Group SBS, Sheet 06, Exercise 01

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In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from itertools import combinations
```

A Linear Regression model is given as $\mathbf{y} = \mathbf{X}\beta + \epsilon_i$ for $i = 1, 2, 3, \ldots.$ where $\epsilon_i \sim (0, \sigma^2 \mathbf{I}_n)$ and iid. $\mathbf{y}$ is of size $n \times 1$ and $\mathbf{X}$ is of size $n \times p$ Thus $\hat{\beta}$ of ML estimator and LS-estimator is given by the formula, $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ where $\mathbf{X}$ is of rank $p + 1$.

In [2]:
```
names = ['X1', 'X2', 'X3', 'X4', 'X5']
X = pd.read_csv("X_potential_drivers.txt", header=None, names=names)
# adding X0
X['X0'] = np.ones(len(X))
# rearranging
X = X[['X0','X1', 'X2', 'X3', 'X4', 'X5']]
# converting to complex datatype
X['X4'] = X['X4'].str.replace('i','j').apply(lambda x: np.complex(x))
# removing the infinity value from the data assuming that it is an outlier
X.drop(100, inplace=True)
```

In [3]:
```
X_start = X.to_numpy()
# imaginary value
X_imag = X_start[:, 4].imag
# seperating real and imaginary part of X4 and adding X4imag as a
# as a new predictor variable
X = np.hstack((X_start.real, X_imag.reshape(len(X_start),1)))

Y = np.loadtxt("Y_snow.txt")
# deleting the y label for the record with infinity value in X
Y = np.delete(Y, [100], axis=0)
```

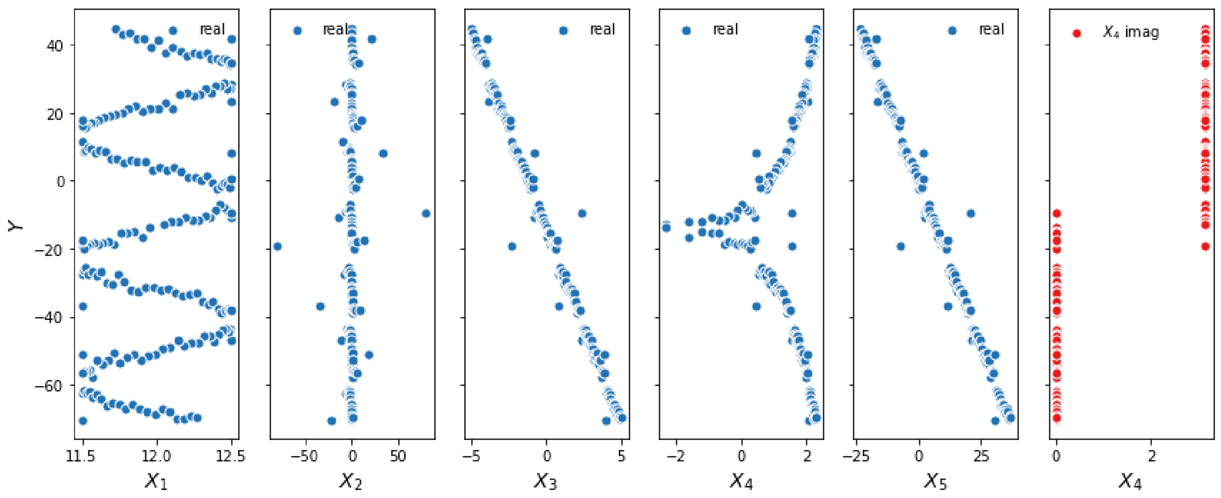
#

Exploratory Data Analysis

In [4]:
```
def plot_pred_response():
    fig, axs = plt.subplots(1, 6, figsize=(12,5), sharey=True)
    axs = axs.flat
    for i, ax in enumerate(axs[:-1]):
        ax.scatter(X[:,i+1], Y, s=50, color='#2171b5', ec="white", label='real')
        ax.set_xlabel(f"$X_{i+1}$", fontsize=14)
        ax.legend(frameon=False)
    axs[-1].scatter(X[:,-1], Y, s=50, color='#e41a1c', ec="white", label='$X_4$ imag
    axs[-1].legend(frameon=False)
    axs[-1].set_xlabel(f"$X_{4}$", fontsize=14)
    axs[0].set_ylabel("$Y$", fontsize=14)
    fig.tight_layout()
```

In [5]:

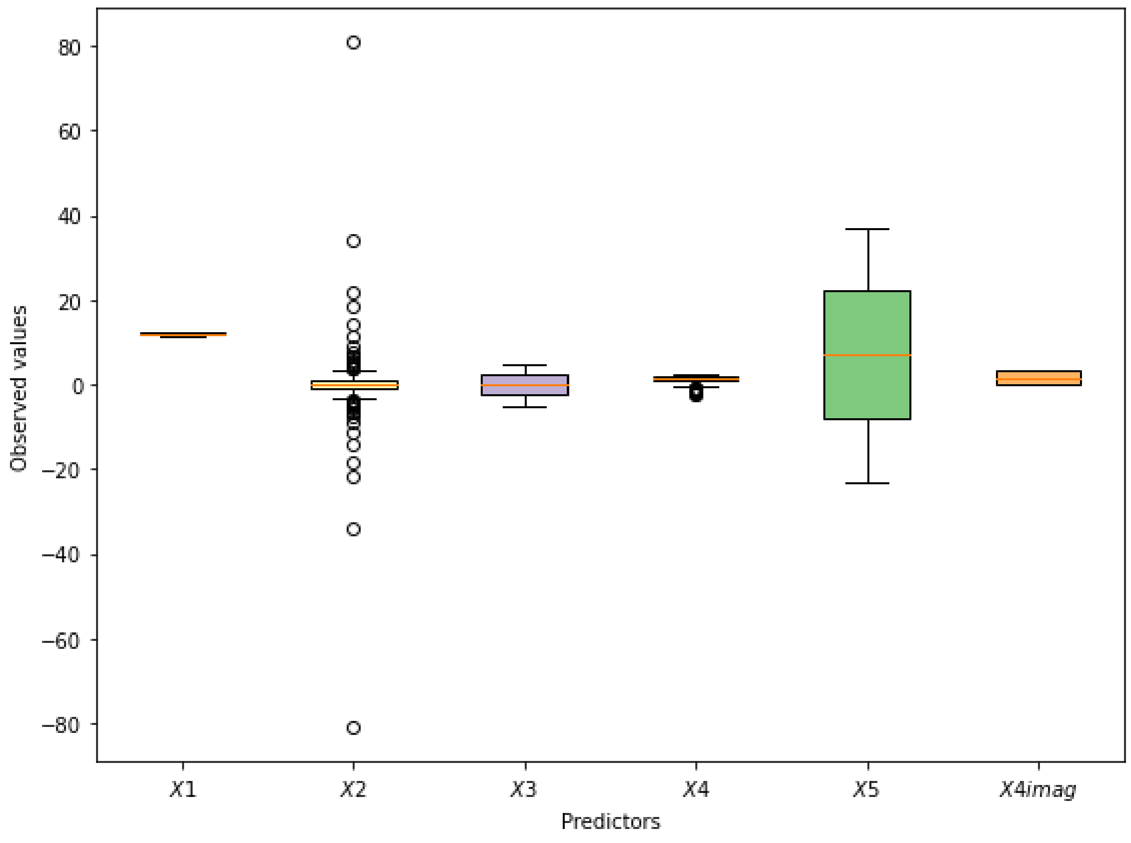
```
plot_pred_response()
```



- There is no linear relationship between X_1 and Y. The relationship is a sinusoidal wave.
- There is no linear relationship between X_2 and Y. The relationship follows a sawtooth curve
- There exists a linear relationship between X_3 and Y, but they are negatively correlated
- There is no linear relationship between X_4 and Y. Y diverges to $-\infty$ and ∞ when X_4 increases.
- There exist a linear relationship between X_3 and Y, but they are negatively correlated. Also it looks like X_5 and X_3 are positively correlated. The values of X_5 are upscaled in comparison to X_3
- Imaginary part of X_4 predictor is a binary variable

In [6]:

```
names_ = names[:]
names_.append("X4 imag")

def plot_outliers():
    fig, axs = plt.subplots(figsize=(8,6), sharey=True)
    bplot = axs.boxplot(X[:,1:].real, patch_artist=True, labels=[f'${name}$' for nam
    colors = ["#8dd3c7", "#ffffb3", "#beaed4", "#fb8072", "#7fc97f", "#fdb462"]
    for patch, color in zip(bplot['boxes'], colors):
        patch.set_facecolor(color)
    axs.set_xlabel('Predictors')
    axs.set_ylabel('Observed values')
    fig.tight_layout()

plot_outliers()
```



- Predictors X_2 and X_4 is having outliers, this is clear from the above exploratory graph as well.

Correlation between predictors and also with response

$$Corr(X,Y) = \frac{E[(X - E[X])(Y - E[Y])]}{\sqrt{Var(X)Var(Y)}}$$

In [7]:

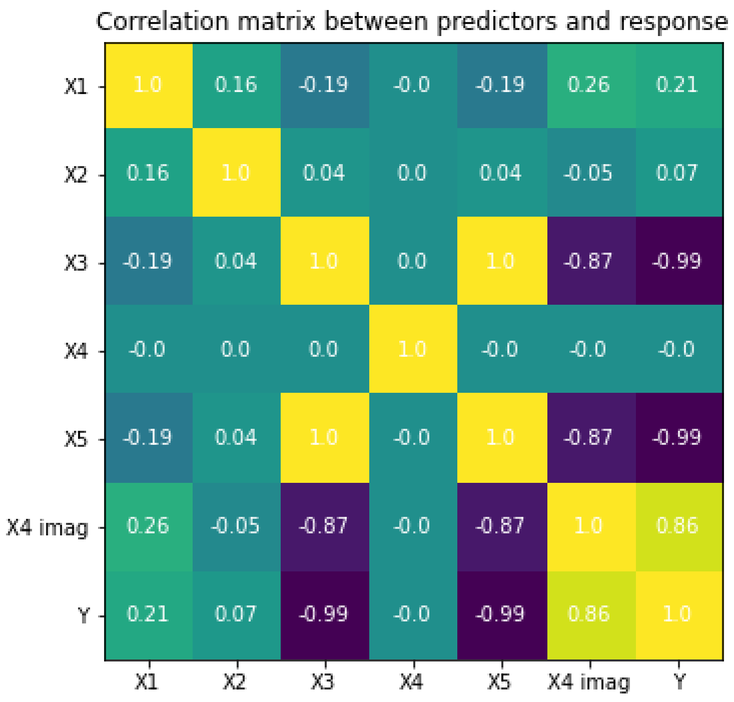
```
# correlation matrix
corr_mat = np.hstack((X[:,1:],Y.reshape(len(Y),1)))

def correlation_matrix(corr_mat):
    # deviations from mean
    x_dev = (corr_mat - np.mean(corr_mat, axis = 0))
    # square of deviations
    x_dev_sqr = np.sum(x_dev**2, axis=0).reshape(corr_mat.shape[1], 1)
    numerator = x_dev.T@x_dev
    denominator = np.sqrt(x_dev_sqr @ x_dev_sqr.T)
    return numerator/denominator
```

In [8]:

```
def plot_heatmap(corr, names):
    """parts of code from matplotlib page"""
    len_names = len(names)
    fig, ax = plt.subplots(figsize=(5.2,5.2))
    ax.imshow(corr)
    # Show all ticks and label them with the respective list entries
    ax.set_xticks(np.arange(len_names))
    ax.set_yticks(np.arange(len_names))
    ax.set_xticklabels(names)
    ax.set_yticklabels(names)
    # Loop over data dimensions and create text annotations.
    for i in range(len_names):
        for j in range(len_names):
            text = ax.text(j, i, np.round(corr[i, j],2),
                           ha="center", va="center", color="w")
        ax.set_title("Correlation matrix between predictors and response")
    fig.tight_layout()
    plt.show()
```

In [9]:

```
name_pred_resp = names_[:]
corr = correlation_matrix(corr_mat)
name_pred_resp.append("Y")
plot_heatmap(corr, name_pred_resp)
```



	X1	X2	X3	X4	X5	X4 imag	Y
X1	1.0	0.16	-0.19	-0.0	-0.19	0.26	0.21
X2	0.16	1.0	0.04	0.0	0.04	-0.05	0.07
X3	-0.19	0.04	1.0	0.0	1.0	-0.87	-0.99
X4	-0.0	0.0	0.0	1.0	-0.0	-0.0	-0.0
X5	-0.19	0.04	1.0	-0.0	1.0	-0.87	-0.99
X4 imag	0.26	-0.05	-0.87	-0.0	-0.87	1.0	0.86
Y	0.21	0.07	-0.99	-0.0	-0.99	0.86	1.0

- As expected from the figures, there is a perfect correlation between X_3 and X_5. Otherwise, no other predictor variables show strong correlation with each other
- There is almost a perfect negative correlation between X_3 and Y and X_5 and Y. From this we can draw the conclusion that X_3 or X_5 will be among the important variables in model building.
- There is no correlation between the real part of X_4 and Y or with other predictor variables

In [10]:

```
class MultipleRegression():

    def __init__(self, scale=True):
        self.scale = scale
        self.X = None
        self.Y = None

    def scale_data(self, X):
        self.X = X
        if self.scale:
            dev = X - np.mean(X, axis=0)
            std = np.std(X, axis = 0)
            np.true_divide(dev, std, out=self.X, where=std != 0)

    def fit_predict(self, X, Y):
        self.Y = Y
        self.X = X
        try:
            coeff = np.linalg.inv(self.X.T @ self.X) @ self.X.T @ self.Y
            y_hat = self.X @ coeff
            return [coeff, y_hat]
        except np.linalg.LinAlgError:
            print("Singular matrix")

    def mse(self, predictions):
        return np.mean((self.Y - predictions)**2)

    def r_squared(self, predictions):
        muY = np.mean(self.Y)
        return np.sum((predictions - muY)**2)/np.sum((self.Y - muY)**2)

    def adj_r_squared(self, X, rsquared):
        n = len(self.X)
        p = self.X.shape[1]
        return 1 - (((n-1)/(n-p)) *(1-rsquared))
```

Approach 1

Best subset selection method based on R^2 adjusted value

In [11]:

```
class BestSubsetSelection(MultipleRegression):

    def run_subset_selection(self, p, X, Y):
        self.models = {}
        # scaling the data to deal with the outliers
        self.scale_data(X)
        X0 = self.X[:, 0].reshape(-1,1)
        for i in range(1, p):
            combs = combinations(np.arange(1, p), i)
            for j in combs:
                X_sub = np.hstack((X0, X[:, j]))
                if isinstance(self.fit_predict(X_sub, Y), list):
                    coeff, pred = self.fit_predict(X_sub, Y)
                    rsquared = self.r_squared(pred)
                    self.models[(0, j)] = [self.mse(pred), rsquared, self.adj_r_squa


    def select_best_models(self, threshold):
        self.best_models = {}
        for key, values in self.models.items():
            if values[-1] > threshold and values[-1] < 1 :
                self.best_models[key] = [round(value, 4) for value in values]
```

In [12]:

```
bss = BestSubsetSelection()
bss.run_subset_selection(p=7, X=X, Y=Y)
```

```
Singular matrix
```

In [13]:

```
bss.select_best_models(threshold=0.9)
print(f"Predictors: [MSE, R2, corrected R2]")
print("------------------------------------")
bm = bss.best_models
for key, value in bm.items():
    # filtering based on MSE
    if value[0] < 1:
        print(key, value)
```

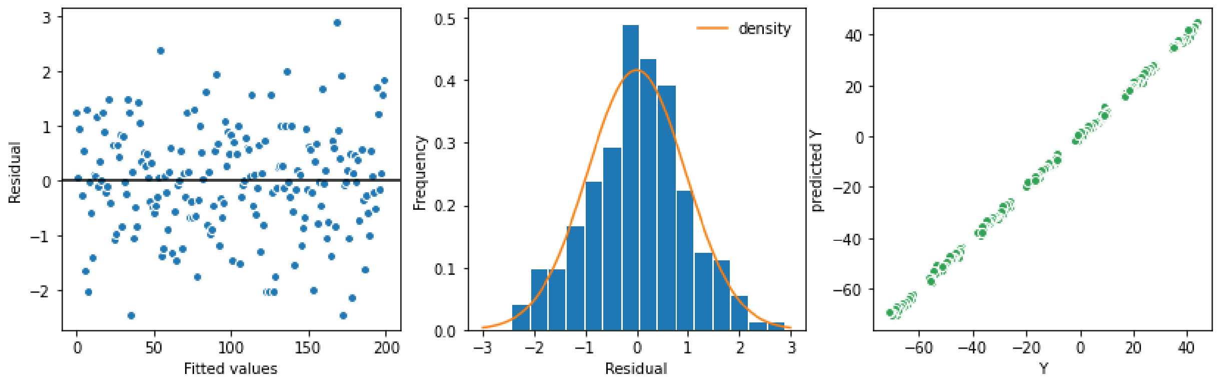
```
Predictors: [MSE, R2, corrected R2]
-----------------------------------
(0, (2, 3)) [0.917, 0.9992, 0.9992]
(0, (2, 5)) [0.917, 0.9992, 0.9992]
(0, (1, 2, 3)) [0.9122, 0.9992, 0.9992]
(0, (1, 2, 5)) [0.9122, 0.9992, 0.9992]
(0, (2, 3, 4)) [0.9169, 0.9992, 0.9992]
(0, (2, 3, 6)) [0.9168, 0.9992, 0.9992]
(0, (2, 4, 5)) [0.9169, 0.9992, 0.9992]
(0, (2, 5, 6)) [0.9168, 0.9992, 0.9992]
(0, (1, 2, 3, 4)) [0.9121, 0.9992, 0.9992]
(0, (1, 2, 3, 6)) [0.9122, 0.9992, 0.9992]
(0, (1, 2, 4, 5)) [0.9121, 0.9992, 0.9992]
(0, (1, 2, 5, 6)) [0.9122, 0.9992, 0.9992]
(0, (2, 3, 4, 6)) [0.9167, 0.9992, 0.9992]
(0, (2, 4, 5, 6)) [0.9167, 0.9992, 0.9992]
(0, (1, 2, 3, 4, 6)) [0.9121, 0.9992, 0.9992]
(0, (1, 2, 4, 5, 6)) [0.9121, 0.9992, 0.9992]
```

From the subset selection method, the model with the least corrected R^2 is selected as the best model. Based on this criteria, we had 32 models. Therefore we looked into the MSE as the next parameter to select the model keeping corrected R^2 fixed. After this filtering criteria we had 16 models to choose from. Therefore, we choose the model with least number of predictors as adding more variables is not considerably decreasing the MSE error. Based on this the best predictor variables for our model are the following.

- model 1: X_0, X_2, X_3
    - model 2: X_0, X_2, X_5

In [14]:

```
from scipy.stats import norm
M_reg = MultipleRegression()
# coefficients and predictions of the best model
coeff, y_hat = M_reg.fit_predict(X[:, [0, 2, 3]], Y)
residual = Y - y_hat


fig, axs = plt.subplots(1, 3, figsize=(14,4))
axs[0].scatter(np.arange(len(Y)), residual, ec='white')
axs[0].axhline(0, color='black');
axs[0].set_ylabel("Residual")
axs[0].set_xlabel("Fitted values")
axs[1].hist(residual, bins=15, ec='white', density=True);
axs[1].set_xlabel("Residual")
axs[1].set_ylabel("Frequency")
x = np.linspace(-3, 3, 100)
axs[1].plot(x, norm.pdf(x, np.mean(residual), np.std(residual)), label='density');
axs[1].legend(frameon=False)
axs[2].scatter(y_hat, Y, color= '#31a354', ec='white')
axs[2].set_xlabel("Y")
axs[2].set_ylabel("predicted Y")
plt.show()
```



Residual plots are a useful graphical tool for identifying non-linearity. Ideally, the residual plot will show no fitted discernible pattern. The presence of a pattern may indicate a problem with some aspect of the linear model [1]. From the figures above we can see that there is no distinguishable pattern from the residual plot, which is a good sign that the model is following linearity assumption. The predicted values of Y and Y also follows a linear relationship, which also points towards a well fitted model.

#

Approach 2

Best model selection using cross validation approach

Compute the the cross-validation error for each model and then select the model for which the resulting estimated test error is smallest.

In [15]:

```
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold
from sklearn.model_selection import train_test_split, cross_val_score
```

In [16]:

```
class CrossValidation():

    def run_cross_validation_subset(self, p, X, Y):
            self.cross_models = {}
            for i in range(1, p):
                combs = combinations(np.arange(p), i)
                for j in combs:
                    X_sub = X[:, j]
                    folds = KFold(n_splits = 5, shuffle = True, random_state = 100)
                    LR = LinearRegression(fit_intercept=False)
                    scores = cross_val_score(LR, X_sub, Y, scoring='neg_root_mean_sq
                    rmse_scores = np.sqrt(np.mean(-scores))
                    self.cross_models[j] = rmse_scores

    def select_best_cross_models(self, threshold):
        self.best_cross_models = {}
        for key, values in self.cross_models.items():
            if values  < threshold:
                self.best_cross_models[key] = round(values, 5)
```

In [17]:

```
CV = CrossValidation()
CV.run_cross_validation_subset(X=X, Y=Y, p=X.shape[1]-1)
CV.select_best_cross_models(threshold=1)
```

In [18]:
```
CV.best_cross_models
```

Out[18]:
```
{(0, 2, 3): 0.98445,
 (0, 2, 5): 0.98445,
 (0, 1, 2, 3): 0.98356,
 (0, 1, 2, 5): 0.98356,
 (0, 2, 3, 4): 0.98529,
 (0, 2, 3, 5): 0.98445,
 (0, 2, 4, 5): 0.98529,
 (0, 1, 2, 3, 4): 0.98421,
 (0, 1, 2, 3, 5): 0.98356,
 (0, 1, 2, 4, 5): 0.98421,
 (0, 2, 3, 4, 5): 0.98529}
```

# From the best cross validation models, the model with the least prediction error on the test data set is taken as the best model. Based on this criteria, we have three models with the least rmse value

- model 1: X_0, X_1, X_2, X_3
    - model 2: X_0, X_1, X_2, X_5
- model 3: X_0, X_1, X_2, X_3, X_5

However keeping X_3 and X_5 together in the model is not necessary as they are perfectly correlated, and not giving any additional information on the dataset fitted. Therefore, the best models are model 1 and model 2.

#

Approach 3

Backward selection approach

We start with all variables in the model, and backward remove the variable with the largest p-value—that is, the variable selection that is the least statistically significant. The new (p − 1)-variable model is fit, and the variable with the largest p-value is removed. This procedure continues until a stopping rule is reached. For instance, we may stop when all remaining variables have a p-value below some threshold [1]. Here we chose the popular threshold, alpha = 0.05.

In [19]:
```
import statsmodels.api as sm

def backward_selection(X, Y, alpha=0.05, col_names=list(range(6))):
    mod = sm.OLS(Y,X)
    fit_ = mod.fit()
    p_values = fit_.summary2().tables[1]['P>|t|']
    X_copy = X.copy()
    if np.any(p_values > 0.05):
        idx = np.argmax(p_values)
        if idx in col_names:
            col_names.remove(idx)
        X_copy = np.delete(X_copy, idx, axis=1)
        return backward_selection(X_copy, Y, col_names)
    return col_names, fit_.summary()
```

In [20]:
```
cols, summary = backward_selection(X, Y)
print("Columns", cols)
print("Summary", summary)
```

```
Columns [0, 2, 3, 5]
Summary                             OLS Regression Results                            
==============================================================================
Dep. Variable:                      y   R-squared:                       0.999
Model:                            OLS   Adj. R-squared:                  0.999
Method:                 Least Squares   F-statistic:                 1.212e+05
Date:                Wed, 15 Dec 2021   Prob (F-statistic):          3.99e-305
Time:                        09:42:20   Log-Likelihood:                -275.13
No. Observations:                 200   AIC:                             556.3
Df Residuals:                     197   BIC:                             566.1
Df Model:                           2                                         
Covariance Type:            nonrobust                                         
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const        -13.9013      0.068   -203.750      0.000     -14.036     -13.767
x1             3.8905      0.068     56.967      0.000       3.756       4.025
x2           -16.7669      0.034   -491.026      0.000     -16.834     -16.700
x3           -16.7669      0.034   -491.026      0.000     -16.834     -16.700
==============================================================================
Omnibus:                        0.367   Durbin-Watson:                   2.002
Prob(Omnibus):                  0.832   Jarque-Bera (JB):                0.186
Skew:                          -0.063   Prob(JB):                        0.911
Kurtosis:                       3.081   Cond. No.                     4.13e+15
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly spe
cified.
[2] The smallest eigenvalue is 2.34e-29. This might indicate that there are
strong multicollinearity problems or that the design matrix is singular.
```

- The backward selection method is useful for selecting the important features. According to this method X_0, X_2, X_3, X_5 are the most important variables. In this selection procedure we used the significance level, alpha = 0.05. If we want to create a model, we could use a model with X_0, X_2, X_3 as features or a model with X_0, X_2, X_5 as features, since X_3 and X_5 are perfectly correlated, we could use one of them in the model.
- From all the three approaches we followed, we can come to the conclusion that the best model can be build using the predictors X_0, X_2, X_3 or X_0, X_2, X_5

Coefficients of best model

In [21]:

```
mr = MultipleRegression()
coeff, pred = mr.fit_predict(X[:,[0, 2,3]], Y)
r2 = mr.r_squared(pred)
r2_corrected = mr.adj_r_squared(X[:,[0, 2,3]], rsquared=r2)
print(f"Coefficients: b0:{coeff[0]}, b2:{coeff[1]},  b3:{coeff[2]}")
print("r2:", r2)
print("Corrected r2:", r2_corrected)
```

```
Coefficients: b0:-13.9012797, b2:3.89047454388653,  b3:-33.53378235959251
r2: 0.9991878139546398
Corrected r2: 0.9991795684110322
```

References

[1]. Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning (ESL)