Московский государственный технический университет им. Н. Э. Баумана

Курс «Технологии машинного обучения»
Отчёт по лабораторной работе №3
«Подготовка обучающей и тестовой выборки, кросс-валидация и подбор гиперпараметров на примере метода ближайших соседей»

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Дата:

Подпись:

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Москва

Импортируем библиотеки

```
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
import matplotlib.ticker as ticker
%matplotlib inline
sns.set(style="ticks")
from operator import itemgetter
import math
from sklearn.metrics import mean_absolute_error, mean_squared_error,
median_absolute_error, r2_score
from sklearn.neighbors import KNeighborsRegressor
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn import svm
from sklearn.metrics import accuracy_score
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import RepeatedKFold
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import KFold
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import RandomizedSearchCV
from sklearn.model_selection import ShuffleSplit
from sklearn.metrics import precision_score, recall_score
```

Импортируем данные

```
data = pd.read_csv('diabetes.csv')

data_1 = data.copy()

data.head()
```

```
   Pregnancies  Glucose  BloodPressure  SkinThickness  Insulin
BMI  \
0            6      148             72             35        0  33.6

1            1       85             66             29        0  26.6

2            8      183             64              0        0  23.3

3            1       89             66             23       94  28.1

4            0      137             40             35      168  43.1


   DiabetesPedigreeFunction  Age  Outcome
0                     0.627   50        1
1                     0.351   31        0
```

```
2                    0.672   32        1
3                    0.167   21        0
4                    2.288   33        1
```

```
data.describe()
```

```
       Pregnancies     Glucose  BloodPressure  SkinThickness
Insulin  \
count   768.000000  768.000000     768.000000     768.000000
768.000000
mean      3.845052  120.894531      69.105469      20.536458
79.799479
std       3.369578   31.972618      19.355807      15.952218
115.244002
min       0.000000    0.000000       0.000000       0.000000
0.000000
25%       1.000000   99.000000      62.000000       0.000000
0.000000
50%       3.000000  117.000000      72.000000      23.000000
30.500000
75%       6.000000  140.250000      80.000000      32.000000
127.250000
max      17.000000  199.000000     122.000000      99.000000
846.000000

              BMI  DiabetesPedigreeFunction         Age     Outcome
count  768.000000                768.000000  768.000000  768.000000
mean    31.992578                  0.471876   33.240885    0.348958
std      7.884160                  0.331329   11.760232    0.476951
min      0.000000                  0.078000   21.000000    0.000000
25%     27.300000                  0.243750   24.000000    0.000000
50%     32.000000                  0.372500   29.000000    0.000000
75%     36.600000                  0.626250   41.000000    1.000000
max     67.100000                  2.420000   81.000000    1.000000
```

Отделяем целевой признак

```
X=data.drop(columns=['Outcome'],axis=1)
Y=data['Outcome']
```

```
print(X)
```

```
     Pregnancies  Glucose  BloodPressure  SkinThickness  Insulin   BMI
\
0              6      148             72             35        0  33.6

1              1       85             66             29        0  26.6

2              8      183             64              0        0  23.3

3              1       89             66             23       94  28.1
```

```
4              0      137              40              35      168  43.1

..           ...      ...             ...             ...      ...   ...

763           10      101              76              48      180  32.9

764            2      122              70              27        0  36.8

765            5      121              72              23      112  26.2

766            1      126              60               0        0  30.1

767            1       93              70              31        0  30.4


     DiabetesPedigreeFunction  Age
0                       0.627   50
1                       0.351   31
2                       0.672   32
3                       0.167   21
4                       2.288   33
..                        ...  ...
763                     0.171   63
764                     0.340   27
765                     0.245   30
766                     0.349   47
767                     0.315   23

[768 rows x 8 columns]
```

```
print(Y)
```

```
0      1
1      0
2      1
3      0
4      1
      ..
763    0
764    0
765    0
766    1
767    0
Name: Outcome, Length: 768, dtype: int64
```

Разделяем на тестовую и тренировочную выборки

```
X_train,X_test,Y_train,Y_test=train_test_split(X,Y,test_size=0.2,strat
ify=Y,random_state=2)
```

```
print(X.shape,X_train.shape,X_test.shape)
```

```
(768, 8) (614, 8) (154, 8)
```

```
print(Y.shape,Y_train.shape,Y_test.shape)
```

```
(768,) (614,) (154,)
```

Модель k близжайших соседей для k = 3

```
knn = KNeighborsClassifier(n_neighbors=3)

knn.fit(X_train, Y_train)
prediction = knn.predict(X_test)
len(prediction), prediction
```

```
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py:228: FutureWarning: Unlike other reduction
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eliminated, and the value None will no longer be accepted. Set
`keepdims` to True or False to avoid this warning.
  mode, _ = stats.mode(_y[neigh_ind, k], axis=1)
```

```
(154,
 array([0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0,
0,
        1, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0,
1,
        0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1,
0,
        0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0,
0,
        1, 1, 0, 0, 1, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0,
        1, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0,
1,
        0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0,
1],
       dtype=int64))
```

```
len(Y_test), Y_test
```

```
(154,
 615    0
 80     0
 148    0
 132    1
 501    0
       ..
 127    0
```

```
185    1
85     0
497    0
86     0
Name: Outcome, Length: 154, dtype: int64)
```

Оцениваем качество модели с произвольно заданным параметром k = 3

```
print(mean_absolute_error(Y_test, prediction))
print(mean_squared_error(Y_test, prediction))
print(median_absolute_error(Y_test, prediction))
print(r2_score(Y_test, prediction))

print(accuracy_score(Y_test, prediction))
```

```
0.3051948051948052
0.3051948051948052
0.0
-0.34037037037037066
0.6948051948051948
```

- **Mean absolute error** - средняя абсолютная ошибка = (чем ближе значение к нулю, тем лучше качество регрессии)
- **Mean squared error** - средняя квадратичная ошибка = (чем ближе значение к нулю, тем лучше качество регрессии)
- **Median absolute error** = (чем ближе значение к нулю, тем лучше качество регрессии)
- **Метрика R2** или коэффициент детерминации = (чем ближе значение к единице, тем лучше качество регрессии)

Grid Search (решетчатый поиск)

```
k_range = np.array(range(0, 26, 5))
param_grid = dict(n_neighbors=k_range)
clf_gs = GridSearchCV(KNeighborsClassifier(), param_grid, cv=5,
scoring='accuracy', return_train_score=False)
clf_gs.fit(X_train,Y_train)
print("tuned hyperparameters :(best parameters) ",clf_gs.best_params_)
print("accuracy :",clf_gs.best_score_)
```

```
tuned hyperparameters :(best parameters)  {'n_neighbors': 20}
accuracy : 0.7361322137811542
```

```
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
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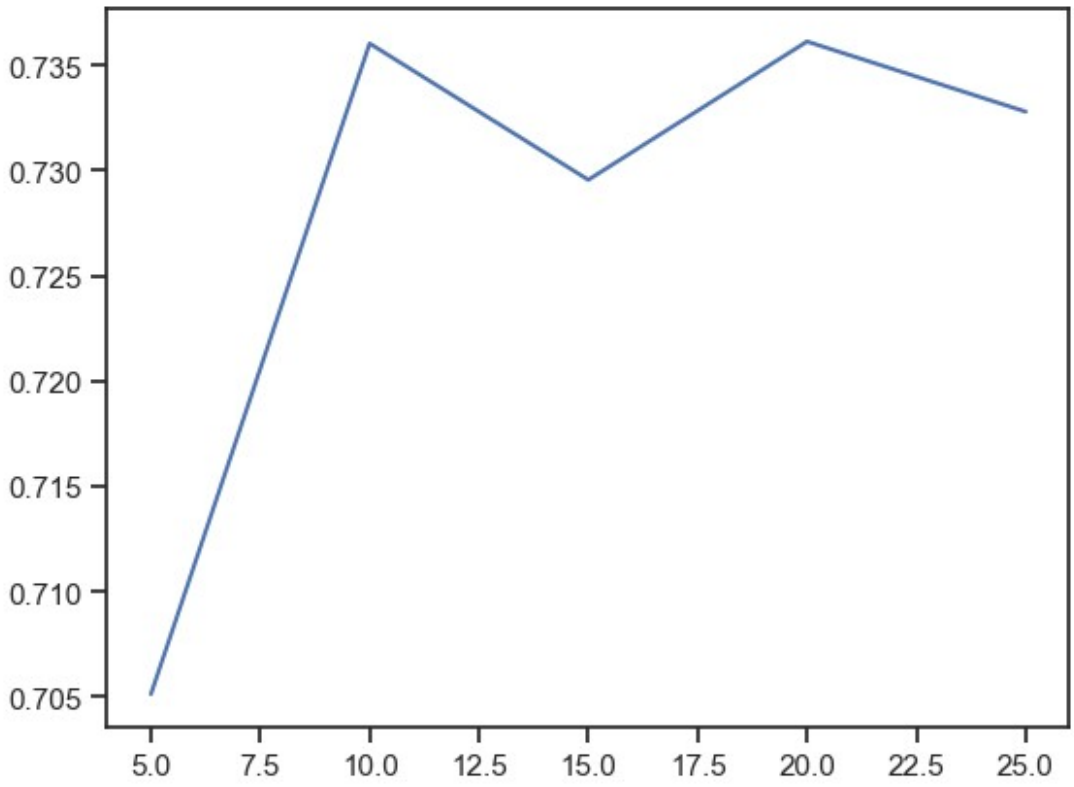
  mode, _ = stats.mode(_y[neigh_ind, k], axis=1)
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\model_selection\
_validation.py:372: FitFailedWarning:
5 fits failed out of a total of 30.
The score on these train-test partitions for these parameters will be
set to nan.
If these failures are not expected, you can try to debug them by
setting error_score='raise'.

Below are more details about the failures:
--------------------------------------------------------------------
----------
5 fits failed with the following error:
Traceback (most recent call last):
  File "C:\Users\shimo\anaconda3\lib\site-packages\sklearn\
model_selection\_validation.py", line 680, in _fit_and_score
    estimator.fit(X_train, y_train, **fit_params)
  File "C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py", line 198, in fit
    return self._fit(X, y)
  File "C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_base.py", line 569, in _fit
    raise ValueError("Expected n_neighbors > 0. Got %d" %
self.n_neighbors)
ValueError: Expected n_neighbors > 0. Got 0

  warnings.warn(some_fits_failed_message, FitFailedWarning)
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\model_selection\
_search.py:969: UserWarning: One or more of the test scores are non-
finite: [       nan 0.70513128 0.73603892 0.72956151 0.73613221
0.73280021]
  warnings.warn(
```

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

```
[<matplotlib.lines.Line2D at 0x1facd3f8be0>]
```



Randomized Search (случайный поиск)

```
clf_rs = RandomizedSearchCV(KNeighborsClassifier(), param_grid, cv=5,
scoring='accuracy')
clf_rs.fit(X_train, Y_train)
print("tuned hyperparameters :(best parameters) ",clf_rs.best_params_)
print("accuracy :",clf_rs.best_score_)
```

```
tuned hyperparameters :(best parameters)  {'n_neighbors': 20}
accuracy : 0.7361322137811542
```

```
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\model_selection\
_search.py:292: UserWarning: The total space of parameters 6 is
smaller than n_iter=10. Running 6 iterations. For exhaustive searches,
use GridSearchCV.
  warnings.warn(
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py:228: FutureWarning: Unlike other reduction
functions (e.g. `skew`, `kurtosis`), the default behavior of `mode`
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behavior will change: the default value of `keepdims` will become
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eliminated, and the value None will no longer be accepted. Set
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  mode, _ = stats.mode(_y[neigh_ind, k], axis=1)
```

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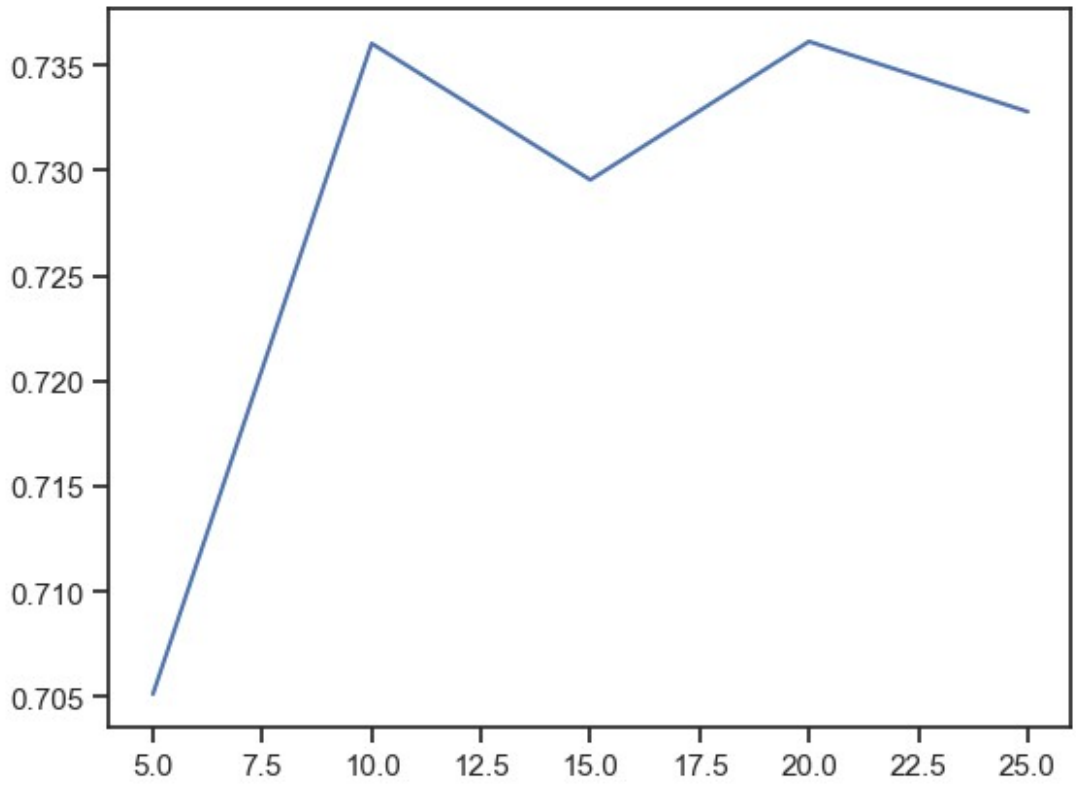
  mode, _ = stats.mode(_y[neigh_ind, k], axis=1)
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\model_selection\
_validation.py:372: FitFailedWarning:
5 fits failed out of a total of 30.
The score on these train-test partitions for these parameters will be
set to nan.
If these failures are not expected, you can try to debug them by
setting error_score='raise'.

Below are more details about the failures:
--------------------------------------------------------------------
----------
5 fits failed with the following error:
Traceback (most recent call last):
  File "C:\Users\shimo\anaconda3\lib\site-packages\sklearn\
model_selection\_validation.py", line 680, in _fit_and_score
    estimator.fit(X_train, y_train, **fit_params)
  File "C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py", line 198, in fit
    return self._fit(X, y)
  File "C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_base.py", line 569, in _fit
    raise ValueError("Expected n_neighbors > 0. Got %d" %
self.n_neighbors)
ValueError: Expected n_neighbors > 0. Got 0

  warnings.warn(some_fits_failed_message, FitFailedWarning)
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\model_selection\
_search.py:969: UserWarning: One or more of the test scores are non-
finite: [       nan 0.70513128 0.73603892 0.72956151 0.73613221
0.73280021]
  warnings.warn(
```

```
plt.plot(k_range, clf_rs.cv_results_['mean_test_score'])
```

```
[<matplotlib.lines.Line2D at 0x1facd473550>]
```



Кросс-валидация

```
cols_x = ['BMI', 'Age', 'Insulin']
col_y = 'Outcome'
scores =
cross_val_score(KNeighborsClassifier(n_neighbors=3),data[cols_x],data[
col_y],cv=4)
```

```
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
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scores

array([0.66666667, 0.66666667, 0.71354167, 0.640625  ])

np.mean(scores)

0.671875

# k-fold
scores=cross_val_score(KNeighborsClassifier(n_neighbors=20),data[cols_
x],data[col_y],cv=KFold(n_splits=4))
np.mean(scores)

C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py:228: FutureWarning: Unlike other reduction
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```

```
0.6888020833333334
```

```
#ShuffleSplit
scores=cross_val_score(KNeighborsClassifier(n_neighbors=20),data[cols_
x],data[col_y],cv=ShuffleSplit(n_splits=5,test_size=0.25))
np.mean(scores)
```

```
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py:228: FutureWarning: Unlike other reduction
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```

```
0.6708333333333334
```

```
knn = KNeighborsClassifier(n_neighbors=3)
knn.fit(X_train, Y_train)
prediction1 = knn.predict(X_test)
```

```
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py:228: FutureWarning: Unlike other reduction
functions (e.g. `skew`, `kurtosis`), the default behavior of `mode`
typically preserves the axis it acts along. In SciPy 1.11.0, this
behavior will change: the default value of `keepdims` will become
False, the `axis` over which the statistic is taken will be
eliminated, and the value None will no longer be accepted. Set
`keepdims` to True or False to avoid this warning.
  mode, _ = stats.mode(_y[neigh_ind, k], axis=1)
```

```
knn = KNeighborsClassifier(n_neighbors=20)
knn.fit(X_train, Y_train)
prediction2 = knn.predict(X_test)
```

```
C:\Users\shimo\anaconda3\lib\site-packages\sklearn\neighbors\
_classification.py:228: FutureWarning: Unlike other reduction
functions (e.g. `skew`, `kurtosis`), the default behavior of `mode`
typically preserves the axis it acts along. In SciPy 1.11.0, this
behavior will change: the default value of `keepdims` will become
False, the `axis` over which the statistic is taken will be
eliminated, and the value None will no longer be accepted. Set
`keepdims` to True or False to avoid this warning.
  mode, _ = stats.mode(_y[neigh_ind, k], axis=1)
```

accuracy — доля правильных ответов алгоритма: precision называется доля правильных ответов модели в пределах класса — это доля объектов действительно принадлежащих данному классу относительно всех объектов которые система отнесла к этому классу

```
print("3 neigbours:")
print(accuracy_score(Y_test, prediction1))
print(precision_score(Y_test, prediction1))
print("20 neigbours:")
print(accuracy_score(Y_test, prediction2))
print(precision_score(Y_test, prediction2))
```

```
3 neigbours:
0.6818181818181818
0.5531914893617021
20 neigbours:
0.6948051948051948
0.6129032258064516
```