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

In [1]:

```
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import accuracy_score, balanced_accuracy_score
from sklearn.metrics import precision_score, recall_score, f1_score, classification_report
from sklearn.model_selection import cross_val_score, cross_validate
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import learning_curve, validation_curve
from sklearn.model_selection import KFold, RepeatedKFold, ShuffleSplit, StratifiedKFold
%matplotlib inline
sns.set(style="ticks")
```

In [2]:

```
data=pd.read_csv('heart.csv', sep=",")
```

In [3]:

```
data.shape
```

Out[3]:

```
(303, 11)
```

In [4]:

```
data.dtypes
```

Out[4]:

```
age         int64
sex         int64
cp          int64
trestbps    int64
chol        int64
restecg     int64
thalach     int64
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
restecg     0
thalach     0
slope       0
ca          0
thal        0
target      0
dtype: int64
```

In [6]:

```
data.head()
```

Out[6]:

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

Разделение выборки на обучающую и тестовую

In [7]:

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

In [8]:

```
# Размер обучающей выборки
X_train.shape, y_train.shape
```

Out[8]:

```
((242, 11), (242,))
```

In [9]:

```
# Размер тестовой выборки
X_test.shape, y_test.shape
```

Out[9]:

```
((61, 11), (61,))
```

Построим базовые модели на основе метода ближайших соседей

In [10]:

```
simple_knn = KNeighborsClassifier(n_neighbors=2)
```

In [11]:

```
simple_knn.fit(X_train, y_train)
```

Out[11]:

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

In [12]:

```
target_1 = simple_knn.predict(X_test)
```

In [13]:

```
#оценка моделей с помощью метрик
accuracy_score(y_test, target_1), \
precision_score(y_test, target_1),  \
recall_score(y_test, target_1)
```

Out[13]:

```
(0.4918032786885246, 0.5, 0.3870967741935484)
```

Построим модели с использованием кросс-валидации

In [14]:

```
#K-fold:работает в соответствии с определпением кросс-валидации
kfold = cross_val_score(KNeighborsClassifier(),
                     data, data['target'],
                     cv=KFold(n_splits=5))
kfold
```

Out[14]:

```
array([0.47540984, 0.63934426, 0.6557377 , 0.4       , 0.31666667])
```

In [15]:

```
#ShuffleSplit: генерирует N случайных перемешиваний данных, в каждом перемешивании заданная доля помещается в тестовую выборку
shufflesplit = cross_val_score(KNeighborsClassifier(),
                     data, data['target'],
                     cv=ShuffleSplit(n_splits=5, test_size=0.2))
shufflesplit
```

Out[15]:

```
array([0.70491803, 0.72131148, 0.67213115, 0.72131148, 0.67213115])
```

In [16]:

```
#StratifiedKFold: предоставляет индексы для разделения данных, вариант KFold
stratifiedkfold = cross_val_score(KNeighborsClassifier(),
                     data, data['target'],
                     cv=StratifiedKFold(n_splits=5))
stratifiedkfold
```

Out[16]:

```
array([0.60655738, 0.6557377 , 0.57377049, 0.73333333, 0.65      ])
```

Подбор гиперпараметра K

In [17]:

```
n_range = np.array(range(1,10,1))
tuned_parameters = [{'n_neighbors': n_range}]
clf_gs = GridSearchCV(KNeighborsClassifier(), tuned_parameters,
                    cv=StratifiedKFold(n_splits=5), scoring='accuracy')
clf_gs.fit(X_train, y_train)
```

```
C:\Users\Dovlat\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[17]:

```
GridSearchCV(cv=StratifiedKFold(n_splits=5, 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=None,
       param_grid=[{'n_neighbors': array([1, 2, 3, 4, 5, 6, 7, 8, 9])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
       scoring='accuracy', verbose=0)
```

In [18]:

```
clf_gs.best_params_
```

Out[18]:

```
{'n_neighbors': 3}
```

Пункт 4 для найденного оптимального значения K

In [19]:

```
simple_knn2 = KNeighborsClassifier(n_neighbors=3)
```

In [20]:

```
simple_knn2.fit(X_train, y_train)
```

Out[20]:

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

In [21]:

```
target_2 = simple_knn2.predict(X_test)
```

In [22]:

```
accuracy_score(y_test, target_2), \
precision_score(y_test, target_2),  \
recall_score(y_test, target_2)
```

Out[22]:

```
(0.5901639344262295, 0.575, 0.7419354838709677)
```

Построить кривые обучения и валидации

In [23]:

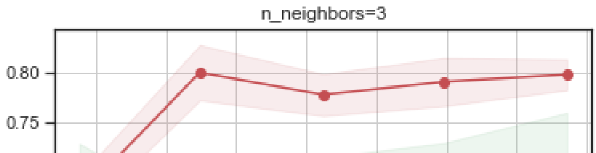
```
def plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
                        n_jobs=None, train_sizes=np.linspace(.1, 1.0, 5)):

    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=0.1,
                     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
```

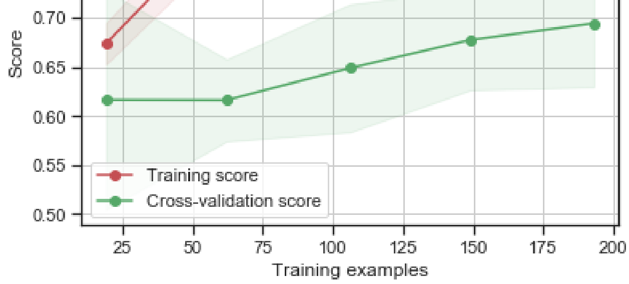
In [24]:

```
plot_learning_curve(KNeighborsClassifier(n_neighbors=3), 'n_neighbors=3',
                    X_train, y_train, cv=StratifiedKFold(n_splits=5))
```

Out[24]:

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





In [25]:

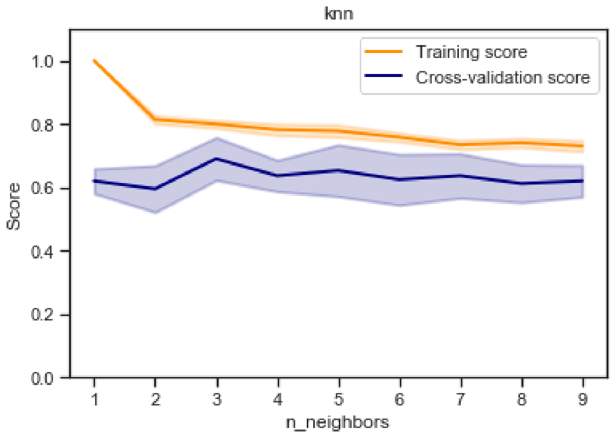
```
def plot_validation_curve(estimator, title, X, y,
                          param_name, param_range, cv,
                          scoring="accuracy"):

    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 [26]:

```
plot_validation_curve(KNeighborsClassifier(), 'knn',
                      X_train, y_train,
                      param_name='n_neighbors', param_range=n_range,
                      cv=StratifiedKFold(n_splits=5), scoring="accuracy")
```

Out[26]:

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


knn
Training score
Cross-validation score
Score
n_neighbors