ТМО ЛР3 ИУ5-63Б Горкунов Николай

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1 *ТМО ЛР3 ИУ5-63Б Горкунов Николай*

2 Подготовка обучающей и тестовой выборки, кросс-валидация и подбор гиперпараметров на примере метода ближайших соседей.

- Выберите набор данных (датасет) для решения задачи классификации или регрессии.
- В случае необходимости проведите удаление или заполнение пропусков и кодирование категориальных признаков.
- С использованием метода train_test_split разделите выборку на обучающую и тестовую.
- Обучите модель ближайших соседей для произвольно заданного гиперпараметра K. Оцените качество модели с помощью подходящих для задачи метрик.
- Произведите подбор гиперпараметра K с использованием GridSearchCV и RandomizedSearchCV и кросс-валидации, оцените качество оптимальной модели. Используйте не менее двух стратегий кросс-валидации.
- Сравните метрики качества исходной и оптимальной моделей.

3 Набор данных: Boston housing dataset

[1]:
```
import warnings
warnings.filterwarnings("ignore")
import pandas as pd
import numpy as np
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, mean_absolute_error
from sklearn.model_selection import GridSearchCV, RandomizedSearchCV
from sklearn.model_selection import cross_val_score, cross_validate
from sklearn.model_selection import KFold, RepeatedKFold, LeaveOneOut,␣
↪LeavePOut, ShuffleSplit, StratifiedKFold
import seaborn as sns
import time
import matplotlib.pyplot as plt
from kaggle.api.kaggle_api_extended import KaggleApi
pd.options.display.max_columns = None
```

[2]:
```
kaggle_api = KaggleApi()
kaggle_api.authenticate()
kaggle_api.dataset_download_files('altavish/boston-housing-dataset', unzip=True)
```

```
Dataset URL: https://www.kaggle.com/datasets/altavish/boston-housing-dataset
```

3.1 Смотрю, что в данных

[3]:
```
df = pd.read_csv('HousingData.csv')
print(df.shape)
df.head()
```

```
(506, 14)
```

[3]:
```
      CRIM    ZN  INDUS  CHAS    NOX     RM   AGE     DIS  RAD  TAX  PTRATIO  \
0  0.00632  18.0   2.31   0.0  0.538  6.575  65.2  4.0900    1  296     15.3
1  0.02731   0.0   7.07   0.0  0.469  6.421  78.9  4.9671    2  242     17.8
2  0.02729   0.0   7.07   0.0  0.469  7.185  61.1  4.9671    2  242     17.8
3  0.03237   0.0   2.18   0.0  0.458  6.998  45.8  6.0622    3  222     18.7
4  0.06905   0.0   2.18   0.0  0.458  7.147  54.2  6.0622    3  222     18.7

        B  LSTAT  MEDV
0  396.90   4.98  24.0
1  396.90   9.14  21.6
2  392.83   4.03  34.7
3  394.63   2.94  33.4
4  396.90    NaN  36.2
```

3.2 Проверяю типы данных

[4]:
```
df.dtypes
```

[4]:
```
CRIM       float64
ZN         float64
INDUS      float64
CHAS       float64
NOX        float64
RM         float64
AGE        float64
DIS        float64
RAD          int64
TAX          int64
PTRATIO    float64
B          float64
LSTAT      float64
MEDV       float64
dtype: object
```

3.3 Проверяю значения категориальных признаков

[5]:
```
df.CHAS.unique()
```

[5]:
```
array([ 0., nan,  1.])
```

3.4 Проверяю пропуски

[6]:
```
df.isna().sum()
```

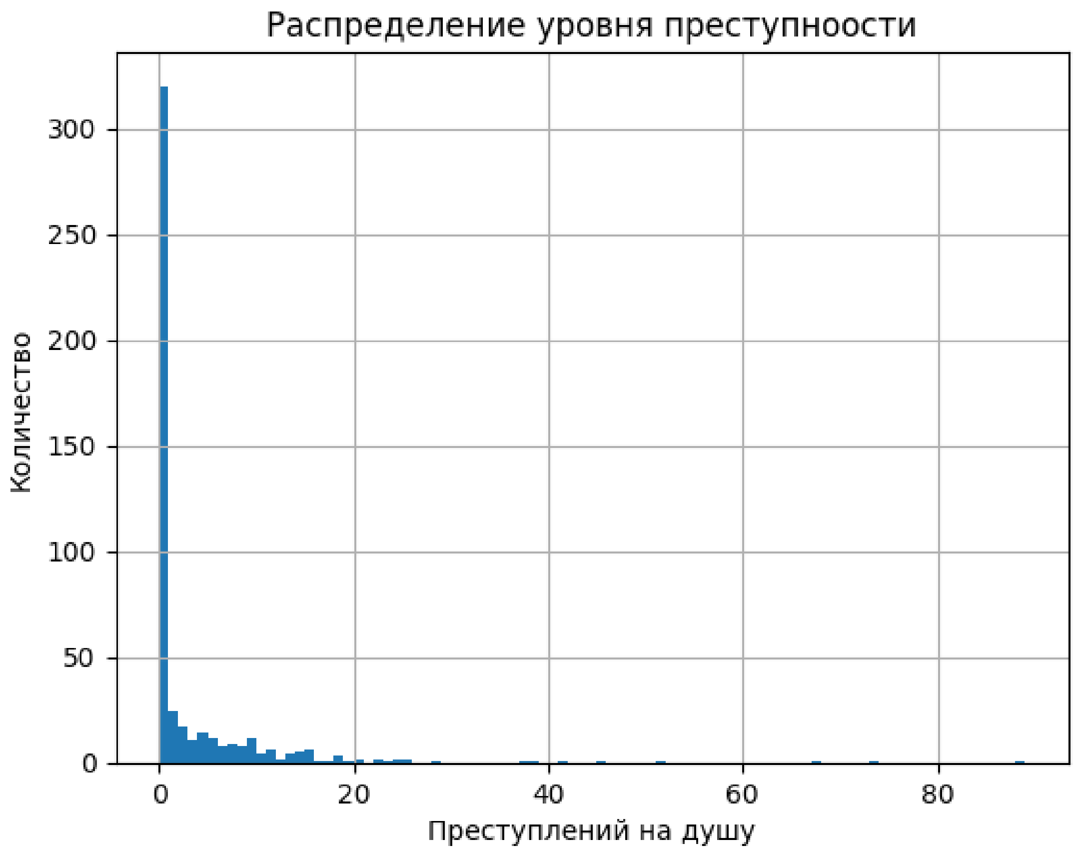
[6]:
```
CRIM       20
ZN         20
INDUS      20
CHAS       20
NOX         0
RM          0
AGE        20
DIS         0
RAD         0
TAX         0
PTRATIO     0
B           0
LSTAT      20
MEDV        0
dtype: int64
```

3.5 Заполняю пропуски в численном признаке "CRIM" в соответствии с описанием "CRIM - per capita crime rate by town"

[7]:
```
df[df.CRIM == 0]
```

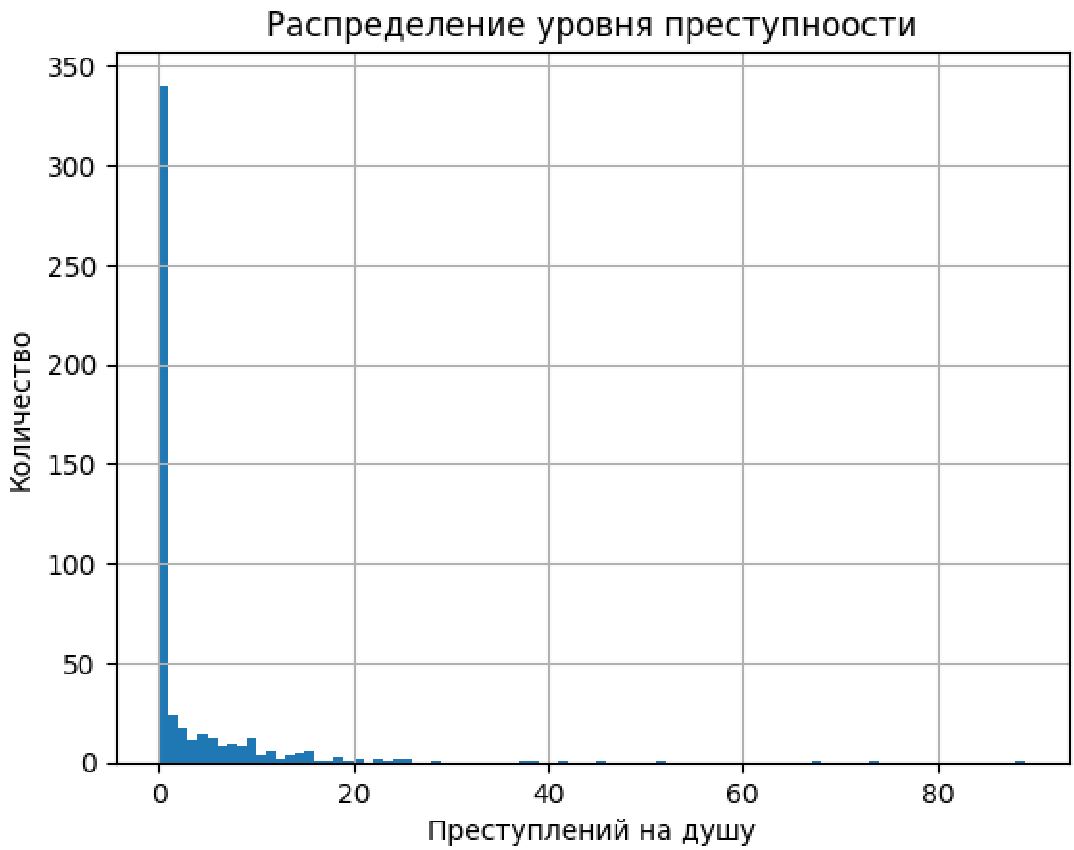
[7]:
```
Empty DataFrame
Columns: [CRIM, ZN, INDUS, CHAS, NOX, RM, AGE, DIS, RAD, TAX, PTRATIO, B, LSTAT,
MEDV]
Index: []
```

[8]:
```
df.CRIM.hist(bins=range(90))
plt.title('Распределение уровня преступноости')
plt.xlabel('Преступлений на душу')
plt.ylabel('Количество')
plt.show()
```



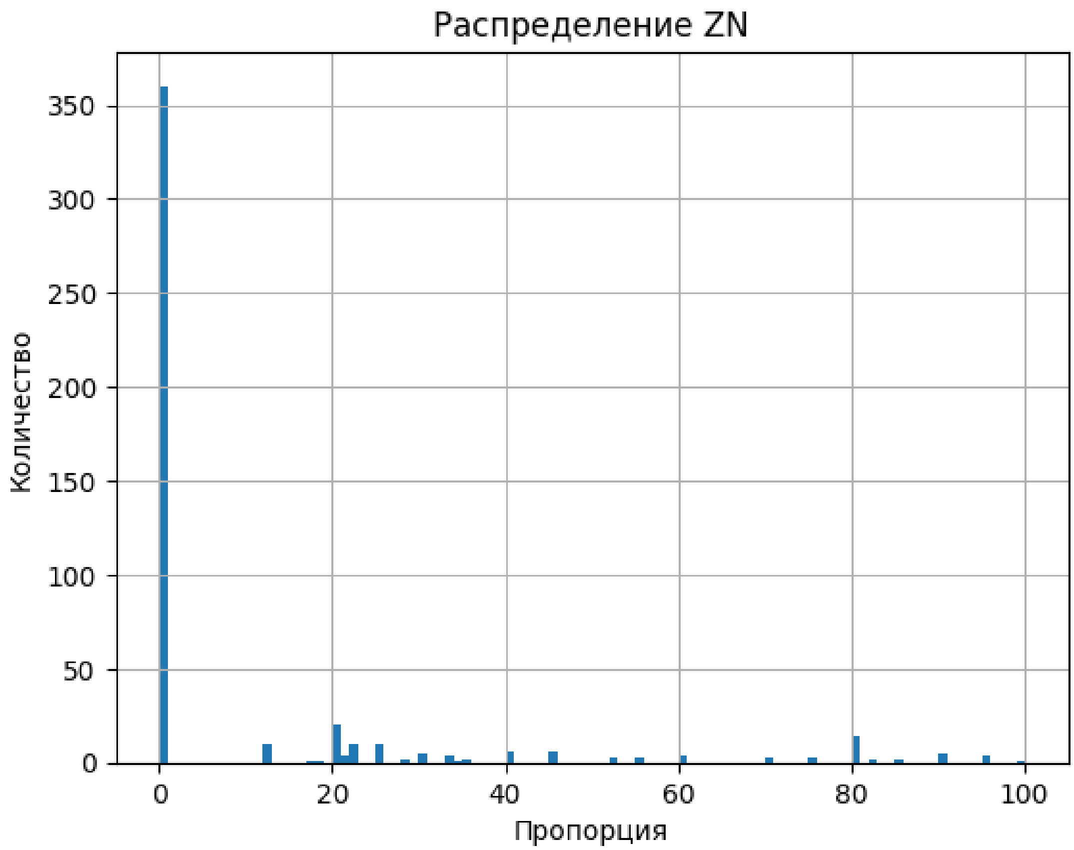
[9]:
```
df = df.fillna(value={"CRIM": 0})

df.CRIM.hist(bins=range(90))
plt.title('Распределение уровня преступноости')
plt.xlabel('Преступлений на душу')
plt.ylabel('Количество')
plt.show()
```



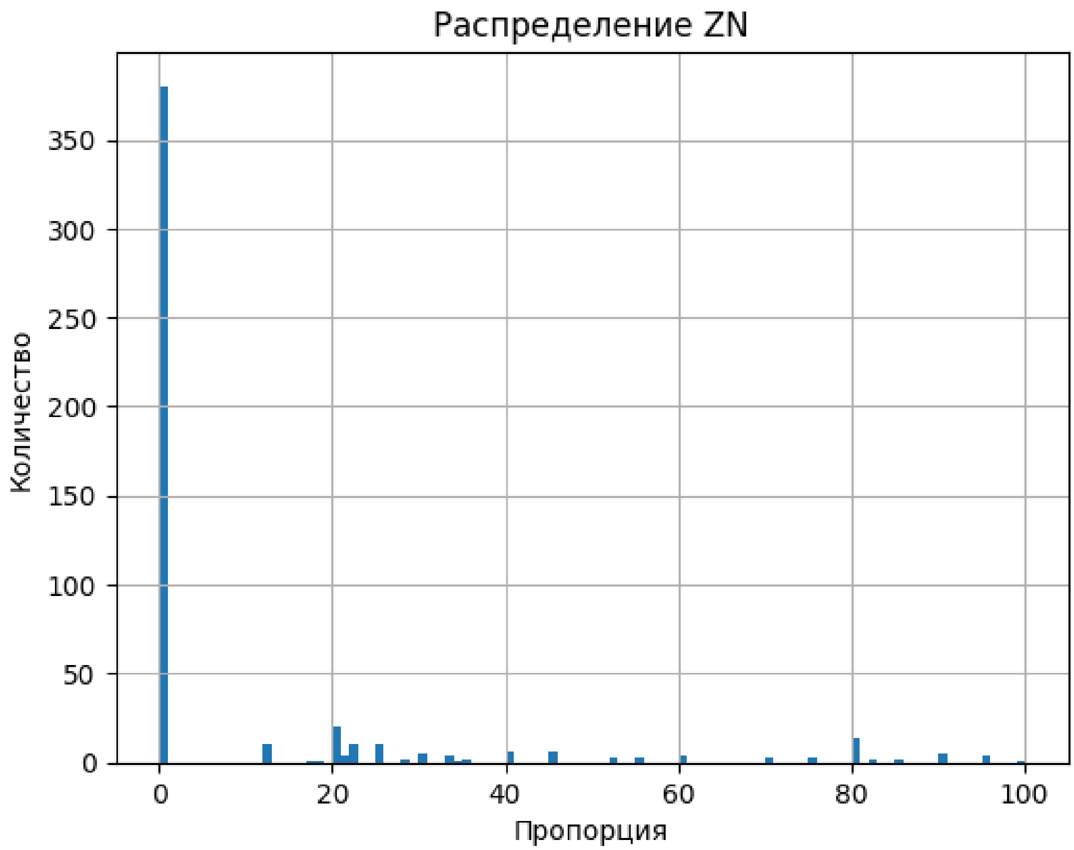
3.6 Заполняю пропуски в численном признаке "ZN" в соответствии с описанием "ZN - proportion of residential land zoned for lots over 25,000 sq.ft."

[10]:
```
df.ZN.hist(bins=range(101))
plt.title('Распределение ZN')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```



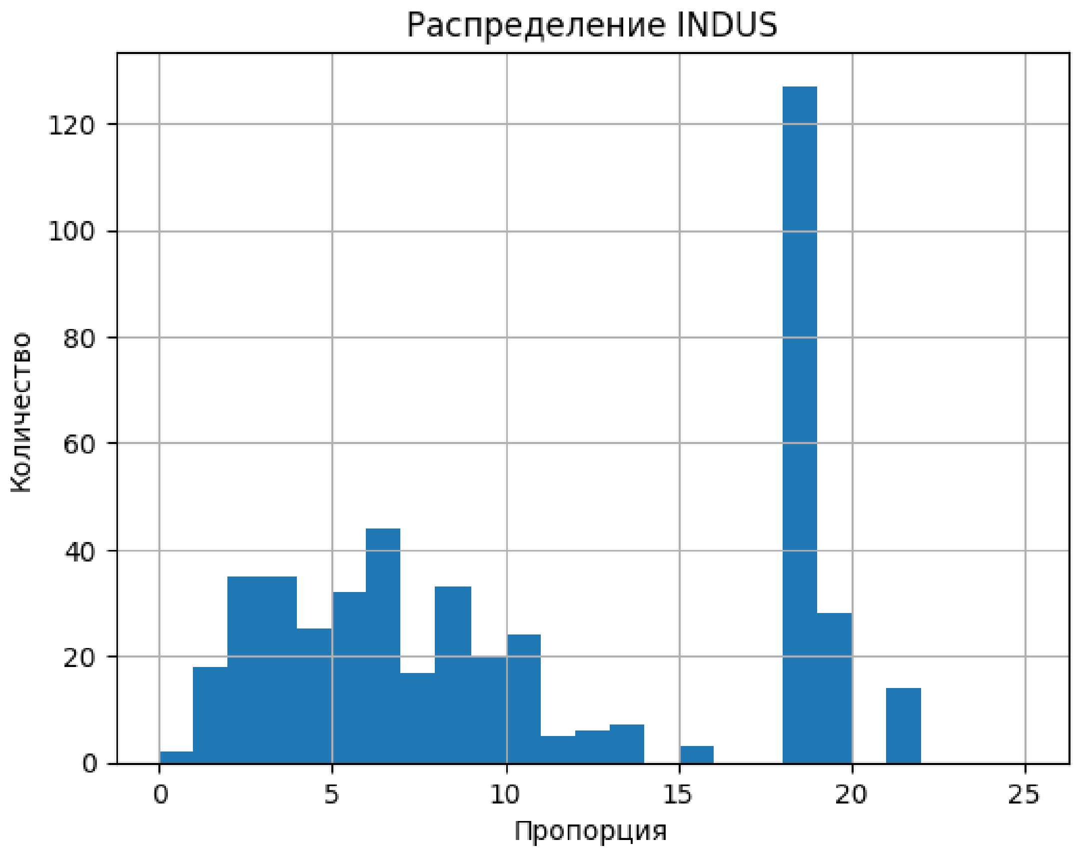
[11]:
```
df = df.fillna(value={"ZN": 0})

df.ZN.hist(bins=range(101))
plt.title('Распределение ZN')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```



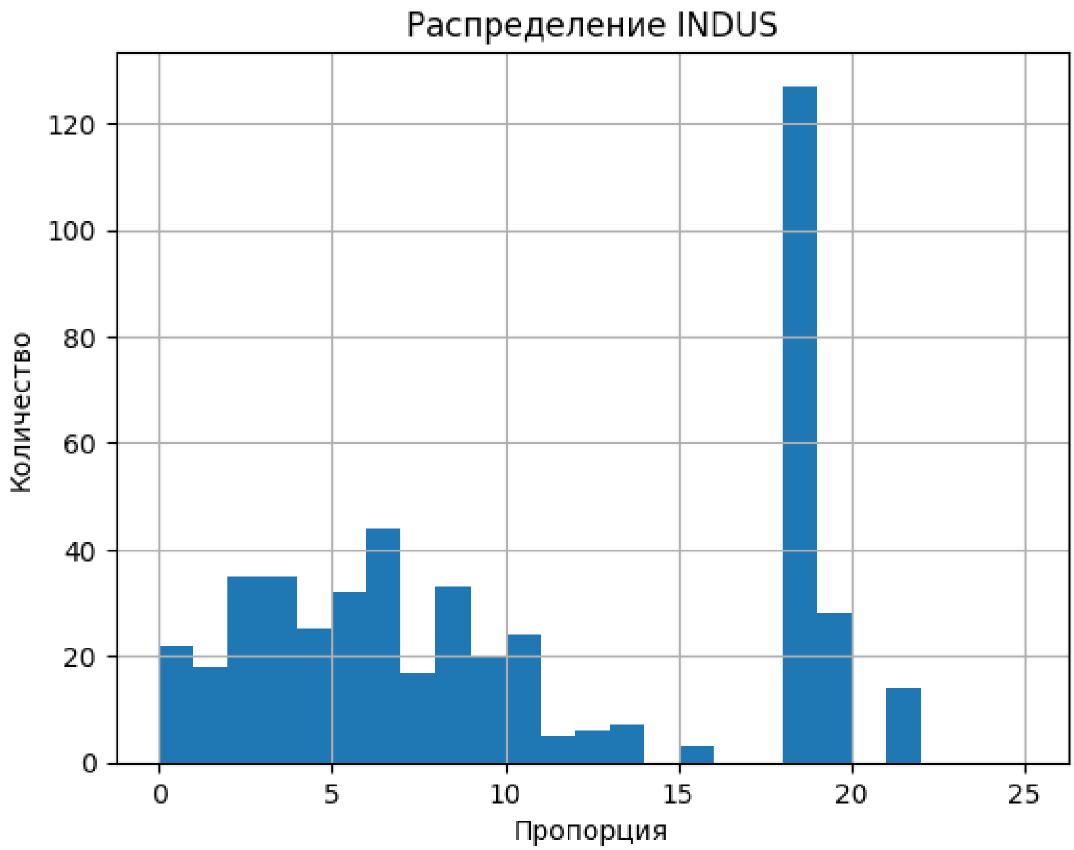
3.7 Заполняю пропуски в численном признаке "INDUS" в соответствии с описанием "INDUS - proportion of non-retail business acres per town."

[12]:
```
df.INDUS.hist(bins=range(26))
plt.title('Распределение INDUS')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```



[13]:
```
df = df.fillna(value={"INDUS": 0})

df.INDUS.hist(bins=range(26))
plt.title('Распределение INDUS')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```

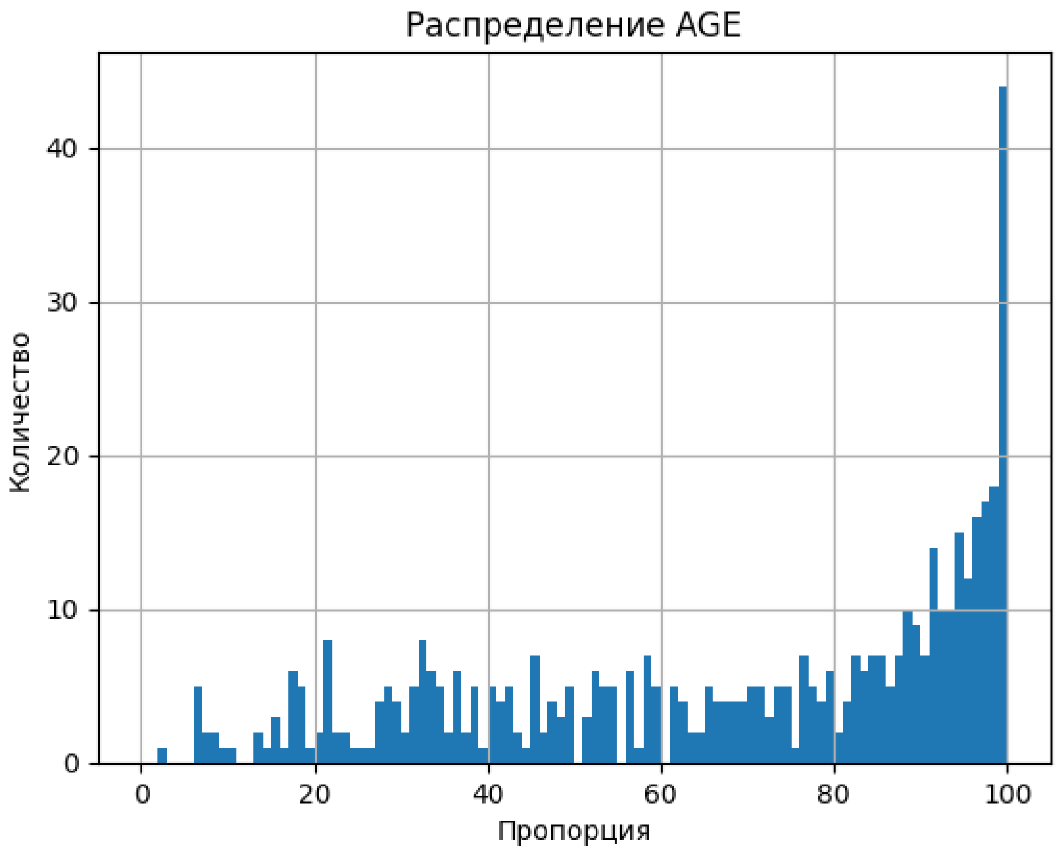


3.8 Не удаляю пропуски в категориальном признаке “CHAS” в соответствии с описанием “CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise)”

[14]:
```
df = df.fillna(value={"CHAS": 2})
```

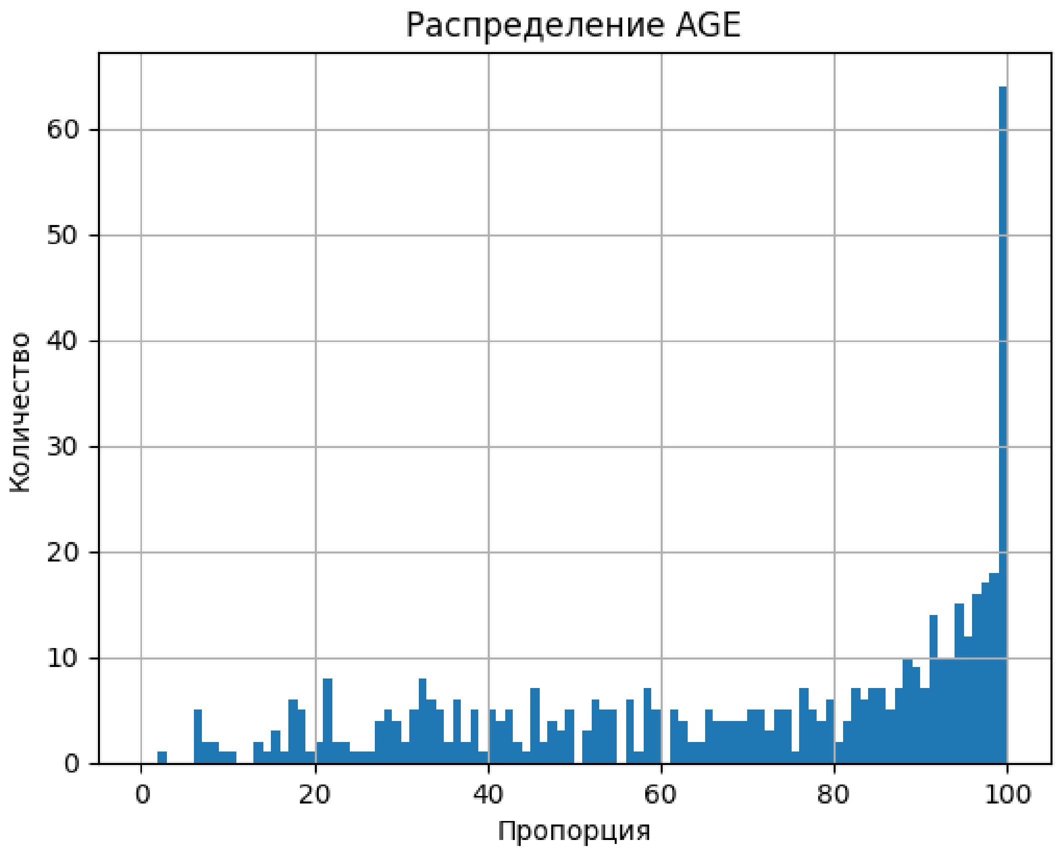
3.9 Заполняю пропуски в численном признаке “AGE” в соответствии с описанием “AGE - proportion of owner-occupied units built prior to 1940”

[15]:
```
df.AGE.hist(bins=range(101))
plt.title('Распределение AGE')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```



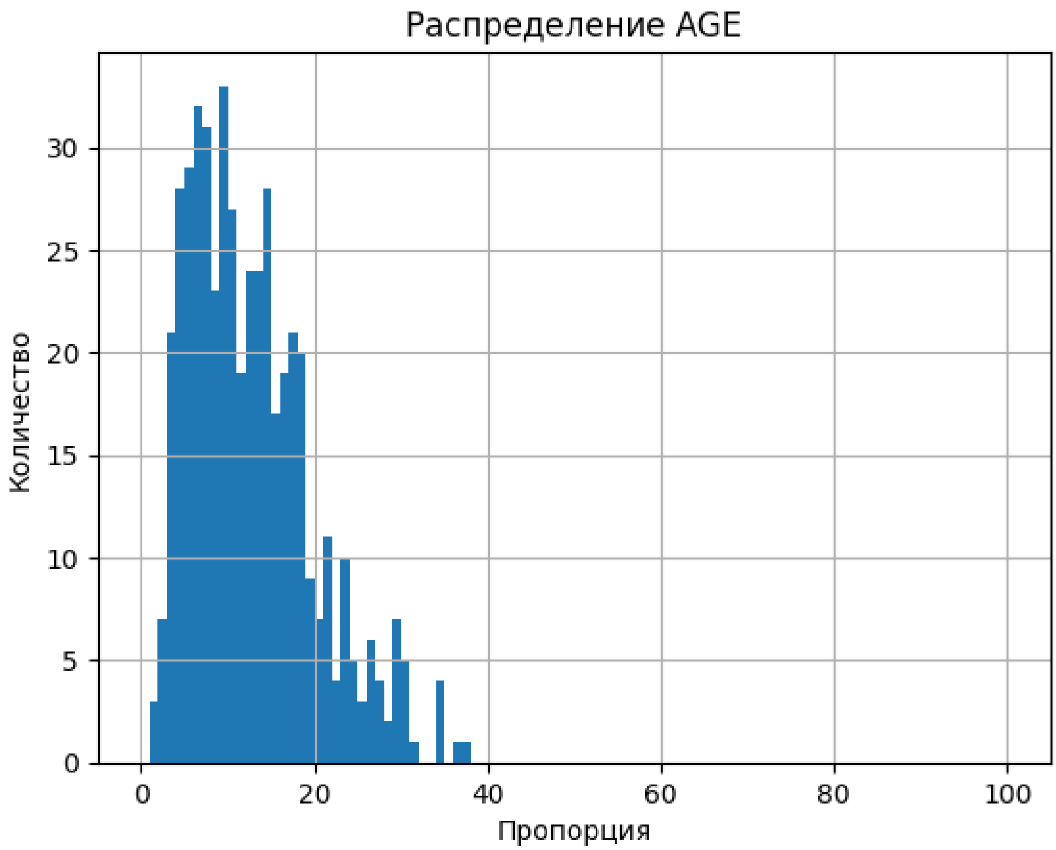
[16]:
```python
df = df.fillna(value={"AGE": 100})

df.AGE.hist(bins=range(101))
plt.title('Распределение AGE')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```



3.10 Заполняю пропуски в численном признаке “LSTAT” в соответствии с описанием “LSTAT - % lower status of the population”

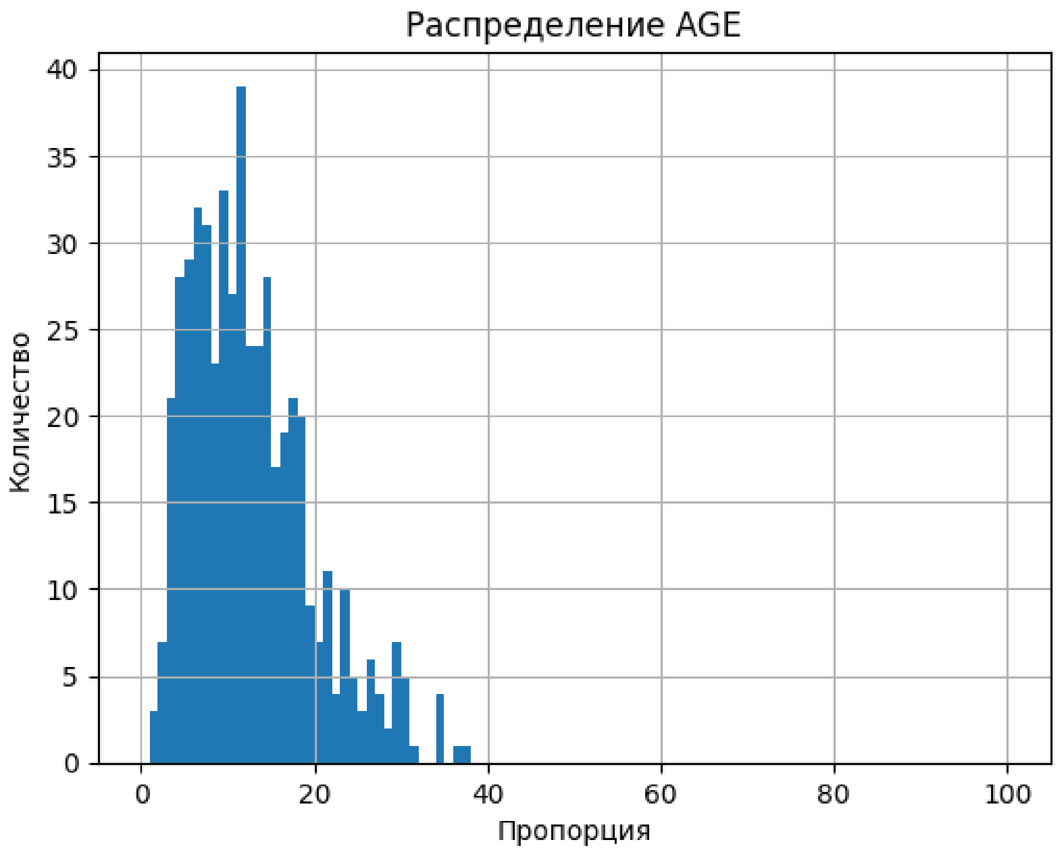
[17]:
```
df.LSTAT.hist(bins=range(101))
plt.title('Распределение AGE')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```



[18]:
```python
med = df.LSTAT.median()
print(med)
df = df.fillna(value={"LSTAT": int(med)})

df.LSTAT.hist(bins=range(101))
plt.title('Распределение AGE')
plt.xlabel('Пропорция')
plt.ylabel('Количество')
plt.show()
```

```
11.43
```



[19]:
```
df.isna().sum()
```

[19]:
```
CRIM       0
ZN         0
INDUS      0
CHAS       0
NOX        0
RM         0
AGE        0
DIS        0
RAD        0
TAX        0
PTRATIO    0
B          0
LSTAT      0
MEDV       0
dtype: int64
```

3.11 Преобразую категориальные признаки (one hot encoding)

[20]:
```
for to_enc in ["CHAS"]:
    one_hot = pd.get_dummies(df[to_enc]).astype(int)
    del df[to_enc]
    df = df.join(one_hot)
df.columns = df.columns.map(str)
df.head()
```

[20]:
```
      CRIM    ZN  INDUS    NOX     RM   AGE     DIS  RAD  TAX  PTRATIO  \
0  0.00632  18.0   2.31  0.538  6.575  65.2  4.0900    1  296     15.3
1  0.02731   0.0   7.07  0.469  6.421  78.9  4.9671    2  242     17.8
2  0.02729   0.0   7.07  0.469  7.185  61.1  4.9671    2  242     17.8
3  0.03237   0.0   2.18  0.458  6.998  45.8  6.0622    3  222     18.7
4  0.06905   0.0   2.18  0.458  7.147  54.2  6.0622    3  222     18.7

        B  LSTAT  MEDV  0.0  1.0  2.0
0  396.90   4.98  24.0    1    0    0
1  396.90   9.14  21.6    1    0    0
2  392.83   4.03  34.7    1    0    0
3  394.63   2.94  33.4    1    0    0
4  396.90  11.00  36.2    1    0    0
```

3.12 Провожу разделение на тестовую и обучающую выборки, обучаю и тестирую KNN для предсказания признака MEDV (регрессия), оцениваю с помощью MAE, MSE

[21]:
```
def exec_time(start, end):
   diff_time = end - start
   m, s = divmod(diff_time, 60)
   h, m = divmod(m, 60)
   s,m,h = int(round(s, 0)), int(round(m, 0)), int(round(h, 0))
   return("{0:02d}:{1:02d}:{2:02d}".format(h, m, s))
```

[22]:
```
y = df.MEDV.copy()
X = df.loc[:, df.columns != "MEDV"].copy()
```

[23]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33,␣
 ↪random_state=42)
```

[24]:
```
model = KNeighborsRegressor(n_neighbors=2)

start = time.time()
model.fit(X_train, y_train)
end = time.time()
fitTime = exec_time(start, end)
```

```python
start = time.time()
y_pred = model.predict(X_test)
end = time.time()
testTime = exec_time(start, end)

start = time.time()
y_train_pred = model.predict(X_train)
end = time.time()
trainTime = exec_time(start, end)

testMAE = mean_absolute_error(y_test, y_pred)
trainMAE = mean_absolute_error(y_train, y_train_pred)
testMSE = mean_squared_error(y_test, y_pred)
trainMSE = mean_squared_error(y_train, y_train_pred)
print("Test MAE = %.4f" % testMAE)
print("Train MAE = %.4f" % trainMAE)
print("Test MSE = %.4f" % testMSE)
print("Train MSE = %.4f" % trainMSE)
```

```
Test MAE = 4.7790
Train MAE = 2.5242
Test MSE = 43.3266
Train MSE = 14.9951
```

[25]:

```python
KNeighborsRegressorMAE = pd.DataFrame({
    "Train MAE" : [trainMAE],
    "Test MAE" : [testMAE],
    "Train MSE" : [trainMSE],
    "Test MSE" : [testMSE],
    "Fit time" : [fitTime],
    "Test time on train df" : [trainTime],
    "Test time on test df" : [testTime],
}, index=["KNeighborsRegressor"])
KNeighborsRegressorMAE
```

[25]:

```
                     Train MAE  Test MAE  Train MSE   Test MSE  Fit time  \
KNeighborsRegressor   2.524189  4.779042  14.995103  43.326647  00:00:00

                    Test time on train df Test time on test df
KNeighborsRegressor              00:00:00             00:00:00
```

3.13 Провожу подбор гиперпараметра K с использованием GridSearchCV и RandomizedSearchCV и кросс-валидации, оцениваю качество оптимальных моделей

3.13.1 GridSearchCV + KFold

[26]:
```
model = KNeighborsRegressor()

param_grid = {
    'n_neighbors': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
}

cv = KFold(n_splits=5, shuffle=True, random_state=42)

grid_search = GridSearchCV(estimator=model, param_grid=param_grid, cv=cv,␣
 ↪scoring='neg_mean_squared_error', n_jobs=-1)

#start = time.time()
grid_search.fit(X_train, y_train)
#end = time.time()
#fitTime = exec_time(start, end)

model = grid_search.best_estimator_

start = time.time()
model.fit(X_train, y_train)
end = time.time()
fitTime = exec_time(start, end)

start = time.time()
y_pred = model.predict(X_test)
end = time.time()
testTime = exec_time(start, end)

start = time.time()
y_train_pred = model.predict(X_train)
end = time.time()
trainTime = exec_time(start, end)

testMAE = mean_absolute_error(y_test, y_pred)
trainMAE = mean_absolute_error(y_train, y_train_pred)
testMSE = mean_squared_error(y_test, y_pred)
trainMSE = mean_squared_error(y_train, y_train_pred)
print("Test MAE = %.4f" % testMAE)
print("Train MAE = %.4f" % trainMAE)
print("Test MSE = %.4f" % testMSE)
print("Train MSE = %.4f" % trainMSE)
```

```
Test MAE = 4.5034
Train MAE = 3.7670
Test MSE = 37.5112
Train MSE = 29.1933
```

[27]:

```
KNeighborsRegressorGridSearchKFoldMAE = pd.DataFrame({
    "Train MAE" : [trainMAE],
    "Test MAE" : [testMAE],
    "Train MSE" : [trainMSE],
    "Test MSE" : [testMSE],
    "Fit time" : [fitTime],
    "Test time on train df" : [trainTime],
    "Test time on test df" : [testTime],
}, index=["KNeighborsRegressorGridSearchKFold"])
KNeighborsRegressorGridSearchKFoldMAE
```

[27]:

```
                                    Train MAE  Test MAE  Train MSE   Test MSE  \
KNeighborsRegressorGridSearchKFold   3.766962  4.503443  29.193296  37.511194

                                    Fit time Test time on train df  \
KNeighborsRegressorGridSearchKFold  00:00:00              00:00:00

                                   Test time on test df
KNeighborsRegressorGridSearchKFold             00:00:00
```

3.13.2 RandomizedSearchCV + RepeatedKFold

[28]:

```
model = KNeighborsRegressor()

param_grid = {
    'n_neighbors': range(1, 31)
}

cv = RepeatedKFold(n_splits=5, n_repeats=3, random_state=42)

random_search = RandomizedSearchCV(estimator=model,␣
 ↪param_distributions=param_grid, cv=cv, scoring='neg_mean_squared_error',␣
 ↪n_jobs=-1, random_state=42)

#start = time.time()
random_search.fit(X_train, y_train)
#end = time.time()
#fitTime = exec_time(start, end)

model = random_search.best_estimator_

start = time.time()
```

```python
model.fit(X_train, y_train)
end = time.time()
fitTime = exec_time(start, end)

start = time.time()
y_pred = model.predict(X_test)
end = time.time()
testTime = exec_time(start, end)

start = time.time()
y_train_pred = model.predict(X_train)
end = time.time()
trainTime = exec_time(start, end)

testMAE = mean_absolute_error(y_test, y_pred)
trainMAE = mean_absolute_error(y_train, y_train_pred)
testMSE = mean_squared_error(y_test, y_pred)
trainMSE = mean_squared_error(y_train, y_train_pred)
print("Test MAE = %.4f" % testMAE)
print("Train MAE = %.4f" % trainMAE)
print("Test MSE = %.4f" % testMSE)
print("Train MSE = %.4f" % trainMSE)
```

```
Test MAE = 4.6490
Train MAE = 4.4235
Test MSE = 40.5287
Train MSE = 39.3962
```

[29]:
```python
KNeighborsRegressorRandomizedSearchRepeatedKFoldMAE = pd.DataFrame({
    "Train MAE" : [trainMAE],
    "Test MAE" : [testMAE],
    "Train MSE" : [trainMSE],
    "Test MSE" : [testMSE],
    "Fit time" : [fitTime],
    "Test time on train df" : [trainTime],
    "Test time on test df" : [testTime],
}, index=["KNeighborsRegressorRandomizedSearchRepeatedKFold"])
KNeighborsRegressorRandomizedSearchRepeatedKFoldMAE
```

[29]:
```
                                                 Train MAE  Test MAE  \
KNeighborsRegressorRandomizedSearchRepeatedKFold     4.4235  4.649035

                                                 Train MSE   Test MSE  \
KNeighborsRegressorRandomizedSearchRepeatedKFold 39.396214  40.528699

                                                 Fit time  \
KNeighborsRegressorRandomizedSearchRepeatedKFold 00:00:00
```

```
                                              Test time on train df  \
KNeighborsRegressorRandomizedSearchRepeatedKFold             00:00:00

                                              Test time on test df
KNeighborsRegressorRandomizedSearchRepeatedKFold            00:00:00
```

3.14 Провожу сравнение исходной и оптимальной моделей

[30]:
```python
AllMAE = pd.concat([KNeighborsRegressorMAE,␣
↪KNeighborsRegressorRandomizedSearchRepeatedKFoldMAE,␣
↪KNeighborsRegressorGridSearchKFoldMAE])
AllMAE.sort_values(by=["Test MSE"])
```

[30]:
```
                                                Train MAE  Test MAE  \
KNeighborsRegressorGridSearchKFold               3.766962  4.503443
KNeighborsRegressorRandomizedSearchRepeatedKFold  4.423500  4.649035
KNeighborsRegressor                              2.524189  4.779042

                                                Train MSE   Test MSE  \
KNeighborsRegressorGridSearchKFold              29.193296  37.511194
KNeighborsRegressorRandomizedSearchRepeatedKFold 39.396214  40.528699
KNeighborsRegressor                             14.995103  43.326647

                                                Fit time  \
KNeighborsRegressorGridSearchKFold              00:00:00
KNeighborsRegressorRandomizedSearchRepeatedKFold 00:00:00
KNeighborsRegressor                             00:00:00

                                              Test time on train df  \
KNeighborsRegressorGridSearchKFold                           00:00:00
KNeighborsRegressorRandomizedSearchRepeatedKFold             00:00:00
KNeighborsRegressor                                          00:00:00

                                              Test time on test df
KNeighborsRegressorGridSearchKFold                          00:00:00
KNeighborsRegressorRandomizedSearchRepeatedKFold            00:00:00
KNeighborsRegressor                                         00:00:00
```