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

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

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1. Лабораторная работа № 4

```
[0]: import numpy as np
     import pandas as pd
     import seaborn as sns
     import matplotlib.pyplot as plt
     %matplotlib inline
     sns.set(style="ticks")
     #from sklearn.datasets import load wine
     #data2 = Load wine()
     def make_dataframe(ds_function):
         ds = ds function()
         df = pd.DataFrame(data= np.c [ds['data'], ds['target']],
                          columns= list(ds['feature names']) + ['target'])
         return df
[0]: #
     #data1.head()
[0]: #for col in data1.columns:
          temp null count = data1[data1[col].isnull()].shape[0]
          print('{} - {}'.format(col, temp null count))
[0]: #data = pd.read csv("diabetes.csv")
     #X=data.iloc[0:,0:8]
     #X.head()
     #y=data.iloc[0:,-1]
     #y.head()
     #x train, x test, y train, y test = train test split(x, y, test size=0.
      \rightarrow 33, random state=324)
[0]: from sklearn.datasets import fetch california housing
```

2. Датасет данных о жилье в Калифорнии(пропуски отсутствуют, нет категориальных признаков для кодирования):

3. Разбиение выборки:

```
[0]: from sklearn.model_selection import train_test_split
#x=data.iloc[0:,0:8]
x=data.data
#x.head()
#y=data.iloc[0:,-1]
y=data.target
#y.head()
x_train, x_test, y_train, y_test = train_test_split(x, y, test_size=0.
→33, random_state=324)
```

4. Обучение модели ближайших соседей с произвольно заданным гиперпараметром:

5. Оценка качества модели с использованием подходящих метрик:

```
[0]: 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

mean_absolute_error(y_test, target2_1)
```

[0]: 0.82001825631239

```
[0]: mean_squared_error(y_test, target2_1)
```

[0]: 1.1360970590205923

```
[0]: median absolute error(y test, target2 1)
[0]: 0.656401
[0]: r2 score(y test, target2 1)
 [0]: 0.146285549833991
     6. Кросс-валидация
 [0]: from sklearn.model selection import cross val score, cross validate
      scores = cross_val_score(KNeighborsRegressor(n_neighbors=5), data.data,P
       →data.target, cv=3)
      #scores
      #np.mean(scores)
[77]: scores
                          0.07663073, -0.00727265])
[77]: array([ 0.08942206,
[78]: np.mean(scores)
[78]: 0.05292671098955367
[79]: #explained variance
      #max error
      #Добавим несколько метрик
      scoring = {'neg_mean_absolute_error',
                 'neg_mean_squared_error',
                 'neg_median_absolute_error',
                 'r2',
                 'max error',
                 'explained variance'}
      scores = cross validate(KNeighborsRegressor(n neighbors=5),
                              data.data, data.target, scoring=scoring,
                              cv=3, return train score=True)
      scores
[79]: {'fit_time': array([0.02059913, 0.01460958, 0.01455784]),
       'score time': array([0.04011416, 0.03742957, 0.03828692]),
       'test explained variance': array([0.09405041, 0.07825933, 0.05755802]),
       'test_max_error': array([-4.04721, -3.95981, -4.33741]),
       'test_neg_mean_absolute_error': array([-0.87302279, -0.79852741, -0.
       \rightarrow 9249041 ]),
       'test_neg_mean_squared_error': array([-1.22757547, -1.10340978, -1.
       →43734607]),
       'test neg_median_absolute_error': array([-0.724501, -0.6243 , -0.7331P
       → ]),
       'test r2': array([ 0.08942206, 0.07663073, -0.00727265]),
```

7. Стратегия 1:

-3.395808]),

→63746003,

-0.64833978, -0.63364302]),

```
[80]: #K-Fold
      from sklearn.model_selection import KFold, RepeatedKFold, LeaveOneOut, 
       →LeavePOut, ShuffleSplit, StratifiedKFold
      kf = KFold(n splits=5)
      scores = cross validate(KNeighborsRegressor(n neighbors=5),
                                data.data, data.target, scoring=scoring,
                                cv=kf, return train score=True)
      scores
[80]: {'fit_time': array([0.03301859, 0.01943374, 0.02062464, 0.0199368,
      0.01965833]),
       'score time': array([0.0273335 , 0.02370882, 0.13579059, 0.02444959,
      0.02442241]),
       'test explained variance': array([ 0.08611725, 0.09408026, 0.
       \rightarrow 13821535,
      -0.01643905, 0.13420392]),
       'test max error': array([-3.83401, -4.04721, -3.9868 , -3.91961, -4.
       \rightarrow 34241]),
       'test neg mean absolute error': array([-0.86581377, -0.7749557 , -0.
       →88992606,
      -0.88476702, -0.93090844]),
       'test_neg_mean_squared_error': array([-1.12793334, -1.08765125, -1.
       \rightarrow 39321723,
      -1.23392298, -1.44103421),
       'test_neg_median_absolute_error': array([-0.7757, -0.5784, -0.6762, -0.
       -7645,
      -0.7321),
       'test r2': array([-0.0499511 , 0.07083077, 0.03149977, -0.05177241,
      0.01106559]),
       'train explained variance': array([0.45104821, 0.46043257, 0.45277795,
      0.47567216, 0.45748092]),
```

'train_max_error': array([-3.395808, -3.452408, -3.512408, -3.452408,

'train neg mean absolute error': array([-0.66201964, -0.66290899, -0.

```
<sup>→</sup>70180463,
      -0.71265573, -0.70082914]),
       'train neg median absolute error': array([-0.5266 , -0.5291 , -0.
       501201,
      -0.5144 , -0.4921 ]),
       'train r2': array([0.44951963, 0.45880618, 0.45084177, 0.47368489,
      0.45616596])}
[0]: #kf = LeaveOneOut()
[0]: \#kf = LeavePOut(2)
      #scores = cross val score(KNeighborsRegressor(n neighbors=2),
                                 data.data, data.target,₽
       →scoring='neg_mean_absolute_error',
                                 cv=kf)
      #scores
     8. Стратегия 2:
[81]: kf = ShuffleSplit(n splits=5, test size=0.25)
      scores = cross_validate(KNeighborsRegressor(n_neighbors=5),
                                data.data, data.target, scoring=scoring,
                                cv=kf, return train score=True)
      scores
[81]: {'fit_time': array([0.02485085, 0.01900673, 0.01945448, 0.02046108,
      0.01931548]),
       'score_time': array([0.02912545, 0.02912283, 0.02868509, 0.02853417,
      0.03168583]),
       'test explained variance': array([0.13594097, 0.13847265, 0.14608201,
      0.12522304, 0.15411858]),
       'test_max_error': array([-4.17581, -4.00781, -3.92221, -4.17401, -3.
       \rightarrow94501]),
       'test neg mean absolute error': array([-0.8367783 , -0.83489776, -0.
       -82009248,
      -0.83760976, -0.82979485]),
       'test_neg_mean_squared_error': array([-1.1689623 , -1.17981427, -1.
       \rightarrow12594811,
      -1.19815902, -1.15452878]),
       'test_neg_median_absolute_error': array([-0.6658 , -0.6606 , -0.6673₽
      -0.6536 , -0.661598]),
       'test_r2': array([0.1327442 , 0.13510542, 0.14302162, 0.12066656, 0.
       \rightarrow14933073]),
       'train_explained_variance': array([0.45254202, 0.44933859, 0.44999685,
      0.45081511, 0.45157425]),
       'train_max_error': array([-3.480008, -3.452408, -3.452408, -3.457408,
```

'train neg mean squared error': array([-0.74283576, -0.7393373 , -0.

```
-3.452408]),
'train_neg_mean_absolute_error': array([-0.6560425 , -0.65519779, -0.

-65850667,
-0.65558237, -0.65295885]),
'train_neg_mean_squared_error': array([-0.72815517, -0.72942896, -0.

-73771273,
-0.72792547, -0.72768498]),
'train_neg_median_absolute_error': array([-0.5236, -0.5225, -0.5214, -0.5194,
-0.5178]),
'train_r2': array([0.45090414, 0.44767233, 0.44841677, 0.44900279,
0.44988072])}
```

9. Стратегия 3:

→66132916,

-0.66601055, -0.66141178]),

[82]: skf = StratifiedKFold(n splits=3)

```
scores = cross validate(KNeighborsRegressor(n neighbors=5),
                                data.data, data.target, scoring=scoring,
                                cv=kf, return train score=True)
      scores
[82]: {'fit_time': array([0.0220511 , 0.01954985, 0.02040076, 0.01952934,
      0.01926112]),
       'score time': array([0.03333974, 0.02903891, 0.02912569, 0.02949739,
      0.028922321),
       'test_explained_variance': array([0.13822771, 0.16750964, 0.16106668,
      0.15542754, 0.14842437]),
       'test max error': array([-3.95961, -3.7574 , -4.34741, -4.02601, -4.
       \rightarrow19861]),
       'test neg mean absolute error': array([-0.83357843, -0.82667521, -0.
       →81878238,
      -0.80976838, -0.81899329]),
       'test_neg_mean_squared_error': array([-1.17316112, -1.15360182, -1.
       \rightarrow 13768852,
      -1.10057008, -1.13360017]),
       'test neg median absolute error': array([-0.667701, -0.658401, -0.6416₽
      -0.6559 , -0.658198]),
       'test_r2': array([0.13659913, 0.16255585, 0.15776543, 0.15381193, 0.
       \rightarrow14463861]),
       'train explained variance': array([0.44746549, 0.44125961, 0.4425836,
      0.44239222, 0.44776412]),
       'train_max_error': array([-3.382408, -3.452408, -3.395808, -3.528408,
      -3.462408]),
       'train_neg_mean_absolute_error': array([-0.65700164, -0.65951543, -0.
```

```
'train neg mean squared error': array([-0.73330957, -0.73798363, -0.
      →74079879,
     -0.75020402, -0.73866955]),
      'train neg median absolute error': array([-0.519 , -0.5227, -0.5235,₽
      \rightarrow -0.5293,
     -0.52781),
      'train r2': array([0.4454824 , 0.43922391, 0.44092892, 0.44087664,
     0.44612142])}
[0]: import sklearn
     sorted(sklearn.metrics.SCORERS.keys())
[0]: ['accuracy',
      'adjusted_mutual_info_score',
      'adjusted_rand_score',
      'average precision',
      'balanced_accuracy',
      'completeness_score',
      'explained variance',
      'f1',
      'f1_macro',
      'f1 micro',
      'f1 samples',
      'f1_weighted',
      'fowlkes mallows score',
      'homogeneity score',
      'jaccard',
      'jaccard_macro',
      'jaccard_micro',
      'jaccard samples',
      'jaccard_weighted',
      'max error',
      'mutual_info_score',
      'neg_brier_score',
      'neg_log_loss',
      'neg_mean_absolute_error',
      'neg_mean_gamma_deviance',
      'neg mean poisson deviance',
      'neg mean squared error',
      'neg_mean_squared_log_error',
      'neg median absolute error',
      'neg root mean squared error',
      'normalized_mutual_info_score',
      'precision',
      'precision macro',
      'precision micro',
      'precision samples',
      'precision weighted',
      'r2',
      'recall',
```

```
'recall_macro',
'recall_micro',
'recall_samples',
'recall_weighted',
'roc_auc',
'roc_auc_ovo',
'roc_auc_ovo_weighted',
'roc_auc_ovr',
'roc_auc_ovr_weighted',
'v measure score']
```

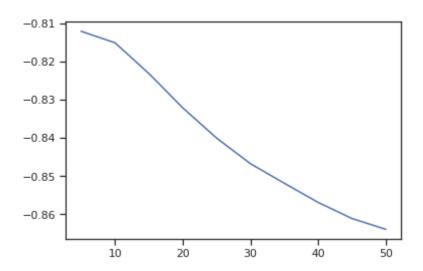
10. Подбор гиперпараметра с GriDSearchCV

```
[83]: n range = np.array(range(5,55,5))
      tuned_parameters = [{'n_neighbors': n_range}]
      tuned parameters
 [83]: [{'n_neighbors': array([ 5, 10, 15, 20, 25, 30, 35, 40, 45, 50])}]
[111]: #test=ShuffleSplit()
      #test
[111]: ShuffleSplit(n splits=10, random state=None, test size=None, P
        →train size=None)
 [99]: from sklearn.model selection import GridSearchCV, RandomizedSearchCV
      from sklearn.model selection import learning curve, validation curve
      #clf_gs = GridSearchCV(KNeighborsRegressor(), tuned_parameters, P
        →cv=LeaveOneOut(), scoring='neg mean absolute error')
      #clf qs.fit(data.data, data.target)
      clf rs = RandomizedSearchCV(KNeighborsRegressor(), tuned_parameters, P
       clf rs.fit(data.data, data.target)
 [99]: RandomizedSearchCV(cv=ShuffleSplit(n_splits=10, random_state=None,
      test_size=None, train_size=None),
                         error score=nan,
                         estimator=KNeighborsRegressor(algorithm='auto', 2
        →leaf size=30,
                                                      metric='minkowski',
                                                      metric_params=None,
                                                       n jobs=None, ₽
        ⊸n neighbors=5,
                                                       p=2, ₽
        →weights='uniform'),
                         iid='deprecated', n_iter=10, n_jobs=None,
                         param distributions=[{'n neighbors': array([ 5, 10, №
        \rightarrow15, 20,
```

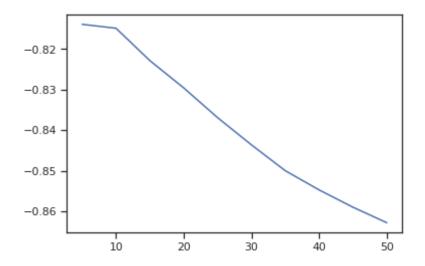
```
25, 30, 35, 40, 45, 50])}],
                          pre_dispatch='2*n_jobs', random state=None,P
        →refit=True,
                          return train score=False, <a>₽</a>
        →scoring='neg_mean_absolute_error',
                          verbose=0)
[107]: clf_rs.best_params_
[107]: {'n neighbors': 5}
[101]: clf_gs = GridSearchCV(KNeighborsRegressor(), tuned_parameters, ₽
        clf gs.fit(data.data, data.target)
[101]: GridSearchCV(cv=ShuffleSplit(n_splits=10, random_state=None, P
        →test size=None,
       train size=None),
                    error_score=nan,
                    estimator=KNeighborsRegressor(algorithm='auto', P
        →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, ₽
        \rightarrow 35, 40,
      45, 50])}],
                    pre dispatch='2*n jobs', refit=True, <a>₽</a>
        →return_train_score=False,
                    scoring='neg mean absolute error', verbose=0)
[109]: clf gs.cv results
[109]: {'mean_fit_time': array([0.02351162, 0.02266765, 0.02260883, 0.02307355,
       0.02268093,
               0.02268136, 0.02261248, 0.02272775, 0.02263823, 0.02278049]),
        'mean score time': array([0.01279907, 0.01530466, 0.01707008, 0.
        \rightarrow01960509,
       0.02129235,
               0.02387059, 0.02496018, 0.02808068, 0.02937937, 0.03181584]),
        'mean test score': array([-0.81203015, -0.81503612, -0.8230933 , -0.
        →83207381,
       -0.84000791,
               -0.846717 , -0.85183971, -0.85686798, -0.86108694, -0.863922
        →]),
        'param n neighbors': masked array(data=[5, 10, 15, 20, 25, 30, 35, 40, ₽
        45, 50
```

```
mask=[False, False, False, False, False, False, Palse, Pal
   →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, 2, 3, 4, 5, 6, 7, 8, 9, 10],
dtype=int32),
   'split0 test score': array([-0.8204379 , -0.8144728 , -0.82442798, -0.
   -83384151,
-0.84408377,
                   -0.85088312, -0.85790902, -0.86335614, -0.86538739, -0.
   →86709766]),
   'split1 test score': array([-0.8132376 , -0.82517394, -0.83646746, -0.
   →84484002,
-0.85354687,
                   -0.86184336, -0.86750736, -0.87176307, -0.87639178, -0.
   \rightarrow87954024]),
   'split2 test score': array([-0.77656432, -0.78454806, -0.7986453 , -0.
   →80949349,
-0.81804306,
                   -0.82517943, -0.82896983, -0.83525805, -0.84008578, -0.
   →84269529]),
   'split3 test score': array([-0.81509895, -0.82747879, -0.83711943, -0.
   34747662,
-0.85568191,
                   -0.86228979, -0.86774153, -0.87112331, -0.87479035, -0.
   →87778043]),
   'split4 test score': array([-0.81860875, -0.81666236, -0.81827355, -0.
   →82565653,
-0.83014141,
                   -0.83881223, -0.84274031, -0.84874638, -0.85390569, -0.
   485658187]),
   'split5 test score': array([-0.82433839, -0.82244156, -0.82784972, -0.
   →8372571 ,
-0.84616749,
                   -0.85107147, -0.85597538, -0.8621645, -0.86794017, -0.
   →87198665]),
   'split6_test_score': array([-0.81934245, -0.81974171, -0.82132706, -0.
   -83047181,
```

```
-0.83815918,
               -0.84354891, -0.84882261, -0.85230448, -0.85496734, -0.
        \rightarrow85767652]),
        'split7 test score': array([-0.80237355, -0.80526664, -0.81919044, -0.
        →82717728,
       -0.83563199,
               -0.84261306, -0.8478305 , -0.85320056, -0.85890744, -0.
        →86393131]),
        'split8 test score': array([-0.81986751, -0.8218043 , -0.82610359, -0.
        →83596837,
       -0.84252003.
               -0.84829952, -0.85426183, -0.85813786, -0.862585 , -0.
        \rightarrow86398928]),
        'split9 test score': array([-0.81043207, -0.81277105, -0.82152852, -0.
        -82855533,
       -0.83610337,
               -0.84262911, -0.84663877, -0.85262543, -0.85590841, -0.
        485794077]),
        'std fit time': array([0.00164925, 0.00042376, 0.00052891, 0.00103466,
       0.00040232,
               0.00043602, 0.00039983, 0.00044322, 0.00039219, 0.00051819),
        'std score time': array([0.00023189, 0.00040602, 0.00013945, 0.
        →00060906,
       0.00029574,
               0.00161806, 0.00020324, 0.00161472, 0.00044112, 0.00178795),
        'std test score': array([0.01320931, 0.01188883, 0.01025086, 0.
        \rightarrow 01017524,
       0.01052357,
               0.01039271, 0.01102818, 0.01040223, 0.0102536, 0.01044196)
[110]: clf_gs.best_estimator_
[110]: KNeighborsRegressor(algorithm='auto', leaf size=30, metric='minkowski',
                           metric params=None, n jobs=None, n neighbors=5, p=2,
                           weights='uniform')
[106]: clf gs.best params
[106]: {'n neighbors': 5}
[103]: plt.plot(n range, clf gs.cv results ['mean test score'])
[103]: [<matplotlib.lines.Line2D at 0x7f59bdcd5198>]
```



[104]: [<matplotlib.lines.Line2D at 0x7f59bdd99550>]



```
[105]: clf_gs.best_estimator_.fit(x_train, y_train)
  target2_1 = clf_gs.best_estimator_.predict(x_test)
  mean_absolute_error(y_test, target2_1)
```

[105]: 0.82001825631239

11. Качество модели с подобранным гиперпараметром такое же, как и с взятым произвольно гиперпараметром, так как мы угадали лучшее значение гиперпараметра изначально

12. Кривые обучения и валидации

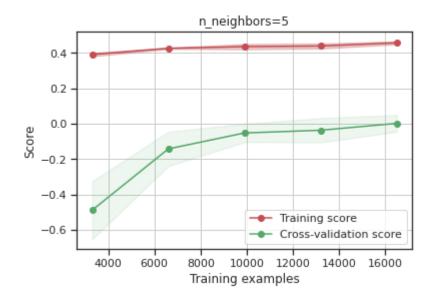
```
[0]: from sklearn.model selection import learning curve, validation curve
[0]: def plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
                             n jobs=None, train sizes=np.linspace(.1, 1.0,₽
      →5)):
         Generate a simple plot of the test and training learning 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), [2]
      →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 all
      ⇔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 12
⇔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 \mathbb{I}
\rightarrow (0, 1].
      Otherwise it is interpreted as absolute sizes of the training 

Output
⇒sets.
      Note that for classification the number of samples usually have 12
-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=0.3,
                    color="r")
  plt.fill between(train sizes, test scores mean - test scores std,
                    test scores mean + test scores std, alpha=0.1, <a>≥</a>

¬color="g")
```

[124]: <module 'matplotlib.pyplot' from '/usr/local/lib/python3.6/distpackages/matplotlib/pyplot.py'>



```
[0]: n_range2 = np.array(range(5,125,5))
```

[131]: <module 'matplotlib.pyplot' from '/usr/local/lib/python3.6/distpackages/matplotlib/pyplot.py'>

