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Факультет «Информатика и управление»

Кафедра ИУ5. Курс «Технологии машинного обучения»

Отчет по лабораторной работе №4:
«Подготовка обучающей и тестовой выборки, кросс-валидация и подбор гиперпараметров на примере метода ближайших соседей»

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Отчет по лабораторной работе №4 "Подготовка обучающей и тестовой выборки, кросс-валидация и подбор гиперпараметров на примере метода ближайших соседей"

In [336]:

```
import numpy as np
import pandas as pd
from sklearn.preprocessing import LabelEncoder
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, classificat
ion_report
from sklearn.metrics import confusion_matrix
from sklearn.metrics import mean_absolute_error, mean_squared_error, mean_square
d_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
import warnings
%matplotlib inline
sns.set(style="ticks")
```

подготовление датасета

In [337]:

```
# сторонняя компания по страхованию путешествий, базирующаяся в Сингапуре
data = pd.read_csv('лр4.csv', sep=',')
```

In [338]:

```
data.head()
```

Out[338]:

	Agency	Agency Type	Distribution Channel	Product Name	Claim	Duration	Destination	Net Sales	Commis (in va
0	CBH	Travel Agency	Offline	Comprehensive Plan	No	186	MALAYSIA	-29.0	9
1	CBH	Travel Agency	Offline	Comprehensive Plan	No	186	MALAYSIA	-29.0	9
2	CWT	Travel Agency	Online	Rental Vehicle Excess Insurance	No	65	AUSTRALIA	-49.5	29
3	CWT	Travel Agency	Online	Rental Vehicle Excess Insurance	No	60	AUSTRALIA	-39.6	23
4	CWT	Travel Agency	Online	Rental Vehicle Excess Insurance	No	79	ITALY	-19.8	11

In [339]:

```
data.shape
```

Out[339]:

```
(63326, 11)
```

In [340]:

```
data.dtypes
```

Out[340]:

```
Agency                    object
Agency Type               object
Distribution Channel      object
Product Name              object
Claim                     object
Duration                   int64
Destination               object
Net Sales                float64
Commision (in value)     float64
Gender                    object
Age                        int64
dtype: object
```

In [341]:

```
# удаление пропусков
data = data.drop(columns='Gender')
data.isnull().sum()
```

Out[341]:

```
Agency                    0
Agency Type               0
Distribution Channel      0
Product Name              0
Claim                     0
Duration                  0
Destination               0
Net Sales                 0
Commision (in value)      0
Age                       0
dtype: int64
```

In [342]:

```
# преобразование типов
cat_coll = []
for col in data.columns:
    if data[col].dtype == 'object':
        cat_coll.append(col)
en_cat = {}
for col in cat_coll:
    le = LabelEncoder()
    data[[col]] = le.fit_transform(data[col])
    en_cat[col] = le
```

In [343]:

```
data.dtypes
```

Out[343]:

```
Agency                     int64
Agency Type                int64
Distribution Channel       int64
Product Name               int64
Claim                      int64
Duration                   int64
Destination                int64
Net Sales                float64
Commision (in value)     float64
Age                        int64
dtype: object
```

In [344]:

```
# разделение выборки на обучающую и тестовую
# разделение исходного датасета на 2: с содержанием независимых и зависимых параметров соответственно
x, y = data[data.columns[range(9)]], data[data.columns[[9]]]
```

In [345]:

```
x.dtypes
```

Out[345]:

```
Agency                     int64
Agency Type                int64
Distribution Channel       int64
Product Name               int64
Claim                      int64
Duration                   int64
Destination                int64
Net Sales                float64
Commision (in value)     float64
dtype: object
```

In [346]:

```
y.dtypes
```

Out[346]:

```
Age    int64
dtype: object
```

In [348]:

```
test_size = 0.2
state = 42
xtrain, xtest, ytrain, ytest = train_test_split(x, y, test_size=test_size, rando
m_state=state)
len(xtrain), len(xtest), len(ytrain), len(ytest)
```

Out[348]:

```
(50660, 12666, 50660, 12666)
```

обучение модели на произвольном гиперпараметре k

In [349]:

```
# значения возраста от 0 до 118, поэтому используется классифаер
print('количество классов:', len(data['Age'].unique()))
```

количество классов: 89

In [350]:

```
# обучение модели для произвольно заданного гиперпараметра k
k = 3
KNeighborsClassifierObj = KNeighborsClassifier(n_neighbors=k)
KNeighborsClassifierObj
```

Out[350]:

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

In [351]:

```
# обучение модели для произвольно заданного гиперпараметра k
KNeighborsClassifierObj.fit(xtrain, ytrain.values.ravel())
```

Out[351]:

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

In [352]:

```
y_pred_train = KNeighborsClassifierObj.predict(xtrain)
y_pred_train
```

Out[352]:

```
array([ 29,  22,  36, ...,  36,  36, 118])
```

In [353]:

```
y_pred_test = KNeighborsClassifierObj.predict(xtest)
y_pred_test
```

Out[353]:

```
array([36, 31, 35, ..., 36, 26, 22])
```

In [354]:

```
ytest['Age'].values
```

Out[354]:

```
array([36, 68, 36, ..., 36, 61, 36])
```

In [355]:

```
# оценивание качество модели классификации
print('train accuracy(%) {}'.format(accuracy_score(ytrain, y_pred_train) * 100))
print('train accuracy(%) {}'.format(accuracy_score(ytest, y_pred_test) * 100))
```

```
train accuracy(%) 53.45637583892617
train accuracy(%) 36.009789988946785
```

In [356]:

```
print('матрица ошибок: строки – истинное, столбцы – предсказанное')
print('train:\n', confusion_matrix(ytrain, y_pred_train))
print('test:\n', confusion_matrix(ytest, y_pred_test))
```

```
матрица ошибок: строки – истинное, столбцы – предсказанное
train:
 [[  0   0   0 ...   0   0   0]
 [  0   3   0 ...   0   0   0]
 [  0   0   1 ...   0   0   0]
 ...
 [  0   0   0 ...   0   0   0]
 [  0   0   0 ...   0   0   0]
 [  0   0   0 ...   0   0 662]]
test:
 [[  0   0   0 ...   0   0   0]
 [  0   0   0 ...   0   0   0]
 [  0   0   0 ...   0   0   0]
 ...
 [  0   0   0 ...   0   0   0]
 [  0   0   0 ...   0   0   0]
 [  0   1   0 ...   0   0 145]]
```

In [357]:

```
warnings.filterwarnings("ignore")
print(precision_score(ytrain, y_pred_train, average='weighted'))
print(precision_score(ytest, y_pred_test, average='weighted'))
```

```
0.5369837479887902
0.33407827460523043
```

In [358]:

```
warnings.filterwarnings("ignore")
print(f1_score(ytrain, y_pred_train, average='weighted'))
print(f1_score(ytest, y_pred, average='weighted'))
```

```
0.5001660212851098
0.3415855080250703
```

оценивание качества с использованием кросс-валидации

In [359]:

```
# автоматически выбирается стратегия
warnings.filterwarnings("ignore")
scores = cross_val_score(KNeighborsClassifierObj, x, y.values.ravel(), cv=3)  # 3 фолда
scores  # дефолтная точность
```

Out[359]:

```
array([0.36716828, 0.35783292, 0.34903691])
```

In [360]:

```
np.mean(scores)
```

Out[360]:

```
0.35801270300862303
```

In [361]:

```
warnings.filterwarnings("ignore")
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, x, y.values.ravel(), scoring=sc
oring, cv=3, return_train_score=True)
scores
```

Out[361]:

```
{'fit_time': array([0.04443002, 0.03210306, 0.04179573]),
 'score_time': array([2.10332513, 2.17887306, 2.0072    ]),
 'test_precision': array([0.31211565, 0.3422917 , 0.33507145]),
 'train_precision': array([0.53744392, 0.53315717, 0.54169843]),
 'test_recall': array([0.36716828, 0.35783292, 0.34903691]),
 'train_recall': array([0.53991089, 0.53506278, 0.54381272]),
 'test_f1': array([0.33180252, 0.34690815, 0.33772616]),
 'train_f1': array([0.50527049, 0.49931282, 0.50993471])}
```

In [362]:

```
# стратегии кросс-валидации
# k-fold
scores = cross_val_score(KNeighborsClassifierObj, x, y.values.ravel(), cv=KFold(
n_splits=8))
scores
```

Out[362]:

```
array([0.42331986, 0.43292067, 0.40879232, 0.39527539, 0.36925215,
       0.34903992, 0.34996841, 0.13885028])
```

In [363]:

```
np.mean(scores)
```

Out[363]:

```
0.3584273752321039
```

In [364]:

```
import warnings
warnings.filterwarnings("ignore")
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, x, y.values.ravel(), scoring=sc
oring, cv=KFold(n_splits=8), return_train_score=True)
scores
```

Out[364]:

```
{'fit_time': array([0.06199241, 0.04982924, 0.04527402, 0.05136704,
0.06994486,
        0.0535481 , 0.04695106, 0.05018783]),
 'score_time': array([0.78344965, 0.84904599, 0.78026295, 0.7718789
6, 0.88731003,
        0.84380794, 0.7876761 , 0.85170388]),
 'test_precision': array([0.4021957 , 0.42366685, 0.38153719, 0.4033
9355, 0.38272103,
        0.34907666, 0.34156568, 0.11046427]),
 'train_precision': array([0.52952924, 0.52388708, 0.52496116, 0.529
09709, 0.52733944,
        0.53372504, 0.53298139, 0.56723542]),
 'test_recall': array([0.42331986, 0.43292067, 0.40879232, 0.3952753
9, 0.36925215,
        0.34903992, 0.34996841, 0.13885028]),
 'train_recall': array([0.52717921, 0.52051976, 0.52914636, 0.530463
82, 0.53271973,
        0.53273777, 0.53653607, 0.56672863]),
 'test_f1': array([0.40850374, 0.42615716, 0.38998112, 0.39508761,
0.37264892,
        0.34484141, 0.34172742, 0.09835689]),
 'train_f1': array([0.49274776, 0.48825839, 0.4945263 , 0.49514389,
0.49691419,
        0.49907789, 0.50304382, 0.53376689])}
```

In [365]:

```
# ShuffleSplit
scores = cross_val_score(KNeighborsClassifierObj, x, y.values.ravel(), cv=Shuffl
eSplit(n_splits=8, test_size=0.2))
scores
```

Out[365]:

```
array([0.36696668, 0.36641402, 0.37083531, 0.35843992, 0.37012474,
       0.36538765, 0.36759829, 0.36507185])
```

In [366]:

```
np.mean(scores)
```

Out[366]:

```
0.36635480814779725
```

In [367]:

```
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, x, y.values.ravel(), scoring=sc
oring, cv=ShuffleSplit(n_splits=8, test_size=0.2), return_train_score=True)
scores
```

Out[367]:

```
{'fit_time': array([0.06298709, 0.0541029 , 0.05324697, 0.05118823,
0.04534888,
        0.04684019, 0.04511309, 0.04306793]),
 'score_time': array([1.47089791, 1.30955911, 1.23071313, 1.4208219
1, 1.34536815,
        1.29949474, 1.26875377, 1.23436594]),
 'test_precision': array([0.33898849, 0.33870243, 0.3558928 , 0.3431
6941, 0.33798552,
        0.34112644, 0.34278456, 0.34014289]),
 'train_precision': array([0.53597169, 0.53467763, 0.53991082, 0.530
92839, 0.53209386,
        0.53129997, 0.53427949, 0.53462289]),
 'test_recall': array([0.36736144, 0.36617717, 0.37691457, 0.3662561
2, 0.36601926,
        0.36554556, 0.36980894, 0.36957208]),
 'train_recall': array([0.53385314, 0.53683379, 0.53624161, 0.532885
91, 0.53452428,
        0.53553099, 0.53426767, 0.5358863 ]),
 'test_f1': array([0.34871206, 0.34699649, 0.35954662, 0.34954222,
0.34718676,
        0.34634674, 0.35090211, 0.35001448]),
 'train_f1': array([0.49956762, 0.5021287 , 0.50160143, 0.49783251,
0.49939902,
        0.49961399, 0.4993428 , 0.50128196])}
```

In [368]:

```
# RepeatedKFold
scores = cross_val_score(KNeighborsClassifierObj, x, y.values.ravel(), cv=Repeat
edKFold(n_splits=3, n_repeats=3), n_jobs=-1)
scores
```

Out[368]:

```
array([0.36591028, 0.36373111, 0.37213379, 0.36785257, 0.36699986,
       0.36678037, 0.36382586, 0.36330475, 0.36606974])
```

In [369]:

```
np.mean(scores)
```

Out[369]:

```
0.36628981310706
```

In [370]:

```
scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
scores = cross_validate(KNeighborsClassifierObj, x, y.values.ravel(), scoring=sc
oring, cv=RepeatedKFold(n_splits=3, n_repeats=3),
                        return_train_score=True, n_jobs=-1)
scores
```

Out[370]:

```
{'fit_time': array([0.10314083, 0.11190295, 0.10741496, 0.07907581,
0.06042886,
        0.07871509, 0.08184385, 0.06535697, 0.06220388]),
 'score_time': array([3.79636908, 4.09066701, 4.01828909, 4.1263489
7, 4.16349101,
        4.7188592 , 4.81816101, 4.95011806, 3.35850906]),
 'test_precision': array([0.33423078, 0.33867559, 0.34067855, 0.3410
9225, 0.33969601,
        0.33419296, 0.33829907, 0.33442165, 0.3348406 ]),
 'train_precision': array([0.53540671, 0.53354868, 0.54068358, 0.539
2429 , 0.53652721,
        0.54200505, 0.53068382, 0.53341513, 0.53575838]),
 'test_recall': array([0.35766735, 0.36875266, 0.36635399, 0.3662892
6, 0.36785257,
        0.3590108 , 0.36752096, 0.36718935, 0.36114269]),
 'train_recall': array([0.54210389, 0.54101428, 0.54085935, 0.539024
56, 0.54165384,
        0.54230423, 0.53966412, 0.54132222, 0.53979345]),
 'test_f1': array([0.34075052, 0.3482693 , 0.34663884, 0.34844736,
0.34776344,
        0.34059248, 0.34767408, 0.34515737, 0.34333964]),
 'train_f1': array([0.50711763, 0.504329  , 0.50413985, 0.50397641,
0.50396608,
        0.50682933, 0.50320821, 0.50496213, 0.50413953])}
```

подбор гиперпараметра к с GridSearchCV и кросс-валидацией

In [371]:

```
n_neigh_values = range(1, 100, 5)
param = [{'n_neighbors': np.array(n_neigh_values)}]
class_grid = GridSearchCV(KNeighborsClassifier(), param, cv=KFold(n_splits=3), s
coring='accuracy',
                          return_train_score=True,
                          n_jobs=-1,
                         )
class_grid.fit(x, y.values.ravel())
# считает ~4 мин
```

Out[371]:

```
GridSearchCV(cv=KFold(n_splits=3, random_state=None, shuffle=False),
             error_score='raise-deprecating',
             estimator=KNeighborsClassifier(algorithm='auto', leaf_s
ize=30,
                                            metric='minkowski',
                                            metric_params=None, n_jo
bs=None,
                                            n_neighbors=5, p=2,
                                            weights='uniform'),
             iid='warn', n_jobs=-1,
             param_grid=[{'n_neighbors': array([ 1,  6, 11, 16, 21,
26, 31, 36, 41, 46, 51, 56, 61, 66, 71, 76, 81,
       86, 91, 96])}],
             pre_dispatch='2*n_jobs', refit=True, return_train_score
=True,
             scoring='accuracy', verbose=0)
```

In [372]:

```
class_grid.best_estimator_
```

Out[372]:

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

In [373]:

```
class_grid.best_score_
```

Out[373]:

```
0.4316236616871427
```

In [374]:

```
class_grid.best_params_
```

Out[374]:

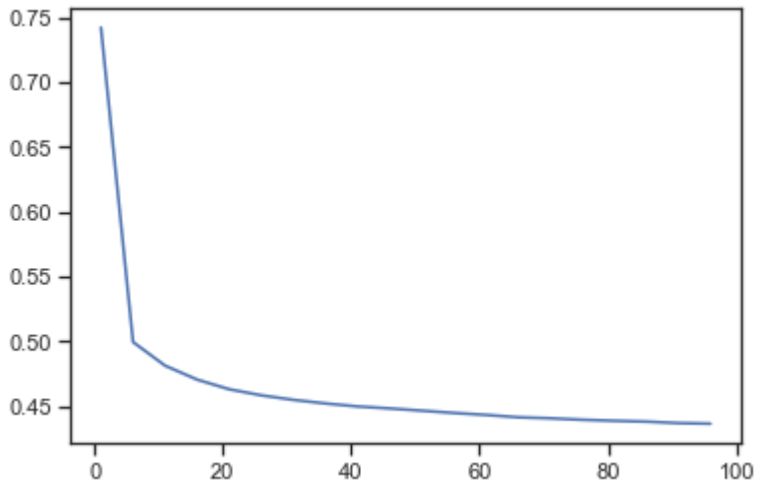
```
{'n_neighbors': 31}
```

In [375]:

```
plt.plot(n_neigh_values, class_grid.cv_results_['mean_train_score'])
```

Out[375]:

```
[<matplotlib.lines.Line2D at 0x11c01e1d0>]
```

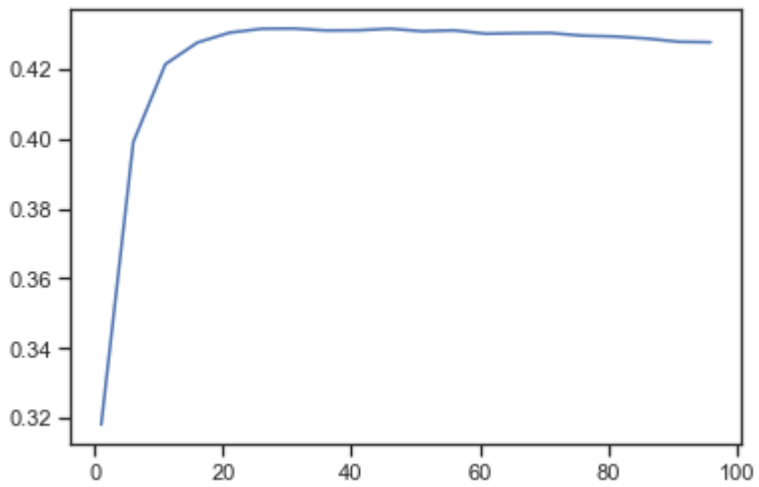


In [376]:

```
plt.plot(n_neigh_values, class_grid.cv_results_['mean_test_score'])
```

Out[376]:

```
[<matplotlib.lines.Line2D at 0x11cd410b8>]
```



возрастание значения accuracy, оптимальный k = 31

повторение для выборок x, y

In [377]:

```
class_grid.best_estimator_.fit(xtrain, ytrain.values.ravel())

newypred_train = class_grid.best_estimator_.predict(xtrain)
newypred_test = class_grid.best_estimator_.predict(xtest)

print('train accuracy (%): {}'.format(accuracy_score(ytrain, y_pred_train) * 100
))
print('test accuracy (%): {}'.format(accuracy_score(ytest, y_pred_test) * 100))

print('new accuracy train (%)): {}'.format(accuracy_score(ytrain, newypred_train
) * 100))
print('new accuracy test (%): {}'.format(accuracy_score(ytest, newypred_test) *
100))
```

```
train accuracy (%): 53.45637583892617
test accuracy (%): 36.009789988946785
new accuracy train (%)): 45.64547966837742
new accuracy test (%): 42.79172588030949
```

кривые обучения и валидации

In [379]:

```
def plotlearn_curve(estimator, title, x, y, ylim=None, cv=None,
                        n_jobs=-1, 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), 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 a 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 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 (0, 1].
        Otherwise it is interpreted as absolute sizes of the training sets.
        Note that for classification the number of samples usually have 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)
```

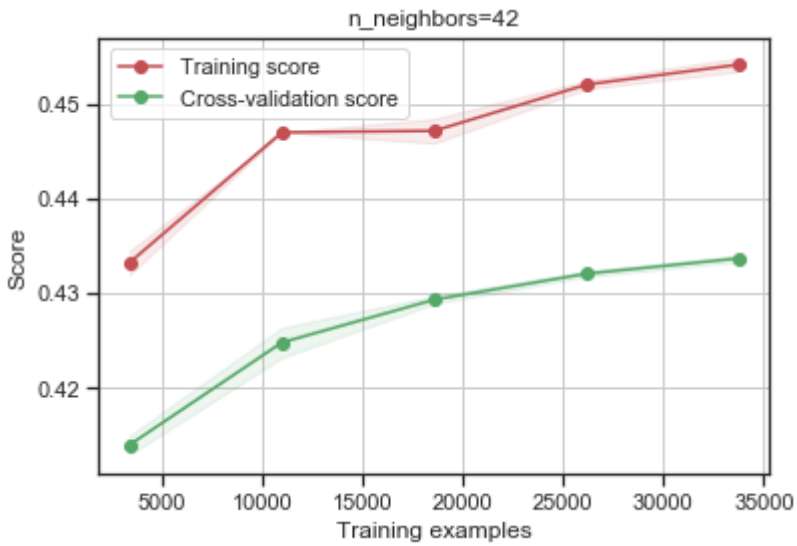
```
    plt.xlabel("Training examples")
    plt.ylabel("Score")
    train_sizes, train_scores, test_scores = learning_curve(
        estimator, x, y, cv=cv, n_jobs=n_jobs, train_sizes=train_sizes)
    train_scores_mean = np.mean(train_scores, axis=1)
    train_scores_std = np.std(train_scores, axis=1)
    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=0.1,
                     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 [381]:

```
plotlearn_curve(class_grid.best_estimator_, 'n_neighbors=42',
                    xtrain, ytrain.values.ravel(), cv=KFold(n_splits=3))
```

Out[381]:

```
<module 'matplotlib.pyplot' from '/Users/a.kurganova/Library/Python/
3.7/lib/python/site-packages/matplotlib/pyplot.py'>
```



In [382]:

```
def plotvalid_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 [383]:

```
plotvalid_curve(KNeighborsClassifier(), 'knn',
                      xtrain, ytrain.values.ravel(),
                      param_name='n_neighbors', param_range=n_neigh_values,
                      cv=KFold(n_splits=3), scoring="accuracy")
```

Out[383]:

```
<module 'matplotlib.pyplot' from '/Users/a.kurganova/Library/Python/
3.7/lib/python/site-packages/matplotlib/pyplot.py'>
```