# medical-insurance-pred-full

April 12, 2024

## 1 Personal Medical Insurance Cost with ML Regression Model

## 1.1 Libraries imports

## Library imports for i/o

```
[1]: # working with structured data
import pandas as pd

# support for arrays, matrices, and mathematical functions to operate on data
structures
import numpy as np

# manipulating file paths and directories
import os.path
```

## Libraries for general purposes

```
# embedding HTML content like visualizations or interactive elements within and Jupyter notebook
from IPython.display import HTML

# generating random strings or for various string manipulation tasks
from string import ascii_letters

# generating random numbers within a specified range
from random import randint
import time
```

### Filtering warnings

```
[3]: import warnings warnings.filterwarnings("ignore")
```

## Matplotlib and Seaborn

Seaborn:

- 1. Seaborn is built on top of Matplotlib and provides a higher-level interface for creating attractive statistical graphics.
- 2. It simplifies the process of creating complex plots such as histograms, KDE plots, and regression plots by providing easy-to-use functions with sensible defaults.
- 3. Seaborn is particularly useful for exploring and visualizing relationships in complex datasets.
- 4. It is well-suited for statistical data analysis and exploratory data visualization.

## Matplotlib:

- 1. Matplotlib is a comprehensive library for creating static, animated, and interactive visualizations in Python.
- 2. It provides a MATLAB-like interface for creating plots and offers fine-grained control over plot customization.
- 3. Matplotlib is highly customizable and can create nearly any type of plot imaginable, although sometimes with more verbose syntax compared to other libraries.
- 4. It is a foundational library for data visualization in Python and is often used for creating publication-quality graphics and embedding plots in various applications.

```
[4]: # statistical data visualization
import seaborn as sns
# for Q-Q plots
import scipy.stats as stats

# creating static, animated, and interactive visualizations
import matplotlib.pyplot as plt
```

### **Plotly Packages**

- 1. Plotly is another library for creating interactive visualizations, with a focus on producing publication-quality graphics.
- 2. It supports a wide range of chart types and offers numerous customization options for fine-tuning plots.
- 3. Plotly also provides an online platform (Chart Studio) for sharing, collaborating on, and hosting Plotly graphs.
- 4. It is well-suited for creating interactive visualizations that can be easily shared and embedded in web applications, reports, and presentations.

### Plot Library for flexible data visualization purposes

- 1. It provides a concise and powerful interface for creating a wide variety of plots, including interactive plots suitable for web applications and dashboards.
- 2. Bokeh emphasizes interactivity and can handle large datasets with ease.
- 3. It is well-suited for creating complex, interactive visualizations for web-based applications and dashboards.

```
[6]: # creating interactive and web-ready visualizations
from bokeh.io import output_notebook, show
from bokeh.plotting import figure
output_notebook()
from bokeh.layouts import gridplot
```

#### Statistical Libraries

[7]: from scipy import stats

## **Data-preprocessing libraries**

```
[8]: # encoding categorical features
from sklearn.preprocessing import LabelEncoder

# generate polynomial and interaction features
from sklearn.preprocessing import PolynomialFeatures

# scale numerical features to a specified range
from sklearn.preprocessing import MinMaxScaler
from sklearn.preprocessing import StandardScaler
```

## Model tuning libraries

```
[9]: # chaining together multiple processing steps into a single object
from sklearn.pipeline import Pipeline

# split the dataset into training and testing sets
from sklearn.model_selection import train_test_split

# regression evaluation metrics
from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error

# cross-validation technics
from sklearn.model_selection import KFold
from sklearn.model_selection import GroupKFold
from sklearn.model_selection import ShuffleSplit
```

### Regression models libraries

```
[10]: from sklearn.linear_model import LinearRegression, Ridge, Lasso
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
```

```
from sklearn.tree import DecisionTreeRegressor, ExtraTreeRegressor
      from sklearn.neighbors import KNeighborsRegressor
      from sklearn.gaussian_process import GaussianProcessRegressor
      import xgboost as xgb
     Model hyperparameter tuning
[11]: from sklearn.model_selection import GridSearchCV
     1.2 Read the Dataset for health insurance
[12]: # path to the original dataset
      df_path ="D://programming//information-technologies-of-smart-systems//
       -calculation-and-graphic work//personal-medical-insurance-cost-prediction//

data//insurance.csv"

[13]: # is there such path?
      print(os.path.exists(df_path))
     True
[14]: # read the health insurance dataset
      df = pd.read_csv(df_path)
     1.3 Exploratory Data Analysis (EDA)
     1.3.1 Data Shapes
[15]: print('columns count - ', len(df.columns), '\n')
      print('columns: ', list(df.columns))
     columns count - 7
     columns: ['age', 'sex', 'bmi', 'children', 'smoker', 'region', 'charges']
[21]: print('Samples count: ', df.shape[0])
     Samples count: 1338
[19]: df.head(10)
[19]:
                             children smoker
                                                             charges
        age
                sex
                        bmi
                                                 region
      0
         19 female 27.900
                                    0
                                              southwest 16884.92400
                                         yes
               male 33.770
                                                          1725.55230
      1
         18
                                    1
                                          no
                                              southeast
```

southeast

4449.46200

3

2

28

male 33.000

```
3
    33
          male 22.705
                                 0
                                            northwest
                                                        21984.47061
                                       no
                 28.880
4
    32
          male
                                 0
                                            northwest
                                                         3866.85520
                                        no
5
    31
        female
                 25.740
                                       no
                                            southeast
                                                         3756.62160
6
    46
        female
                 33.440
                                 1
                                            southeast
                                                         8240.58960
                                       no
7
    37
        female
                27.740
                                 3
                                            northwest
                                                         7281.50560
                                       nο
                                 2
8
    37
          male
                29.830
                                            northeast
                                                         6406.41070
                                       nο
9
    60
        female
                25.840
                                 0
                                            northwest
                                                        28923.13692
                                       nο
```

## **Data Types**

[22]: df.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1338 entries, 0 to 1337
Data columns (total 7 columns):

#	Column	Non-l	Null Count	Dtype
0	age	1338	non-null	int64
1	sex	1338	non-null	object
2	bmi	1338	non-null	float64
3	children	1338	non-null	int64
4	smoker	1338	non-null	object
5	region	1338	non-null	object
6	charges	1338	non-null	float64
<pre>dtypes: float64(2),</pre>			int64(2),	object(3)
memory usage: 73.3+			KB	

### **Descriptive Statistics**

[23]: df.describe(include='0') # for categorical variables

```
[23]:
                sex smoker
                                 region
                                    1338
      count
               1338
                       1338
      unique
                           2
                                       4
                   2
      top
               male
                              southeast
                         no
      freq
                676
                       1064
                                     364
```

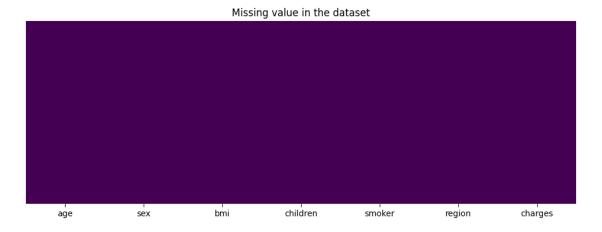
[24]: df.describe(exclude='0') # for numerical variables

```
[24]:
                                    bmi
                                            children
                                                            charges
                      age
                                                        1338.000000
      count
             1338.000000
                           1338.000000
                                         1338.000000
               39.207025
                             30.663397
                                            1.094918
                                                       13270.422265
      mean
      std
               14.049960
                              6.098187
                                            1.205493
                                                       12110.011237
      min
               18.000000
                             15.960000
                                            0.000000
                                                        1121.873900
      25%
               27.000000
                             26.296250
                                            0.000000
                                                        4740.287150
      50%
               39.000000
                             30.400000
                                            1.000000
                                                        9382.033000
      75%
               51.000000
                             34.693750
                                            2.000000
                                                       16639.912515
      max
               64.000000
                             53.130000
                                            5.000000
                                                       63770.428010
```

## 1.3.2 Check for missing value

## There is no missing value in the data:)

```
[25]: # no missing data visualisation
plt.figure(figsize=(12,4))
sns.heatmap(df.isnull(),cbar=False,cmap='viridis',yticklabels=False)
plt.title('Missing value in the dataset')
```



## 1.3.3 Plots for data exploring

## General mixed plots

```
[40]: selected_cols = [col for col in df.columns if col]

# generate random colors for each selected column
colors = ['mediumvioletred']
for i in range(len(selected_cols)):
        colors.append('#%06X' % randint(0, 0xFFFFFF))

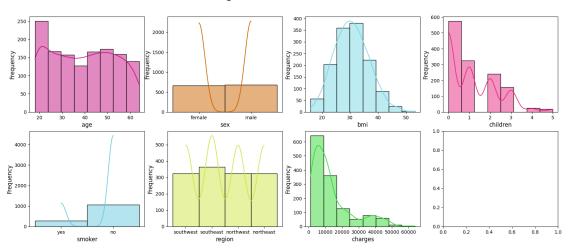
# determine the number of subplots based on the selected columns
num_subplots = len(selected_cols)
```

```
num_rows = (num_subplots - 1) // 5 + 1
num_cols = min(4, num_subplots)
# create the figure and axes for subplots
fig, axes = plt.subplots(num_rows, num_cols, figsize=(20, num_rows * 4),__

¬facecolor='white')
fig.suptitle("Histograms of Various Features", size=24)
for i in range(num_rows):
    for j in range(num_cols):
        idx = i * num_cols + j
        if idx < num_subplots:</pre>
            sns.histplot(df[selected_cols[idx]], ax=axes[i, j],__

color=colors[idx], kde=True, bins=8)
            axes[i, j].set_xlabel(selected_cols[idx], fontsize=12) # Set_
 \rightarrow x-axis label font size
            axes[i, j].set_ylabel("Frequency", fontsize=12)
                                                                        # Set_
 \hookrightarrow y-axis label font size
#plt.tight_layout(rect=[0, 0.03, 1, 0.95])
plt.show()
```

### Histograms of Various Features



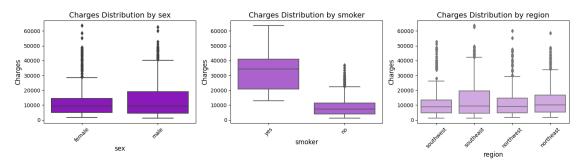
There's something insanely beautiful about bmi distribution, isn't there? The average BMI in patients is 30.

```
[50]: # selecting categorical columns from the DataFrame
    categorical_cols = df.select_dtypes(include=['object']).columns
# extracting column names into a list
```

```
selected_cols = [col for col in categorical_cols]
# calculating the number of subplots needed
num_subplots = len(selected_cols)
num\_rows = (num\_subplots - 1) // 3 + 1
num_cols = min(3, num_subplots)
# creating the subplot grid and setting figure size
fig, axes = plt.subplots(num_rows, num_cols, figsize=(15, num_rows * 5),__

¬facecolor='white')
# adding a title to the figure
fig.suptitle("Charges Distribution Across Various Categorical Features",
 ⇔size=20)
# generating a palette of colors for visualization
colors = sns.light_palette('darkviolet', n_colors=len(selected_cols)+1,__
 ⇔reverse=True)
# plotting boxplots for each selected categorical feature
for idx, col in enumerate(selected_cols):
   row = idx // num_cols
   col idx = idx % num cols
   ax = axes[idx] if num_rows == 1 else axes[row, col_idx]
   sns.boxplot(x=col, y='charges', data=df, ax=ax, palette=[colors[idx]])
   ax.set_title(f'Charges Distribution by {col}', fontsize=14)
   ax.set xlabel(col, fontsize=12)
   ax.set_ylabel("Charges", fontsize=12)
   ax.tick_params(axis='x', rotation=45)
# removing excess empty subplots if there are any
for ax in axes.flat[num_subplots:]:
   ax.remove()
# adjusting layout for better visualization
plt.tight_layout(rect=[0, 0.03, 1, 0.95])
# displaying the plot
plt.show()
```

### Charges Distribution Across Various Categorical Features



```
[54]: # selecting numerical columns from the DataFrame
      numerical_cols = df.select_dtypes(include=['float64', 'int64', 'int32']).columns
      # excluding the 'charges' column from the selected numerical features
      selected_cols = [col for col in numerical_cols if col != 'charges']
      # calculating the number of subplots needed
      num_subplots = len(selected_cols)
      num_rows = (num_subplots - 1) // 3 + 1
      num_cols = min(3, num_subplots)
      # creating the subplot grid and setting figure size
      fig, axes = plt.subplots(num_rows, num_cols, figsize=(15, num_rows * 5),__

¬facecolor='white')
      # adding a title to the figure
      fig.suptitle("Scatter Plots of Numerical Features vs Charges with Polynomial ⊔

    Lines", size=20)

      # generating a palette of colors for visualization
      palette = sns.husl_palette(n_colors=len(selected_cols), s=0.7, l=0.6)
      \# plotting scatter plots with polynomial lines for each selected numerical \sqcup
       \hookrightarrow feature
      for idx, col in enumerate(selected_cols):
          if num_rows == 1 or num_cols == 1:
              ax = axes[idx]
          else:
              row = idx // num_cols
              col_idx = idx % num_cols
              ax = axes[row, col_idx]
          sns.scatterplot(x=col, y='charges', data=df, ax=ax, color=palette[idx])
```

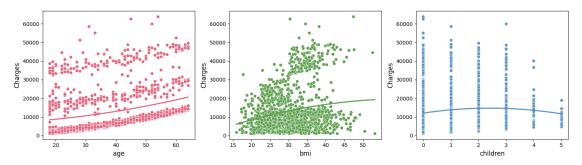
```
sns.regplot(x=col, y='charges', data=df, ax=ax, scatter=False, order=2, color=palette[idx], ci=None)
    ax.set_xlabel(col, fontsize=12)
    ax.set_ylabel("Charges", fontsize=12)

# removing excess empty subplots if there are any
for ax in axes.flat[num_subplots:]:
    ax.remove()

# adjusting layout for better visualization
plt.tight_layout(rect=[0, 0.03, 1, 0.95])

# displaying the plot
plt.show()
```

Scatter Plots of Numerical Features vs Charges with Polynomial Lines



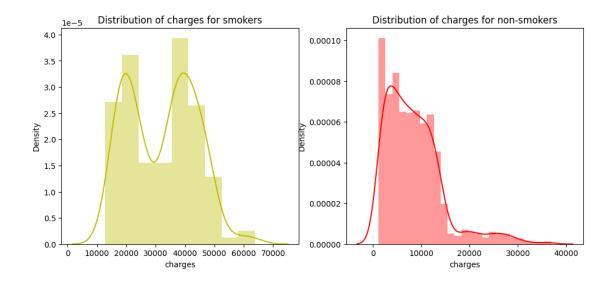
**Distribution for smokers** Smoking patients spend more on treatment.

```
[114]: f= plt.figure(figsize=(12,5))

ax=f.add_subplot(121)
sns.distplot(df[(df.smoker == 1)]["charges"],color='y',ax=ax)
ax.set_title('Distribution of charges for smokers')

ax=f.add_subplot(122)
sns.distplot(df[(df.smoker == 0)]['charges'],color='r',ax=ax)
ax.set_title('Distribution of charges for non-smokers')
```

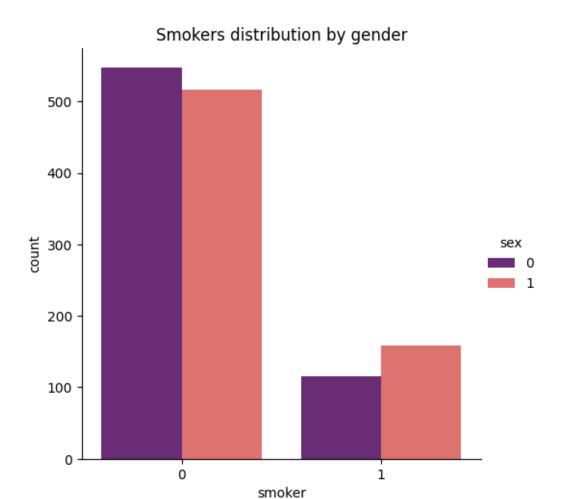
[114]: Text(0.5, 1.0, 'Distribution of charges for non-smokers')



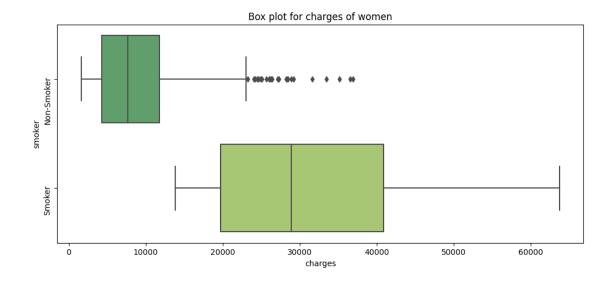
Exploring dependencies of gender distribution and smoking Please note that women are coded with the symbol "0" and men - "1". Thus non-smoking people and the truth more. Also we can notice that more male smokers than women smokers. It can be assumed that the total cost of treatment in men will be more than in women, given the impact of smoking.

```
[112]: sns.catplot(x="smoker", kind="count", hue = 'sex', palette="magma", data=df)
plt.title("Smokers distribution by gender")
# plt.xticks([0, 1], ['Non-Smoker', 'Smoker'])
```

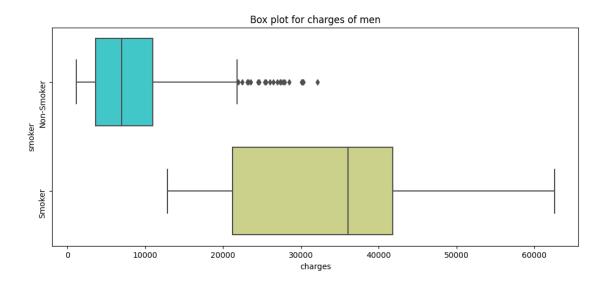
[112]: Text(0.5, 1.0, 'Smokers distribution by gender')



```
plt.figure(figsize=(12,5))
plt.title("Box plot for charges of women")
sns.boxplot(y="smoker", x="charges", data = df[(df.sex == 0)], orient="h", upalette = 'summer')
# adding annotations to clarify y-axis labels
plt.yticks([0, 1], ['Non-Smoker', 'Smoker'], rotation = 90)
```

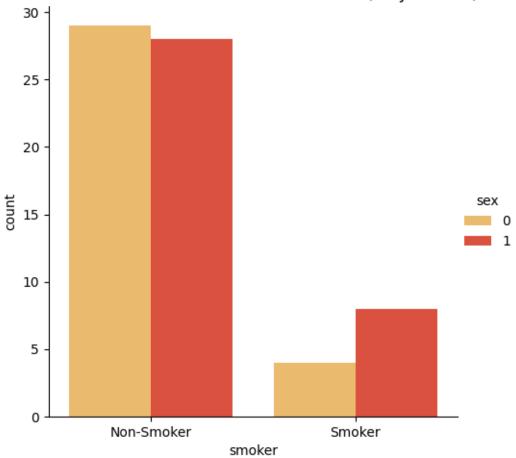


```
[227]: plt.figure(figsize=(12,5))
plt.title("Box plot for charges of men")
sns.boxplot(y="smoker", x="charges", data = df[(df.sex == 1)] , orient="h", use palette = 'rainbow')
# adding annotations to clarify y-axis labels
plt.yticks([0, 1], ['Non-Smoker', 'Smoker'], rotation = 90)
```



## Exploring dependencies between gender distribution (y.o. 18), smoking and charges

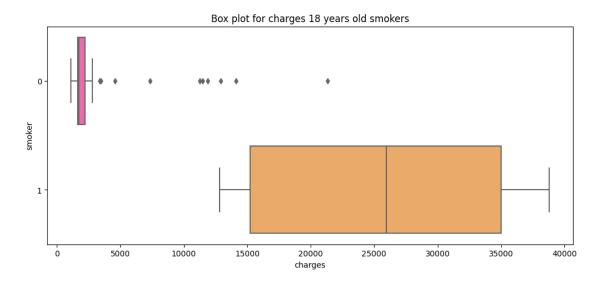
## The number of smokers and non-smokers (18 years old)



As we can see, even at the age of 18 smokers spend much more on treatment than non-smokers. Among non-smokers we are seeing some "tails". I can assume that this is due to serious diseases or accidents. Now let's see how the cost of treatment depends on the age of smokers and non-smokers patients.

```
[223]: plt.figure(figsize=(12,5))
plt.title("Box plot for charges 18 years old smokers")
```

```
sns.boxplot(y="smoker", x="charges", data = df[(df.age == 18)] , orient="h", u palette = 'spring')
```

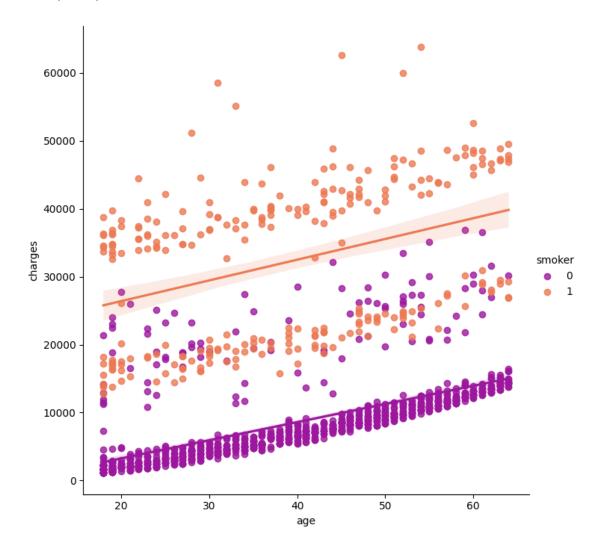


In non-smokers, the cost of treatment increases with age. That makes sense. In smoking people, we do not see such dependence. I think that it is not only in smoking but also in the peculiarities of the dataset. Such a strong effect of Smoking on the cost of treatment would be more logical to judge having a set of data with a large number of records and signs. Let's pay attention to bmi. I am surprised that this figure but affects the cost of treatment in patients. Or are we on a diet for nothing?

```
[240]: sns.lmplot(x="age", y="charges", hue="smoker", data=df, palette='plasma', height=7)
```

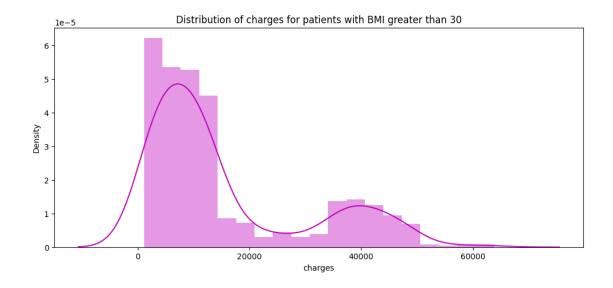
```
ax.set_title('Smokers and non-smokers')
```

[240]: Text(0.5, 1.0, 'Smokers and non-smokers')

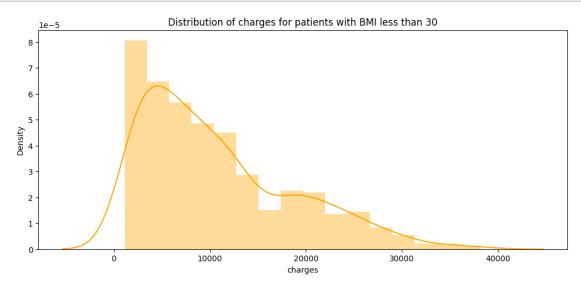


**Plot distributing by bmi** Let's start to explore distribution of bmi. First, let's look at the distribution of costs in patients with BMI greater than 30 and less than 30.

```
[245]: plt.figure(figsize=(12,5))
   plt.title("Distribution of charges for patients with BMI greater than 30")
   ax = sns.distplot(df[(df.bmi >= 30)]['charges'], color = 'm')
```

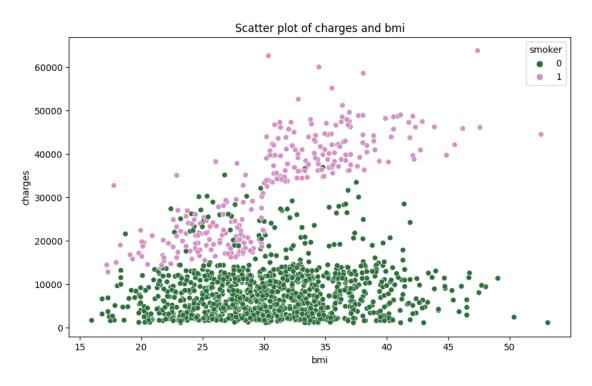


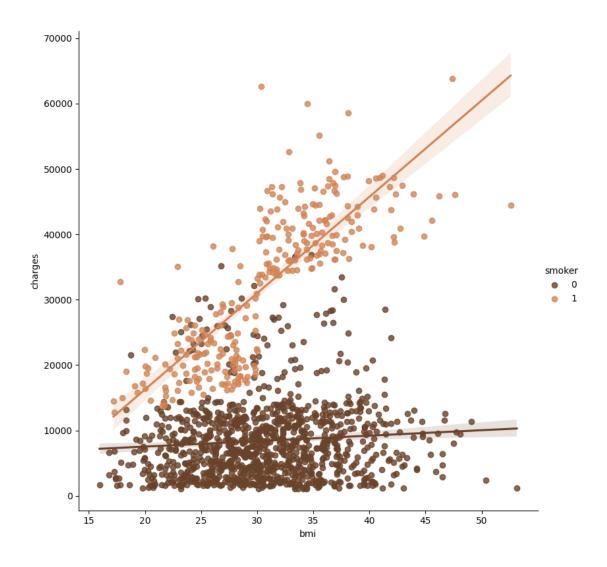
```
[247]: plt.figure(figsize=(12,5))
  plt.title("Distribution of charges for patients with BMI less than 30")
  ax = sns.distplot(df[(df.bmi < 30)]['charges'], color = 'orange')</pre>
```



Patients with BMI above 30 spend more on treatment.

[250]: <seaborn.axisgrid.FacetGrid at 0x1c0ea9a5210>





Age Analysis: Turning Age into Categorical Variables: 1. Young Adult: from 18 - 35 2. Senior Adult: from 36 - 55 3. Elder: 56 or older 4. Share of each Category: Young Adults (42.9%), Senior Adults (41%) and Elder (16.1%)

## Is there a Relationship between BMI and Age

- 1. BMI frequency: Most of the BMI frequency is concentrated between 27 33.
- 2. Correlations Age and charges have a correlation of 0.29 while bmi and charges have a correlation of 0.19
- 3. Relationship betweem BMI and Age: The correlation for these two variables is 0.10 which is not that great. Therefore, we can disregard that age has a huge influence on BMI.

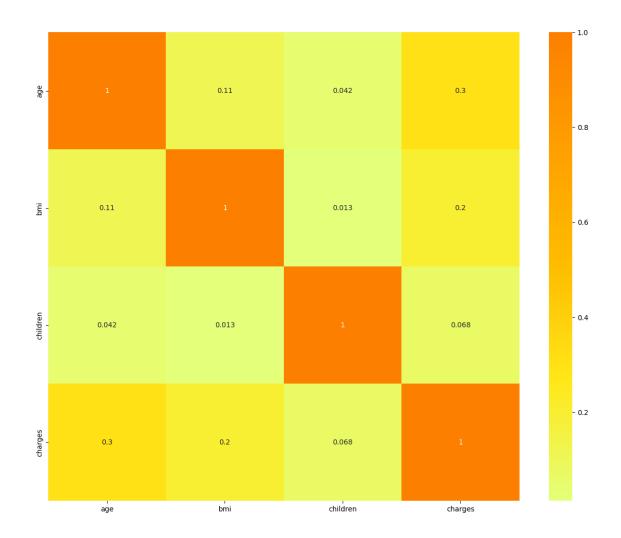
```
[252]: # extracting BMI values for different age categories
       young_adults = df["bmi"].loc[df["age_cat"] == "Young Adult"].values
       senior_adult = df["bmi"].loc[df["age_cat"] == "Senior Adult"].values
       elders = df["bmi"].loc[df["age_cat"] == "Elder"].values
       # creating Box plots for each age category
       trace0 = go.Box(
           y=young adults,
           name='Young Adults',
           boxmean=True,
           marker=dict(
               color='rgb(214, 12, 140)',
           )
       trace1 = go.Box(
           y=senior_adult,
           name='Senior Adults',
           boxmean=True,
           marker=dict(
               color='rgb(0, 128, 128)',
           )
       )
       trace2 = go.Box(
```

```
y=elders,
    name='Elders',
    boxmean=True,
    marker=dict(
        color='rgb(247, 186, 166)',
    )
)
# combining data into a list
data = [trace0, trace1, trace2]
# creating layout for the plot
layout = go.Layout(
   title="Body Mass Index <br > by Age Category",
    xaxis=dict(title="Age Category", titlefont=dict(size=16)),
    yaxis=dict(title="Body Mass Index", titlefont=dict(size=16))
)
# creating the figure and plotting it
fig = go.Figure(data=data, layout=layout)
iplot(fig)
```

## Correlation plot without categorical variables

```
[59]: # features for matrix
col_for_corr = ['age', 'bmi', 'children', 'charges']

# correlation matrix calculation
corr = df[col_for_corr].corr()
sns.heatmap(corr, cmap = 'Wistia', annot= True)
```



### 1.4 Feature engineering

Feature engineering is the process of selecting and transforming variables (features) to improve model performance in machine learning tasks. It involves creating new features, selecting relevant ones, and encoding categorical variables, among other techniques.

Importance of Feature Engineering: - Improved Model Performance. Well-engineered features can lead to better model accuracy and generalization. - Better Interpretability. Properly engineered features can make models more interpretable and understandable. - Reduced Overfitting. Feature engineering can help in reducing overfitting by providing the model with more relevant information.

### Techniques in Feature Engineering

- 1. **Imputation**. Handling missing values in the dataset using techniques like mean, median, or mode imputation.
- 2. **Feature Scaling**. Scaling features to a similar range, such as normalization or standardization, to prevent bias in models.

- 3. **Feature Encoding**. Converting categorical variables into numerical format, such as one-hot encoding or label encoding.
- 4. **Feature Transformation**. Transforming features using techniques like logarithm, square root, or Box-Cox transformation to make them more suitable for modeling.
- 5. **Feature Selection**. Selecting the most relevant features using techniques like correlation analysis, feature importance, or recursive feature elimination.
- 6. **Interaction Features**. Creating new features by combining existing ones, such as product or ratio features, to capture interaction effects.
- 7. **Dimensionality Reduction**. Reducing the number of features using techniques like Principal Component Analysis (PCA) or Singular Value Decomposition (SVD) to simplify the model.

## 1.4.1 Encoding Categorical Features with LabelEncoder()

Categorical variables are non-numeric variables that represent categories or groups. Label encoding is a technique used to convert categorical variables into numerical format, where each category is assigned a unique integer.

```
[15]: # sex feature
       le = LabelEncoder()
       le.fit(df.sex.drop_duplicates())
       df.sex = le.transform(df.sex)
[16]: # get the mapping between original categories and encoded values
       encoded_mapping = dict(zip(le.classes_, le.transform(le.classes_)))
       print(encoded mapping)
      {'female': 0, 'male': 1}
[167]: df.head(5)
[167]:
                            children smoker
          age
               sex
                       bmi
                                                 region
                                                             charges
                    27.900
       0
           19
                                   0
                                              southwest 16884.92400
                 0
                                         yes
       1
           18
                 1 33.770
                                   1
                                              southeast
                                                          1725.55230
       2
           28
                 1 33.000
                                   3
                                              southeast
                                                          4449.46200
       3
                                   0
           33
                 1 22.705
                                              northwest 21984.47061
                                         no
       4
           32
                    28.880
                                   0
                                         no
                                              northwest
                                                          3866.85520
[17]: # smoker or not feature
       le.fit(df.smoker.drop duplicates())
       df.smoker = le.transform(df.smoker)
[169]: # get the mapping between original categories and encoded values
       encoded_mapping = dict(zip(le.classes_, le.transform(le.classes_)))
       print(encoded_mapping)
      {'no': 0, 'yes': 1}
```

```
[65]: df.head(5)
[65]:
                              children
                        bmi
                                        smoker
                                                    region
                                                                 charges
          age
                sex
       0
           19
                  0
                     27.900
                                     0
                                                 southwest
                                                             16884.92400
       1
           18
                     33.770
                                     1
                                                 southeast
                                                              1725.55230
       2
           28
                     33.000
                                     3
                                                 southeast
                                              0
                                                              4449.46200
       3
           33
                  1
                     22.705
                                     0
                                                 northwest
                                                             21984.47061
       4
           32
                  1
                     28.880
                                                 northwest
                                                              3866.85520
      A few words about coding "region". In general, categorical variables with large variability are best
      encoded using OneHotEncoder and so on. But in this case, nothing will change, because there is
      no special order in which the regions would be listed
[18]: # region feature
       le.fit(df.region.drop_duplicates())
       df.region = le.transform(df.region)
[171]: # get the mapping between original categories and encoded values
       encoded_mapping = dict(zip(le.classes_, le.transform(le.classes_)))
       print(encoded_mapping)
      {'northeast': 0, 'northwest': 1, 'southeast': 2, 'southwest': 3}
[82]:
       df.head(5)
[82]:
          age
                sex
                        bmi
                              children
                                        smoker
                                                 region
                                                              charges
       0
           19
                  0
                     27.900
                                     0
                                              1
                                                       3
                                                          16884.92400
       1
           18
                  1
                     33.770
                                     1
                                              0
                                                       2
                                                           1725.55230
                                     3
                                              0
       2
           28
                     33.000
                                                      2
                                                           4449.46200
                  1
       3
           33
                     22.705
                                     0
                                              0
                                                       1
                                                          21984.47061
                  1
       4
                     28.880
                                     0
                                              0
                                                       1
                                                           3866.85520
           32
[172]:
      df.info()
      <class 'pandas.core.frame.DataFrame'>
      RangeIndex: 1338 entries, 0 to 1337
      Data columns (total 7 columns):
       #
            Column
                      Non-Null Count
                                        Dtype
                       _____
            _____
                                        ____
                       1338 non-null
                                        int64
       0
            age
       1
            sex
                      1338 non-null
                                        int32
       2
            bmi
                      1338 non-null
                                        float64
            children 1338 non-null
       3
                                        int64
       4
                      1338 non-null
            smoker
                                        int32
       5
            region
                       1338 non-null
                                        int32
            charges
                      1338 non-null
                                        float64
      dtypes: float64(2), int32(3), int64(2)
      memory usage: 57.6 KB
```

### Save the new encoded dataset

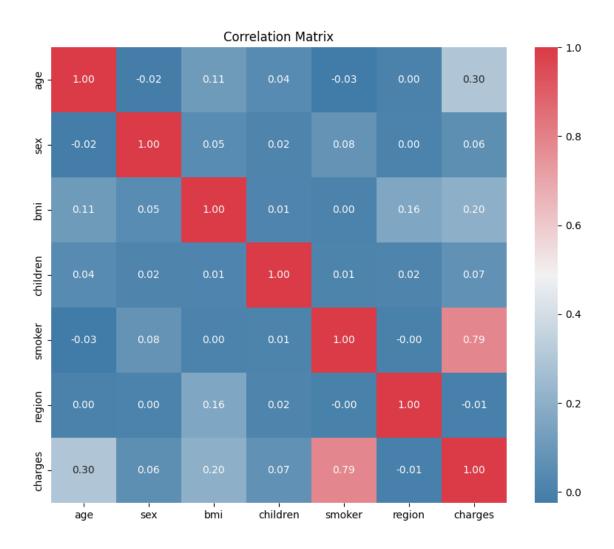
```
[173]: df_encoded = df.copy()
df_encoded.to_csv('.//data//explore//insurance_encoded.csv', index=False)
```

```
[12]: # is there such path?
print(os.path.exists(dataset_encoded_path))
```

True

```
[13]: df_encoded= pd.read_csv(dataset_encoded_path)
```

### Correlation plot with encoded categorical variables



```
[19]: # corelation matrix in text output
corr = df.corr()
print("Correlation Matrix:")
print(corr)
```

## Correlation Matrix:

	age	sex	bmi	children	smoker	region	charges
	O						•
age	1.000000	-0.020856	0.109272	0.042469	-0.025019	0.002127	0.299008
sex	-0.020856	1.000000	0.046371	0.017163	0.076185	0.004588	0.057292
bmi	0.109272	0.046371	1.000000	0.012759	0.003750	0.157566	0.198341
children	0.042469	0.017163	0.012759	1.000000	0.007673	0.016569	0.067998
smoker	-0.025019	0.076185	0.003750	0.007673	1.000000	-0.002181	0.787251
region	0.002127	0.004588	0.157566	0.016569	-0.002181	1.000000	-0.006208
charges	0.299008	0.057292	0.198341	0.067998	0.787251	-0.006208	1.000000

### 1.4.2 Outlier Engineering

Outliers are data points that significantly differ from other observations in a dataset. Outlier engineering involves identifying and handling these outliers to prevent them from adversely affecting model performance.

## Techniques for Outlier Engineering

#### 1. Identification:

- Statistical Methods: Use statistical techniques such as Z-score, interquartile range (IQR), or modified Z-score to identify outliers.
- Visualization: Plotting techniques like box plots, scatter plots, or histograms can help visually identify outliers.
- Domain Knowledge: Leverage domain knowledge to identify anomalies that may be outliers in the dataset.

### 2. Handling Outliers:

- Removal. Exclude outliers from the dataset if they are deemed to be errors or anomalies.
- Transformation. Apply transformations such as log transformation or Winsorization to mitigate the impact of outliers.
- Imputation. Impute outliers with more representative values using techniques like mean, median, or nearest neighbors.

## 3. Model-Specific Approaches:

- Robust Models. Use robust machine learning algorithms that are less sensitive to outliers, such as robust regression or tree-based models.
- Weighted Models. Assign different weights to outliers or downsample them to reduce their influence on the model.

### 4. Ensemble Methods:

• Ensemble techniques like bagging or boosting can help in reducing the impact of outliers by combining predictions from multiple models.

```
[211]: # function to create histogram, Q-Q plot and

def diagnostic_plots(df, variable):
    # function takes a dataframe (df) and
    # the variable of interest as arguments

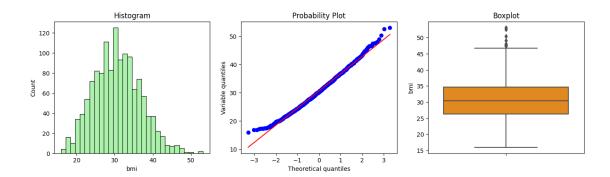
# define figure size
    plt.figure(figsize=(16, 4))

# histogram
    plt.subplot(1, 3, 1)
    sns.histplot(df[variable], bins=30, color='lightgreen')
    plt.title('Histogram')

# Q-Q plot
    plt.subplot(1, 3, 2)
    stats.probplot(df[variable], dist="norm", plot=plt)
    plt.ylabel('Variable quantiles')
```

```
plt.gca().get_lines()[0].set_color('blue')
             # boxplot
             plt.subplot(1, 3, 3)
             sns.boxplot(y=df[variable], color='darkorange')
             plt.title('Boxplot')
             plt.show()
[118]: # display unique values of each feature
        df.nunique()
[118]: age
                         47
        sex
                          2
        bmi
                       548
        children
                          6
        smoker
                          2
                          4
        region
        charges
                      1337
        dtype: int64
[212]: # let's find outliers in age
        diagnostic_plots(df, 'age')
                          Histogram
                                                      Probability Plot
                                                                                     Boxplot
              140
              120
              100
                                            60
                                                                         50
              80
                                          Variable o
               60
                                                                         30
               40
                                                     -1 0 1
Theoretical quantiles
```

```
[213]: # let's find outliers in bmi
diagnostic_plots(df, 'bmi')
```



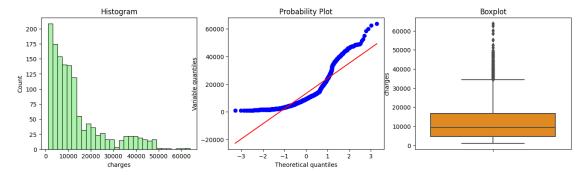
BMI (Body Mass Index) can definitely be greater than 50. BMI is a measure of body fat based on a person's weight and height, calculated by dividing weight in kilograms by height in meters squared. It's a useful tool for assessing whether someone is underweight, normal weight, overweight, or obese.

A BMI of 50 or above would indicate extreme obesity (Obese Class III). While less common, it's certainly possible for individuals to have BMIs in this range, especially in cases of severe obesity. However, it's important to note that BMI is just one indicator of health and doesn't account for factors like muscle mass, bone density, or distribution of fat, so it's not always a perfect measure of an individual's health status.

```
[137]: bmi_gt_50 = df[df['bmi'] > 50][['bmi', 'sex', 'charges', 'smoker']]
print(bmi_gt_50)
```

	DIIIT	Ser	charges	PHOYET
847	50.38	1	2438.0552	0
1047	52.58	1	44501.3982	1
1317	53.13	1	1163.4627	0

[214]: # let's find outliers in charges diagnostic\_plots(df, 'charges')



Charges are greater than 35000 for smokers.

```
bmi
              sex
                        charges
                                  smoker
14
      42.130
                    39611.75770
19
      35.300
                    36837.46700
                 1
                                       1
      31.920
23
                 0
                    37701.87680
                                       1
29
      36.300
                 1
                    38711.00000
                                       1
30
      35.600
                    35585.57600
                                       1
      30.360
                    62592.87309
1300
                                       1
1301
     30.875
                    46718.16325
                                       1
1303 27.800
                    37829.72420
                                       1
                 1
      34.700
                    36397.57600
1313
                                       1
1323
     40.370
                    43896.37630
                                       1
```

[130 rows x 4 columns]

	bmi	sex	charges	smoker
14	42.130	1	39611.75770	1
19	35.300	1	36837.46700	1
23	31.920	0	37701.87680	1
29	36.300	1	38711.00000	1
30	35.600	1	35585.57600	1
•••			•••	
1300	30.360	1	62592.87309	1
1301	30.875	1	46718.16325	1
1303	27.800	1	37829.72420	1
1313	34.700	0	36397.57600	1
1323	40.370	0	43896.37630	1

[133 rows x 4 columns]

### 1.4.3 Numeric Data Standardization

MinMaxScaler () MinMaxScaler transforms features by scaling each feature to a given range.

This estimator scales and translates each feature individually such that it is in the given range on the training set, e.g. between zero and one.

```
The transformation is given by: 1. Xstd = (X - Xmin(axis=0)) / (Xmax(axis=0) - Xmin(axis=0))
2. Xscaled = Xstd * (max - min) + min
```

where  $\min$ ,  $\max$  = feature\_range.

This transformation is often used as an alternative to zero mean, unit variance scaling.

MinMaxScaler doesn't reduce the effect of outliers, but it linearly scales them down into a fixed range, where the largest occurring data point corresponds to the maximum value and the smallest one corresponds to the minimum value. For an example visualization, refer to Compare MinMaxScaler with other scalers.

```
[53]: # standardization: with the MinMaxScaler() from sklearn
      # set up the scaler
      scaler = MinMaxScaler()
      # fit the scaler to the train set, it will learn the parameters
      scaler.fit(df_encoded[['age', 'bmi', 'charges']])
      # transform train and test sets
      MinMaxScaled = scaler.transform(df_encoded[['age', 'bmi', 'charges']])
[54]: # the scaler stores the min of the features, learned from train set
      scaler.data_min_
[54]: array([ 18.
                          15.96 , 1121.8739])
[55]: # the scaler stores the max of the features, learned from train set
      scaler.data_max_
[55]: array([6.4000000e+01, 5.3130000e+01, 6.3770428e+04])
[56]: # access the range of each feature
      scaler.data_range_
[56]: array([4.60000000e+01, 3.71700000e+01, 6.26485541e+04])
[57]: MinMaxScaled
[57]: array([[0.02173913, 0.3212268, 0.25161076],
                        , 0.47914985, 0.00963595],
             [0.2173913, 0.45843422, 0.05311516],
             [0.
                        , 0.56201238, 0.00810808],
             [0.06521739, 0.26472962, 0.01414352],
             [0.93478261, 0.35270379, 0.44724873]])
[58]: df_encoded_MinMaxScaler = df_encoded.copy()
[59]: # let's transform the returned NumPy arrays to dataframes for the rest of
      # the demo
```

```
MinMaxScaled = pd.DataFrame(MinMaxScaled, columns=['age', 'bmi', 'charges'])
[61]: # check contents of scaled columnss
     MinMaxScaled.head(5)
[61]:
             age
                       bmi
                             charges
     0 0.021739 0.321227 0.251611
     1 0.000000 0.479150 0.009636
     2 0.217391 0.458434 0.053115
     3 0.326087 0.181464 0.333010
     4 0.304348 0.347592 0.043816
[63]: # replace the data in the df_encoded_MinMaxScaler variable using the data from
      ⇔the MinMaxScaled variable
     df encoded_MinMaxScaler['age'] = MinMaxScaled['age']
     df encoded_MinMaxScaler['bmi'] = MinMaxScaled['bmi']
     df_encoded_MinMaxScaler['charges'] = MinMaxScaled['charges']
[64]: # check content of copy of dataset with scaled features
     df_encoded_MinMaxScaler.head(5)
[64]:
             age sex
                            bmi children smoker region
                                                           charges
     0 0.021739
                    0 0.321227
                                        0
                                                        3 0.251611
     1 0.000000
                    1 0.479150
                                        1
                                                0
                                                        2 0.009636
                  1 0.458434
     2 0.217391
                                                0
                                                       2 0.053115
     3 0.326087 1 0.181464
                                        0
                                                0
                                                       1 0.333010
     4 0.304348
                    1 0.347592
                                        0
                                                0
                                                        1 0.043816
[65]: df_encoded_MinMaxScaler.to_csv('.//data//explore//
       ⇔insurance_encoded_MinMaxScaler.csv', index=False)
[66]: ds_encoded_MinMaxScaler_path = "D://programming//
       dinformation-technologies-of-smart-systems//calculation-and-graphic work//
       opersonal-medical-insurance-cost-prediction//data//explore//
       →insurance_encoded_MinMaxScaler.csv"
[67]: # is there such path?
     if os.path.exists(ds_encoded_MinMaxScaler_path):
         print("File exists at the specified path.")
     else:
         print("File does not exist at the specified path.")
     File exists at the specified path.
[68]: df_encoded_MinMaxScaler= pd.read_csv(ds_encoded_MinMaxScaler_path)
```

**StandardScaler()** Standardisation involves centering the variable at zero, and standardising the variance to 1. The procedure involves subtracting the mean of each observation and then dividing by the standard deviation:

```
z = (x - xmean) / std
```

The result of the above transformation is z, which is called the z-score, and represents how many standard deviations a given observation deviates from the mean. A z-score specifies the location of the observation within a distribution (in numbers of standard deviations respect to the mean of the distribution). The sign of the z-score (+ or - ) indicates whether the observation is above (+) or below ( - ) the mean.

The shape of a standardised (or z-scored normalised) distribution will be identical to the original distribution of the variable. If the original distribution is normal, then the standardised distribution will be normal. But, if the original distribution is skewed, then the standardised distribution of the variable will also be skewed. In other words, standardising a variable does not normalize the distribution of the data and if this is the desired outcome, we should implement any of the techniques discussed in section 7 of the course.

```
[24]: # standardization: with the StandardScaler() from sklearn

# set up the scaler
scaler = StandardScaler()

# fit the scaler to the train set, it will learn the parameters
scaler.fit(df_encoded[['age', 'bmi', 'charges']])

# transform train and test sets
StandardScaled = scaler.transform(df_encoded[['age', 'bmi', 'charges']])
```

```
[25]: # the scaler stores the mean of the features, learned from train set print("Mean of features:", scaler.mean_)

# the scaler stores the standard deviation deviation of the features, # learned from train set print("Standard deviation of features:", scaler.scale_)
```

Mean of features: [ 39.20702541 30.66339686 13270.42226514] Standard deviation of features: [1.40447090e+01 6.09590764e+00 1.21054850e+04]

```
[26]: StandardScaled
```

```
[44]: df_encoded_StandardScaler = df_encoded.copy()
[62]: df_encoded_StandardScaler.head(5)
[62]:
                             bmi
                                  children
                                            smoker region
                                                             charges
              age
      0 -1.438764
                     0 - 0.453320
                                                 1
                                                         3 0.298584
      1 -1.509965
                     1 0.509621
                                         1
                                                 0
                                                         2 -0.953689
      2 -0.797954
                     1 0.383307
                                         3
                                                 0
                                                         2 -0.728675
      3 -0.441948
                     1 -1.305531
                                         0
                                                 0
                                                         1 0.719843
                                                         1 -0.776802
      4 -0.513149
                     1 -0.292556
                                         0
                                                 0
[45]: # let's transform the returned NumPy arrays to dataframes
      # for the rest of the demo
      StandardScaled = pd.DataFrame(StandardScaled, columns=['age', 'bmi', 'charges'])
[46]: # check contents of scaled columns
      StandardScaled.head(5)
[46]:
                        bmi
                              charges
              age
      0 -1.438764 -0.453320 0.298584
      1 -1.509965 0.509621 -0.953689
      2 -0.797954 0.383307 -0.728675
      3 -0.441948 -1.305531 0.719843
      4 -0.513149 -0.292556 -0.776802
[47]: # replace the data in the df_encoded_StandardScaler variable using the data_
      ⇔from the StandardScaled variable
      df_encoded_StandardScaler['age'] = StandardScaled['age']
      df_encoded_StandardScaler['bmi'] = StandardScaled['bmi']
      df_encoded_StandardScaler['charges'] = StandardScaled['charges']
[48]: # check content of copy of dataset with scaled features
      df_encoded_StandardScaler.head(5)
[48]:
                             bmi
                                  children
                                            smoker region
                                                             charges
                  sex
              age
      0 -1.438764
                                                         3 0.298584
                     0 -0.453320
                                         0
                                                 1
                                                         2 -0.953689
      1 -1.509965
                     1 0.509621
                                         1
                                                 0
      2 -0.797954
                     1 0.383307
                                         3
                                                 0
                                                         2 - 0.728675
      3 -0.441948
                     1 -1.305531
                                         0
                                                 0
                                                         1 0.719843
      4 -0.513149
                     1 -0.292556
                                                         1 -0.776802
                                         0
                                                 0
[49]: df encoded StandardScaler.to csv('.//data//explore//
       →insurance_encoded_StandardScaler.csv', index=False)
[50]:
```

```
ds_encoded_StandardScaler_path = "D://programming//

information-technologies-of-smart-systems//calculation-and-graphic work//

personal-medical-insurance-cost-prediction//data//explore//

insurance_encoded_StandardScaler.csv"
```

```
[51]: # is there such path?
if os.path.exists(ds_encoded_StandardScaler_path):
    print("File exists at the specified path.")
else:
    print("File does not exist at the specified path.")
```

File exists at the specified path.

For **Polynomial Regression**, feature scaling is often less critical compared to some other algorithms like SVMs or Neural Networks. However, it can still be beneficial in certain scenarios. Here's a brief overview of how feature scaling can affect Polynomial Regression:

**StandardScaler:** - StandardScaler scales features to have a mean of 0 and a standard deviation of 1. This can be useful if the features have different scales or units and you want to center them around zero. - Polynomial features can sometimes lead to multicollinearity, where features are highly correlated. Standardizing the features can mitigate multicollinearity to some extent.

MinMaxScaler: + MinMaxScaler scales features to a specified range, typically between 0 and 1. It preserves the relationships between the data points and can be useful if you want to bound the features within a specific range. + It can also help in cases where the polynomial features are bounded within a certain range and you want to maintain that range in the scaled data.

No Scaling: \* In some cases, particularly if the features are already on similar scales or if the polynomial features are generated in a way that preserves the original scale, you may choose not to scale the features at all. \* Additionally, if interpretability of the coefficients is important, you might prefer not to scale the features.

It's often a good idea to experiment with both scalers and evaluate their impact on the model's performance using cross-validation or other validation techniques.

## 1.5 Modelling

### 1.5.1 Regression

Regression in machine learning is a type of supervised learning task where the goal is to predict a continuous output variable based on one or more input features. In simpler terms, regression models try to find the relationship between independent variables (features) and dependent variables (target) and use this relationship to make predictions.

Key points about regression in machine learning: 1. Continuous Output: Unlike classification, where the output is a discrete label or category, regression predicts a continuous value. For example, predicting house prices, stock prices, temperature, or sales figures are all regression problems. 2. Linear Regression: One of the simplest and most commonly used regression techniques is linear regression, where the relationship between the input features and the target variable is modeled as a linear equation. The goal is to find the best-fitting line (or hyperplane in higher dimensions) that minimizes the difference between the actual and predicted values. 3. Non-linear Regression:

In many real-world scenarios, the relationship between the input features and the target variable may not be linear. In such cases, more complex regression techniques like polynomial regression, decision tree regression, random forest regression, support vector regression, or neural network regression can be used to capture non-linear patterns. 4. **Evaluation Metrics**: Regression models are evaluated using metrics that quantify the difference between the actual and predicted values. Common evaluation metrics for regression include Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), R-squared (coefficient of determination), and others. 5. **Overfitting and Underfitting**: Like other machine learning models, regression models can suffer from overfitting (capturing noise in the training data) or underfitting (failing to capture the underlying patterns). Techniques such as regularization, cross-validation, and feature selection can help mitigate these issues. 6. **Feature Engineering**: Feature engineering plays a crucial role in regression tasks. It involves selecting, transforming, or creating new features from the raw data to improve the model's predictive performance. Techniques like scaling, normalization, encoding categorical variables, handling missing values, and creating interaction terms can be applied to preprocess the data before training the regression model.

Overall, regression is a fundamental technique in machine learning that finds numerous applications in various domains such as finance, healthcare, marketing, and engineering for making predictions and understanding relationships between variables.

### 1.5.2 Baseline regression models with default hyperparameters

```
[72]: # get list of all features
       df_encoded.columns
[72]: Index(['age', 'sex', 'bmi', 'children', 'smoker', 'region', 'charges'],
       dtype='object')
[117]: # Split the DataFrame into features (X) and target (y)
       X = df_encoded[['age', 'sex', 'bmi', 'children', 'smoker', 'region']] # features
       y = df_encoded['charges'] # target
[118]: | # Split the transformed data into training and testing sets
       X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,__
        →random_state=42)
[119]: # initialize regression models with specific random states
       lm = LinearRegression()
       ridge = Ridge(random state = 42)
       lasso = Lasso(random state = 42)
       knn = KNeighborsRegressor()
       rf = RandomForestRegressor(random state = 42)
       xgbt = xgb.XGBRegressor(random_state = 42)
       dtree = DecisionTreeRegressor(random state = 42)
       gbr = GradientBoostingRegressor(random_state = 42)
       etr = ExtraTreeRegressor(random_state = 42)
```

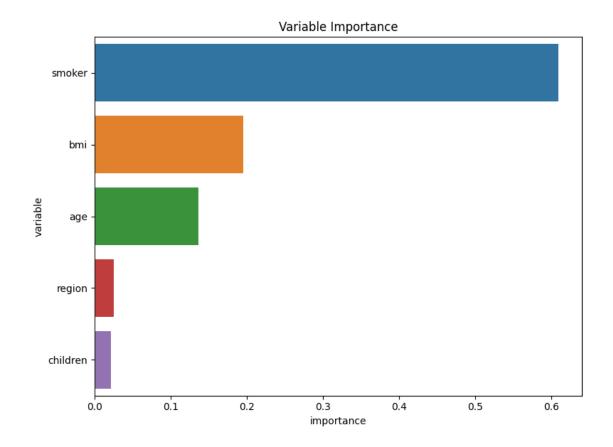
```
# list of all regression models
       algo = [xgbt, lm, ridge, lasso, knn, rf, dtree, gbr, etr]
       result = []
       for i in algo:
               start = time.process_time()
               # fit the model on the training data and calculate performance metrics
              ml_model = i.fit(X_train,y_train)
               result.append([str(i).split("(")[0] + str("_baseline"), ml_model.
        score(X_train, y_train), ml_model.score(X_test, y_test),
                         np.sqrt(mean_squared_error(y_train, ml_model.
        →predict(X_train))),
                         np.sqrt(mean_squared_error(y_test, ml_model.predict(X_test))),
                         mean_absolute_error(y_train, ml_model.predict(X_train)),
                         mean_absolute_error(y_test, ml_model.predict(X_test)),
                         r2_score(y_train, ml_model.predict(X_train)),
                         r2_score(y_test, ml_model.predict(X_test))]),
               print(str(i).split("(")[0]," \t", "{}".format(round(time.
        ⇒process_time()-start,3)),"sec")
       # create DataFrame from the result list and set the index as Algorithm
       result = pd.DataFrame(result, columns = ["Algorithm", "Train_Score", _

¬"Test_Score", "Train_Rmse",
                                                "Test_Rmse", "Train_Mae", "Test_Mae", "
        Guide Train R2", "Test R2"]).sort_values("Test_Rmse").set_index("Algorithm")
       result
      XGBRegressor
                       1.078 sec
      LinearRegression
                              0.0 sec
                       0.172 sec
      Ridge
      Lasso
                       0.156 sec
                              0.328 sec
      KNeighborsRegressor
      RandomForestRegressor
                                       0.688 sec
      DecisionTreeRegressor
                                       0.016 sec
      GradientBoostingRegressor
                                       0.109 sec
      ExtraTreeRegressor
                              0.016 sec
[119]:
                                           Train_Score Test_Score
                                                                     Train_Rmse \
      Algorithm
       GradientBoostingRegressor_baseline
                                                          0.877973 3836.065033
                                              0.898046
      RandomForestRegressor_baseline
                                              0.974309
                                                          0.864261 1925.624128
      XGBRegressor_baseline
                                                          0.850168
                                                                    919.765561
                                              0.994139
      LinearRegression_baseline
                                                          0.783346 6105.789320
                                              0.741705
      Lasso_baseline
                                              0.741705
                                                          0.783320 6105.790345
                                              0.741684
                                                          0.783085 6106.033325
      Ridge_baseline
```

```
DecisionTreeRegressor_baseline
                                       0.998308
                                                   0.684357
                                                              494.205984
ExtraTreeRegressor_baseline
                                       0.998308
                                                   0.671399
                                                              494.205984
KNeighborsRegressor_baseline
                                       0.393768
                                                   0.144504 9354.125544
                                       Test_Rmse
                                                                  Test_Mae \
                                                    Train_Mae
Algorithm
                                                  2101.361701
GradientBoostingRegressor_baseline
                                     4352.538932
                                                               2447.951558
RandomForestRegressor_baseline
                                     4590.573539 1053.588715 2533.674644
XGBRegressor baseline
                                     4822.991168
                                                   499.339156 2791.832518
LinearRegression_baseline
                                     5799.587091 4208.762029 4186.508898
                                                  4209.135074 4187.244900
Lasso baseline
                                     5799.943043
Ridge_baseline
                                     5803.084710 4218.431488 4198.141005
DecisionTreeRegressor_baseline
                                     7000.231682
                                                    29.572515 3154.705669
ExtraTreeRegressor_baseline
                                     7142.470320
                                                    29.572515 3310.218896
KNeighborsRegressor_baseline
                                    11524.523708 6491.688549 7953.210498
                                    Train_R2
                                               Test_R2
Algorithm
GradientBoostingRegressor_baseline
                                    0.898046 0.877973
RandomForestRegressor_baseline
                                    0.974309 0.864261
XGBRegressor_baseline
                                    0.994139 0.850168
LinearRegression baseline
                                    0.741705 0.783346
Lasso_baseline
                                    0.741705 0.783320
Ridge baseline
                                    0.741684 0.783085
DecisionTreeRegressor_baseline
                                    0.998308 0.684357
ExtraTreeRegressor baseline
                                    0.998308 0.671399
KNeighborsRegressor_baseline
                                    0.393768 0.144504
```

#### Feature importance

```
[ ]: rankings = ml_model.feature_importances_.tolist()
```



#### 1.5.3 Baseline regression models with PolynomialFeatures matrix of 2

```
[141]: # Split the DataFrame into features (X) and target (y)
X = df_encoded[['age', 'sex', 'bmi', 'children', 'smoker', 'region']] # features
y = df_encoded['charges'] # target
```

- [144]: # initialize regression models with specific random states

  lm = LinearRegression()

```
ridge = Ridge(random_state = 42)
lasso = Lasso(random state = 42)
knn = KNeighborsRegressor()
rf = RandomForestRegressor(random_state = 42)
xgbt = xgb.XGBRegressor(random_state = 42)
dtree = DecisionTreeRegressor(random_state = 42)
gbr = GradientBoostingRegressor(random_state = 42)
etr = ExtraTreeRegressor(random_state = 42)
# list of all regression models
algo = [xgbt, lm, ridge, lasso, knn, rf, dtree, gbr, etr]
result = []
for i in algo:
        start = time.process_time()
        # fit the model on the training data and calculate performance metrics
        ml_model = i.fit(X_train,y_train)
        result.append([str(i).split("(")[0] + str("_baseline"), ml_model.
  score(X_train, y_train), ml_model.score(X_test, y_test),
                  np.sqrt(mean_squared_error(y_train, ml_model.
  →predict(X_train))),
                  np.sqrt(mean_squared_error(y_test, ml_model.predict(X_test))),
                  mean_absolute_error(y_train, ml_model.predict(X_train)),
                  mean_absolute_error(y_test, ml_model.predict(X_test)),
                  r2 score(y train, ml model.predict(X train)),
                   r2_score(y_test, ml_model.predict(X_test))]),
        print(str(i).split("(")[0]," \t", "{}".format(round(time.
 ⇔process_time()-start,3)),"sec")
# create DataFrame from the result list and set the index as Algorithm
result = pd.DataFrame(result, columns = ["Algorithm", "Train Score", |

¬"Test_Score", "Train_Rmse",
                                          "Test Rmse", "Train Mae", "Test Mae", "
 →"Train_R2", "Test_R2"]).sort_values("Test_Rmse").set_index("Algorithm")
result
XGBRegressor
                1.312 sec
LinearRegression
                        0.0 sec
Ridge
                0.156 sec
                0.172 sec
Lasso
                        0.406 sec
KNeighborsRegressor
RandomForestRegressor
                                 1.422 sec
DecisionTreeRegressor
                                 0.016 sec
GradientBoostingRegressor
                                 0.312 sec
ExtraTreeRegressor
                        0.016 sec
```

```
[144]:
                                           Train_Score Test_Score
                                                                     Train_Rmse \
      Algorithm
      GradientBoostingRegressor baseline
                                                                    3531.079729
                                             0.913613
                                                          0.882020
      RandomForestRegressor_baseline
                                                                    1915.426618
                                              0.974581
                                                          0.869866
      Ridge baseline
                                              0.840397
                                                          0.868124
                                                                    4799.589844
      Lasso_baseline
                                              0.840507
                                                          0.867811
                                                                    4797.941643
      LinearRegression baseline
                                              0.837402
                                                          0.864922
                                                                   4844.420432
      XGBRegressor_baseline
                                             0.996256
                                                         0.852146
                                                                    735.134486
      DecisionTreeRegressor_baseline
                                             0.998308
                                                         0.801469
                                                                    494.205984
      ExtraTreeRegressor_baseline
                                             0.998308
                                                          0.744335
                                                                    494.205984
      KNeighborsRegressor_baseline
                                             0.346751
                                                          0.119860 9710.090728
                                             Test_Rmse
                                                                         Test_Mae \
                                                          Train_Mae
      Algorithm
      GradientBoostingRegressor_baseline
                                            4279.741000
                                                        1957.139704
                                                                     2409.996822
      RandomForestRegressor_baseline
                                            4494.788638
                                                        1053.655276 2413.199889
      Ridge_baseline
                                            4524.765957
                                                        2921.514403 2732.520621
      Lasso_baseline
                                            4530.143241 2925.518663 2726.472040
      LinearRegression_baseline
                                            4579.378770 3035.118503 2876.026334
                                                         347.089509 2635.593164
      XGBRegressor baseline
                                            4791.052846
      DecisionTreeRegressor_baseline
                                            5551.726579
                                                           29.572515 2308.392866
      ExtraTreeRegressor baseline
                                                           29.572515 2829.846888
                                            6300.129213
      KNeighborsRegressor_baseline
                                           11689.335127 6799.720735 8219.705903
                                           Train_R2
                                                      Test_R2
      Algorithm
      GradientBoostingRegressor_baseline
                                          0.913613 0.882020
      RandomForestRegressor_baseline
                                           0.974581 0.869866
                                           0.840397 0.868124
      Ridge_baseline
      Lasso_baseline
                                           0.840507 0.867811
      LinearRegression_baseline
                                           0.837402 0.864922
      XGBRegressor_baseline
                                          0.996256 0.852146
      DecisionTreeRegressor baseline
                                           0.998308 0.801469
      ExtraTreeRegressor_baseline
                                           0.998308 0.744335
      KNeighborsRegressor_baseline
                                           0.346751 0.119860
```

# 1.5.4 Baseline regression models with MinMaxScaler data without PolynomialFeatures

[91]: # Split the transformed data into training and testing sets

```
[92]: # initialize regression models with specific random states
      lm = LinearRegression()
      ridge = Ridge(random_state = 42)
      lasso = Lasso(random_state = 42)
      knn = KNeighborsRegressor()
      rf = RandomForestRegressor(random_state = 42)
      xgbt = xgb.XGBRegressor(random_state = 42)
      dtree = DecisionTreeRegressor(random_state = 42)
      gbr = GradientBoostingRegressor(random_state = 42)
      etr = ExtraTreeRegressor(random_state = 42)
      #rnr = RadiusNeighborsRegressor(random_state = 42)
      # svr = SVR(random_state = 42)
      gpr = GaussianProcessRegressor(random_state = 42)
      # list of all regression models
      algo = [xgbt, lm, ridge, lasso, knn, rf, dtree, gbr, etr, gpr]
      result = []
      for i in algo:
              start = time.process_time()
              # fit the model on the training data and calculate performance metrics
              ml_model = i.fit(X_train,y_train)
              result.append([str(i).split("(")[0] + str("_baseline"), ml_model.
       score(X_train, y_train), ml_model.score(X_test, y_test),
                        np.sqrt(mean_squared_error(y_train, ml_model.
       →predict(X_train))),
                        np sqrt(mean_squared_error(y_test, ml_model.predict(X_test))),
                        mean_absolute_error(y_train, ml_model.predict(X_train)),
                        mean_absolute_error(y_test, ml_model.predict(X_test)),
                        r2_score(y_train, ml_model.predict(X_train)),
                        r2_score(y_test, ml_model.predict(X_test))]),
              print(str(i).split("(")[0]," \t", "{}".format(round(time.
       ⇔process_time()-start,3)),"sec")
      # create DataFrame from the result list and set the index as Algorithm
      result = pd.DataFrame(result, columns = ["Algorithm", "Train_Score", __

¬"Test_Score", "Train_Rmse",
                                               "Test_Rmse", "Train_Mae", "Test_Mae", u

¬"Train_R2", "Test_R2"]).sort_values("Test_Rmse").set_index("Algorithm")

      result
```

Ridge 0.141 sec Lasso 0.172 sec 0.516 secKNeighborsRegressor RandomForestRegressor 0.516 sec DecisionTreeRegressor 0.016 sec GradientBoostingRegressor 0.109 sec ExtraTreeRegressor 0.016 sec GaussianProcessRegressor 1.016 sec [92]: Train\_Score Test\_Score Train\_Rmse Algorithm 0.898046 GradientBoostingRegressor\_baseline 0.877973 0.061232 RandomForestRegressor\_baseline 0.974440 0.863972 0.030658 XGBRegressor baseline 0.852686 0.014861 0.993995 LinearRegression\_baseline 0.741705 0.783346 0.097461 Ridge\_baseline 0.741643 0.783118 0.097473 ExtraTreeRegressor baseline 0.771167 0.007889 0.998308 KNeighborsRegressor\_baseline 0.803382 0.735285 0.085032 DecisionTreeRegressor\_baseline 0.998308 0.727382 0.007889 Lasso\_baseline 0.000000 -0.000919 0.191766 GaussianProcessRegressor\_baseline 0.976524 -55.113747 0.029382 Test\_Rmse Train\_Mae Test\_Mae Train\_R2 \ Algorithm GradientBoostingRegressor\_baseline 0.069475 0.033542 0.039074 0.898046 RandomForestRegressor\_baseline 0.073353 0.016765 0.040546 0.974440 XGBRegressor baseline 0.007866 0.043728 0.993995 0.076335 LinearRegression\_baseline 0.092573 0.067181 0.066825 0.741705 Ridge baseline 0.092622 0.067076 0.066686 0.741643 ExtraTreeRegressor baseline 0.095140 0.000472 0.042052 0.998308 KNeighborsRegressor\_baseline 0.102328 0.051107 0.063950 0.803382 DecisionTreeRegressor\_baseline 0.048087 0.998308 0.103844 0.000472 0.198977 Lasso baseline 0.143667 0.153129 0.000000 GaussianProcessRegressor baseline 1.489833 0.013307 0.578576 0.976524  $Test_R2$ Algorithm GradientBoostingRegressor\_baseline 0.877973 RandomForestRegressor\_baseline 0.863972 XGBRegressor\_baseline 0.852686 LinearRegression\_baseline 0.783346 Ridge baseline 0.783118 ExtraTreeRegressor\_baseline 0.771167 KNeighborsRegressor\_baseline 0.735285

0.172 sec

LinearRegression

0.727382

-0.000919

DecisionTreeRegressor\_baseline

Lasso\_baseline

# 1.5.5 Baseline regression models with StandardScaler data without PolynomialFeatures

```
[133]: # Split the DataFrame into features (X) and target (y)
      X = df_encoded_StandardScaler[['age', 'sex', 'bmi', 'children', 'smoker', _
        y = df_encoded_StandardScaler['charges'] # target
 []: # Split the transformed data into training and testing sets
      X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,__
        →random_state=42)
[135]: # initialize regression models with specific random states
      lm = LinearRegression()
      ridge = Ridge(random_state = 42)
      lasso = Lasso(random_state = 42)
      knn = KNeighborsRegressor()
      rf = RandomForestRegressor(random_state = 42)
      xgbt = xgb.XGBRegressor(random_state = 42)
      dtree = DecisionTreeRegressor(random_state = 42)
      gbr = GradientBoostingRegressor(random_state = 42)
      etr = ExtraTreeRegressor(random_state = 42)
      #rnr = RadiusNeighborsRegressor(random_state = 42)
       # svr = SVR(random_state = 42)
      gpr = GaussianProcessRegressor(random_state = 42)
       # list of all regression models
      algo = [xgbt, lm, ridge, lasso, knn, rf, dtree, gbr, etr, gpr]
      result = []
      for i in algo:
              start = time.process_time()
               # fit the model on the training data and calculate performance metrics
              ml_model = i.fit(X_train,y_train)
              result.append([str(i).split("(")[0] + str("_baseline"), ml_model.
        ⇒score(X_train, y_train), ml_model.score(X_test, y_test),
                        np.sqrt(mean_squared_error(y_train, ml_model.
        →predict(X_train))),
                        np.sqrt(mean_squared_error(y_test, ml_model.predict(X_test))),
                        mean_absolute_error(y_train, ml_model.predict(X_train)),
                        mean_absolute_error(y_test, ml_model.predict(X_test)),
                        r2_score(y_train, ml_model.predict(X_train)),
```

XGBRegressor 1.078 sec LinearRegression 0.0 sec Ridge 0.172 sec Lasso 0.172 sec KNeighborsRegressor 0.438 sec RandomForestRegressor 0.516 sec DecisionTreeRegressor 0.031 sec GradientBoostingRegressor 0.156 sec ExtraTreeRegressor 0.016 sec

GaussianProcessRegressor 0.922 sec

[135]:		Train_Score	Test_Sco	re Train_Rmse	١
	Algorithm				
	<pre>GradientBoostingRegressor_baseline</pre>	0.898046	0.8775	0.316887	
	RandomForestRegressor_baseline	0.974276	0.86511	19 0.159173	
	XGBRegressor_baseline	0.994077	0.85046	0.076379	
	LinearRegression_baseline	0.741705	0.78334	16 0.504382	
	Ridge_baseline	0.741684	0.78308	0.504402	
	KNeighborsRegressor_baseline	0.795118	0.71014	19 0.449214	
	DecisionTreeRegressor_baseline	0.998308	0.70961	0.040825	
	ExtraTreeRegressor_baseline	0.998308	0.66977	76 0.040825	
	Lasso_baseline	0.000000	-0.00091	19 0.992434	
	GaussianProcessRegressor_baseline	0.997850	-12424.38727	71 0.046013	
		${\tt Test\_Rmse}$	Train_Mae	Test_Mae \	
	Algorithm				
	GradientBoostingRegressor_baseline	0.360173	0.173588	0.202335	
	RandomForestRegressor_baseline	0.378014	0.087103	0.208042	
	XGBRegressor_baseline	0.398018	0.041398	0.230354	
	LinearRegression_baseline	0.479088	0.347674	0.345836	
	Ridge_baseline	0.479376	0.348439	0.346760	
	KNeighborsRegressor_baseline	0.554139	0.269205	0.322244	
	DecisionTreeRegressor_baseline	0.554648	0.002443	0.246004	
	ExtraTreeRegressor_baseline	0.591474	0.002443	0.274660	
	Lasso_baseline	1.029749	0.743511	0.792479	
	GaussianProcessRegressor_baseline	114.732592	0.003875 3	32.749994	

	$Train_R2$	Test_R2
Algorithm		
<pre>GradientBoostingRegressor_baseline</pre>	0.898046	0.877550
RandomForestRegressor_baseline	0.974276	0.865119
XGBRegressor_baseline	0.994077	0.850465
LinearRegression_baseline	0.741705	0.783346
Ridge_baseline	0.741684	0.783085
KNeighborsRegressor_baseline	0.795118	0.710149
DecisionTreeRegressor_baseline	0.998308	0.709617
ExtraTreeRegressor_baseline	0.998308	0.669776
Lasso_baseline	0.000000	-0.000919
GaussianProcessRegressor_baseline	0.997850	-12424.387271

# 1.5.6 Baseline regression models without 'children' feature and with PolynomialFeatures

```
[154]: # deleting feature 'children'
       X = df_encoded.drop(['charges','children'], axis = 1)
       Y = df_encoded.charges # target
       # creating an instance of PolynomialFeatures with degree 2
       quad = PolynomialFeatures (degree = 2)
       # transforming the input features X into quadratic polynomial features
       # this generates new features that are combinations of the original features up_
        ⇔to degree 2
       x_quad = quad.fit_transform(X)
       X_train, X_test, Y_train, Y_test = train_test_split(x_quad, Y, test_size=0.2,_
        →random_state=42)
       lm = LinearRegression()
       ridge = Ridge(random_state = 42)
       lasso = Lasso(random_state = 42)
       knn = KNeighborsRegressor()
       rf = RandomForestRegressor(random_state = 42)
       xgbt = xgb.XGBRegressor(random_state = 42)
       dtree = DecisionTreeRegressor(random_state = 42)
       gbr = GradientBoostingRegressor(random_state = 42)
       etr = ExtraTreeRegressor(random_state = 42)
       # list of all regression models
       algo = [xgbt, lm, ridge, lasso, knn, rf, dtree, gbr, etr]
       result = []
       for i in algo:
```

```
start = time.process_time()
       # fit the model on the training data and calculate performance metrics
       ml_model = i.fit(X_train,y_train)
       result.append([str(i).split("(")[0] + str("_baseline"), ml_model.
 ⇒score(X_train, y_train), ml_model.score(X_test, y_test),
                 np.sqrt(mean_squared_error(y_train, ml_model.
 →predict(X_train))),
                 np.sqrt(mean_squared_error(y_test, ml_model.predict(X_test))),
                 mean_absolute_error(y_train, ml_model.predict(X_train)),
                 mean_absolute_error(y_test, ml_model.predict(X_test)),
                 r2_score(y_train, ml_model.predict(X_train)),
                 r2_score(y_test, ml_model.predict(X_test))]),
       ⇔process_time()-start,3)),"sec")
# create DataFrame from the result list and set the index as Algorithm
result = pd.DataFrame(result, columns = ["Algorithm", "Train_Score", __

¬"Test_Score", "Train_Rmse",
                                       "Test_Rmse", "Train_Mae", "Test_Mae", u

¬"Train_R2", "Test_R2"]).sort_values("Test_Rmse").set_index("Algorithm")

result
```

RandomForestRegressor 0.781 sec GradientBoostingRegressor 0.281 sec LinearRegression 0.0 sec

[154]:		Train_Score	Test_Score	Train_Rmse	\
	Algorithm				
	GradientBoostingRegressor_baseline	0.906376	0.873384	3676.018847	
	LinearRegression_baseline	0.835682	0.862207	4869.972761	
	RandomForestRegressor_baseline	0.973032	0.856412	1972.897358	
		Test_Rmse	Train_Mae	Test_Mae	\
	Algorithm				
	GradientBoostingRegressor_baseline	4433.625698	2083.829667	2519.561704	
	LinearRegression_baseline	4625.173407	2983.118678	2823.290299	
	RandomForestRegressor_baseline	4721.430221	1108.386813	2657.723463	
		Train_R2 Test_R2			
	Algorithm				
	GradientBoostingRegressor_baseline	0.906376 0.	873384		
	LinearRegression_baseline	0.835682 0.	862207		
	RandomForestRegressor_baseline	0.973032 0.	856412		

1.5.7 Baseline regression models without 'region' feature and with PolynomialFeatures

```
[169]: # deleting feature 'region'
      X = df_encoded.drop(['charges', 'region'], axis = 1)
      Y = df encoded.charges
      # creating an instance of PolynomialFeatures with degree 2
      quad = PolynomialFeatures (degree = 2)
      # transforming the input features X into quadratic polynomial features
      # this generates new features that are combinations of the original features up_
       →to degree 2
      x_quad = quad.fit_transform(X)
      ⇒random state=42)
      lm = LinearRegression()
      ridge = Ridge(random_state = 42)
      lasso = Lasso(random_state = 42)
      knn = KNeighborsRegressor()
      rf = RandomForestRegressor(random_state = 42)
      xgbt = xgb.XGBRegressor(random_state = 42)
      dtree = DecisionTreeRegressor(random state = 42)
      gbr = GradientBoostingRegressor(random_state = 42)
      etr = ExtraTreeRegressor(random_state = 42)
      # list of all regression models
      algo = [xgbt, lm, ridge, lasso, knn, rf, dtree, gbr, etr]
      # list for results of previous best models
      result = []
      for i in algo:
              start = time.process_time()
              # fit the model on the training data and calculate performance metrics
              ml_model = i.fit(X_train,y_train)
              result.append([str(i).split("(")[0] + str("_baseline"), ml_model.
        score(X_train, y_train), ml_model.score(X_test, y_test),
                        np.sqrt(mean_squared_error(y_train, ml_model.
        →predict(X_train))),
                       np.sqrt(mean_squared_error(y_test, ml_model.predict(X_test))),
                        mean_absolute_error(y_train, ml_model.predict(X_train)),
                        mean absolute error(y test, ml model.predict(X test)),
                        r2_score(y_train, ml_model.predict(X_train)),
                        r2 score(y test, ml model.predict(X test))]),
```

```
print(str(i).split("(")[0]," \t", "{}".format(round(time.
        ⇔process_time()-start,3)),"sec")
       # create DataFrame from the result list and set the index as Algorithm
       result = pd.DataFrame(result, columns = ["Algorithm", "Train_Score", __

¬"Test_Score", "Train_Rmse",

                                                "Test_Rmse", "Train_Mae", "Test_Mae", u
        →"Train_R2", "Test_R2"]).sort_values("Test_Rmse").set_index("Algorithm")
       result
      XGBRegressor
                       1.016 sec
      LinearRegression
                               0.0 sec
      Ridge
                       0.125 sec
      Lasso
                       0.172 sec
                               0.391 sec
      KNeighborsRegressor
      RandomForestRegressor
                                       1.188 sec
      DecisionTreeRegressor
                                       0.016 sec
                                       0.25 sec
      GradientBoostingRegressor
      ExtraTreeRegressor
                               0.016 sec
[169]:
                                           Train_Score Test_Score
                                                                     Train_Rmse \
       Algorithm
       GradientBoostingRegressor_baseline
                                                                    3612.890453
                                              0.909564
                                                          0.884762
       Ridge baseline
                                              0.837345
                                                          0.867382
                                                                    4845.256885
      Lasso_baseline
                                              0.837453
                                                          0.866962
                                                                    4843.651407
      LinearRegression baseline
                                              0.837456
                                                          0.866944
                                                                    4843.610528
                                                          0.860197
       RandomForestRegressor_baseline
                                              0.972708
                                                                    1984.746067
       XGBRegressor_baseline
                                              0.995600
                                                          0.840341
                                                                     796.868123
       DecisionTreeRegressor_baseline
                                              0.998308
                                                          0.755805
                                                                     494.205984
       ExtraTreeRegressor_baseline
                                              0.998308
                                                          0.729844
                                                                     494.205984
       KNeighborsRegressor_baseline
                                              0.393287
                                                          0.157401
                                                                    9357.834084
                                              Test_Rmse
                                                           Train_Mae
                                                                          Test_Mae \
       Algorithm
       GradientBoostingRegressor_baseline
                                            4229.719923
                                                         1994.232121
                                                                      2402.180667
       Ridge_baseline
                                            4537.480504
                                                         2941.739688 2781.345595
                                                         2945.426050 2779.964683
      Lasso baseline
                                            4544.673041
      LinearRegression_baseline
                                            4544.969862 2946.198677 2783.356805
       RandomForestRegressor baseline
                                            4658.787101 1082.612897 2455.683798
       XGBRegressor_baseline
                                            4978.639363
                                                          395.158384 2720.287917
```

Train\_R2 Test\_R2

29.572515

11437.329081 6543.612219 8062.165955

2694.995542

29.572515 3028.218157

6157.183038

6476.221024

Algorithm

DecisionTreeRegressor baseline

ExtraTreeRegressor\_baseline

KNeighborsRegressor\_baseline

GradientBoostingRegressor\_baseline 0.909564 0.884762

```
Ridge_baseline
                                   0.837345 0.867382
                                   0.837453 0.866962
Lasso_baseline
LinearRegression_baseline
                                   0.837456 0.866944
                                   0.972708 0.860197
RandomForestRegressor_baseline
XGBRegressor_baseline
                                   0.995600 0.840341
DecisionTreeRegressor_baseline
                                   0.998308 0.755805
ExtraTreeRegressor_baseline
                                   0.998308 0.729844
KNeighborsRegressor_baseline
                                   0.393287 0.157401
```

#### 1.5.8 Final model choice

```
[23]: X = df_encoded.drop(['charges', 'region'], axis = 1)
      Y = df encoded.charges
      # quad = PolynomialFeatures (degree = 2)
      # x_quad = quad.fit_transform(X)
      X_train,X_test,Y_train,Y_test = train_test_split(X,Y, test_size=0.2,_
       →random state = 0)
      plr = GradientBoostingRegressor(random_state = 42).fit(X_train,Y_train)
      Y_train_pred = plr.predict(X_train)
      Y_test_pred = plr.predict(X_test)
      # Calculating metrics
      score_train = plr.score(X_train, Y_train)
      score_test = plr.score(X_test, Y_test)
      mse_train = mean_squared_error(Y_train, Y_train_pred)
      mse_test = mean_squared_error(Y_test, Y_test_pred)
      mae_train = mean_absolute_error(Y_train, Y_train_pred)
      mae_test = mean_absolute_error(Y_test, Y_test_pred)
      r2_train = r2_score(Y_train, Y_train_pred)
      r2_test = r2_score(Y_test, Y_test_pred)
      # Function to format score_train in desired pattern
      def format score(score):
          return "{:.6f}".format(score)
      # Displaying metrics in a grid
      metrics df = pd.DataFrame({
          'Metric': ['Score', 'MSE', 'MAE', 'R2'],
          'Train Data': [format score(score_train), mse_train, mae_train, r2_train],
          'Test Data': [format_score(score_test), mse_test, mae_test, r2_test]
```

```
print(metrics_df)
```

```
        Metric
        Train Data
        Test Data

        0 Score
        0.895655
        0.897123

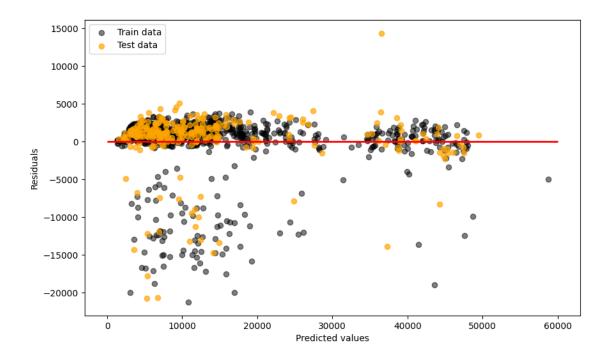
        1 MSE 14959484.462928
        16370815.053277

        2 MAE 2123.736738
        2366.20557

        3 R2 0.895655
        0.897123
```

Scatter plot of predicted values versus residuals (the difference between predicted and actual values) for both the training and test data sets

```
[19]: # Set the figure size
     plt.figure(figsize=(10,6))
      # Plot the residuals for the training data
      plt.scatter(Y_train_pred, Y_train_pred - Y_train,
                  c='black', marker='o', s=35, alpha=0.5,
                  label='Train data')
      # Plot the residuals for the test data
      plt.scatter(Y_test_pred, Y_test_pred - Y_test,
                  c='orange', marker='o', s=35, alpha=0.7,
                  label='Test data')
      # Label the x and y axes
      plt.xlabel('Predicted values')
      plt.ylabel('Residuals')
      # Add a legend
      plt.legend(loc='upper left')
      # Add a horizontal line at y=0 for reference
      plt.hlines(y=0, xmin=0, xmax=60000, lw=2, color='red')
      # Show the plot
      plt.show()
```



#### Feature importance for Gradient Boosting Regressor

#### 1.5.9 Cross-validation technics

**K-fold validation** When evaluating different settings ("hyperparameters") for estimators, such as the CV setting that must be manually set for an SVM, there is still a risk of overfitting on the test set because the parameters can be tweaked until the estimator performs optimally. This way, knowledge about the test set can "leak" into the model and evaluation metrics no longer report on generalization performance. To solve this problem, yet another part of the dataset can be held out as a so-called "validation set": training proceeds on the training set, after which evaluation is done on the validation set, and when the experiment seems to be successful, final evaluation can be done on the test set.

However, by partitioning the available data into three sets, we drastically reduce the number of

samples which can be used for learning the model, and the results can depend on a particular random choice for the pair of (train, validation) sets.

A solution to this problem is a procedure called cross-validation (CV for short). A test set should still be held out for final evaluation, but the validation set is no longer needed when doing CV. In the basic approach, called k-fold CV, the training set is split into k smaller sets (other approaches are described below, but generally follow the same principles). The following procedure is followed for each of the k "folds":

```
[187]: # Define feature matrix X and target variable Y
       X = df_encoded.drop(['charges', 'region'], axis=1)
       Y = df_encoded['charges']
       # Transform features using polynomial features if necessary
       quad = PolynomialFeatures(degree=2)
       X_quad = quad.fit_transform(X)
       # Split the data into training and testing sets
       X_train, X_test, Y_train, Y_test = train_test_split(X_quad, Y, test_size=0.2,_
        →random_state=0)
       # Initialize the model
       model = GradientBoostingRegressor(random state=42)
       # RandomForestRegressor(random_state = 42)
       # LinearRegression()
       # Ridge(random_state = 42)
       # GradientBoostingRegressor(random_state=42)
       # Lasso(random_state = 42)
       # Perform k-fold cross-validation
       kf = KFold(n_splits=5, shuffle=True, random_state=42)
       train_scores, test_scores, train_mse, test_mse, train_mae, test_mae, train_r2,_u
        stest_r2 = [], [], [], [], [], [], []
       for train_index, test_index in kf.split(X_quad):
           X_train, X_test = X_quad[train_index], X_quad[test_index]
           Y_train, Y_test = Y.iloc[train_index], Y.iloc[test_index]
           model.fit(X_train, Y_train)
           Y_train_pred = model.predict(X_train)
           Y_test_pred = model.predict(X_test)
           train_scores.append(model.score(X_train, Y_train))
           test_scores.append(model.score(X_test, Y_test))
           train_mse.append(mean_squared_error(Y_train, Y_train_pred))
           test_mse.append(mean_squared_error(Y_test, Y_test_pred))
```

```
train_mae.append(mean_absolute_error(Y_train, Y_train_pred))
   test_mae.append(mean_absolute_error(Y_test, Y_test_pred))
   train_r2.append(r2_score(Y_train, Y_train_pred))
   test_r2.append(r2_score(Y_test, Y_test_pred))
# Calculate average performance metrics across all folds
avg_train_score = np.mean(train_scores)
avg_test_score = np.mean(test_scores)
avg_train_mse = np.mean(train_mse)
avg_test_mse = np.mean(test_mse)
avg_train_mae = np.mean(train_mae)
avg_test_mae = np.mean(test_mae)
avg_train_r2 = np.mean(train_r2)
avg_test_r2 = np.mean(test_r2)
# Print the results
print('Average Score train data: %.5f, Average Score test data: %.5f' %_
 ⇔(avg_train_score, avg_test_score))
print('Average MSE train data: %.5f, Average MSE test data: %.5f' %_
 ⇔(avg_train_mse, avg_test_mse))
print('Average MAE train data: %.5f, Average MAE test data: %.5f' %__

(avg_train_mae, avg_test_mae))
print('Average R2 train data: %.5f, Average R2 test data: %.5f' %_
```

```
Average Score train data: 0.91739, Average Score test data: 0.85188
Average MSE train data: 12083975.90761, Average MSE test data: 21101318.40206
Average MAE train data: 1891.18876, Average MAE test data: 2524.18689
Average R2 train data: 0.91739, Average R2 test data: 0.85188
```

Random permutations cross-validation The ShuffleSplit iterator will generate a user defined number of independent train / test dataset splits. Samples are first shuffled and then split into a pair of train and test sets.

It is possible to control the randomness for reproducibility of the results by explicitly seeding the random\_state pseudo random number generator.

```
[194]: # Define your DataFrame and preprocessing steps
X = df_encoded.drop(['charges','region'], axis=1)
y = df_encoded['charges']
# Initialize ShuffleSplit with desired parameters
```

```
shuffle_split = ShuffleSplit(n_splits=5, test_size=0.2, random_state=42)
# Initialize lists to store evaluation metrics
train_scores, test_scores, train_mse, test_mse, train_mae, test_mae, train_r2,__
 →test_r2 = [], [], [], [], [], [], []
# Iterate through ShuffleSplit splits
for train_index, test_index in shuffle_split.split(X):
    X_train, X_test = X.iloc[train_index], X.iloc[test_index]
    y_train, y_test = y.iloc[train_index], y.iloc[test_index]
    # Initialize and fit model
    plr = GradientBoostingRegressor(random_state=42).fit(X_train, y_train)
    # Predict on training and test sets
    y_train_pred = plr.predict(X_train)
    y_test_pred = plr.predict(X_test)
    # Calculate evaluation metrics
    train_score = plr.score(X_train, y_train)
    test score = plr.score(X test, y test)
    train_mse_score = mean_squared_error(y_train, y_train_pred)
    test_mse_score = mean_squared_error(y_test, y_test_pred)
    train_mae_score = mean_absolute_error(y_train, y_train_pred)
    test_mae_score = mean_absolute_error(y_test, y_test_pred)
    train_r2_score = r2_score(y_train, y_train_pred)
    test_r2_score = r2_score(y_test, y_test_pred)
    # Append metrics to lists
    train_scores.append(train_score)
    test_scores.append(test_score)
    train mse.append(train mse score)
    test_mse.append(test_mse_score)
    train mae.append(train mae score)
    test_mae.append(test_mae_score)
    train_r2.append(train_r2_score)
    test_r2.append(test_r2_score)
# Calculate mean and standard deviation of evaluation metrics
mean_train_score = np.mean(train_scores)
mean_test_score = np.mean(test_scores)
mean_train_mse = np.mean(train_mse)
mean_test_mse = np.mean(test_mse)
mean_train_mae = np.mean(train_mae)
mean_test_mae = np.mean(test_mae)
mean_train_r2 = np.mean(train_r2)
mean_test_r2 = np.mean(test_r2)
```

```
std_train_score = np.std(train_scores)
std_test_score = np.std(test_scores)
std_train_mse = np.std(train_mse)
std_test_mse = np.std(test_mse)
std_train_mae = np.std(train_mae)
std_test_mae = np.std(test_mae)
std_train_r2 = np.std(train_r2)
std test r2 = np.std(test r2)
# Print the mean and standard deviation of evaluation metrics
print("Mean train score: {:.5f} +/- {:.5f}".format(mean_train_score, __
 ⇔std train score))
print("Mean test score: {:.5f} +/- {:.5f}".format(mean_test_score,__
 ⇔std_test_score))
print("Mean train MSE: {:.5f} +/- {:.5f}".format(mean_train_mse, std_train_mse))
print("Mean test MSE: {:.5f} +/- {:.5f}".format(mean_test_mse, std_test_mse))
print("Mean train MAE: {:.5f} +/- {:.5f}".format(mean_train_mae, std_train_mae))
print("Mean test MAE: {:.5f} +/- {:.5f}".format(mean_test_mae, std_test_mae))
print("Mean train R^2: {:.5f} +/- {:.5f}".format(mean_train_r2, std_train_r2))
print("Mean test R^2: {:.5f} +/- {:.5f}".format(mean_test_r2, std_test_r2))
```

```
Mean train score: 0.90242 +/- 0.01112
Mean test score: 0.85730 +/- 0.04462
Mean train MSE: 14224739.00574 +/- 1271403.97849
Mean test MSE: 20427228.90336 +/- 5363680.73304
Mean train MAE: 2042.63645 +/- 142.04313
Mean test MAE: 2452.22782 +/- 238.02025
Mean train R^2: 0.90242 +/- 0.01112
Mean test R^2: 0.85730 +/- 0.04462
```

### 1.6 Model tuning

https://en.wikipedia.org/wiki/Hyperparameter\_optimization

### 1.6.1 Parameters vs Hyperparameters

Let's now define what are hyperparameters, but before doing that let's consider the difference between a parameter and a hyperparameter.

A parameter can be considered to be intrinsic or internal to the model and can be obtained after the model has learned from the data. Examples of parameters are regression coefficients in linear regression, support vectors in support vector machines and weights in neural networks.

A hyperparameter can be considered to be extrinsic or external to the model and can be set arbitrarily by the practitioner. Examples of hyperparameters include the k in k-nearest neighbors, number of trees and maximum number of features in random forest, learning rate and momentum in neural networks, the C and gamma parameters in support vector machines.

#### 1.6.2 Hyperparameter tuning

As there are no universal best hyperparameters to use for any given problem, hyperparameters are typically set to default values. However, the optimal set of hyperparameters can be obtained from manual empirical (trial-and-error) hyperparameter search or in an automated fashion via the use of optimization algorithm to maximize the fitness function.

Two common hyperparameter tuning methods include grid search and random search. As the name implies, a grid search entails the creation of a grid of possible hyperparameter values whereby models are iteratively built for all of these hyperparameter combinations in a brute force manner. In a random search, not all hyperparameter combinations are used, but instead each iteration makes use of a random hyperparameter combination.

Building a Baseline Gradient Boosting Regressor Here, we will first start by building a baseline Gradient Boosting Regressor that will serve as a baseline for comparative purpose with the model using the optimal set of hyperparameters. For the baseline model, we will set a default hyperparameters of Gradient Boosting Regressor.

```
[24]: X = df_encoded.drop(['charges', 'region'], axis = 1)
      Y = df encoded.charges
      X_train,X_test,Y_train,Y_test = train_test_split(X,Y, test_size=0.2,_
       →random_state = 0)
      plr = GradientBoostingRegressor(random_state = 42).fit(X_train,Y_train)
      Y_train_pred = plr.predict(X_train)
      Y_test_pred = plr.predict(X_test)
      # calculating metrics
      score_train = plr.score(X_train, Y_train)
      score_test = plr.score(X_test, Y_test)
      mse_train = mean_squared_error(Y_train, Y_train_pred)
      mse_test = mean_squared_error(Y_test, Y_test_pred)
      mae train = mean absolute error(Y train, Y train pred)
      mae_test = mean_absolute_error(Y_test, Y_test_pred)
      r2_train = r2_score(Y_train, Y_train_pred)
      r2_test = r2_score(Y_test, Y_test_pred)
      # function to format score_train in desired pattern
      def format score(score):
          return "{:.6f}".format(score)
      # displaying metrics in a grid
      metrics_df = pd.DataFrame({
```

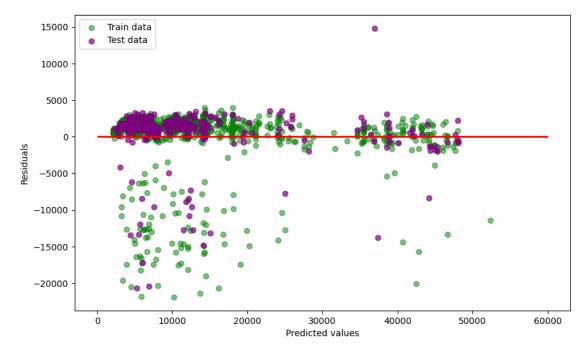
```
'Metric': ['Score', 'MSE', 'MAE', 'R2'],
          'Train Data': [format_score(score_train), mse_train, mae_train, r2_train],
          'Test Data': [format score(score_test), mse_test, mae_test, r2_test]
      })
      print(metrics_df)
       Metric
                    Train Data
                                       Test Data
     0 Score
                       0.895655
                                        0.897123
               14959484.462928 16370815.053277
     1
          MSE
     2
          MAE
                                      2366.20557
                    2123.736738
     3
           R2
                       0.895655
                                        0.897123
[25]: # display baseline model params
      plr.get_params()
[25]: {'alpha': 0.9,
       'ccp_alpha': 0.0,
       'criterion': 'friedman_mse',
       'init': None,
       'learning_rate': 0.1,
       'loss': 'squared_error',
       'max_depth': 3,
       'max_features': None,
       'max_leaf_nodes': None,
       'min_impurity_decrease': 0.0,
       'min_samples_leaf': 1,
       'min_samples_split': 2,
       'min_weight_fraction_leaf': 0.0,
       'n_estimators': 100,
       'n iter no change': None,
       'random state': 42,
       'subsample': 1.0,
       'tol': 0.0001,
       'validation_fraction': 0.1,
       'verbose': 0,
       'warm_start': False}
```

**Hyperparameter Tuning** Now we will be performing the tuning of hyperparameters of the random forest model.

```
[37]: # grid with all param to tune on model
param_grid = {
    'n_estimators': [10, 50, 100, 150, 200],
    'max_depth': [2, 3, 5, 7, 9, 11],
    'learning_rate': [0.01, 0.1, 0.3],
    'min_samples_split': [2, 5, 10, 13],
```

```
'min_samples_leaf': [1, 2, 4, 5]
      }
[38]: # create new GridSearchCV object
      grid_search = GridSearchCV(estimator=GradientBoostingRegressor(random_state=42),
                                 param_grid=param_grid,
                                 scoring='neg_mean_squared_error', #
                                 cv=5, #
                                                                  CPU
                                 n_jobs=-1) #
[39]: # release Grid Search
      grid_search.fit(X_train, Y_train)
[39]: GridSearchCV(cv=5, estimator=GradientBoostingRegressor(random_state=42),
                   n_{jobs}=-1,
                   param_grid={'learning_rate': [0.01, 0.1, 0.3],
                               'max_depth': [2, 3, 5, 7, 9, 11],
                                'min_samples_leaf': [1, 2, 4, 5],
                               'min_samples_split': [2, 5, 10, 13],
                                'n_estimators': [10, 50, 100, 150, 200]},
                   scoring='neg_mean_squared_error')
[53]: # display best tuned hyperparameters
      print("Best hyperparameters:", grid_search.best_params_)
     Best hyperparameters: {'learning_rate': 0.1, 'max_depth': 3, 'min_samples_leaf':
     4, 'min_samples_split': 13, 'n_estimators': 50}
[50]: # define features for model
      X = df_encoded.drop(['charges', 'region', 'sex'], axis = 1)
      Y = df_encoded.charges
      # split dataset
      X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.2,_
       →random state = 0)
      plr = GradientBoostingRegressor(random_state = 42, learning_rate = 0.1, __
       ⇒max_depth = 3, min_samples_leaf = 4, min_samples_split = 13, n_estimators =
       →50).fit(X_train,Y_train)
      # train model
      Y_train_pred = plr.predict(X_train)
      Y_test_pred = plr.predict(X_test)
      # calculating metrics
      score_train = plr.score(X_train, Y_train)
```

```
score_test = plr.score(X_test, Y_test)
      mse_train = mean_squared_error(Y_train, Y_train_pred)
      mse_test = mean_squared_error(Y_test, Y_test_pred)
      mae_train = mean_absolute_error(Y_train, Y_train_pred)
      mae_test = mean_absolute_error(Y_test, Y_test_pred)
      r2_train = r2_score(Y_train, Y_train_pred)
      r2_test = r2_score(Y_test, Y_test_pred)
      # function to format score_train in desired pattern
      def format score(score):
          return "{:.6f}".format(score)
      # displaying metrics in a grid
      metrics_df = pd.DataFrame({
          'Metric': ['Score', 'MSE', 'MAE', 'R2'],
          'Train Data': [format_score(score_train), mse_train, mae_train, r2_train],
          'Test Data': [format_score(score_test), mse_test, mae_test, r2_test]
      })
      print(metrics_df)
                    Train Data
                                       Test Data
       Metric
     0 Score
                       0.873020
                                        0.899796
     1
          MSE 18204620.074767 15945425.744968
     2
                   2353.121722
          MAE
                                       2375.0363
     3
           R2
                        0.87302
                                        0.899796
     Result Analysis
                                                                            (0.87)
                                               (R2)
     0.90
                 ),
                             : 1.
                                                  (MSE)
                                                                                15,955,774.
                                                           $15,955
             . 2.
                               (MAE)
                                                             2,374.
                                                     $2,374.
                                     Gradient Boosting Regressor
[51]: # Set the figure size
      plt.figure(figsize=(10,6))
      # Plot the residuals for the training data
      plt.scatter(Y_train_pred, Y_train_pred - Y_train,
                  c='green', marker='o', s=35, alpha=0.5,
```



### Feature importance for Final Gradient Boosting Regressor

