, 0.74190375,
       0.75067427, 0.75778509, 0.75067154, 0.75074637, 0.74840578,
       0.75728266, 0.75095983, 0.74679527, 0.74028282, 0.74621629,
       0.74865586, 0.7550299 , 0.74886829, 0.73800867]),
 'test_recall': array([0.53731343, 0.50746269, 0.5       , 0.46616541, 0.47368421,
       0.55639098, 0.54135338, 0.44360902, 0.55639098, 0.53383459,
       0.53383459, 0.51879699, 0.49253731, 0.52238806, 0.52238806,
       0.53383459, 0.4962406 , 0.4887218 , 0.51879699, 0.51879699,
       0.48120301, 0.5037594 , 0.56390977, 0.55639098]),
 'train_recall': array([0.75494881, 0.75085324, 0.75290102, 0.74556617, 0.74693042,
       0.75716235, 0.74556617, 0.74761255, 0.75170532, 0.74215553,
       0.75306958, 0.75511596, 0.75153584, 0.75221843, 0.75017065,
       0.75648022, 0.75238745, 0.74693042, 0.74693042, 0.75238745,
       0.74829468, 0.7585266 , 0.75034106, 0.73806276]),
 'test_f1': array([0.53599349, 0.49833054, 0.49431945, 0.47085686, 0.46513048,
       0.53517011, 0.52733707, 0.44215581, 0.55627343, 0.52906589,
       0.53059412, 0.50524834, 0.48587007, 0.51362311, 0.52775955,
       0.52236987, 0.4980235 , 0.48105271, 0.51143039, 0.5022196 ,
       0.4761986 , 0.49427739, 0.56911375, 0.55369479]),
 'train_f1': array([0.7501476 , 0.74544578, 0.7485189 , 0.7422911 , 0.74247865,
       0.75417334, 0.7417451 , 0.74405862, 0.74652516, 0.73847935,
       0.74884735, 0.74955797, 0.74769256, 0.74766462, 0.74564042,
       0.75316421, 0.74787142, 0.7423968 , 0.74112355, 0.74687262,
       0.74493458, 0.75340032, 0.74539455, 0.73464243])}
```

Подбор гиперпараметра K с использованием GridSearchCV и кросс-валидации

In [32]:
```
from sklearn.model_selection import GridSearchCV
parameters = [{'n_neighbors': np.array(range(1, 51))}]
clf_gs = GridSearchCV(KNeighborsClassifier(), parameters, cv=KFold(n_splits=100), scoring='accuracy',
                      n_jobs=-1,
                      verbose=10
                     )
clf_gs.fit(X, y.values.ravel())
```

```
Fitting 100 folds for each of 50 candidates, totalling 5000 fits
```

```
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=-1)]: Done   2 tasks      | elapsed:    1.2s
[Parallel(n_jobs=-1)]: Done   9 tasks      | elapsed:    1.3s
[Parallel(n_jobs=-1)]: Done  16 tasks      | elapsed:    1.3s
[Parallel(n_jobs=-1)]: Done  25 tasks      | elapsed:    1.4s
[Parallel(n_jobs=-1)]: Batch computation too fast (0.1972s.) Setting batch_size=2.
[Parallel(n_jobs=-1)]: Done  34 tasks      | elapsed:    1.5s
[Parallel(n_jobs=-1)]: Done  45 tasks      | elapsed:    1.6s
[Parallel(n_jobs=-1)]: Done  65 tasks      | elapsed:    1.9s
[Parallel(n_jobs=-1)]: Done  91 tasks      | elapsed:    2.1s
[Parallel(n_jobs=-1)]: Done 117 tasks      | elapsed:    2.4s
[Parallel(n_jobs=-1)]: Done 147 tasks      | elapsed:    2.8s
[Parallel(n_jobs=-1)]: Done 177 tasks      | elapsed:    3.1s
[Parallel(n_jobs=-1)]: Done 211 tasks      | elapsed:    3.5s
[Parallel(n_jobs=-1)]: Done 245 tasks      | elapsed:    3.9s
[Parallel(n_jobs=-1)]: Done 283 tasks      | elapsed:    4.3s
[Parallel(n_jobs=-1)]: Done 321 tasks      | elapsed:    4.8s
[Parallel(n_jobs=-1)]: Done 363 tasks      | elapsed:    5.3s
[Parallel(n_jobs=-1)]: Done 405 tasks      | elapsed:    5.8s
[Parallel(n_jobs=-1)]: Done 451 tasks      | elapsed:    6.3s
[Parallel(n_jobs=-1)]: Done 497 tasks      | elapsed:    6.8s
[Parallel(n_jobs=-1)]: Done 547 tasks      | elapsed:    7.4s
[Parallel(n_jobs=-1)]: Done 597 tasks      | elapsed:    7.9s
[Parallel(n_jobs=-1)]: Done 651 tasks      | elapsed:    8.6s
[Parallel(n_jobs=-1)]: Done 705 tasks      | elapsed:    9.3s
[Parallel(n_jobs=-1)]: Done 763 tasks      | elapsed:   10.0s
[Parallel(n_jobs=-1)]: Done 821 tasks      | elapsed:   10.7s
[Parallel(n_jobs=-1)]: Done 883 tasks      | elapsed:   11.4s
[Parallel(n_jobs=-1)]: Done 945 tasks      | elapsed:   12.3s
[Parallel(n_jobs=-1)]: Done 1011 tasks      | elapsed:   13.1s
[Parallel(n_jobs=-1)]: Done 1077 tasks      | elapsed:   13.9s
[Parallel(n_jobs=-1)]: Done 1147 tasks      | elapsed:   14.8s
[Parallel(n_jobs=-1)]: Done 1217 tasks      | elapsed:   15.6s
[Parallel(n_jobs=-1)]: Done 1291 tasks      | elapsed:   16.5s
[Parallel(n_jobs=-1)]: Done 1365 tasks      | elapsed:   17.3s
[Parallel(n_jobs=-1)]: Done 1443 tasks      | elapsed:   18.3s
[Parallel(n_jobs=-1)]: Done 1521 tasks      | elapsed:   19.2s
[Parallel(n_jobs=-1)]: Done 1603 tasks      | elapsed:   20.2s
[Parallel(n_jobs=-1)]: Done 1685 tasks      | elapsed:   21.2s
[Parallel(n_jobs=-1)]: Done 1771 tasks      | elapsed:   22.4s
[Parallel(n_jobs=-1)]: Done 1857 tasks      | elapsed:   23.6s
```

```
[Parallel(n_jobs=-1)]: Done 1947 tasks      | elapsed:   25.1s
[Parallel(n_jobs=-1)]: Done 2037 tasks      | elapsed:   26.4s
[Parallel(n_jobs=-1)]: Done 2131 tasks      | elapsed:   27.6s
[Parallel(n_jobs=-1)]: Done 2225 tasks      | elapsed:   28.8s
[Parallel(n_jobs=-1)]: Done 2323 tasks      | elapsed:   30.2s
[Parallel(n_jobs=-1)]: Done 2421 tasks      | elapsed:   31.7s
[Parallel(n_jobs=-1)]: Done 2523 tasks      | elapsed:   33.1s
[Parallel(n_jobs=-1)]: Done 2625 tasks      | elapsed:   34.6s
[Parallel(n_jobs=-1)]: Done 2731 tasks      | elapsed:   36.2s
[Parallel(n_jobs=-1)]: Done 2837 tasks      | elapsed:   37.7s
[Parallel(n_jobs=-1)]: Done 2947 tasks      | elapsed:   39.2s
[Parallel(n_jobs=-1)]: Done 3057 tasks      | elapsed:   40.7s
[Parallel(n_jobs=-1)]: Done 3171 tasks      | elapsed:   42.8s
[Parallel(n_jobs=-1)]: Done 3285 tasks      | elapsed:   44.7s
[Parallel(n_jobs=-1)]: Done 3403 tasks      | elapsed:   46.4s
[Parallel(n_jobs=-1)]: Done 3521 tasks      | elapsed:   48.5s
[Parallel(n_jobs=-1)]: Done 3643 tasks      | elapsed:   50.2s
[Parallel(n_jobs=-1)]: Done 3765 tasks      | elapsed:   52.0s
[Parallel(n_jobs=-1)]: Done 3891 tasks      | elapsed:   53.9s
[Parallel(n_jobs=-1)]: Done 4017 tasks      | elapsed:   56.3s
[Parallel(n_jobs=-1)]: Done 4147 tasks      | elapsed:   58.3s
[Parallel(n_jobs=-1)]: Done 4277 tasks      | elapsed:  1.0min
[Parallel(n_jobs=-1)]: Done 4411 tasks      | elapsed:  1.0min
[Parallel(n_jobs=-1)]: Done 4545 tasks      | elapsed:  1.1min
[Parallel(n_jobs=-1)]: Done 4683 tasks      | elapsed:  1.1min
[Parallel(n_jobs=-1)]: Done 4821 tasks      | elapsed:  1.1min
[Parallel(n_jobs=-1)]: Done 4963 tasks      | elapsed:  1.2min
[Parallel(n_jobs=-1)]: Done 4985 out of 5000 | elapsed:  1.2min remaining:    0.2s
[Parallel(n_jobs=-1)]: Done 5000 out of 5000 | elapsed:  1.2min finished
```

Out[32]:
```
GridSearchCV(cv=KFold(n_splits=100, random_state=None, shuffle=False),
       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'),
       fit_params=None, iid='warn', n_jobs=-1,
       param_grid=[{'n_neighbors': array([ 1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 1
7,
       18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34,
       35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
       scoring='accuracy', verbose=10)
```

In [33]:
```
clf_gs.best_estimator_
```

Out[33]:
```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
           metric_params=None, n_jobs=None, n_neighbors=42, p=2,
           weights='uniform')
```

In [34]:
```
clf_gs.best_score_
```

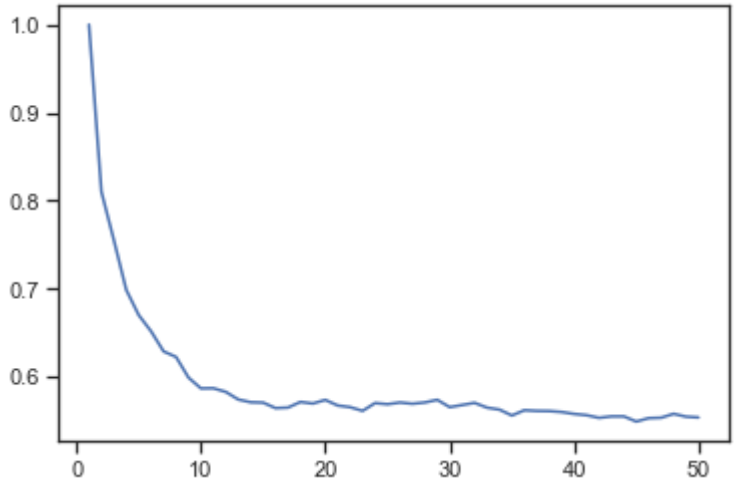
Out[34]:
```
0.5190744215134458
```

In [35]:
```
clf_gs.best_params_
```

Out[35]:
```
{'n_neighbors': 42}
```

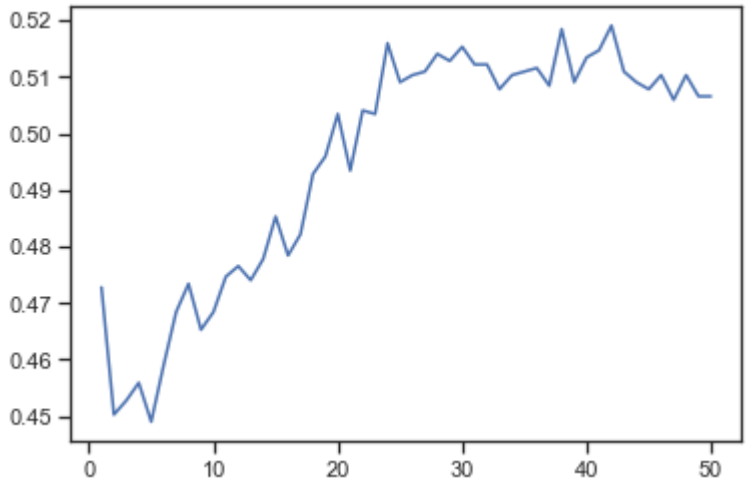
In [36]:
```
plt.plot(range(1, 51), clf_gs.cv_results_['mean_train_score'])
```

Out[36]:
```
[<matplotlib.lines.Line2D at 0x10ae5ddd8>]
```



In [37]:
```
plt.plot(range(1, 51), clf_gs.cv_results_['mean_test_score'])
```

Out[37]:
```
[<matplotlib.lines.Line2D at 0x10a162e48>]
```



Значение Accuracy выросло, оптимальный K = 42.

Повторим для выборок X и y.

In [38]:
```
clf_gs.best_estimator_.fit(xTrain, yTrain.values.ravel())

yPredictedTrainNew = clf_gs.best_estimator_.predict(xTrain)
yPredictedTestNew = clf_gs.best_estimator_.predict(xTest)

print('Accuracy (train): {} %'.format(accuracy_score(yTrain, yPredictedTrain) * 100))
print('Accuracy (test): {} %'.format(accuracy_score(yTest, yPredictedTest) * 100))

print('New accuracy (train): {} %'.format(accuracy_score(yTrain, yPredictedTrainNew) * 100))
print('New accuracy (test): {} %'.format(accuracy_score(yTest, yPredictedTestNew) * 100))
```

```
Accuracy (train): 74.12040656763097 %
Accuracy (test): 45.3125 %
New accuracy (train): 55.27756059421422 %
New accuracy (test): 51.87500000000001 %
```

Кривые обучения и валидации

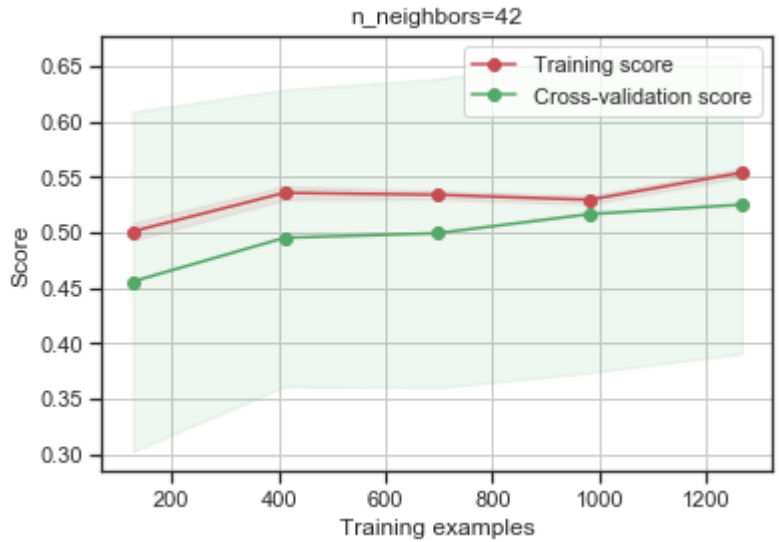
In [39]:
```
from sklearn.model_selection import learning_curve, validation_curve
```

In [40]:
```
def plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
                        n_jobs=-1, train_sizes=np.linspace(.1, 1.0, 5)):
    """
    Generate a simple plot of the test and training learning curve.

    Parameters
    ----------
    estimator : object type that implements the "fit" and "predict" methods
        An object of that type which is cloned for each validation.

    title : string
        Title for the chart.

    X : array-like, shape (n_samples, n_features)
        Training vector, where n_samples is the number of samples and
        n_features is the number of features.

    y : array-like, shape (n_samples) or (n_samples, n_features), optional
        Target relative to X for classification or regression;
        None for unsupervised learning.

    ylim : tuple, shape (ymin, ymax), optional
        Defines minimum and maximum yvalues plotted.

    cv : int, cross-validation generator or an iterable, optional
        Determines the cross-validation splitting strategy.
        Possible inputs for cv are:
          - None, to use the default 3-fold cross-validation,
          - integer, to specify the number of folds.
          - :term:`CV splitter`,
          - An iterable yielding (train, test) splits as arrays of indices.

        For integer/None inputs, if ``y`` is binary or multiclass,
        :class:`StratifiedKFold` used. If the estimator is not a classifier
        or if ``y`` is neither binary nor multiclass, :class:`KFold` is used.

        Refer :ref:`User Guide <cross_validation>` for the various
        cross-validators that can be used here.

    n_jobs : int or None, optional (default=None)
        Number of jobs to run in parallel.
```

```
        ``None`` means 1 unless in a :obj:`joblib.parallel_backend` context.
        ``-1`` means using all processors. See :term:`Glossary <n_jobs>`
        for more details.

    train_sizes : array-like, shape (n_ticks,), dtype float or int
        Relative or absolute numbers of training examples that will be used to
        generate the learning curve. If the dtype is float, it is regarded as a
        fraction of the maximum size of the training set (that is determined
        by the selected validation method), i.e. it has to be within (0, 1].
        Otherwise it is interpreted as absolute sizes of the training sets.
        Note that for classification the number of samples usually have to
        be big enough to contain at least one sample from each class.
        (default: np.linspace(0.1, 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=0.1,
                     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 [41]:
```
plot_learning_curve(clf_gs.best_estimator_, 'n_neighbors=42',
                    xTrain, yTrain.values.ravel(), cv=KFold(n_splits=100))
```

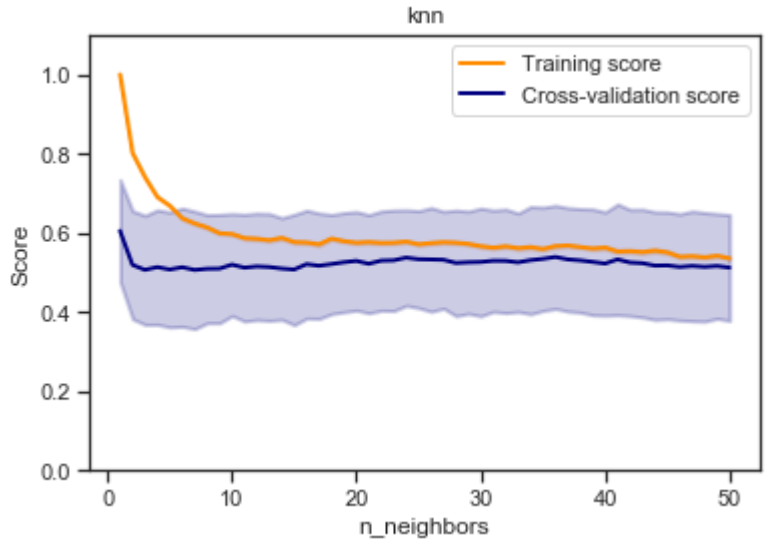
Out[41]:
```
<module 'matplotlib.pyplot' from '/Users/artyom.andreev/Study/.venv/lib/python3.7/site-packages/matplotlib/pyplot.py'>
```



In [42]:
```
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("Score")
    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=0.2,
                     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 [43]:
```
plot_validation_curve(KNeighborsClassifier(), 'knn',
                      xTrain, yTrain.values.ravel(),
                      param_name='n_neighbors', param_range=range(1, 51),
                      cv=KFold(n_splits=100), scoring="accuracy")
```

Out[43]:
```
<module 'matplotlib.pyplot' from '/Users/artyom.andreev/Study/.venv/lib/python3.7/site-packages/matplotlib/pyplot.py'>
```



In [ ]: