mohs-hardness-prediction

December 10, 2023

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import plotly.express as px
from sklearn.preprocessing import StandardScaler, LabelEncoder
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression , Ridge , Lasso
from sklearn.metrics import mean_squared_error,r2_score
from sklearn.metrics import mean_absolute_error , r2_score
from xgboost import XGBRegressor
import warnings
warnings.filterwarnings('ignore')
```

EDA

[2]:
```
df=pd.read_csv("/content/train.csv")
df.shape
```

[2]:
```
(10407, 13)
```

[3]:
```
df.head()
```

[3]:
```
   id  allelectrons_Total  density_Total  allelectrons_Average  val_e_Average  \
0   0               100.0       0.841611                  10.0            4.8
1   1               100.0       7.558488                  10.0            4.8
2   2                76.0       8.885992                  15.6            5.6
3   3               100.0       8.795296                  10.0            4.8
4   4               116.0       9.577996                  11.6            4.8

   atomicweight_Average  ionenergy_Average  el_neg_chi_Average  \
0             20.612526           11.08810               2.766
1             20.298893           12.04083               2.755
2             33.739258           12.08630               2.828
3             20.213349           10.94850               2.648
4             24.988133           11.82448               2.766

   R_vdw_element_Average  R_cov_element_Average  zaratio_Average  \
```

```
0                 1.732                 0.860         0.496070
1                 1.631                 0.910         0.492719
2                 1.788                 0.864         0.481478
3                 1.626                 0.936         0.489272
4                 1.682                 0.896         0.492736

   density_Average  Hardness
0          0.91457       6.0
1          0.71760       6.5
2          1.50633       2.5
3          0.78937       6.0
4          1.86481       6.0
```

[4]:
```
df.tail()
```

[4]:
```
          id  allelectrons_Total  density_Total  allelectrons_Average  \
10402  10402               128.0       7.558488             12.000000
10403  10403                30.0       1.743160             10.000000
10404  10404               196.0      30.920000             24.500000
10405  10405                38.0       1.553160             12.666667
10406  10406               288.0      24.655328             11.142857

       val_e_Average  atomicweight_Average  ionenergy_Average  \
10402       4.000000             26.385218          11.330440
10403       5.333333             20.766935          14.163933
10404       5.500000             53.490297          10.074300
10405       4.666667             26.621687          11.290033
10406       4.571429             22.536126          10.960357

       el_neg_chi_Average  R_vdw_element_Average  R_cov_element_Average  \
10402            2.644000               1.631000               0.892000
10403            3.090000               1.556667               0.866667
10404            2.295000               1.545000               1.120000
10405            2.743333               1.756667               0.980000
10406            2.792143               1.772857               0.940000

       zaratio_Average  density_Average  Hardness
10402         0.496070          1.79607       4.0
10403         0.480390          0.81480       5.0
10404         0.469715          2.11540       1.8
10405         0.486507          0.77755       6.0
10406         0.493919          0.97737       6.5
```

[5]:
```
df.columns.to_list()
```

[5]:
```
['id',
 'allelectrons_Total',
```

```
 'density_Total',
 'allelectrons_Average',
 'val_e_Average',
 'atomicweight_Average',
 'ionenergy_Average',
 'el_neg_chi_Average',
 'R_vdw_element_Average',
 'R_cov_element_Average',
 'zaratio_Average',
 'density_Average',
 'Hardness']
```

[6]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 10407 entries, 0 to 10406
Data columns (total 13 columns):
 #   Column                 Non-Null Count  Dtype
---  ------                 --------------  -----
 0   id                     10407 non-null  int64
 1   allelectrons_Total     10407 non-null  float64
 2   density_Total          10407 non-null  float64
 3   allelectrons_Average   10407 non-null  float64
 4   val_e_Average          10407 non-null  float64
 5   atomicweight_Average   10407 non-null  float64
 6   ionenergy_Average      10407 non-null  float64
 7   el_neg_chi_Average     10407 non-null  float64
 8   R_vdw_element_Average  10407 non-null  float64
 9   R_cov_element_Average  10407 non-null  float64
 10  zaratio_Average        10407 non-null  float64
 11  density_Average        10407 non-null  float64
 12  Hardness               10407 non-null  float64
dtypes: float64(12), int64(1)
memory usage: 1.0 MB
```

[7]:
```
df.isna().sum()
```

[7]:
```
id                     0
allelectrons_Total     0
density_Total          0
allelectrons_Average   0
val_e_Average          0
atomicweight_Average   0
ionenergy_Average      0
el_neg_chi_Average     0
R_vdw_element_Average  0
R_cov_element_Average  0
```

```
zaratio_Average          0
density_Average          0
Hardness                 0
dtype: int64
```

[8]:
```
df.duplicated().sum()
```

[8]:
```
0
```

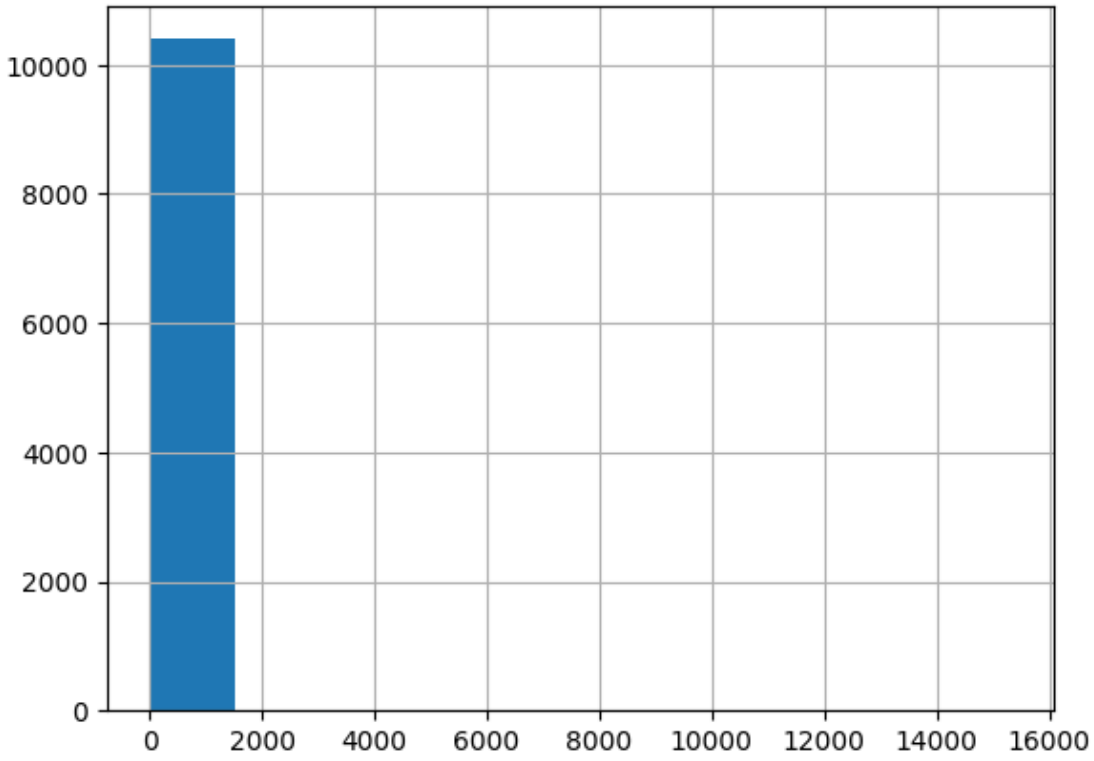
[9]:
```
df.describe()
```

[9]:
```
                id  allelectrons_Total  density_Total  allelectrons_Average  \
count  10407.00000        10407.000000   10407.000000          10407.000000
mean    5203.00000          128.053516      14.491342             17.033222
std     3004.38646          224.123776      15.972877             10.468734
min        0.00000            0.000000       0.000000              0.000000
25%     2601.50000           68.000000       7.558488             10.000000
50%     5203.00000          100.000000      10.650000             12.600000
75%     7804.50000          131.000000      16.676996             22.000000
max    10406.00000        15300.000000     643.093804             67.000000

       val_e_Average  atomicweight_Average  ionenergy_Average  \
count   10407.000000          10407.000000       10407.000000
mean        4.546789             37.507703          10.938308
std         0.690864             26.012313           1.408276
min         0.000000              0.000000           0.000000
25%         4.000000             20.298893          10.590660
50%         4.714286             26.203827          11.202760
75%         4.800000             48.719500          11.670725
max         6.000000            167.400000          15.245810

       el_neg_chi_Average  R_vdw_element_Average  R_cov_element_Average  \
count        10407.000000           10407.000000           10407.000000
mean             2.607662               1.731330               0.944132
std              0.334906               0.192481               0.180017
min              0.000000               0.000000               0.000000
25%              2.530000               1.672500               0.864000
50%              2.706000               1.732727               0.915556
75%              2.805000               1.800000               0.981667
max              3.443000               2.250000               1.615840

       zaratio_Average  density_Average      Hardness
count     10407.000000     10407.000000  10407.000000
mean          0.493349         2.132984      4.647126
std           0.063080         1.936656      1.680525
min           0.000000         0.000000      1.000000
25%           0.476196         0.814800      3.000000
```

```
50%          0.488550          1.351550       5.500000
75%          0.496070          2.741550       6.000000
max          0.825990         10.970000      10.000000
```

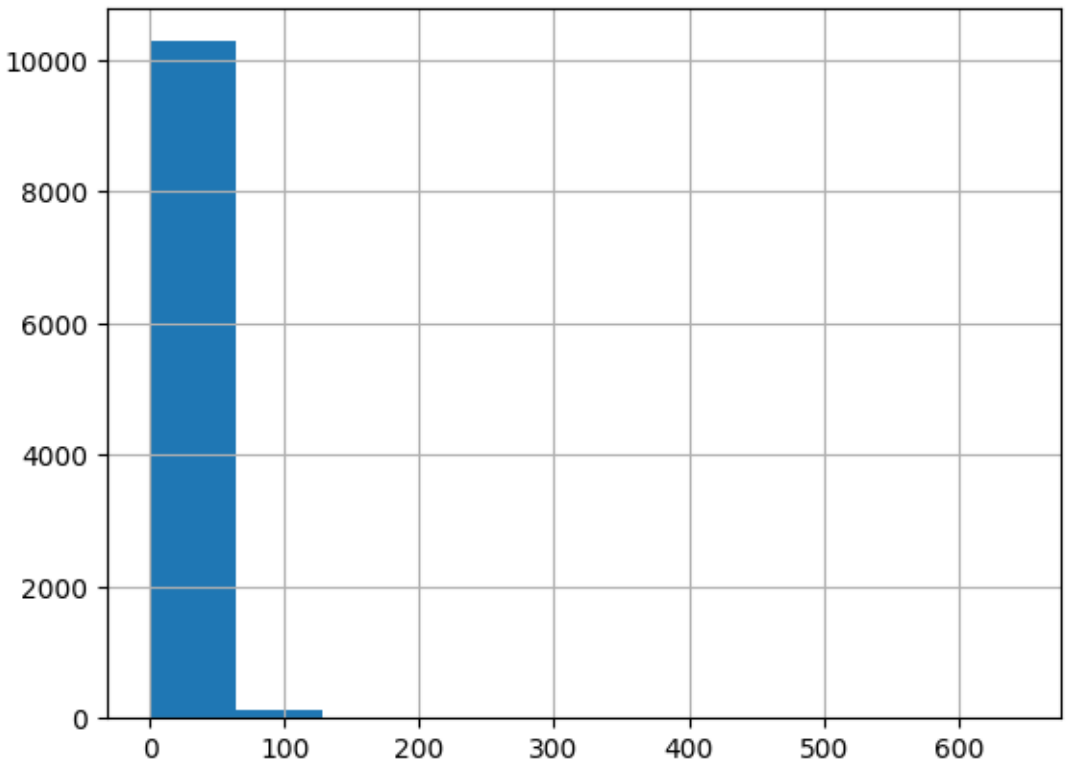
[11]:
```
df['allelectrons_Total'].hist()
```

[11]: <Axes: >



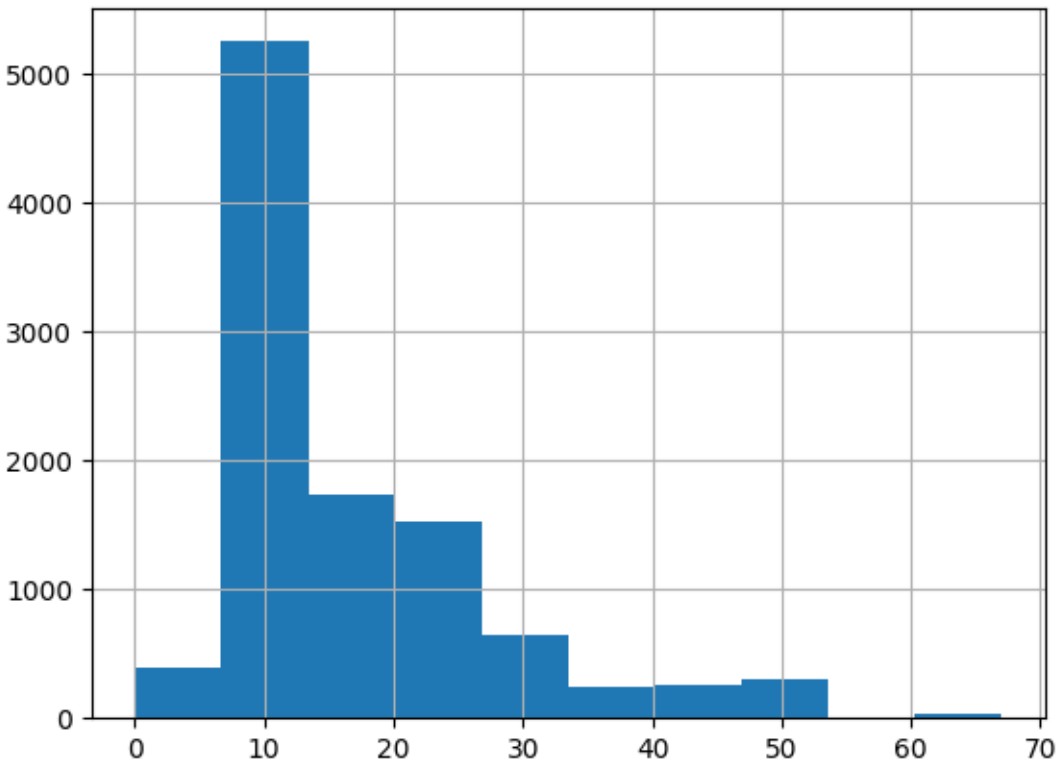
[12]:
```
df['density_Total'].hist()
```

[12]: <Axes: >



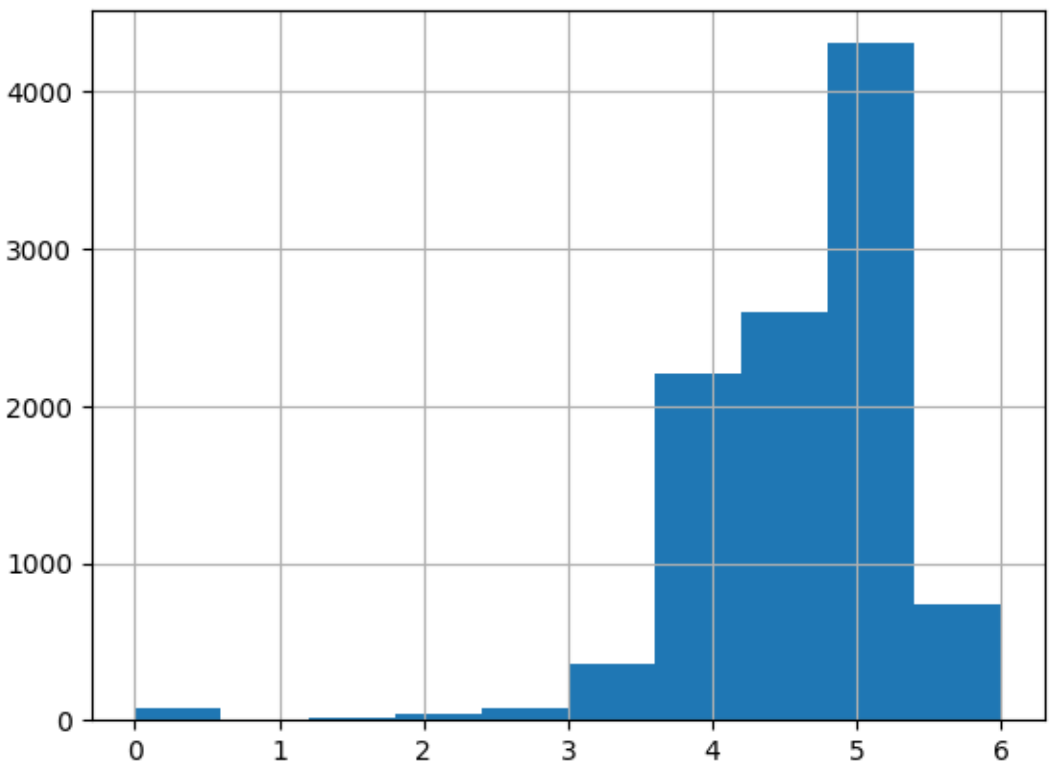
[13]:
```
df['allelectrons_Average'].hist()
```

[13]: <Axes: >



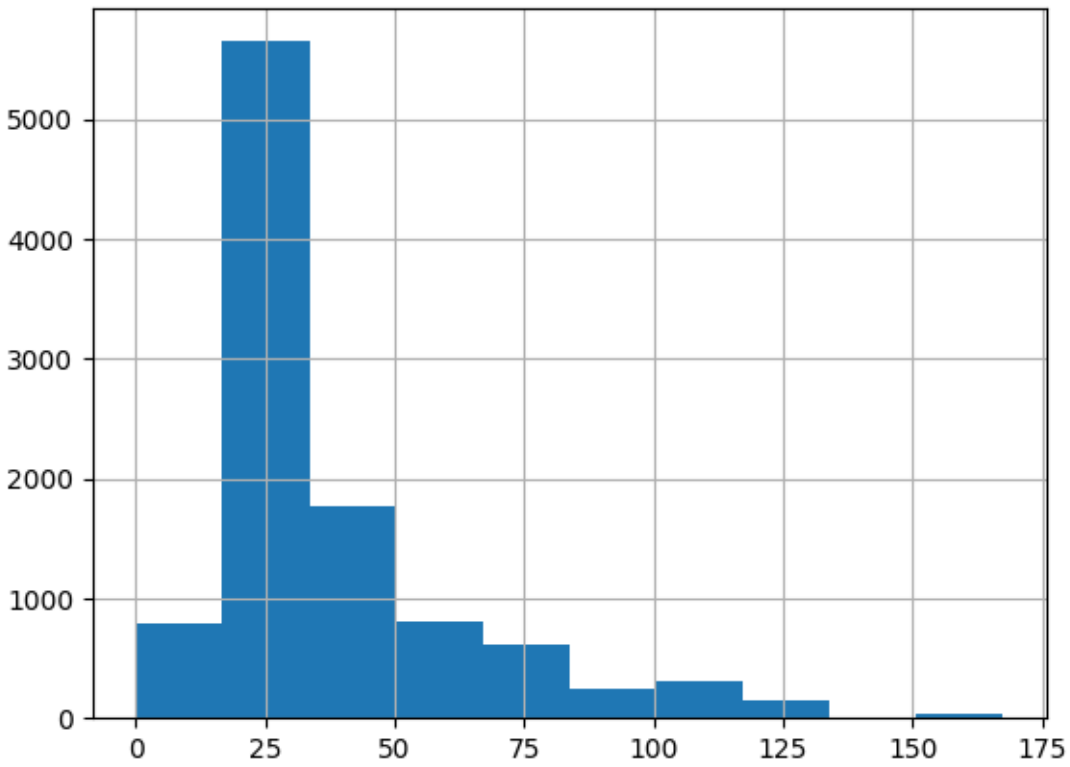
[14]:
```
df['val_e_Average'].hist()
```

[14]: <Axes: >



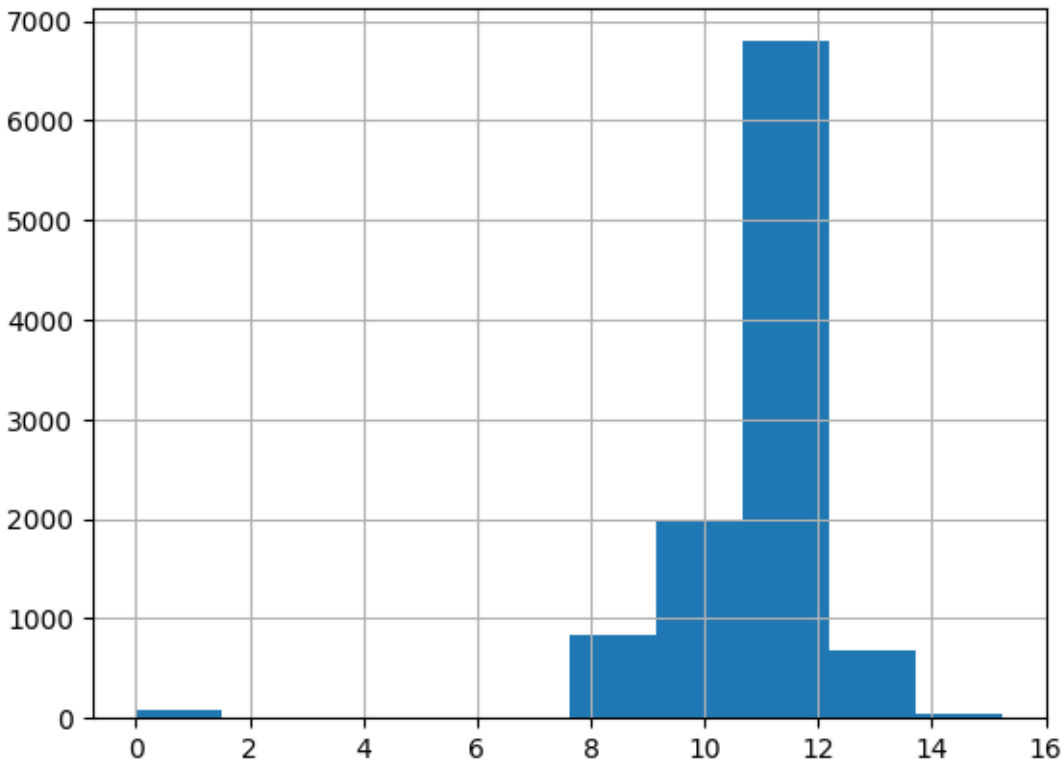
[15]:
```
df['atomicweight_Average'].hist()
```

[15]: <Axes: >



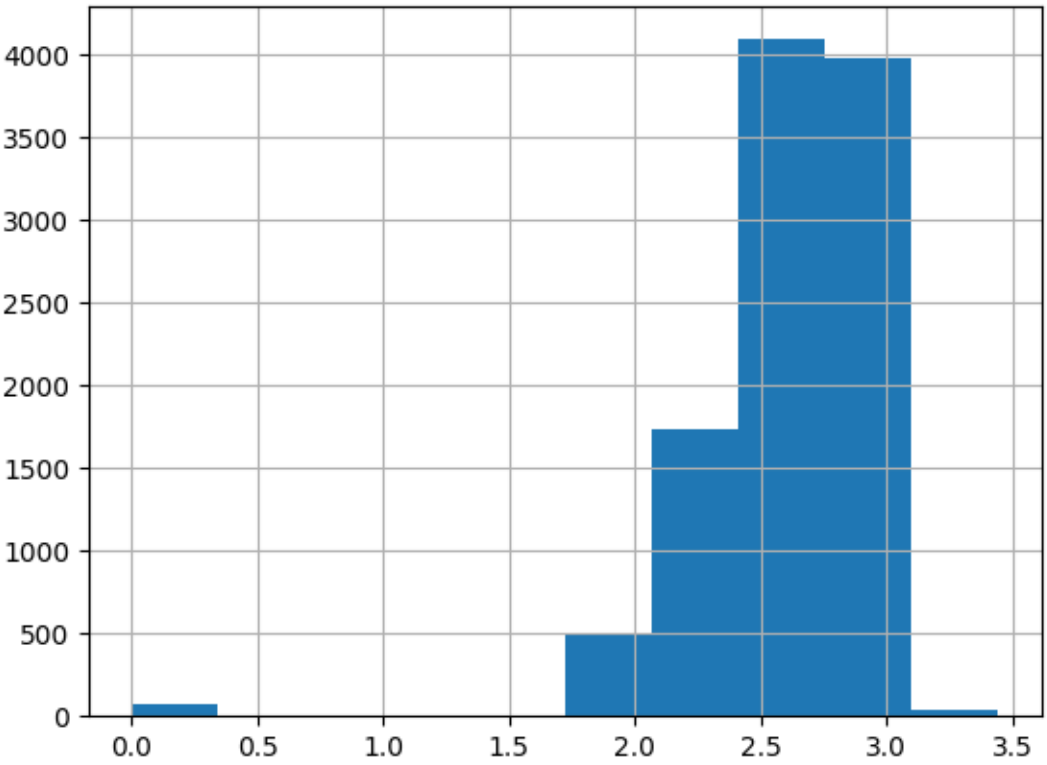
[16]:
```
df['ionenergy_Average'].hist()
```

[16]: <Axes: >



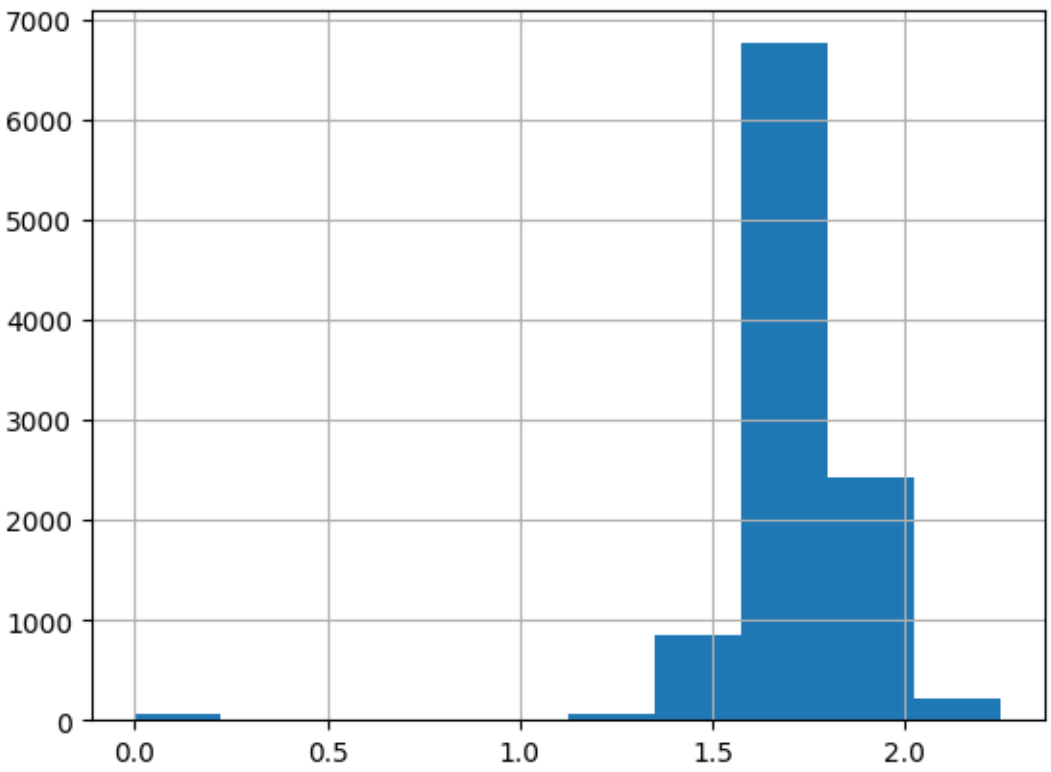
[17]:
```
df['el_neg_chi_Average'].hist()
```

[17]: <Axes: >



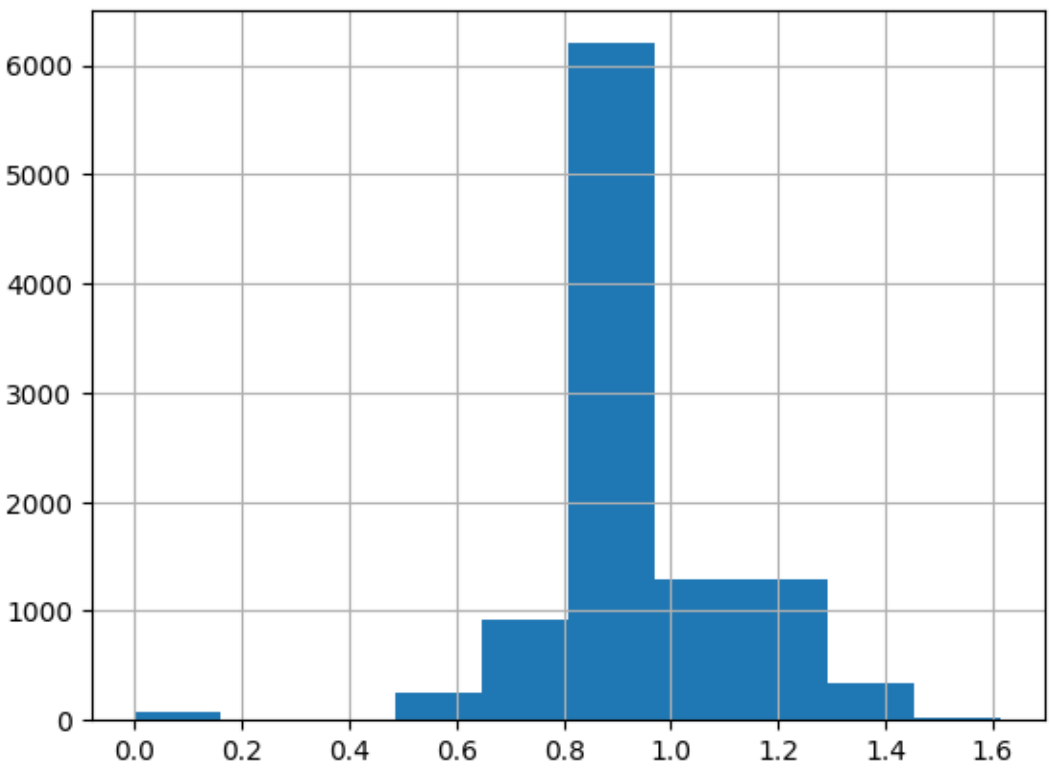
[18]:
```
df['R_vdw_element_Average'].hist()
```

[18]: <Axes: >



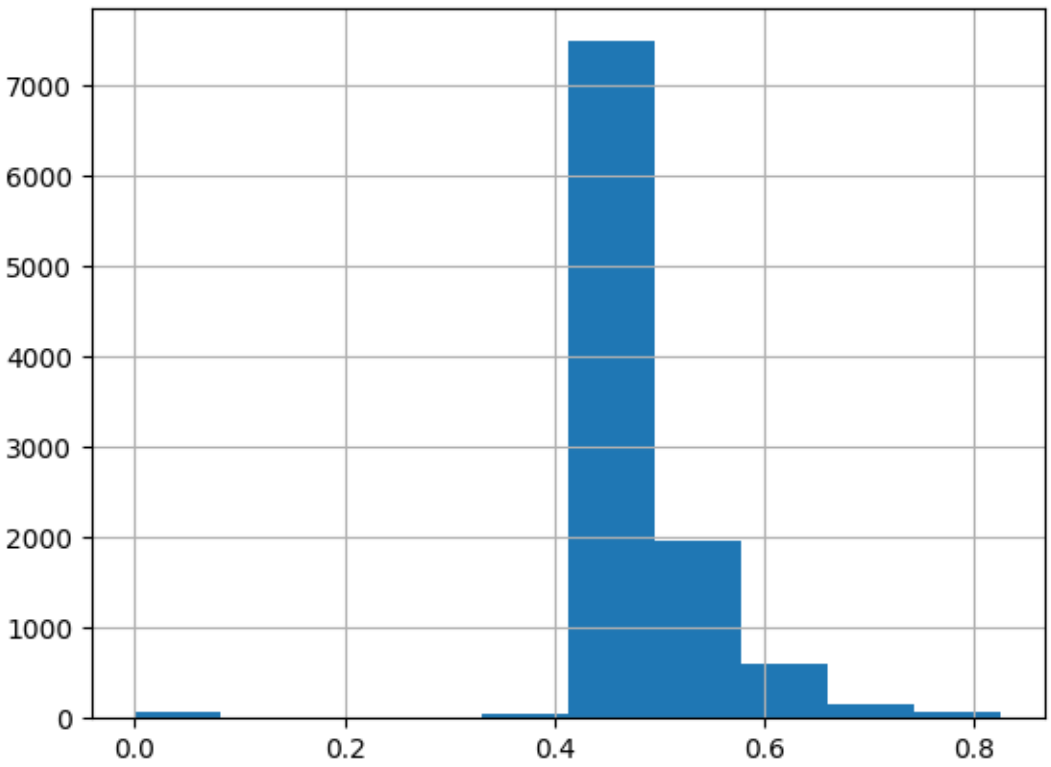
[19]:
```
df['R_cov_element_Average'].hist()
```

[19]: <Axes: >



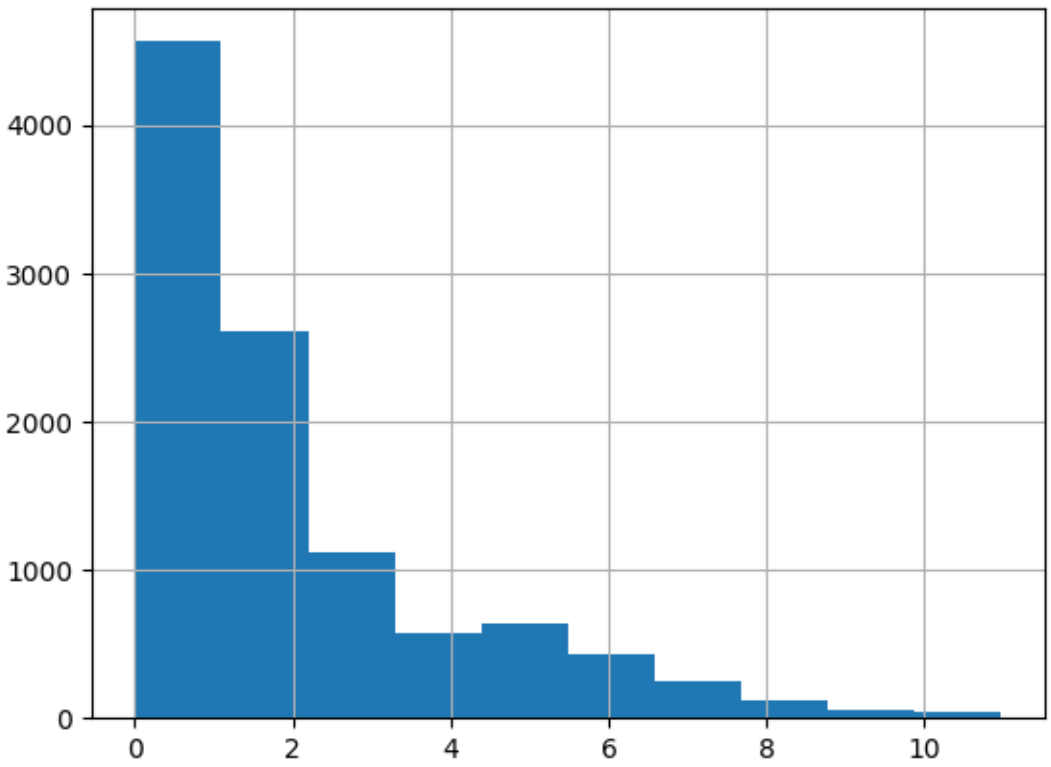
[20]:
```
df['zaratio_Average'].hist()
```

[20]: <Axes: >



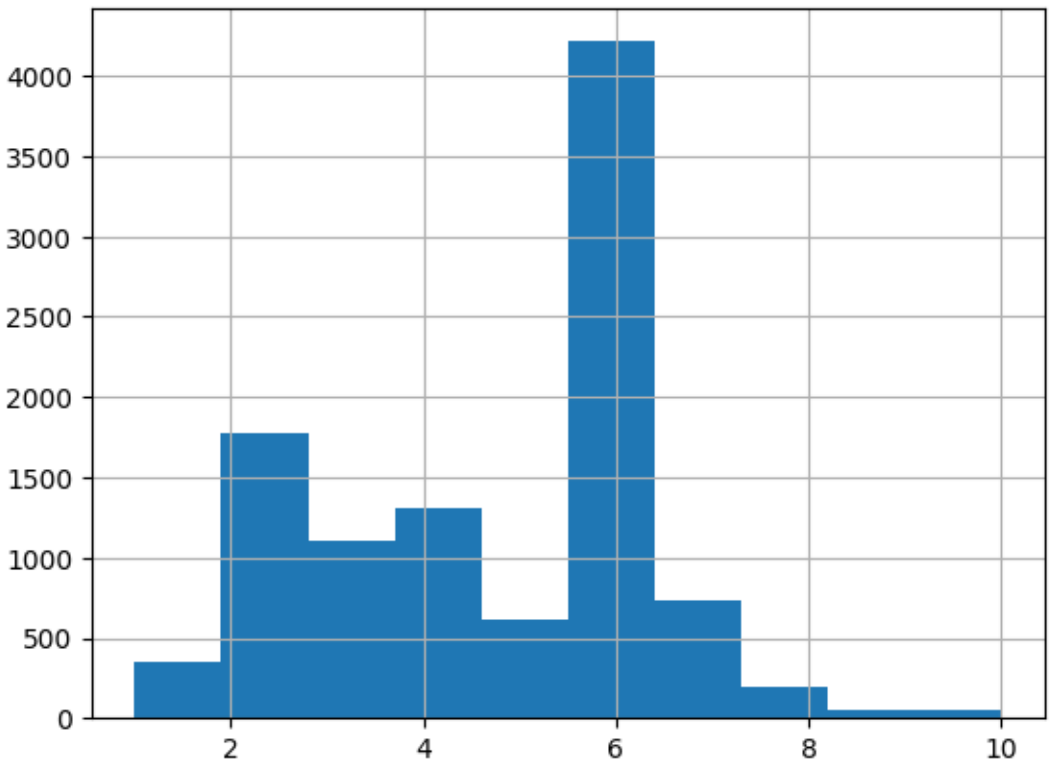
[21]:
```
df['density_Average'].hist()
```

[21]: <Axes: >

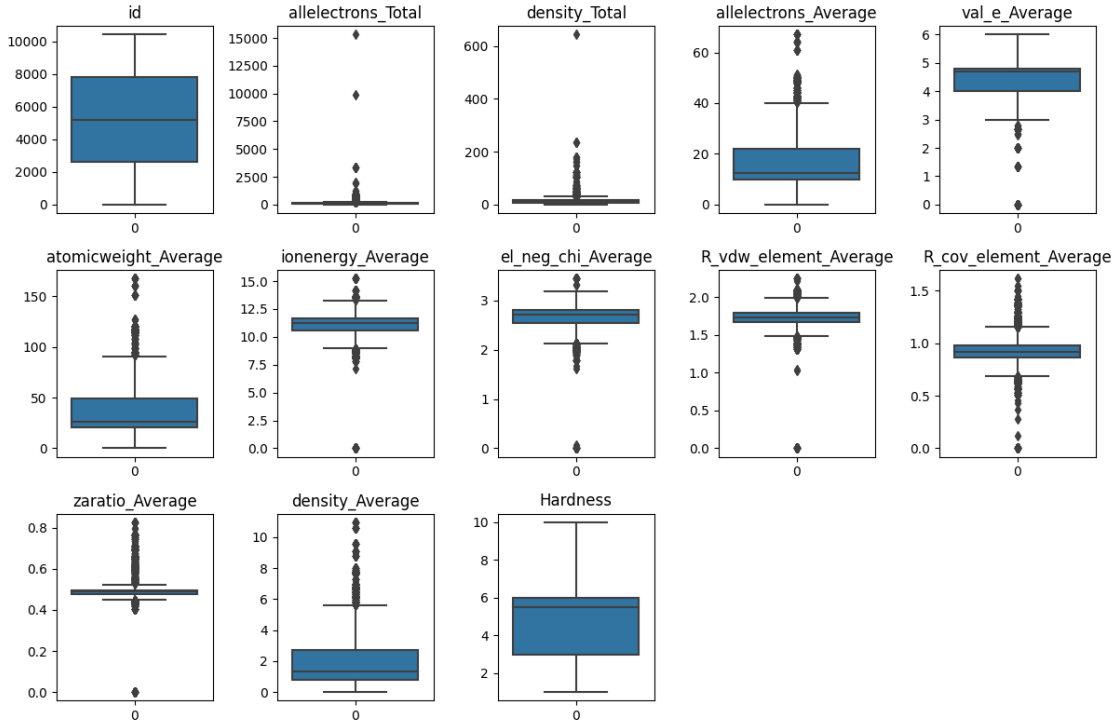


[22]:
```
df['Hardness'].hist()
```

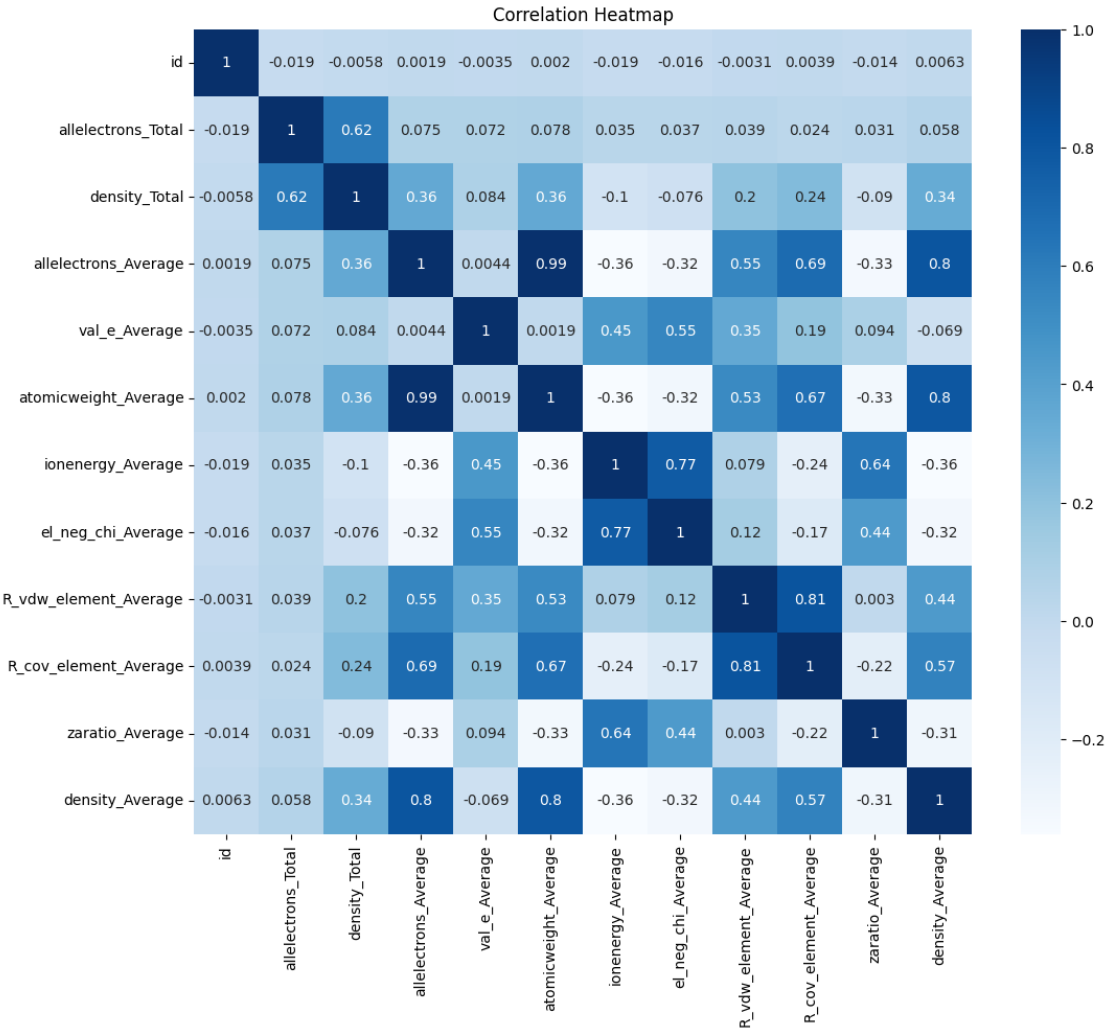
[22]: <Axes: >



[23]:
```
plt.figure(figsize=(12, 8))
for feature in df.columns.to_list():
    plt.subplot(3, 5, df.columns.to_list().index(feature) + 1)
    sns.boxplot(data=df[feature])
    plt.title(feature)
plt.tight_layout()
plt.show()
```



[24]:
```
correlation_matrix = df.drop(columns='Hardness').corr()
plt.figure(figsize=(12, 10))
sns.heatmap(correlation_matrix, annot=True, cmap='Blues')
plt.title('Correlation Heatmap')
plt.show()
```



[25]:
```
df.columns.tolist()
```

[25]:
```
['id',
 'allelectrons_Total',
 'density_Total',
 'allelectrons_Average',
 'val_e_Average',
 'atomicweight_Average',
 'ionenergy_Average',
 'el_neg_chi_Average',
 'R_vdw_element_Average',
 'R_cov_element_Average',
 'zaratio_Average',
 'density_Average',
 'Hardness']
```

[26]:
```
print(df['Hardness'].corr(df['atomicweight_Average']))

print(df['Hardness'].corr(df['density_Average']))
```

```
-0.4029480903545386
-0.36077994780940886
```

[27]:
```
print(df['Hardness'].corr(df['allelectrons_Average']))

print(df['Hardness'].corr(df['density_Average']))
```

```
-0.40049583707006514
-0.36077994780940886
```

[28]:
```
print(df['Hardness'].corr(df['allelectrons_Average']))

print(df['Hardness'].corr(df['atomicweight_Average']))
```

```
-0.40049583707006514
-0.4029480903545386
```

[29]:
```
print(df['Hardness'].corr(df['zaratio_Average']))

print(df['Hardness'].corr(df['atomicweight_Average']))
```

```
0.05524788101979068
-0.4029480903545386
```

[30]:
```
print(df['Hardness'].corr(df['density_Average']))

print(df['Hardness'].corr(df['atomicweight_Average']))
```

```
-0.36077994780940886
-0.4029480903545386
```

[31]:
```
df.drop(columns= ['allelectrons_Average','density_Average'] , axis=1 , inplace=␣
↪True)
```

scal data

[32]:
```
X=df.drop('Hardness',axis=1)
y=df['Hardness']
```

[33]:
```
scaler = StandardScaler()

# Fit the scaler to your data
scaler.fit(X)
```

```
# Transform your data
X_scaled = scaler.transform(X)
```

spilt

[34]:
```
X_train , X_test , y_train , y_test = train_test_split(X_scaled ,y ,test_size=0.
↪2 , random_state=42 )
print("X_train shape:", X_train.shape)
print("y_train shape:", y_train.shape)
print("X_test shape:", X_test.shape)
print("y_test shape:", y_test.shape)
```

```
X_train shape: (8325, 10)
y_train shape: (8325,)
X_test shape: (2082, 10)
y_test shape: (2082,)
```

baseline

[35]:
```
y_mean = y_train.mean()
y_pred_baseline= [y_mean] * len(y_train)
print("Mean apt price:", y_mean)

print("Baseline MAE:", mean_absolute_error(y_train,y_pred_baseline))
```

```
Mean apt price: 4.65015015015015
Baseline MAE: 1.4952898123348572
```

model

[38]:
```
model = LinearRegression()
model.fit(X_train, y_train)
```

[38]:
```
LinearRegression()
```

[39]:
```
reg_y_pred_test = model.predict(X_test)
y_pred_train=model.predict(X_train)
reg_acc_train = r2_score(y_train , y_pred_train)
reg_acc_test = r2_score(y_test , reg_y_pred_test)

print("Training Accuracy:", round(reg_acc_train, 4))
print("Test Accuracy:", round(reg_acc_test, 4))
```

```
Training Accuracy: 0.2437
Test Accuracy: 0.2238
```

[40]:
```
rge =Ridge()

rge.fit(X_train , y_train)
```

[40]:
```
Ridge()
```

[41]:
```
print(rge.score(X_train , y_train))
print(rge.score(X_test , y_test))
```

```
0.24370076851565425
0.22383992595806435
```

[42]:
```
xgb = XGBRegressor(n_estimators= 1000 , max_depth= 3 , learning_rate = 0.01)
xgb.fit(X_train , y_train);
```

[43]:
```
print (xgb.score(X_train , y_train))
print (xgb.score(X_test , y_test))
```

```
0.49629772613292567
0.4458401964892629
```

[44]:
```
test=pd.read_csv("/content/test.csv")
```

[45]:
```
test.shape
```

[45]:
```
(6939, 12)
```

[46]:
```
test.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 6939 entries, 0 to 6938
Data columns (total 12 columns):
 #   Column                 Non-Null Count  Dtype
---  ------                 --------------  -----
 0   id                     6939 non-null   int64
 1   allelectrons_Total     6939 non-null   float64
 2   density_Total          6939 non-null   float64
 3   allelectrons_Average   6939 non-null   float64
 4   val_e_Average          6939 non-null   float64
 5   atomicweight_Average   6939 non-null   float64
 6   ionenergy_Average      6939 non-null   float64
 7   el_neg_chi_Average     6939 non-null   float64
 8   R_vdw_element_Average  6939 non-null   float64
 9   R_cov_element_Average  6939 non-null   float64
 10  zaratio_Average        6939 non-null   float64
 11  density_Average        6939 non-null   float64
dtypes: float64(11), int64(1)
memory usage: 650.7 KB
```

[47]:
```
scaler = StandardScaler()

# Fit the scaler to your data
```

```
scaler.fit(test)

# Transform your data
test_scaled = scaler.transform(test)
```

[54]:
```
test_encoded = pd.get_dummies(test)
```

[49]:
```
submisson =test[["id"]]
```

[51]:
```
submisson.head()
```

[51]:
```
      id
0  10407
1  10408
2  10409
3  10410
4  10411
```

```
<google.colab._quickchart_helpers.SectionTitle at 0x7a54b5955210>
```

```
from matplotlib import pyplot as plt
_df_0['id'].plot(kind='hist', bins=20, title='id')
plt.gca().spines[['top', 'right',]].set_visible(False)
```

```
<google.colab._quickchart_helpers.SectionTitle at 0x7a54b59551e0>
```

```
from matplotlib import pyplot as plt
import seaborn as sns
def _plot_series(series, series_name, series_index=0):
  from matplotlib import pyplot as plt
  import seaborn as sns
  palette = list(sns.palettes.mpl_palette('Dark2'))
  counted = (series['id']
               .value_counts()
             .reset_index(name='counts')
             .rename({'index': 'id'}, axis=1)
             .sort_values('id', ascending=True))
  xs = counted['id']
  ys = counted['counts']
  plt.plot(xs, ys, label=series_name, color=palette[series_index % len(palette)])

fig, ax = plt.subplots(figsize=(10, 5.2), layout='constrained')
df_sorted = _df_1.sort_values('id', ascending=True)
_plot_series(df_sorted, '')
sns.despine(fig=fig, ax=ax)
plt.xlabel('id')
_ = plt.ylabel('count()')
```

```
<google.colab._quickchart_helpers.SectionTitle at 0x7a54b5954af0>
```

```
from matplotlib import pyplot as plt
_df_2['id'].plot(kind='line', figsize=(8, 4), title='id')
plt.gca().spines[['top', 'right']].set_visible(False)
```

[52]:
```
submisson.to_csv("submisson2.csv" , index = False)
```

[ ]:
```

```