Московский государственный технический университет имени 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»

Выполнил:

Студент ИУ5-24М

Черната Н. С.

Москва, 2020

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.

```
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_Ver1.1.csv")
data
```

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
...
...
...
...
0.73
499
500
327
113
4
4.5
4.5
9.04
0
0.84
500 rows × 9 columns

```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 500 entries, 0 to 499
Data columns (total 9 columns):
```

```
 #   Column             Non-Null Count  Dtype  
---  ------             --------------  -----  
 0   Serial No.         500 non-null    int64  
 1   GRE Score          500 non-null    int64  
 2   TOEFL Score        500 non-null    int64  
 3   University Rating  500 non-null    int64  
 4   SOP                500 non-null    float64
 5   LOR                500 non-null    float64
 6   CGPA               500 non-null    float64
 7   Research           500 non-null    int64  
 8   Chance of Admit    500 non-null    float64
dtypes: float64(4), int64(5)
memory usage: 35.3 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
```

```
(500, 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
      ... 
495    1.0
496    1.0
497    1.0
498    1.0
499    1.0
Name: isAdmit, Length: 500, dtype: float64
```

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

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

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

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

```
((500, 8), (500,))
```

```
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
```

```
((200, 8), (300, 8), (200,), (300,))
```

```
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)
```

```
(0.79, 0.6533333333333333)
```

```
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)
```

```
(0.83, 0.6966666666666667)
```

```
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, 0.82)
```

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

```
(array([0.35, 0.52, 0.71, 0.6 , 0.77]), 0.5900000000000001)
```

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

```
(array([0.08450704, 0.52      , 0.71      , 0.43661972, 0.69333333]),
 0.4888920187793427)
```

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

```
(array([0.31428571, 0.83985765, 0.12698413]), 0.427042497505131)
```

```
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([0.00699782, 0.00499678, 0.00399804, 0.00399756,
0.00499845]),
 'score_time': array([0.01299381, 0.0109942 , 0.00799537, 0.00799584,
0.00799394]),
 'test_accuracy': array([0.35, 0.52, 0.71, 0.6 , 0.77]),
 'train_accuracy': array([0.865 , 0.8625, 0.8975, 0.855 , 0.8625]),
 'test_jaccard': array([0.08450704, 0.52      , 0.71      , 0.43661972,
0.69333333]),
 'train_jaccard': array([0.83685801, 0.83333333, 0.86900958, 0.82477341,
0.83333333]),
 'test_f1': array([0.15584416, 0.68421053, 0.83040936, 0.60784314,
0.81889764]),
 'train_f1': array([0.91118421, 0.90909091, 0.92991453, 0.90397351,
0.90909091])}

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

Wall time: 3.89 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., 1., 1., 1., 1., 0.,
        1., 1., 1., 1., 1., 1., 1., 0., 1., 1., 0., 1., 1., 1., 1., 0., 1.,
        1., 1., 1., 1., 1., 0., 1., 1., 0., 0., 0., 1., 1., 1., 1., 1., 1.,
        1., 1., 0., 1., 1., 0., 1., 1., 1., 0., 0., 0., 0., 1., 1., 0., 1.,
        1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 0., 1., 1., 1.,
        1., 1., 0., 0., 1., 1., 1., 1., 1., 1., 1., 1., 0., 1., 1., 1., 0.,
        0., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 0., 0.,
        0., 1., 1., 1., 1., 1., 1.]),
 0.824)
```

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

```
array([0.76, 0.77, 0.81, 0.62, 0.74])
```

```
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)
```

```
Wall time: 503 ms
```

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

```
clf_gs.cv_results_
```

```
{'mean_fit_time': array([0.00539775, 0.00439777, 0.00360117, 0.00439715,
0.00319815,
        0.00319843, 0.00399475, 0.00579686, 0.00499306, 0.00459676]),
 'std_fit_time': array([0.00048992, 0.00101884, 0.00048532, 0.00135525,
0.00039971,
        0.00040043, 0.00062511, 0.0020421 , 0.00063718, 0.00079986]),
 'mean_score_time': array([0.00659523, 0.00419726, 0.00499401, 0.00479727,
0.0043973 ,
        0.00400066, 0.00439377, 0.00579667, 0.00620103, 0.0057972 ]),
 'std_score_time': array([1.01912224e-03, 4.00114443e-04, 6.31988295e-04,
1.16610586e-03,
        4.89375878e-04, 7.27704123e-06, 5.00204961e-04, 9.79326166e-04,
        7.52164723e-04, 1.16565645e-03]),
 '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([0.8  , 0.825, 0.825, 0.8  , 0.8  , 0.8  , 0.8  ,
0.8  , 0.8  ,
        0.8  ]),
 'split1_test_score': array([0.875, 0.9  , 0.825, 0.8  , 0.8  , 0.8  , 0.8  ,
0.8  , 0.8  ,
        0.8  ]),
 'split2_test_score': array([0.875, 0.85 , 0.8  , 0.825, 0.8  , 0.8  , 0.8  ,
0.8  , 0.8  ,
        0.8  ]),
 'split3_test_score': array([0.725, 0.725, 0.75 , 0.775, 0.775, 0.775, 0.775,
0.775, 0.775,
        0.775]),
 'split4_test_score': array([0.775, 0.75 , 0.775, 0.75 , 0.775, 0.775, 0.775,
0.775, 0.775,
        0.775]),
 'mean_test_score': array([0.81 , 0.81 , 0.795, 0.79 , 0.79 , 0.79 , 0.79 ,
0.79 , 0.79 ,
        0.79 ]),
 'std_test_score': array([0.05830952, 0.06442049, 0.02915476, 0.0254951 ,
0.01224745,
        0.01224745, 0.01224745, 0.01224745, 0.01224745, 0.01224745]),
 'rank_test_score': array([ 2,  1,  3, 10,  4,  4,  4,  4,  4,  4])}
```

```
clf_gs.best_estimator_
```

```
KNeighborsClassifier(n_neighbors=10)
```

```
clf_gs.best_score_
```

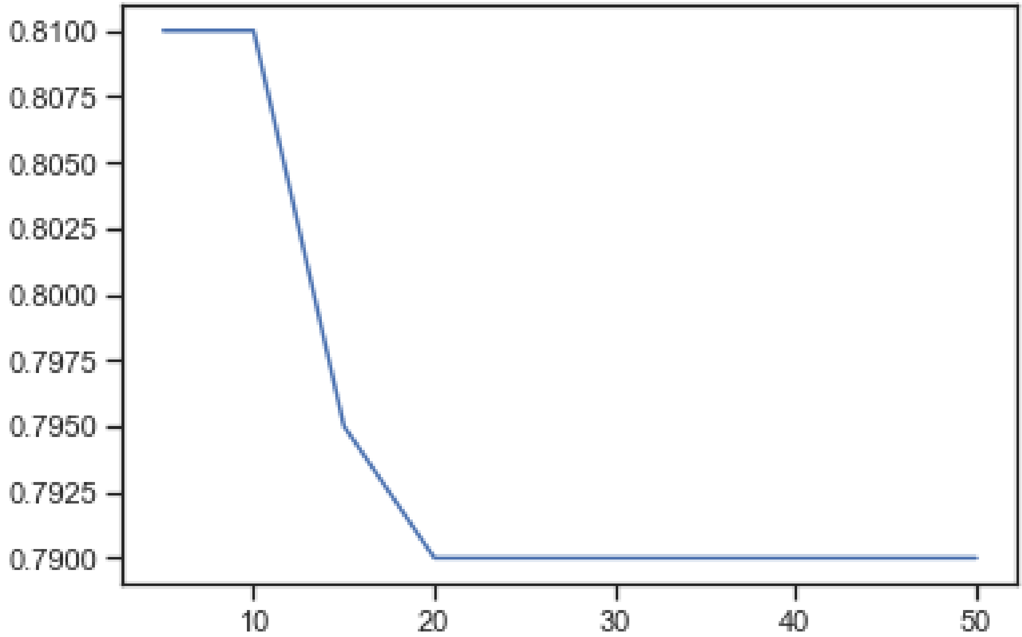
```
0.8100000000000002
```

```
clf_gs.best_params_
```

```
{'n_neighbors': 10}
```

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

```
[<matplotlib.lines.Line2D at 0x29560f902b0>]
```



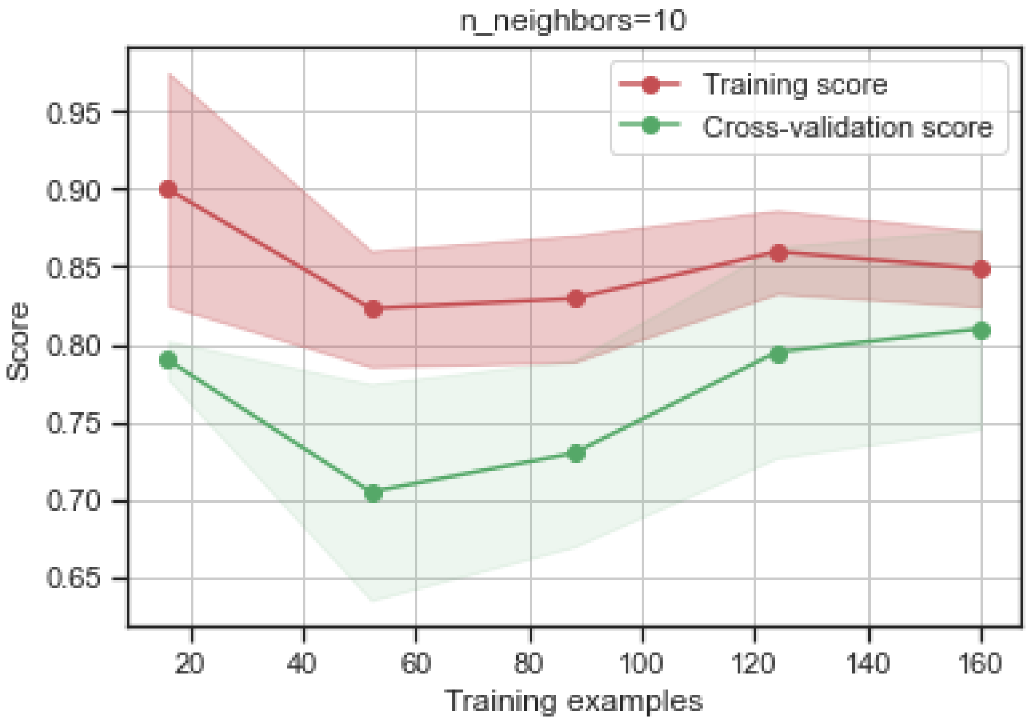

```
def
plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
                        n_jobs=None, train_sizes=np.linspace(.1, 1.0, 5)):
    plt.figure()
    plt.title(title)
    if ylim is not None:
        plt.ylim(*ylim)
    plt.xlabel("Training examples")
    plt.ylabel("Score")
    train_sizes,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

<module 'matplotlib.pyplot' from
'c:\\users\\ncher\\appdata\\local\\programs\\python\\python36\\lib\\site-
packages\\matplotlib\\pyplot.py'>
```




```
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' from
'c:\\users\\ncher\\appdata\\local\\programs\\python\\python36\\lib\\site-
packages\\matplotlib\\pyplot.py'>
```