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Факультет «Информатика и системы управления»

Кафедра ИУ5 «Системы обработки информации и управления»

Лабораторная работа №4
по дисциплине «Технология машинного обучения» на тему:

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

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Задание:

1. Выберите набор данных (датасет) для решения задачи классификации или регресии.
2. В случае необходимости проведите удаление или заполнение пропусков и кодирование категориальных признаков.
3. С использованием метода train_test_split разделите выборку на обучающую и тестовую.
4. Обучите модель ближайших соседей для произвольно заданного гиперпараметра K. Оцените качество модели с помощью трех подходящих для задачи метрик.
5. Постройте модель и оцените качество модели с использованием кросс-валидации. Проведите эксперименты с тремя различными стратегиями кросс-валидации.
6. Произведите подбор гиперпараметра K с использованием GridSearchCV и кросс-валидации.
7. Повторите пункт 4 для найденного оптимального значения гиперпараметра K. Сравните качество полученной модели с качеством модели, полученной в пункте 4.
8. Постройте кривые обучения и валидации.

In [1]:

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

Загрузка и первичный анализ данных

In [2]:

```
data = pd.read_csv('heart.csv')
data.head()
```

Out[2]:

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	target
0	63	1	3	145	233	1	0	150	0	2.3	0	0	1	1
1	37	1	2	130	250	0	1	187	0	3.5	0	0	2	1
2	41	0	1	130	204	0	0	172	0	1.4	2	0	2	1
3	56	1	1	120	236	0	1	178	0	0.8	2	0	2	1
4	57	0	0	120	354	0	1	163	1	0.6	2	0	2	1

In [3]:

```
data.shape
```

Out[3]:

```
(303, 14)
```

In [4]:

```
data.dtypes
```

Out[4]:

```
age           int64
sex           int64
cp            int64
trestbps      int64
chol          int64
fbs           int64
restecg       int64
thalach       int64
exang         int64
oldpeak     float64
slope         int64
ca            int64
thal          int64
target        int64
dtype: object
```

In [5]:

```
data.isnull().sum()
```

Out[5]:

```
age         0
sex         0
cp          0
trestbps    0
chol        0
fbs         0
restecg     0
```

```
thalach     0
exang       0
oldpeak     0
slope       0
ca          0
thal        0
target      0
dtype: int64
```

In [6]:

```
total_count = data.shape[0]
print('Всего строк: {}'.format(total_count))
```

```
Всего строк: 303
```

In [7]:

```
import numpy as np
import pandas as pd
from typing import Dict, Tuple
from scipy import stats
from sklearn.datasets import load_iris, load_boston
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsRegressor, KNeighborsClassifier
from sklearn.metrics import accuracy_score, balanced_accuracy_score
from sklearn.metrics import precision_score, recall_score, f1_score, classification_report
from sklearn.metrics import confusion_matrix
from sklearn.metrics import mean_absolute_error, mean_squared_error, mean_squared_log_error, median_absolute_error, r2_score
from sklearn.metrics import roc_curve, roc_auc_score
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
sns.set(style="ticks")
```

In [8]:

```
target = data.target
X_train, X_test, y_train, y_test = train_test_split(
    data, target, test_size=0.2, random_state=1)
```

In [9]:

```
X_train.head()
```

Out[9]:

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	target
62	52	1	3	118	186	0	0	190	0	0.0	1	0	1	1
127	67	0	2	152	277	0	1	172	0	0.0	2	1	2	1
111	57	1	2	150	126	1	1	173	0	0.2	2	1	3	1
287	57	1	1	154	232	0	0	164	0	0.0	2	1	2	0
108	50	0	1	120	244	0	1	162	0	1.1	2	0	2	1

In [10]:

```
X_test.head()
```

Out[10]:

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	target
204	62	0	0	160	164	0	0	145	0	6.2	0	3	3	0
159	56	1	1	130	221	0	0	163	0	0.0	2	0	3	1
219	48	1	0	130	256	1	0	150	1	0.0	2	2	3	0
174	60	1	0	130	206	0	0	132	1	2.4	1	2	3	0
184	50	1	0	150	243	0	0	128	0	2.6	1	0	3	0

In [11]:

```
y_train.head()
```

Out[11]:

```
62     1
127    1
111    1
287    0
108    1
Name: target, dtype: int64
```

In [12]:

```
y_test.head()
```

Out[12]:

```
204    0
159    1
219    0
174    0
184    0
Name: target, dtype: int64
```

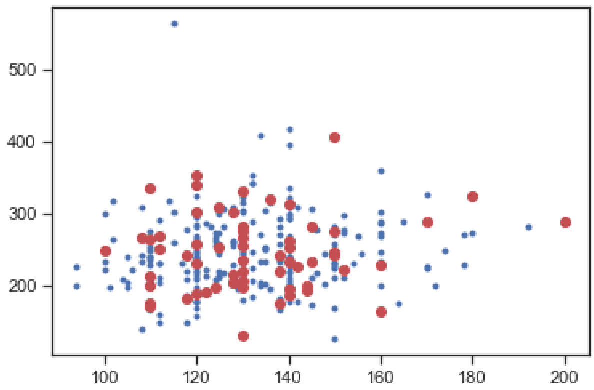
In [13]:

```
total_count_data_X_train = X_train.shape[0]
total_count_data_X_test = X_test.shape[0]
total_count_data_y_train = y_train.shape[0]
total_count_data_y_test = y_test.shape[0]
print('Всего строк train: {}, test: {} '.format(total_count_data_X_train, total_count_data_X_test))
```

Всего строк train: 242, test: 61

In [14]:

```
plt.plot(X_train['trestbps'], X_train['chol'], 'b.', \
        X_test['trestbps'], X_test['chol'], 'ro')
plt.show()
```



Фаза обучения

In [15]:

```
X_train[['trestbps','chol']]
```

Out[15]:

	trestbps	chol
62	118	186
127	152	277
111	150	126

	trestbps	chol
287	154	232
108	120	244
85	115	564
167	140	268
120	130	303
180	132	353
39	160	360
131	134	271
234	130	322
107	138	236
285	140	311
17	150	226
170	130	256
192	120	188
168	130	254
42	104	208
90	124	255
132	120	295
243	152	274
5	140	192
93	132	288
38	155	269
106	160	234
105	120	211
67	130	234
291	114	318
247	160	246
...	...	...
115	120	215
292	170	225
216	130	263
264	110	206
209	140	177
1	130	250
22	140	226
7	120	263
141	115	303
86	118	277
241	174	249
215	132	341
68	120	220
50	130	256
156	130	253
252	138	294
254	160	273
276	146	218
178	120	177
281	128	204
237	140	293
71	94	227

	trestbps	chol
129	128	269
144	140	197
133	110	235
203	180	274
255	142	309
72	130	204
235	140	299
37	150	232

242 rows × 2 columns

In [16]:

```
# первая строка тестовой выборки
data_test_0 = [x for x in X_test[['trestbps','chol']].iloc[0]]
data_test_0
```

Out[16]:

```
[160, 164]
```

In [17]:

```
from sklearn.neighbors import KNeighborsRegressor, KNeighborsClassifier
```

In [18]:

```
KNeighborsClassifierObj = KNeighborsClassifier(n_neighbors=3)
KNeighborsClassifierObj
```

Out[18]:

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

In [19]:

```
KNeighborsClassifierObj.fit(X_train[['trestbps','chol']], X_train['target'])
KNeighborsClassifierObj.predict(X_test[['trestbps','chol']])
```

Out[19]:

```
array([0, 0, 0, 1, 1, 1, 0, 1, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 0, 1, 1,
       0, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 0, 1, 0, 0, 1, 1, 1, 0, 0,
       1, 0, 1, 0, 0, 0, 1, 1, 1, 0, 0, 1, 1, 1, 0, 1, 0], dtype=int64)
```

In [20]:

```
KNeighborsRegressorObj = KNeighborsRegressor()
KNeighborsRegressorObj
```

Out[20]:

```
KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='minkowski',
          metric_params=None, n_jobs=None, n_neighbors=5, p=2,
          weights='uniform')
```

In [21]:

```
KNeighborsRegressorObj.fit(X_train[['trestbps','chol']], X_train['target'])
KNeighborsRegressorObj.predict(X_test[['trestbps','chol']])
```

Out[21]:

```
array([0.4, 0.6, 0.4, 0.8, 0.8, 0.6, 0.2, 0.6, 0.6, 0.6, 0.6, 0.6, 0.4,
       0.6, 0.6, 0.8, 0.6, 0.6, 0.8, 0.2, 0.6, 0.8, 0.4, 0.6, 0.4, 0.6,
       0.8, 0.2, 0.4, 0.6, 0.6, 0.8, 1. , 0.4, 0.4, 0.6, 0.6, 0.2, 0.4,
       0.8, 0.8, 0.8, 0.6, 0.2, 0.6, 0.2, 0.8, 0.2, 0.4, 0.2, 0.8, 1. ,
       0.8, 0.4, 0.4, 0.6, 0.8, 0.4, 0.4, 0.6, 0.4])
```

In [22]:

```
def class_proportions(array: np.ndarray) -> Dict[int, Tuple[int, float]]:
    """
    Вычисляет пропорции классов
    array - массив, содержащий метки классов
    """
    # Получение меток классов и количества меток каждого класса
    labels, counts = np.unique(array, return_counts=True)
    # Превращаем количество меток в процент их встречаемости
    # делим количество меток каждого класса на общее количество меток
    counts_perc = counts/array.size
    # Теперь sum(counts)==1.0
    # Создаем результирующий словарь,
    # ключом словаря является метка класса,
    # а значением словаря процент встречаемости метки
    res = dict()
    for label, count2 in zip(labels, zip(counts, counts_perc)):
        res[label] = count2
    return res

def print_class_proportions(array: np.ndarray):
    """
    Вывод пропорций классов
    """
    proportions = class_proportions(array)
    if len(proportions)>0:
        print('Метка \t Количество \t Процент встречаемости')
    for i in proportions:
        val, val_perc = proportions[i]
        val_perc_100 = round(val_perc * 100, 2)
        print('{} \t {} \t \t {}%'.format(i, val, val_perc_100))
```

In [23]:

```
print_class_proportions(y_train)
```

```
Метка  Количество   Процент встречаемости
0   108     44.63%
1   134     55.37%
```

In [24]:

```
print_class_proportions(y_test)
```

```
Метка  Количество   Процент встречаемости
0   30     49.18%
1   31     50.82%
```

Построим базовые модели на основе метода ближайших соседей

In [25]:

```
cl1_1 = KNeighborsClassifier(n_neighbors=2)
cl1_1.fit(X_train, y_train)
target1_1 = cl1_1.predict(X_test)
target1_1
```

Out[25]:

```
array([0, 0, 1, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 1, 0, 1, 1, 0, 1, 0,
       0, 0, 1, 1, 0, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 0, 1, 0, 0, 0,
       1, 1, 1, 0, 1, 0, 1, 1, 0, 0, 1, 1, 0, 0, 1, 0, 0], dtype=int64)
```

In [26]:

```
cl1_2 = KNeighborsClassifier(n_neighbors=10)
cl1_2.fit(X_train, y_train)
target1_2 = cl1_2.predict(X_test)
target1_2
```

Out[26]:

```
array([1, 1, 0, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 0, 1, 1, 0, 0,
       0, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1, 0, 1, 0,
       1, 1, 1, 0, 1, 0, 1, 1, 0, 0, 1, 1, 1, 0, 1, 0, 0], dtype=int64)
```

In [27]:

```
cl1_3 = KNeighborsClassifier(n_neighbors=5)
cl1_3.fit(X_train, y_train)
target1_3 = cl1_2.predict(X_test)
target1_3
```

Out[27]:

```
array([1, 1, 0, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 0, 1, 1, 0, 0,
       0, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1, 0, 1, 0,
       1, 1, 1, 0, 1, 0, 1, 1, 0, 0, 1, 1, 1, 0, 1, 0, 0], dtype=int64)
```

In [28]:

```
# 5 ближайших соседа
accuracy_score(y_test, target1_3)
```

Out[28]:

```
0.5737704918032787
```

In [29]:

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

Out[29]:

```
0.4918032786885246
```

In [30]:

```
# 10 ближайших соседа
accuracy_score(y_test, target1_2)
```

Out[30]:

```
0.5737704918032787
```

Метрики качества классификации

In [32]:

```
#процент совпадений
print_accuracy_score_for_classes(y_test, target1_1)
```

```
Метка   Accuracy
0   0.6
1   0.3870967741935484
```

In [33]:

```
# процент совпадений
print_accuracy_score_for_classes(y_test, target1_2)
```

```
Метка   Accuracy
0   0.5
1   0.6451612903225806
```

In [34]:

```
balanced_accuracy_score(y_test, target1_1)
```

Out[34]:

```
0.4935483870967742
```

In [35]:

```
balanced_accuracy_score(y_test, target1_2)
```

Out[35]:

0.5725806451612903

Матрица ошибок

In [37]:

```
confusion_matrix(y_test, target1_1, labels=[0, 1])
# 0 0 - верные 0
# 0 1 - предсказана 1 но истинное значение 0
# 1 0 - предсказан 0 но истинное значение 1
# 1 1 - верные 1
```

Out[37]:

```
array([[18, 12],
       [19, 12]], dtype=int64)
```

In [38]:

```
confusion_matrix(y_test, target1_2, labels=[0, 1])
```

Out[38]:

```
array([[15, 15],
       [11, 20]], dtype=int64)
```

In [39]:

```
# Вывод матрицы ошибок в графическом виде
# https://scikit-learn.org/stable/auto_examples/model_selection/plot_confusion_matrix.html#sphx-glr-auto-examples-model-selection-plot-confusio
n-matrix-py
from sklearn.utils.multiclass import unique_labels
def plot_confusion_matrix(y_true, y_pred, classes,
                          normalize=False,
                          title=None,
                          cmap=plt.cm.Blues):
    """
    This function prints and plots the confusion matrix.
    Normalization can be applied by setting `normalize=True`.
    """
    if not title:
        if normalize:
            title = 'Normalized confusion matrix'
        else:
            title = 'Confusion matrix, without normalization'

    # Compute confusion matrix
    cm = confusion_matrix(y_true, y_pred)
    # Only use the labels that appear in the data
    classes = classes[unique_labels(y_true, y_pred)]
    if normalize:
        cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]
        print("Normalized confusion matrix")
    else:
        print('Confusion matrix, without normalization')

    fig, ax = plt.subplots()
    im = ax.imshow(cm, interpolation='nearest', cmap=cmap)
    ax.figure.colorbar(im, ax=ax)
    # We want to show all ticks...
    ax.set(xticks=np.arange(cm.shape[1]),
           yticks=np.arange(cm.shape[0]),
           # ... and label them with the respective list entries
           xticklabels=classes, yticklabels=classes,
           title=title,
           ylabel='True label',
           xlabel='Predicted label')
```

```
    # Rotate the tick labels and set their alignment.
    plt.setp(ax.get_xticklabels(), rotation=45, ha="right",
             rotation_mode="anchor")

    # Loop over data dimensions and create text annotations.
    fmt = '.2f' if normalize else 'd'
    thresh = cm.max() / 2.
    for i in range(cm.shape[0]):
        for j in range(cm.shape[1]):
            ax.text(j, i, format(cm[i, j], fmt),
                    ha="center", va="center",
                    color="white" if cm[i, j] > thresh else "black")
    fig.tight_layout()
    return ax
```

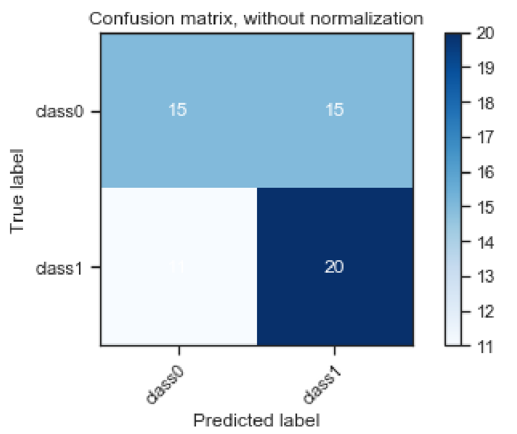
In [40]:

```
plot_confusion_matrix(y_test, target1_2,
                      classes=np.array(['class0', 'class1']),
                      title='Confusion matrix, without normalization')
```

Confusion matrix, without normalization

Out[40]:

<matplotlib.axes._subplots.AxesSubplot at 0x26d1b6c75c0>



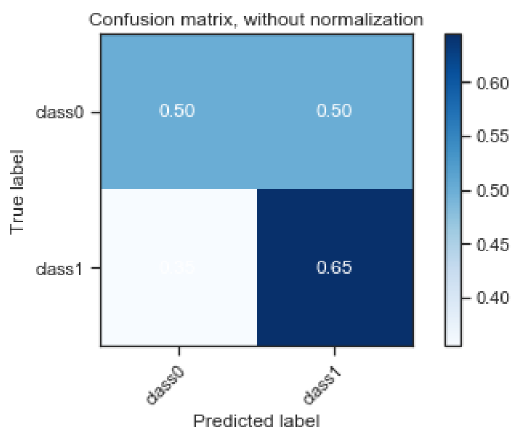
In [41]:

```
#с нормализацией
plot_confusion_matrix(y_test, target1_2,
                      classes=np.array(['class0', 'class1']),
                      normalize=True,
                      title='Confusion matrix, without normalization')
```

Normalized confusion matrix

Out[41]:

<matplotlib.axes._subplots.AxesSubplot at 0x26d1b79c710>



In [42]:

```
# По умолчанию метрики считаются для 1 класса бинарной классификации
# Для 2 ближайших соседей
# 0 0 - верные 0
# 0 1 - предсказана 1 но истинное значение 0
# 1 0 - предсказан 0 но истинное значение 1
# 1 1 - верные 1
# точность = 0 0 / (0 0 + 0 1)
# полнота = 0 0 / (0 0 + 1 0)
precision_score(y_test, target1_1), recall_score(y_test, target1_1)
```

Out[42]:

(0.5, 0.3870967741935484)

In [43]:

```
# Для 10 ближайших соседей
precision_score(y_test, target1_2), recall_score(y_test, target1_2)
```

Out[43]:

(0.5714285714285714, 0.6451612903225806)

In [44]:

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

Out[44]:

0.4918032786885246

In [45]:

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

Out[45]:

0.49324324324324326

In [46]:

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

Out[46]:

0.4933540097474524

Кросс-валидация

In [47]:

```
from IPython.display import Image
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.datasets import load_iris, load_boston
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, ShuffleSplit, StratifiedKFold
from sklearn.metrics import accuracy_score, balanced_accuracy_score
from sklearn.metrics import precision_score, recall_score, f1_score, classification_report
from sklearn.metrics import confusion_matrix
from sklearn.metrics import mean_absolute_error, mean_squared_error, mean_squared_log_error, 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 seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
sns.set(style="ticks")
```

In [48]:

```
# Значение метрики accuracy для 3 фолдов
scores = cross_val_score(KNeighborsClassifier(n_neighbors=2),
                    X_train, y_train, cv=3)
scores
```

Out[48]:

```
array([0.64197531, 0.55555556, 0.6125    ])
```

In [49]:

```
np.mean(scores)
```

Out[49]:

```
0.603343621399177
```

In [50]:

```
scoring = {'precision': 'precision_weighted',
         'recall': 'recall_weighted'}
```

In [51]:

```
scores = cross_validate(KNeighborsClassifier(n_neighbors=2),
                    X_train, y_train, scoring=scoring,
                   cv=3, return_train_score=True)
scores
```

Out[51]:

```
{'fit_time': array([0.00799656, 0.01199412, 0.01199532]),
 'score_time': array([0.05598092, 0.04798961, 0.05598402]),
 'test_precision': array([0.68808026, 0.5862069 , 0.6322695 ]),
 'test_recall': array([0.64197531, 0.55555556, 0.6125    ]),
 'train_precision': array([0.88819876, 0.86239847, 0.85744235]),
 'train_recall': array([0.85093168, 0.80124224, 0.79012346])}
```

Стратегии кросс-валидации

In [52]:

```
X = ["a", "b", "c"]
kf = KFold(n_splits=3)
for train, test in kf.split(X):
    print("%s %s" % (train, test))
```

```
[1 2] [0]
[0 2] [1]
[0 1] [2]
```

In [53]:

```
X = range(12)
kf = KFold(n_splits=3)
for train, test in kf.split(X):
    print("%s %s" % (train, test))
```

```
[ 4  5  6  7  8  9 10 11] [0 1 2 3]
[ 0  1  2  3  8  9 10 11] [4 5 6 7]
[0 1 2 3 4 5 6 7] [ 8  9 10 11]
```

In [54]:

```
scores = cross_val_score(KNeighborsClassifier(n_neighbors=2),
```

```
                  X_train, y_train,
                  cv=KFold(n_splits=3))
scores
```

Out[54]:

```
array([0.66666667, 0.58024691, 0.6375    ])
```

In [55]:

```
scores = cross_validate(KNeighborsClassifier(n_neighbors=2),
                 X_train, y_train, scoring=scoring,
                 cv=KFold(n_splits=3), return_train_score=True)
scores
```

Out[55]:

```
{'fit_time': array([0.01199579, 0.01199794, 0.00799394]),
 'score_time': array([0.06797695, 0.05198073, 0.05050278]),
 'test_precision': array([0.69753086, 0.59273784, 0.702853  ]),
 'test_recall': array([0.66666667, 0.58024691, 0.6375    ]),
 'train_precision': array([0.88601824, 0.87317784, 0.84795322]),
 'train_recall': array([0.8447205 , 0.81987578, 0.77777778])}
```

In [56]:

```
X = range(12)
# Эквивалент KFold(n_splits=n)
kf = LeaveOneOut()
for train, test in kf.split(X):
    print("%s %s" % (train, test))
```

```
[ 1  2  3  4  5  6  7  8  9 10 11] [0]
[ 0  2  3  4  5  6  7  8  9 10 11] [1]
[ 0  1  3  4  5  6  7  8  9 10 11] [2]
[ 0  1  2  4  5  6  7  8  9 10 11] [3]
[ 0  1  2  3  5  6  7  8  9 10 11] [4]
[ 0  1  2  3  4  6  7  8  9 10 11] [5]
[ 0  1  2  3  4  5  7  8  9 10 11] [6]
[ 0  1  2  3  4  5  6  8  9 10 11] [7]
[ 0  1  2  3  4  5  6  7  9 10 11] [8]
[ 0  1  2  3  4  5  6  7  8 10 11] [9]
[ 0  1  2  3  4  5  6  7  8  9 11] [10]
[ 0  1  2  3  4  5  6  7  8  9 10] [11]
```

In [57]:

```
scores = cross_val_score(KNeighborsClassifier(n_neighbors=2),
                  X_train, y_train,
                  cv=LeaveOneOut())
scores
```

Out[57]:

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

In [58]:

```
scores = cross_validate(KNeighborsClassifier(n_neighbors=2),
                 X_train, y_train, scoring=scoring,
                 cv=LeaveOneOut(), return_train_score=True)
scores
```

```
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\metrics\classification.py:1143: UndefinedMetricWarning: Precision is ill-defined and being set to 0.0 in labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\metrics\classification.py:1145: UndefinedMetricWarning: Recall is ill-defined and being set to 0.0 in labels with no true samples.
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```

```
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```

```
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  'recall', 'true', average, warn_for)
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  'precision', 'predicted', average, warn_for)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\metrics\classification.py:1145: UndefinedMetricWarning: Recall is ill-defined and being set to 0.0 in labels with no true samples.
  'recall', 'true', average, warn_for)
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In [59]:

```
X = range(12)
kf = RepeatedKFold(n_splits=3, n_repeats=2)
for train, test in kf.split(X):
    print("%s %s" % (train, test))
```

```
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[0 1 2 4 5 6 7 9] [ 3  8 10 11]
[ 0  2  3  4  7  8 10 11] [1 5 6 9]
[ 0  1  2  5  6  8  9 10] [ 3  4  7 11]
[ 1  3  4  5  6  7  9 11] [ 0  2  8 10]
```

In [60]:

```
scores = cross_val_score(KNeighborsClassifier(n_neighbors=2),
                         X_train, y_train,
                         cv=RepeatedKFold(n_splits=3, n_repeats=2))
scores
```

Out[60]:

```
array([0.62962963, 0.60493827, 0.55      , 0.60493827, 0.55555556,
       0.5875    ])
```

In [61]:

```
scores = cross_validate(KNeighborsClassifier(n_neighbors=2),
                        X_train, y_train, scoring=scoring,
                        cv=RepeatedKFold(n_splits=3, n_repeats=2), return_train_score=True)
scores
```

Out[61]:

```
{'fit_time': array([0.01199389, 0.00799465, 0.00990367, 0.00798225, 0.01199389,
        0.00799584]),
 'score_time': array([0.05598545, 0.04798555, 0.04497457, 0.05198073, 0.04798126,
        0.05198169]),
 'test_precision': array([0.62793512, 0.53847789, 0.63312369, 0.67766464, 0.59885991,
        0.67051332]),
 'test_recall': array([0.61728395, 0.51851852, 0.5625    , 0.61728395, 0.58024691,
        0.6125    ]),
 'train_precision': array([0.90400903, 0.88135378, 0.85796806, 0.85824578, 0.88179548,
        0.86093305]),
 'train_recall': array([0.8757764 , 0.83850932, 0.7962963 , 0.79503106, 0.83850932,
        0.7962963 ])}
```

Оптимизация гиперпараметров

In [62]:

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

Out[62]:

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

In [63]:

```python
clf_gs = GridSearchCV(KNeighborsClassifier(), tuned_parameters, cv=5, scoring='accuracy')
clf_gs.fit(X_train, y_train)
```

```
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\model_selection\_search.py:841: DeprecationWarning: The default of the `iid` parameter will ch
ange from True to False in version 0.22 and will be removed in 0.24. This will change numeric results when test-set sizes are unequal.
  DeprecationWarning)
```

Out[63]:

```
GridSearchCV(cv=5, 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=None,
       param_grid=[{'n_neighbors': array([ 5, 10, 15, 20, 25, 30, 35, 40, 45, 50])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
       scoring='accuracy', verbose=0)
```

In [64]:

```python
clf_gs.cv_results_
```

```
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('mean_train_score
'), which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('split0_train_score'
), which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('split1_train_score'
), which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('split2_train_score'
), which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('split3_train_score'
), which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('split4_train_score'
), which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('std_train_score'),
which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
```

Out[64]:

```
{'mean_fit_time': array([0.00959811, 0.0088809 , 0.0099956 , 0.00879827, 0.00799465,
        0.0084341 , 0.00879841, 0.0079999 , 0.0088491 , 0.0087903 ]),
 'mean_score_time': array([0.0183907 , 0.01720943, 0.01684523, 0.02079229, 0.01999383,
        0.01838856, 0.01919079, 0.01839261, 0.01718173, 0.01839061]),
 'mean_test_score': array([0.64876033, 0.59917355, 0.6322314 , 0.63636364, 0.63636364,
        0.64049587, 0.64049587, 0.62396694, 0.61983471, 0.61983471]),
 'mean_train_score': array([0.77481197, 0.72418389, 0.71492113, 0.69938783, 0.70045069,
        0.68386515, 0.68489085, 0.67251415, 0.67563359, 0.6652443 ]),
 '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}],
 'rank_test_score': array([ 1, 10,  6,  4,  4,  2,  2,  7,  8,  8]),
 'split0_test_score': array([0.67346939, 0.59183673, 0.67346939, 0.65306122, 0.65306122,
        0.67346939, 0.65306122, 0.63265306, 0.57142857, 0.65306122]),
 'split0_train_score': array([0.76165803, 0.75129534, 0.7357513 , 0.68393782, 0.69948187,
        0.67357513, 0.68911917, 0.66321244, 0.69430052, 0.66321244]),
```

```
'split1_test_score': array([0.55102041, 0.57142857, 0.57142857, 0.53061224, 0.6122449 ,
       0.6122449 , 0.6122449 , 0.57142857, 0.57142857, 0.53061224]),
 'split1_train_score': array([0.80829016, 0.73056995, 0.72020725, 0.73056995, 0.7357513 ,
       0.71502591, 0.70984456, 0.72020725, 0.70984456, 0.69430052]),
 'split2_test_score': array([0.65306122, 0.59183673, 0.6122449 , 0.6122449 , 0.63265306,
       0.6122449 , 0.6122449 , 0.59183673, 0.63265306, 0.6122449 ]),
 'split2_train_score': array([0.77202073, 0.70984456, 0.70984456, 0.68911917, 0.68911917,
       0.65803109, 0.65284974, 0.64248705, 0.64248705, 0.62176166]),
 'split3_test_score': array([0.77083333, 0.66666667, 0.75      , 0.79166667, 0.75      ,
       0.75      , 0.72916667, 0.70833333, 0.70833333, 0.66666667]),
 'split3_train_score': array([0.75773196, 0.69587629, 0.71649485, 0.69587629, 0.69072165,
       0.67525773, 0.66494845, 0.64948454, 0.64948454, 0.65463918]),
 'split4_test_score': array([0.59574468, 0.57446809, 0.55319149, 0.59574468, 0.53191489,
       0.55319149, 0.59574468, 0.61702128, 0.61702128, 0.63829787]),
 'split4_train_score': array([0.77435897, 0.73333333, 0.69230769, 0.6974359 , 0.68717949,
       0.6974359 , 0.70769231, 0.68717949, 0.68205128, 0.69230769]),
 'std_fit_time': array([1.95925716e-03, 1.54909700e-03, 1.26295895e-03, 1.60174521e-03,
       2.76812082e-06, 1.54012682e-03, 1.60048059e-03, 3.00445252e-06,
       1.57724289e-03, 1.60193761e-03]),
 'std_score_time': array([0.00196171, 0.00161872, 0.00178927, 0.00160144, 0.00252647,
       0.00230067, 0.00299268, 0.00196279, 0.0015929 , 0.00195513]),
 'std_test_score': array([0.07458736, 0.03463726, 0.07168026, 0.08685051, 0.06969305,
       0.06634816, 0.04799612, 0.04695049, 0.05037006, 0.04845921]),
 'std_train_score': array([0.01785238, 0.01932077, 0.01415242, 0.01632552, 0.01814527,
       0.02001264, 0.02273677, 0.02831331, 0.02585536, 0.02677323])}
```

In [65]:

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

Out[65]:

```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
           metric_params=None, n_jobs=None, n_neighbors=5, p=2,
           weights='uniform')
```

In [66]:

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

Out[66]:

```
0.6487603305785123
```

In [67]:

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

Out[67]:

```
{'n_neighbors': 5}
```

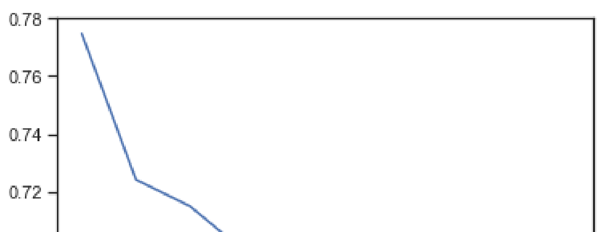
In [68]:

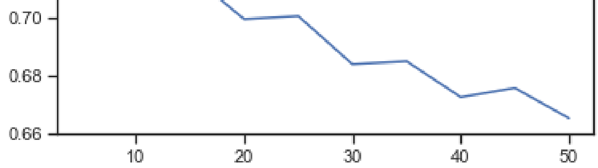
```
# Изменение качества на обучающей выборке
plt.plot(n_range, clf_gs.cv_results_['mean_train_score'])
```

```
C:\Users\cveto\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:125: FutureWarning: You are accessing a training score ('mean_train_score
'), which will not be available by default any more in 0.21. If you need training scores, please set return_train_score=True
  warnings.warn(*warn_args, **warn_kwargs)
```

Out[68]:

```
[<matplotlib.lines.Line2D at 0x26d1b7f2828>]
```



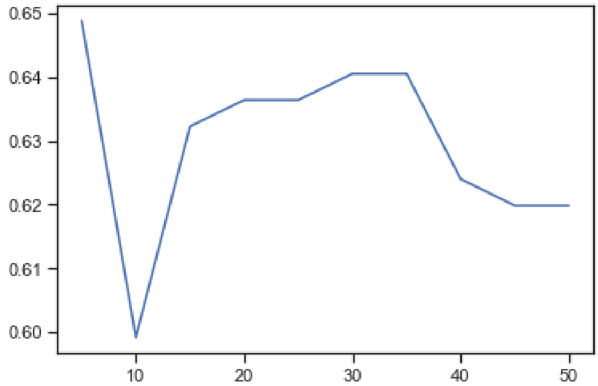


In [69]:

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

Out[69]:

[<matplotlib.lines.Line2D at 0x26d1bb299b0>]



In [70]:

```
cl1_3 = KNeighborsClassifier(n_neighbors=5)
cl1_3.fit(X_train, y_train)
target1_3 = cl1_2.predict(X_test)
target1_3
```

Out[70]:

```
array([1, 1, 0, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 0, 1, 1, 0, 0,
       0, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1, 0, 1, 0,
       1, 1, 1, 0, 1, 0, 1, 1, 0, 0, 1, 1, 1, 0, 1, 0, 0], dtype=int64)
```

In [71]:

```
accuracy_score(y_test, target1_3)
```

Out[71]:

0.5737704918032787

Построение кривых

In [72]:

```
def plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
                        n_jobs=None, 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
```

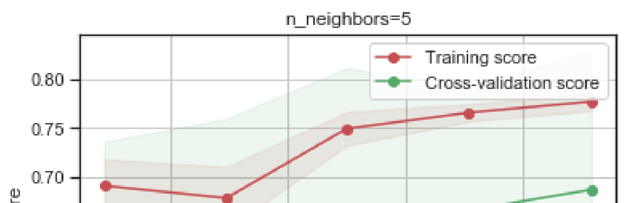
```
        Target relative to X for classification or regression;
        None for unsupervised learning.

    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
```

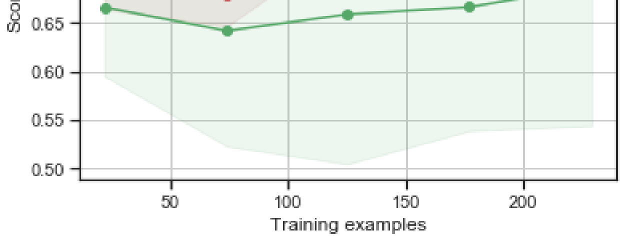
In [73]:

```
plot_learning_curve(KNeighborsClassifier(n_neighbors=5), 'n_neighbors=5',
                    X_train, y_train, cv=20)
```

Out[73]:

<module 'matplotlib.pyplot' from 'C:\\Users\\cveto\\Anaconda3\\lib\\site-packages\\matplotlib\\pyplot.py'>





In [74]:

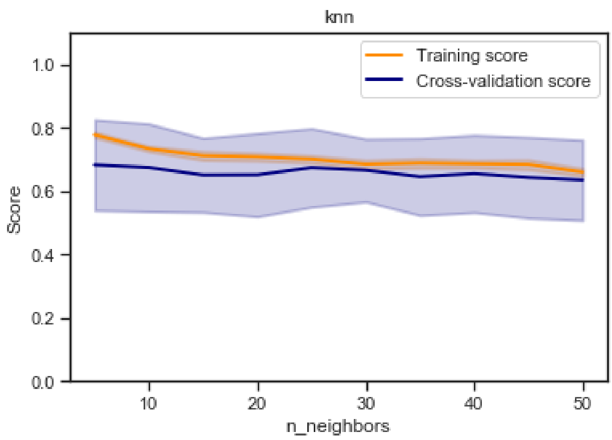
```
def plot_validation_curve(estimator, title, X, y,
                          param_name, param_range, cv,
                          scoring="accuracy"):

    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 [75]:

```
plot_validation_curve(KNeighborsClassifier(), 'knn',
                      X_train, y_train,
                      param_name='n_neighbors', param_range=n_range,
                      cv=20, scoring="accuracy")
```

Out[75]:

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



In [ ]: