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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. Описание задания

Цель лабораторной работы: изучение сложных способов подготовки выборки и подбора гиперпараметров на примере метода ближайших соседей.

# 2. 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.

# 3. Ход выполнения лабораторной работы

## 3.1. Выбор датасета

В качестве исходных данных выбираем датасет Heart Disease UCI (https://www.kaggle.com/ronitf/heart-disease-uci). 303 записи, 14 признаков, целевой признак относится к наличию болезни сердца у пациента: 0 - нет болезни сердца, 1 - есть.

```
In [0]: from google.colab import drive, files
        drive.mount('/content/drive')
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/con
```

```
In [0]: from google.colab import files
        import os
        import numpy as np
        import pandas as pd
        import seaborn as sns
        import matplotlib.pyplot as plt
        %matplotlib inline
        os.listdir()
        data = pd.read_csv('drive/My Drive/mmo_datasets/heart.csv',
                        sep=",", encoding="iso-8859-1")
```

In [0]:
```
total_count = data.shape[0]
num_cols = []
for col in data.columns:
    # Количество пустых значений
    temp_null_count = data[data[col].isnull()].shape[0]
    dt = str(data[col].dtype)
    if temp_null_count>0:
        num_cols.append(col)
        temp_perc = round((temp_null_count / total_count) * 100.0, 2)
        print('Колонка {}. Тип данных {}. Количество пустых значений {}, {}%.'
              .format(col, dt, temp_null_count, temp_perc))

data_cleared = data
```

In [0]:
```
uniquevalues = np.unique(data_cleared['target'].values)
uniquevalues
```

Out[0]: array([0, 1])

In [0]:
```
data_cleared.head(10)
```

Out[0]:

| | age | sex | cp | trestbps | chol | fbs | restecg | thalach | exang | oldpeak | slope \ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 63 | 1 | 3 | 145 | 233 | 1 | 0 | 150 | 0 | 2.3 | 0 |
| 1 | 37 | 1 | 2 | 130 | 250 | 0 | 1 | 187 | 0 | 3.5 | 0 |
| 2 | 41 | 0 | 1 | 130 | 204 | 0 | 0 | 172 | 0 | 1.4 | 2 |
| 3 | 56 | 1 | 1 | 120 | 236 | 0 | 1 | 178 | 0 | 0.8 | 2 |
| 4 | 57 | 0 | 0 | 120 | 354 | 0 | 1 | 163 | 1 | 0.6 | 2 |
| 5 | 57 | 1 | 0 | 140 | 192 | 0 | 1 | 148 | 0 | 0.4 | 1 |
| 6 | 56 | 0 | 1 | 140 | 294 | 0 | 0 | 153 | 0 | 1.3 | 1 |
| 7 | 44 | 1 | 1 | 120 | 263 | 0 | 1 | 173 | 0 | 0.0 | 2 |
| 8 | 52 | 1 | 2 | 172 | 199 | 1 | 1 | 162 | 0 | 0.5 | 2 |
| 9 | 57 | 1 | 2 | 150 | 168 | 0 | 1 | 174 | 0 | 1.6 | 2 |

| | ca | thal | target |
|---|---|---|---|
| 0 | 0 | 1 | 1 |
| 1 | 0 | 2 | 1 |
| 2 | 0 | 2 | 1 |
| 3 | 0 | 2 | 1 |
| 4 | 0 | 2 | 1 |
| 5 | 0 | 1 | 1 |
| 6 | 0 | 2 | 1 |
| 7 | 0 | 3 | 1 |
| 8 | 0 | 3 | 1 |
| 9 | 0 | 2 | 1 |

## 3.2. train_test_split

In [0]:
```
target = data_cleared['target']
data_cleared = data_cleared.drop('target', axis=1)
```

In [0]:
```
data_cleared.head(10)
```

```
Out[0]:    age  sex  cp  trestbps  chol  fbs  restecg  thalach  exang  oldpeak  slope  \
        0   63    1   3       145   233    1        0      150      0      2.3      0
        1   37    1   2       130   250    0        1      187      0      3.5      0
        2   41    0   1       130   204    0        0      172      0      1.4      2
        3   56    1   1       120   236    0        1      178      0      0.8      2
        4   57    0   0       120   354    0        1      163      1      0.6      2
        5   57    1   0       140   192    0        1      148      0      0.4      1
        6   56    0   1       140   294    0        0      153      0      1.3      1
        7   44    1   1       120   263    0        1      173      0      0.0      2
        8   52    1   2       172   199    1        1      162      0      0.5      2
        9   57    1   2       150   168    0        1      174      0      1.6      2

           ca  thal
        0   0     1
        1   0     2
        2   0     2
        3   0     2
        4   0     2
        5   0     1
        6   0     2
        7   0     3
        8   0     3
        9   0     2
```

```
In [0]: from sklearn.model_selection import train_test_split
        X_train, X_test, Y_train, Y_test = train_test_split(
            data_cleared,
            target,
            test_size=0.2,
            random_state=1
        )
```

```
In [0]: X_train.shape, Y_train.shape
```

```
Out[0]: ((242, 13), (242,))
```

```
In [0]: X_test.shape, Y_test.shape
```

```
Out[0]: ((61, 13), (61,))
```

## 3.3. Обучение для произвольного параметра K

```
In [0]: from sklearn.neighbors import KNeighborsRegressor, KNeighborsClassifier
```

```
In [0]: knn_model = KNeighborsClassifier(n_neighbors=5)
        knn_model.fit(X_train, Y_train)
        predicted = knn_model.predict(X_test)
        predicted
```

```
Out[0]: array([0, 1, 1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 0, 0,
               0, 1, 1, 1, 1, 1, 0, 0, 1, 1, 1, 1, 1, 1, 1, 0, 1, 0, 1, 0, 1, 0,
               1, 1, 1, 0, 1, 0, 1, 1, 0, 0, 1, 1, 1, 0, 1, 0, 0])
```

In [0]: 
```
from sklearn.metrics import accuracy_score
accuracy_score(Y_test, predicted)
```

Out[0]: 0.5737704918032787

In [0]: 
```
from sklearn.metrics import balanced_accuracy_score
balanced_accuracy_score(Y_test, predicted)
```

Out[0]: 0.5720430107526882

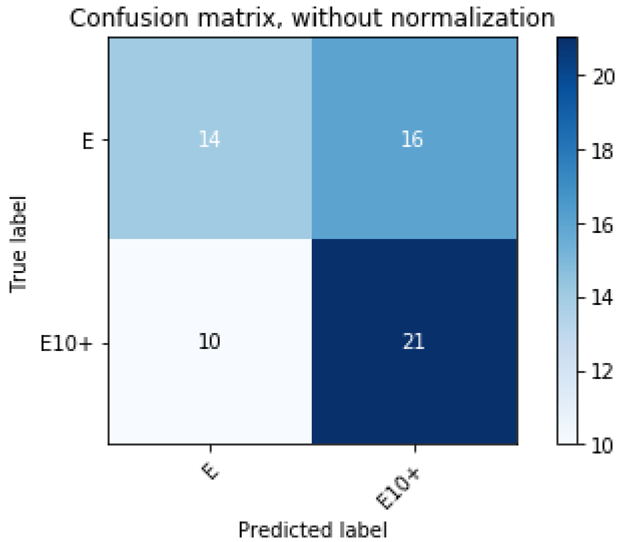
In [0]: 
```
# https://scikit-learn.org/stable/auto_examples/model_selection/plot_confusion_matrix
from sklearn.utils.multiclass import unique_labels
def plot_confusion_matrix(y_true, y_pred, classes,
                          normalize=False,
                          title=None,
                          cmap=plt.cm.Blues):
    """
    This function prints and plots the confusion matrix.
    Normalization can be applied by setting `normalize=True`.
    """
    if not title:
        if normalize:
            title = 'Normalized confusion matrix'
        else:
            title = 'Confusion matrix, without normalization'

    # Compute confusion matrix
    cm = confusion_matrix(y_true, y_pred)
    # Only use the labels that appear in the data
    classes = classes[unique_labels(y_true, y_pred)]
    if normalize:
        cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]
        print("Normalized confusion matrix")
    else:
        print('Confusion matrix, without normalization')

    fig, ax = plt.subplots()
    im = ax.imshow(cm, interpolation='nearest', cmap=cmap)
    ax.figure.colorbar(im, ax=ax)
    # We want to show all ticks...
    ax.set(xticks=np.arange(cm.shape[1]),
           yticks=np.arange(cm.shape[0]),
           # ... and label them with the respective list entries
           xticklabels=classes, yticklabels=classes,
           title=title,
           ylabel='True label',
           xlabel='Predicted label')

    # Rotate the tick labels and set their alignment.
    plt.setp(ax.get_xticklabels(), rotation=45, ha="right",
             rotation_mode="anchor")
```

```
    # Loop over data dimensions and create text annotations.
    fmt = '.2f' if normalize else 'd'
    thresh = cm.max() / 2.
    for i in range(cm.shape[0]):
        for j in range(cm.shape[1]):
            ax.text(j, i, format(cm[i, j], fmt),
                    ha="center", va="center",
                    color="white" if cm[i, j] > thresh else "black")
    fig.tight_layout()
    return ax
```

```
In [0]: plot_confusion_matrix(Y_test, predicted,
                              classes=np.array(['E', 'E10+', 'M', 'T']),
                              title='Confusion matrix, without normalization')
```

Confusion matrix, without normalization

Out[0]: <matplotlib.axes._subplots.AxesSubplot at 0x7f13d7451240>




```
In [0]: from sklearn.metrics import precision_score, recall_score, f1_score
        (precision_score(Y_test, predicted, average='weighted'),
         recall_score(Y_test, predicted, average='weighted'))
```

Out[0]: (0.5753212228622065, 0.5737704918032787)

```
In [0]: f1_score(Y_test, predicted, average='weighted')
```

Out[0]: 0.5688953176899175

### 3.4. Построение модели и оценка с помощью кросс-валидации

In [0]:
```
from sklearn.model_selection import KFold, ShuffleSplit, StratifiedShuffleSplit
from sklearn.model_selection import cross_val_score, cross_validate

scoring = {'precision': 'precision_weighted',
           'recall': 'recall_weighted',
           'f1': 'f1_weighted'}
```

In [0]:
```
scores1 = cross_validate(KNeighborsClassifier(n_neighbors=2),
                          data_cleared,
                          target,
                          scoring=scoring,
                          cv=KFold(n_splits=3),
                          return_train_score=True
                         )
scores1
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/metrics/classification.py:1145: UndefinedMetricW
  'recall', 'true', average, warn_for)
/usr/local/lib/python3.6/dist-packages/sklearn/metrics/classification.py:1145: UndefinedMetricW
  'recall', 'true', average, warn_for)
/usr/local/lib/python3.6/dist-packages/sklearn/metrics/classification.py:1145: UndefinedMetricW
  'recall', 'true', average, warn_for)
/usr/local/lib/python3.6/dist-packages/sklearn/metrics/classification.py:1145: UndefinedMetricW
  'recall', 'true', average, warn_for)
```

Out[0]:
```
{'fit_time': array([0.0035882 , 0.00298381, 0.00277495]),
 'score_time': array([0.01822829, 0.01480269, 0.0153482 ]),
 'test_f1': array([0.28813559, 0.55414336, 0.62585034]),
 'test_precision': array([1.        , 0.69316227, 1.        ]),
 'test_recall': array([0.16831683, 0.56435644, 0.45544554]),
 'train_f1': array([0.80387838, 0.79945524, 0.89967881]),
 'train_precision': array([0.86178676, 0.86071429, 0.93169995]),
 'train_recall': array([0.82673267, 0.80693069, 0.89108911])}
```

In [0]:
```
scores2 = cross_validate(KNeighborsClassifier(n_neighbors=2),
                          data_cleared,
                          target,
                          scoring=scoring,
                          cv=ShuffleSplit(n_splits=5, test_size=0.25),
                          return_train_score=True
                         )
scores2
```

Out[0]:
```
{'fit_time': array([0.00568986, 0.00283527, 0.00285411, 0.00288081, 0.0028367 ]),
 'score_time': array([0.01616049, 0.01285553, 0.01286197, 0.01299715, 0.0131793 ]),
 'test_f1': array([0.59090453, 0.43465982, 0.54309958, 0.49336384, 0.54641813]),
 'test_precision': array([0.65233425, 0.50489204, 0.55322831, 0.58439201, 0.62388664]),
 'test_recall': array([0.59210526, 0.44736842, 0.55263158, 0.52631579, 0.55263158]),
 'train_f1': array([0.77611602, 0.82921815, 0.78953072, 0.80197881, 0.77611602]),
```

```
 'train_precision': array([0.85151099, 0.87616921, 0.85960413, 0.86379331, 0.85151099]),
 'train_recall': array([0.78414097, 0.83259912, 0.79295154, 0.8061674 , 0.78414097])}
```

```
In [0]: scores3 = cross_validate(KNeighborsClassifier(n_neighbors=2),
                              data_cleared,
                              target,
                              scoring=scoring,
                              cv=StratifiedShuffleSplit(n_splits=5, test_size=0.2),
                              return_train_score=True
                             )
        scores3
```

```
Out[0]: {'fit_time': array([0.00362515, 0.00277042, 0.00277781, 0.00282669, 0.00318956]),
 'score_time': array([0.01695871, 0.01117134, 0.01135397, 0.01128387, 0.01146054]),
 'test_f1': array([0.61222806, 0.60401357, 0.61928718, 0.5710147 , 0.53801583]),
 'test_precision': array([0.66323471, 0.62287796, 0.64371954, 0.58848816, 0.55409836]),
 'test_recall': array([0.62295082, 0.60655738, 0.62295082, 0.57377049, 0.54098361]),
 'train_f1': array([0.81073333, 0.78385644, 0.79288886, 0.77931087, 0.80184646]),
 'train_precision': array([0.86803519, 0.85601355, 0.85991995, 0.85409652, 0.86392588]),
 'train_recall': array([0.81404959, 0.7892562 , 0.79752066, 0.78512397, 0.80578512])}
```

```
In [0]: print("%s, %s, %s" % (np.mean(scores1["test_precision"]),
                            np.mean(scores2["test_precision"]),
                            np.mean(scores3["test_precision"])))
```

```
0.8977207579912921, 0.5837466496118905, 0.6144837452406424
```

Лучшую точность модели получилось достичь с использованием стратегии кросс-валидации KFold.

## 3.5. Подбор гиперпараметра K с использованием GridSearchCV и кросс-валидации

```
In [0]: n_range = np.array(range(2,32,2))
        tuned_parameters = [{'n_neighbors': n_range}]
        tuned_parameters
```

```
Out[0]: [{'n_neighbors': array([ 2,  4,  6,  8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30])}]
```

```
In [0]: from sklearn.model_selection import GridSearchCV

        clf_gs = GridSearchCV(KNeighborsClassifier(),
                            tuned_parameters,
                            cv=ShuffleSplit(n_splits=5, test_size=0.25),
                            scoring='accuracy')
        clf_gs.fit(X_train, Y_train)
```

```
Out[0]: GridSearchCV(cv=ShuffleSplit(n_splits=5, random_state=None, test_size=0.25, train_s
       error_score='raise-deprecating',
       estimator=KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
           metric_params=None, n_jobs=None, n_neighbors=5, p=2,
```

```
               weights='uniform'),
             fit_params=None, iid='warn', n_jobs=None,
             param_grid=[{'n_neighbors': array([ 2,  4,  6,  8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28
             pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
             scoring='accuracy', verbose=0)
```

```
In [0]: clf_gs.best_params_
```

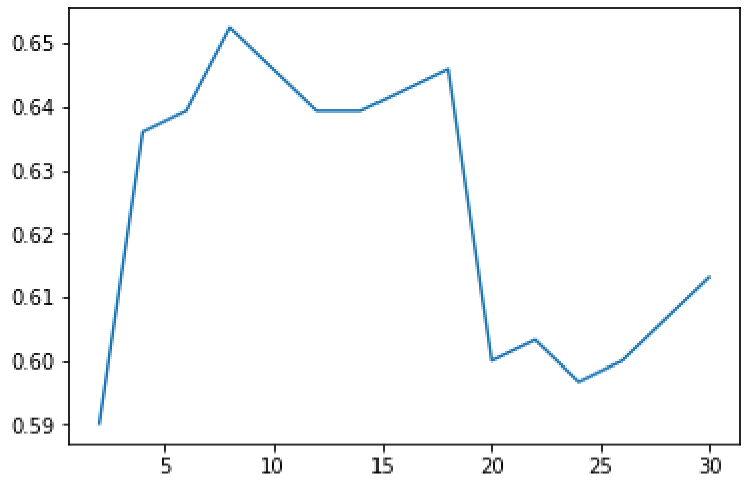
```
Out[0]: {'n_neighbors': 8}
```

```
In [0]: clf_gs.best_estimator_
```

```
Out[0]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
               metric_params=None, n_jobs=None, n_neighbors=8, p=2,
               weights='uniform')
```

```
In [0]: plt.plot(n_range, clf_gs.cv_results_['mean_test_score'])
```

```
Out[0]: [<matplotlib.lines.Line2D at 0x7f13d6f41940>]
```




## 3.6. Сравнение качества обучения моделей

```
In [0]: knn_best_model = KNeighborsClassifier(n_neighbors=24)
        knn_best_model.fit(X_train, Y_train)
        predicted_best = knn_best_model.predict(X_test)
        predicted_best
```

```
Out[0]: array([1, 1, 1, 1, 0, 1, 0, 1, 0, 1, 1, 0, 0, 0, 1, 1, 1, 0, 1, 0, 0, 0,
             0, 0, 1, 1, 0, 1, 1, 1, 1, 1, 1, 1, 0, 1, 0, 1, 1, 0, 1, 0, 1, 0,
             1, 1, 0, 1, 1, 0, 1, 1, 0, 0, 1, 1, 1, 0, 1, 0, 0])
```

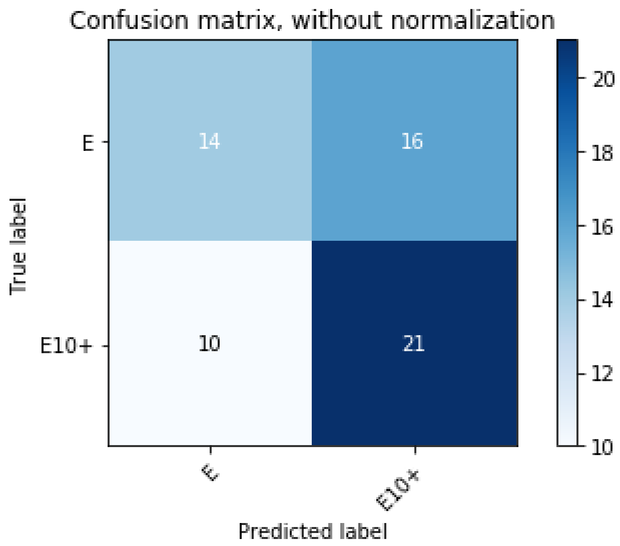
```
In [0]: (accuracy_score(Y_test, predicted),
         accuracy_score(Y_test, predicted_best))
```

```
Out[0]: (0.5737704918032787, 0.6557377049180327)
```

```
In [0]: plot_confusion_matrix(Y_test, predicted,
                              classes=np.array(['E', 'E10+', 'M', 'T']),
                              title='Confusion matrix, without normalization')
```

Confusion matrix, without normalization

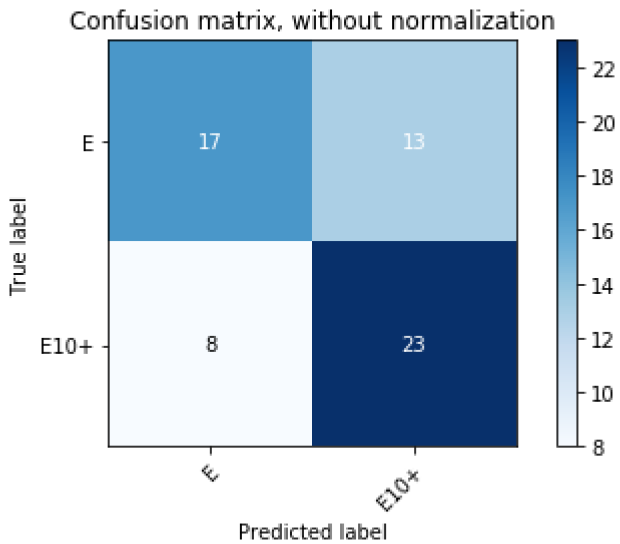
```
Out[0]: <matplotlib.axes._subplots.AxesSubplot at 0x7f13d6f4a320>
```




```
In [0]: plot_confusion_matrix(Y_test, predicted_best,
                              classes=np.array(['E', 'E10+', 'M', 'T']),
                              title='Confusion matrix, without normalization')
```

Confusion matrix, without normalization

```
Out[0]: <matplotlib.axes._subplots.AxesSubplot at 0x7f13d6eeacf8>
```



```
In [0]: (precision_score(Y_test, predicted, average='weighted'),
        precision_score(Y_test, predicted_best, average='weighted'))
```

```
Out[0]: (0.5753212228622065, 0.6591074681238616)
```

```
In [0]: (recall_score(Y_test, predicted, average='weighted'),
        recall_score(Y_test, predicted_best, average='weighted'))
```

```
Out[0]: (0.5737704918032787, 0.6557377049180327)
```

```
In [0]: (f1_score(Y_test, predicted, average='weighted'),
        f1_score(Y_test, predicted_best, average='weighted'))
```

```
Out[0]: (0.5688953176899175, 0.65293502680339)
```

Таким образом, подбор гиперпараметра позволил улучшить результаты оценки модели посредством всех представленных метрик.

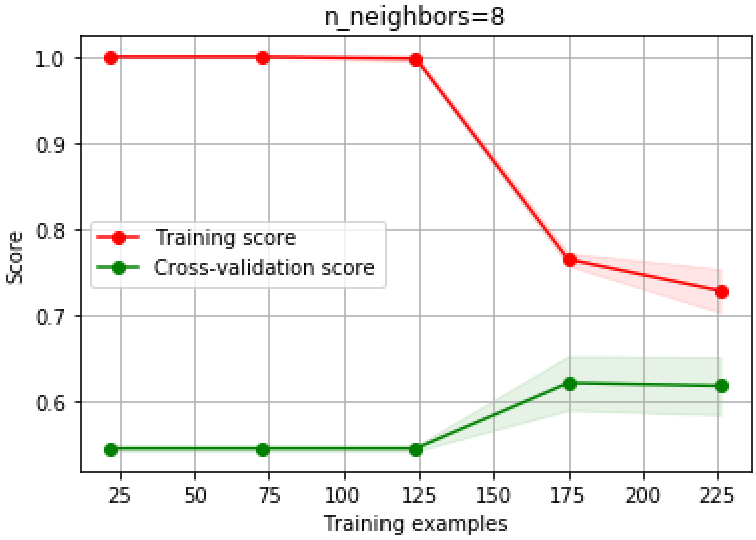
## 3.7. Кривые обучения и валидации

```
In [0]: from sklearn.model_selection import learning_curve, validation_curve


        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=0.1,
                             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

    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("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 [0]:
```
plot_learning_curve(KNeighborsClassifier(n_neighbors=8),
                    'n_neighbors=8',
                    data_cleared,
                    target,
                    cv=4
                   )
```

Out[0]:
```
<module 'matplotlib.pyplot' from '/usr/local/lib/python3.6/dist-packages/matplotlib/pyp
```




```
In [0]: n_range2 = np.array(range(2,24,2))

        plot_validation_curve(KNeighborsClassifier(), 'knn',
                              data_cleared,
                              target,
                              param_name='n_neighbors',
                              param_range=n_range2,
                              cv=4,
                              scoring="accuracy"
                             )
```

Out[0]: <module 'matplotlib.pyplot' from '/usr/local/lib/python3.6/dist-packages/matplotlib/pyp