Московский государственный технический университет им. Н.Э. Баумана
Кафедра «Системы обработки информации и управления»

Лабораторная работа №4 по курсу «Методы машинного обучения» на тему «Подготовка обучающей и тестовой выборки, кросс-валидация и подбор гиперпараметров на примере метода ближайших соседей»

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

data = pd.read_csv("data/Admission_Predict.csv")
data
```

Out[3]:

	Serial No.	GRE Score	TOEFL Score	University Rating	SOP	LOR	CGPA	Research	Chance of Admit
0	1	337	118	4	4.5	4.5	9.65	1	0.92
1	2	324	107	4	4.0	4.5	8.87	1	0.76
2	3	316	104	3	3.0	3.5	8.00	1	0.72
3	4	322	110	3	3.5	2.5	8.67	1	0.80
4	5	314	103	2	2.0	3.0	8.21	0	0.65
...	...	...	...	...	...	...	...	...	...
395	396	324	110	3	3.5	3.5	9.04	1	0.82
396	397	325	107	3	3.0	3.5	9.11	1	0.84
397	398	330	116	4	5.0	4.5	9.45	1	0.91
398	399	312	103	3	3.5	4.0	8.78	0	0.67
399	400	333	117	4	5.0	4.0	9.66	1	0.95

400 rows × 9 columns

```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 400 entries, 0 to 399
Data columns (total 9 columns):
 #   Column             Non-Null Count  Dtype  
---  ------             --------------  -----  
 0   Serial No.         400 non-null    int64  
 1   GRE Score          400 non-null    int64  
 2   TOEFL Score        400 non-null    int64  
 3   University Rating  400 non-null    int64  
 4   SOP                400 non-null    float64
 5   LOR                400 non-null    float64
 6   CGPA               400 non-null    float64
 7   Research           400 non-null    int64  
 8   Chance of Admit    400 non-null    float64
dtypes: float64(4), int64(5)
memory usage: 28.2 KB
```

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

```
Serial No.           0
GRE Score            0
TOEFL Score          0
University Rating    0
SOP                  0
LOR                  0
CGPA                 0
Research             0
Chance of Admit      0
dtype: int64
```

```
data.shape
```

```
(400, 9)
```

```
data.loc[data['Chance of Admit '] < 0.65, 'isAdmit'] = 0
data.loc[data['Chance of Admit '] >= 0.65, 'isAdmit'] = 1
data.isAdmit
```

```
0      1.0
1      1.0
2      1.0
3      1.0
4      1.0
      ...
395    1.0
396    1.0
397    1.0
398    1.0
399    1.0
Name: isAdmit, Length: 400, dtype: float64
```

```
np.unique(data.isAdmit)
```

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

```
target = data.iloc[:, -1]
new_data = data.iloc[:, :-2]
```

```
new_data.shape, target.shape
```

```
((400, 8), (400,))
```

```
data_X_train, data_X_test, data_y_train, data_y_test =
train_test_split(
    new_data, target, test_size=0.6, random_state=1
)
```

```
data_X_train.shape, data_X_test.shape, data_y_train.shape,
data_y_test.shape
```

```
((160, 8), (240, 8), (160,), (240,))
```

```
cl1_1 = KNeighborsClassifier(n_neighbors=50)
cl1_1.fit(data_X_train, data_y_train)
target1_0 = cl1_1.predict(data_X_train)
target1_1 = cl1_1.predict(data_X_test)
```

```
accuracy_score(data_y_train, target1_0), accuracy_score(data_y_test,
target1_1)
```

```
(0.775, 0.6791666666666667)
```

```
cl1_2 = KNeighborsClassifier(n_neighbors=15)
cl1_2.fit(data_X_train, data_y_train)
target2_0 = cl1_2.predict(data_X_train)
target2_1 = cl1_2.predict(data_X_test)
accuracy_score(data_y_train, target2_0), accuracy_score(data_y_test,
target2_1)
```

```
(0.8, 0.7416666666666667)
```

```
cl1_3 = KNeighborsClassifier(n_neighbors=3)
cl1_3.fit(data_X_train, data_y_train)
target3_0 = cl1_3.predict(data_X_train)
target3_1 = cl1_3.predict(data_X_test)
accuracy_score(data_y_train, target3_0), accuracy_score(data_y_test,
target3_1)
```

```
(0.925, 0.8416666666666667)
```

```
scores1 = cross_val_score(KNeighborsClassifier(n_neighbors=15),
                          new_data, target,
                          cv=5)
scores1, np.mean(scores1)
```

```
(array([0.3125, 0.375 , 0.725 , 0.7125, 0.7125]), 0.5675)
```

```
scores2 = cross_val_score(KNeighborsClassifier(n_neighbors=15),
                          new_data, target,
                          cv=5, scoring='jaccard')
scores2, np.mean(scores2)
```

```
(array([0.05172414, 0.32432432, 0.72151899, 0.7125    , 0.7125    ]),
 0.5045134899194261)
```

```
scores3 = cross_val_score(KNeighborsClassifier(n_neighbors=15),
                          new_data, target,
                          cv=3, scoring='f1')
scores3, np.mean(scores3)
```

```
(array([0.30088496, 0.83842795, 0.83333333]), 0.6575487455612663)
```

```
scoring = {
    'accuracy': 'accuracy',
    'jaccard': 'jaccard',
    'f1': 'f1'
}

scores = cross_validate(KNeighborsClassifier(n_neighbors=15),
                        new_data, target, scoring=scoring,
                        cv=5, return_train_score=True)
scores
```

```
{'fit_time': array([0.00293589, 0.00228405, 0.00289893, 0.00178099,
0.00226808]),
 'score_time': array([0.00762486, 0.00671482, 0.0059588 , 0.00602603,
0.00486207]),
 'test_accuracy': array([0.3125, 0.375 , 0.725 , 0.7125, 0.7125]),
 'train_accuracy': array([0.875   , 0.85    , 0.86875 , 0.896875,
0.846875]),
 'test_jaccard': array([0.05172414, 0.32432432, 0.72151899,
0.7125    , 0.7125    ]),
 'train_jaccard': array([0.84848485, 0.82222222, 0.84150943,
0.87007874, 0.82051282]),
 'test_f1': array([0.09836066, 0.48979592, 0.83823529, 0.83211679,
0.83211679]),
 'train_f1': array([0.91803279, 0.90243902, 0.91393443, 0.93052632,
0.90140845])}
```

```
%%time
scores = cross_val_score(KNeighborsClassifier(n_neighbors=15),
                         new_data, target,
                         cv=LeaveOneOut())
scores, np.mean(scores)
```

```
CPU times: user 1.29 s, sys: 6.52 ms, total: 1.29 s
Wall time: 1.3 s
```

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

```
        0., 1., 1., 0., 0., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
1., 1.,
        1., 1., 0., 1., 1., 0., 1., 1., 1., 0., 1., 1., 1., 1., 1.,
1., 1.,
        0., 1., 1., 1., 1., 1., 0., 1., 1., 1., 0., 1., 0., 1., 1.,
1., 1.,
        0., 1., 1., 1., 1., 0., 1., 1., 1., 1., 1., 1., 0., 1.,
1., 0.,
        1., 1., 1., 1., 1., 1., 1., 1., 1.]),
 0.835)
```

```
kf = KFold(n_splits=5)
scores = cross_val_score(KNeighborsClassifier(n_neighbors=10),
                         new_data, target,
                         cv=kf)
scores
```

```
array([0.625 , 0.8375, 0.85  , 0.825 , 0.675 ])
```

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

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

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

```
CPU times: user 218 ms, sys: 3.27 ms, total: 222 ms
Wall time: 221 ms
```

```
GridSearchCV(cv=5, error_score=nan,
             estimator=KNeighborsClassifier(algorithm='auto',
leaf_size=30,
```

```
                                          metric='minkowski',
                                          metric_params=None,
n_jobs=None,
                                          n_neighbors=5, p=2,
                                          weights='uniform'),
             iid='deprecated', n_jobs=None,
             param_grid=[{'n_neighbors': array([ 5, 10, 15, 20, 25,
30, 35, 40, 45, 50])}],
             pre_dispatch='2*n_jobs', refit=True,
return_train_score=False,
             scoring='accuracy', verbose=0)

clf_gs.cv_results_

{'mean_fit_time': array([0.00224361, 0.00239301, 0.00187006,
0.00147581, 0.00148458,
        0.0014236 , 0.00161104, 0.0015831 , 0.00143313, 0.00150428]),
 'std_fit_time': array([2.95497784e-04, 3.89381702e-04,
3.07080709e-05, 5.95586599e-05,
        4.83124293e-05, 4.01606171e-05, 1.48780330e-04,
1.96596150e-04,
        5.30786373e-05, 8.59239654e-05]),
 'mean_score_time': array([0.00285563, 0.00336461, 0.00227323,
0.00210838, 0.00206318,
        0.00195217, 0.00198469, 0.0020319 , 0.00205312, 0.00211654]),
 'std_score_time': array([0.00035558, 0.00097058, 0.00020221,
0.00022293, 0.00019277,
        0.00014798, 0.00010986, 0.00014462, 0.00017963, 0.00022913]),
 '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([0.78125, 0.8125 , 0.75   , 0.75   , 0.75
, 0.75   , 0.75   ,
        0.75   , 0.75   , 0.75   ]),
 'split1_test_score': array([0.84375, 0.78125, 0.8125 , 0.78125,
0.78125, 0.78125, 0.78125,
        0.78125, 0.78125, 0.78125]),
 'split2_test_score': array([0.75   , 0.84375, 0.71875, 0.8125 ,
0.78125, 0.78125, 0.78125,
        0.78125, 0.78125, 0.78125]),
 'split3_test_score': array([0.5625 , 0.5625 , 0.59375, 0.78125,
0.78125, 0.78125, 0.78125,
        0.78125, 0.78125, 0.78125]),
 'split4_test_score': array([0.78125, 0.78125, 0.78125, 0.78125,
0.78125, 0.78125, 0.78125,
        0.78125, 0.78125, 0.78125]),
 'mean_test_score': array([0.74375, 0.75625, 0.73125, 0.78125,
0.775  , 0.775  , 0.775  ,
        0.775  , 0.775  , 0.775  ]),
 'std_test_score': array([0.09560662, 0.09960861, 0.07551904,
0.01976424, 0.0125    ,
        0.0125    , 0.0125    , 0.0125    , 0.0125    , 0.0125    ]),
 'rank_test_score': array([ 9,  8, 10,  1,  2,  2,  2,  2,  2,  2],
dtype=int32)}
```

```
clf_gs.best_estimator_
```

```
KNeighborsClassifier(algorithm='auto', leaf_size=30,
metric='minkowski',
                     metric_params=None, n_jobs=None, n_neighbors=20,
p=2,
                     weights='uniform')
```

```
clf_gs.best_score_
```

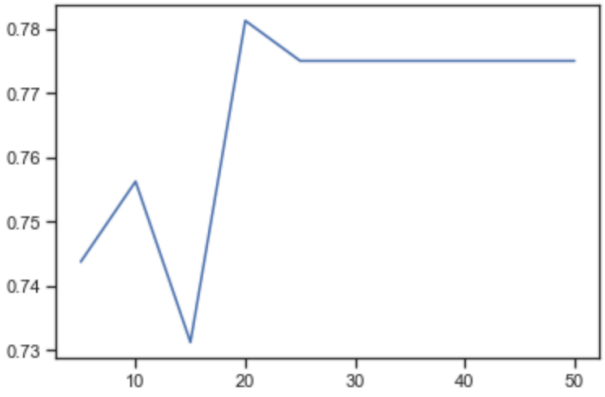
```
0.78125
```

```
clf_gs.best_params_
```

```
{'n_neighbors': 20}
```

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

Out[28]: [<matplotlib.lines.Line2D at 0x126cd6b50>]



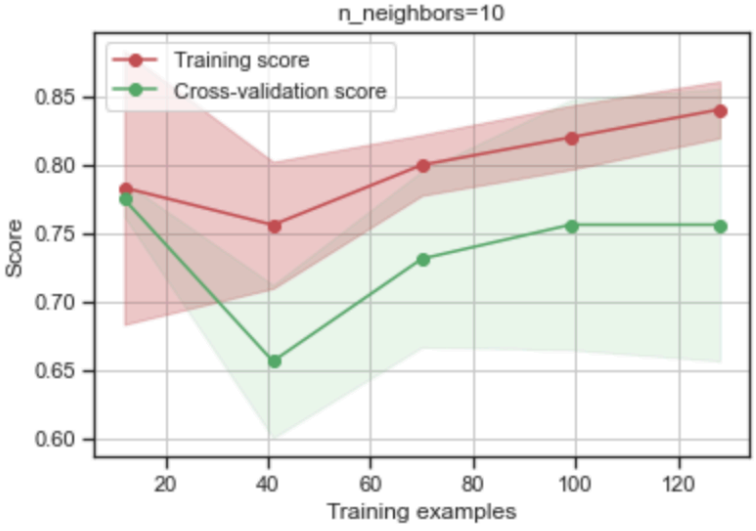

```
def plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
                        n_jobs=None, train_sizes=np.linspace(.1, 1.0,
5)):
    plt.figure()
    plt.title(title)
    if ylim is not None:
        plt.ylim(*ylim)
    plt.xlabel("Training examples")
    plt.ylabel("Score")
    train_sizes, 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=0.3,
                        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

plot_learning_curve(KNeighborsClassifier(n_neighbors=10),
'n_neighbors=10',
                    data_X_train, data_y_train, cv=5)
```



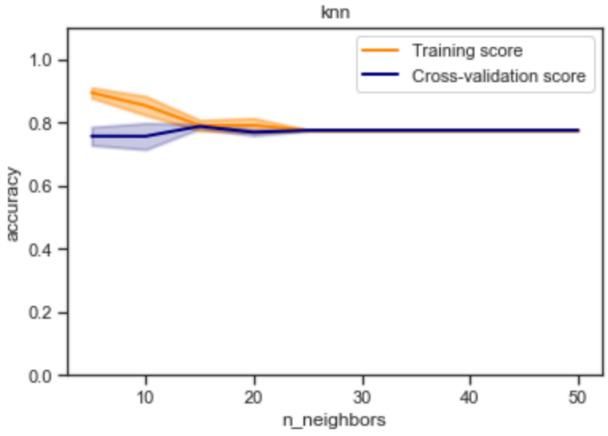

```
def plot_validation_curve(estimator, title, X, y,
                          param_name, param_range, cv,
                          scoring="accuracy"):
```

```
    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

plot_validation_curve(KNeighborsClassifier(), 'knn',
                      data_X_train, data_y_train,
                      param_name='n_neighbors', param_range=n_range,
                      cv=3, scoring="accuracy")
```

```
<module 'matplotlib.pyplot'>
```


knn
Training score
Cross-validation score
accuracy
n_neighbors
0.0
0.2
0.4
0.6
0.8
1.0
10
20
30
40
50