

HW2 – DS for Mechanical Systems

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October/19/2021

Homework #2

0.1 Problem 1 (20 points)

Given the data in [this dataset](#), it consists of 2 columns and 200 rows. If we treat the first column as x , and the second column as y , we want to build a simple linear regression model: $y = \beta_0 + \beta_1 x$ to fit the data:

1. What is the point estimate of the intercept β_0 and the slope β_1 , respectively?
 - Point Estimate: Intercept $\beta_0 = -31.8043$ and the slope $\beta_1 = 16.2056$.
2. What is the standard error for the intercept and the slope, respectively?
 - Standard Error: Intercept $\beta_0 = 5.7635$ and the slope $\beta_1 = 0.5484$.
3. Is the result significant, i.e., the slope is significantly different from zero?

OLS Regression Results						
=====						
Dep. Variable:	y	R-squared:	0.814			
Model:	OLS	Adj. R-squared:	0.813			
Method:	Least Squares	F-statistic:	864.6			
Date:	Mon, 18 Oct 2021	Prob (F-statistic):	3.61e-74			
Time:	07:07:48	Log-Likelihood:	-1157.0			
No. Observations:	200	AIC:	2318.			
Df Residuals:	198	BIC:	2325.			
Df Model:	1					
Covariance Type:	nonrobust					
=====						
	coef	std err	t	P> t	[0.025	0.975]

Intercept	-31.8043	5.764	-5.518	0.000	-43.170	-20.438
x	16.2056	0.551	29.404	0.000	15.119	17.292
=====						
Omnibus:	2.158	Durbin-Watson:	1.638			
Prob(Omnibus):	0.340	Jarque-Bera (JB):	1.747			
Skew:	0.071	Prob(JB):	0.418			
Kurtosis:	2.565	Cond. No.	10.8			
=====						

- From the OLS Regression results, the 95% Confidence Interval for $\beta_0 = [-43.170, -20.438]$ and 95% Confidence Interval for $\beta_1 = [15.119, 17.292]$. The P-Value for both the Intercept and Independent variable is tending to 0, and this means the null hypothesis can be rejected. Since the Class Intervals do not have zero, the correlation between the two doesn't exist. Thus, we can conclude that the slope β_1 is significantly different from Zero.

4. What is the R^2 of your model?
 - $R^2 = 0.8137$.
5. For a new x value of 10, with your fitted model, what is the predicted y, and its 95% confidence interval?
 - Predicted y-value for x = 10: 130.2520

1.) ⑤ $x = 10$, $\bar{x} = 2.5$

$\hat{y} = 130.2520$ $n = 200$

Sample $S_x^2 = 103.627$
 $S_x = 10.179741$

$Z = 1.96 = 95\% \text{ confidence}$

new value of $x = 10$

$\sigma = \text{population sigma} = S_x \times \sqrt{n} \Rightarrow S_x \times \sqrt{200} \Rightarrow 143.962$

$$CI = \left(\hat{y} - Z \cdot \frac{\sigma}{\sqrt{n}} \sqrt{1 + \frac{(x - \bar{x})^2}{(n-1)S_x^2}}, \hat{y} + Z \cdot \frac{\sigma}{\sqrt{n}} \sqrt{1 + \frac{(x - \bar{x})^2}{(n-1)S_x^2}} \right)$$

$CI \Rightarrow$

$$130.252 \pm 1.96 \times 143.962 \sqrt{\frac{1}{200} + \frac{(10 - 2.5)^2}{199 \times 103.109}}$$

$\Rightarrow \boxed{130.252 \pm 24.8049}$

$y_{\min} \Rightarrow \underline{105.447}$

$y_{\max} \Rightarrow \underline{155.0784}$

- From Code: Y min = 116.6153533 & Y max = 143.888859

0.2 Problem 2 (20 points)

Using the same dataset, now we want to build a different linear regression model as: $y = \beta_0 + \beta_1 x + \beta_2 x^2$ to fit the data:

1. What is the point estimate of the β_0 , β_1 , and β_2 , respectively?
 - Point Estimate: $\beta_0 = -18.0505$, $\beta_1 = 16.9156$ and $\beta_2 = -0.1420$.
2. What is the standard error for the three coefficients, respectively?
 - Standard Error: $\beta_0 = 8.138$, $\beta_1 = 0.622$ and $\beta_2 = 0.060$.
3. Are β_1 and β_2 significantly different from zero?
 - From the OLS Regression results, the 95% Confidence Interval for $\beta_0 = [-34.100, -2.001]$, 95% Confidence Interval for $\beta_1 = [15.689, 18.142]$ and the 95% Confidence Interval for $\beta_2 = [-0.260, -0.024]$. The P-Value for β_0 , β_1 and β_2 are 0.028, 0.000 and 0.019, and since the P-Values are < (less than) 0.05, means the null hypothesis can be rejected. Since the Class Intervals do not have zero, the correlation between the three doesn't exist. Thus, we can conclude that β_1 and β_2 are significantly different from Zero.

4. What is the R^2 of your model?
- $R^2 = 0.8188$.

0.3 Problem 3 (10 bonus points)

Show that, for the simple linear regression $y = \beta_0 + \beta_1 x + \epsilon$, if the error term ϵ is assumed to follow a normal distribution of $N(0, \sigma^2)$, then maximizing the likelihood leads to minimizing the mean squared error of $\sum_{i=1} (y_i - \hat{y}_i)^2$, where $\hat{y}_i = \beta_0 + \beta_1 x_i$.

(Hint: what is the likelihood of observing an error of particular error ϵ_i ?)

Problem 3

$$y = \beta_0 + \beta_1 x + \epsilon \quad \epsilon \sim N(0, \sigma^2)$$

$$MSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \hat{y}_i = \beta_0 + \beta_1 x_i$$

For any input (x_i, y_i) , ~~error~~ $\epsilon_i = y_i - (\beta_0 + \beta_1 x_i)$
 $\Rightarrow y_i - \hat{y}_i$

Assume \Rightarrow

$$\epsilon_i = y_i - \hat{y}_i \sim N(0, \sigma^2)$$

For any ϵ_i , $f(\epsilon_i) = \frac{1}{\sqrt{2\pi} \sigma} e^{-\frac{1}{2\sigma^2} \epsilon_i^2}$

likelihood function \Rightarrow

$$L(0, \sigma^2, \epsilon_1, \epsilon_2, \dots, \epsilon_n) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n \epsilon_i^2}$$

$$\Rightarrow \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n \epsilon_i^2}$$

log likelihood function \Rightarrow

$$l = -\frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n \epsilon_i^2$$

log likelihood function

$$l = -\frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n \epsilon_i^2$$

diff w.r.t $\sigma^2 \Rightarrow \frac{dl}{d\sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{i=1}^n \epsilon_i^2 = 0$

$$\frac{1}{2(\sigma^2)^2} \sum_{i=1}^n \epsilon_i^2 = \frac{n}{2\sigma^2}$$

Rearrange \Rightarrow

$$\boxed{\frac{1}{n} \sum_{i=1}^n \epsilon_i^2 = \sigma^2} \quad \text{--- (*)}$$

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^n \epsilon_i^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \Rightarrow \frac{1}{n} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2$$

differentiate $\frac{dl}{d\sigma^2}$ w.r.t $d\sigma^2 \Rightarrow$

$$\frac{d^2 l}{(d\sigma^2)^2} = \frac{n}{2\sigma^4} - \frac{1}{(\sigma^2)^3} \sum_{i=1}^n \epsilon_i^2$$

substituting (*) \Rightarrow

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^n \epsilon_i^2$$

$$\Rightarrow \frac{n}{2 \times \left(\frac{1}{n} \sum_{i=1}^n \epsilon_i^2\right)^2} - \frac{1}{\left(\frac{1}{n} \sum_{i=1}^n \epsilon_i^2\right)^3} \sum_{i=1}^n \epsilon_i^2$$

$$\Rightarrow \frac{n^3}{2 \left(\sum_{i=1}^n \epsilon_i^2\right)^2} - \frac{n^3}{\left(\sum_{i=1}^n \epsilon_i^2\right)^2} = \frac{-n^3}{2 \left(\sum_{i=1}^n \epsilon_i^2\right)^2} < 0$$

\therefore likelihood error term is maximized when ~~mean~~ MSE is min.

squared

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

when
 Thus Maximum likelihood is maximized the Mean square error is minimum

$$\sigma^2 = \frac{1}{n} \sum_{i=0}^n (y_i - \hat{y}_i)^2 \rightarrow \text{Mean square error} \rightarrow \text{MSE} \rightarrow \sigma^2$$

$$f(y_1, \dots, y_n) = \frac{1}{\sqrt{2\pi n} \sigma} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

\therefore when $e^{-(\min)}$ lead to maximizing likelihood

• Simple linear regression $y = \beta_0 + \beta_1 x + E$, if the error term E is assumed to normal distribution of $N(0, \sigma^2)$, then maximizing the likelihood leads to maximizing the mean squared error of $\sum_{i=1}^n (y_i - \hat{y}_i)^2$, where $\hat{y}_i = \beta_0 + \beta_1 x_i$

Linear regression $\Rightarrow y = \beta_0 + \beta_1 x + E = f(x)$
 $E \rightarrow$ error term.

$E \rightarrow N(0, \sigma^2)$ - assumed to normal distribution.

Prove that \Rightarrow ~~M.L.E~~ Maximizing M.L.E = minimizes Mean squared error.

We have 3 unknown parameters β_0 , β_1 and σ^2 and they need to be estimated by using a given sample.

$$\text{MEAN SQUARE ERROR} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \text{1} \quad \text{2} \quad \hat{y}_i = \beta_0 + \beta_1 x_i \quad \text{2}$$

For any input $(x_i, y_i) \Rightarrow E_i = y_i - (\beta_0 + \beta_1 x_i) \quad \text{3}$

$$E_i = y_i - \hat{y}_i \sim N(0, \sigma^2)$$

For any input $(x_i, y_i) \Rightarrow \epsilon_i = y_i - (\beta_0 + \beta_1 x_i)$ — (3)

$$\epsilon_i = y_i - \hat{y}_i \sim N(0, \sigma^2)$$

For a fixed x_i , the distribution of y_i is equal to $N(f(x_i), \sigma^2)$ with p.d.f

$$f(y) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y - f(x_i))^2}{2\sigma^2}}$$

and the likelihood function of the sequence y_1, \dots, y_n is:

$$\begin{aligned} f(y_1, \dots, y_n) &= \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n \times e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - f(x_i))^2} \\ &= \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2} \quad \text{--- (4)} \end{aligned}$$

For points x_1, \dots, x_n which is fixed and non random and deal with randomness from the error ϵ .

The maximum likelihood function?

To maximize the likelihood, we need to ~~minimize~~ ^{maximize} the maximum likelihood estimates of β_0 , β_1 and σ^2 .

Maximum likelihood function:- From equation (4)

$$f(y_1, \dots, y_n) = \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2}$$

To maximize the function $f(y_1, \dots, y_n)$, we need to minimize from equation (4).

$$\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 \quad \text{--- (5)}$$

because $\left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n \rightarrow \text{constant}$

$\frac{-1}{2\sigma^2} \rightarrow \text{constant.}$

\therefore From equation (5) $\Rightarrow \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$

we need to minimize it

Minimizing equation (5) $\Rightarrow \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$

From equation (2) $\hat{y}_{i,0} = \beta_0 + \beta_1 x_i$ put in (5)

we need to minimize it

Minimizing equation (5) $\Rightarrow \sum_{i=0}^n (Y_i - \beta_0 - \beta_1 X_i)^2$

from equation (2) $\hat{y}_i = \beta_0 + \beta_1 x_i$ put in (5)

$$\sum_{i=0}^n (Y_i - (\beta_0 + \beta_1 x_i))^2 \Rightarrow \sum_{i=0}^n (Y_i - \hat{y}_i)^2 \text{ should be minimized}$$

Thus by maximizing the M.L.E \Rightarrow the equation
likelihood $\sum_{i=0}^n (Y_i - \hat{y}_i)^2$

needs to be minimized.

$$\therefore \sum_{i=0}^n (Y_i - \hat{y}_i)^2 = \text{Mean square error} \Rightarrow \text{equation (1)}$$

\therefore Thus proved,

Maximizing likelihood leads to minimizing the mean squared error.

Another way:-

From equation (4)

$$f(y_1, \dots, y_n) = \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2}$$
 is the

Maximum likelihood estimator (MLE).

$$\text{Mean square error} \Rightarrow \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \rightarrow \text{equation (1)}$$

So ~~to~~ minimizing mean square error

$$\therefore \text{differentiating eq. n (1)} \Rightarrow \frac{d(\text{MSE})}{dx} = \frac{1}{n} \frac{d}{dx} \left(\sum_{i=1}^n (y_i - \hat{y}_i)^2 \right)$$

$$\hat{y}_i = \beta_0 + \beta_1 x_i \Rightarrow \text{equation to the above equation.}$$

$$\frac{d(\text{MSE})}{dx} = \frac{1}{n} \frac{d}{dx} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2$$

So minimizing it \Rightarrow The derivative should be equated to zero

$$\frac{d(\text{MSE})}{dx} = 0 \Rightarrow \frac{1}{n} \frac{d}{dx} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2 = 0$$

To minimizing it \Rightarrow The derivative should be equated to zero.

$$\frac{d}{d\alpha} (MSE) = 0 \Rightarrow \frac{1}{n} \frac{d}{d\alpha} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2 = 0$$

$$\sum_{i=1}^n \frac{d}{d\alpha} (y_i - (\beta_0 + \beta_1 x_i))^2 = 0 \rightarrow (6)$$

Equation (6) $\Rightarrow f(y_1, \dots, y_n) = \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 + \beta_1 x_i)^2}$

Applying \ln :

$$l = -\frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 + \beta_1 x_i)^2 \quad (7)$$

From (6) Residual sum of squares :-

$$RSS(\beta) = \sum_{i=1}^N (y_i - f(x_i))^2$$

$$\Rightarrow \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2$$

Dealing in terms of matrices. The geometry of least squares fitting in the \mathbb{R}^{p+1} dimension space.

Denote by X the $N \times (p+1)$ matrix with each row an input vector and similarly let y be the vector of outputs in the training set.

Residual sum of squares $\Rightarrow \text{RSS}(\beta) = (y - X\beta)^T (y - X\beta)$

$$\frac{\partial \text{RSS}}{\partial \beta} = -2X^T(y - X\beta)$$

$$-\frac{\partial^2 \text{RSS}}{\partial \beta \partial \beta^T} \Rightarrow 2X^T X$$

Assuming that X has a full column rank, hence $X^T X$ is a positive definite, we set derivative to zero $\Rightarrow X^T(y - X\beta) = 0$
 \therefore unique sol. $\hat{\beta} = (X^T X)^{-1} X^T y$

The training inputs $\Rightarrow \hat{y} = X\hat{\beta} = X(X^T X)^{-1} X^T y$.

Thus the minimizing MSE leads to maximizing

$$\text{Zero} \Rightarrow X^T (y - X\beta) = 0$$

$$\therefore \text{unique sol. is } \hat{\beta} = (X^T X)^{-1} X^T y$$

$$\text{The training inputs } \Rightarrow \hat{y} = X\hat{\beta} = X(X^T X)^{-1} X^T y.$$

Thus the minimizing MSE leads to maximizing MSE

\therefore from equation (6) & (4)

Thus minimizing mean square error \Rightarrow leads to

$$\text{of } \frac{\partial}{\partial x} \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2 = 0 \quad \rightarrow (7)$$

(Leads to zero)

$$\ln f(y_1, \dots, y_n) \Rightarrow \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n e^{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2}$$

Minimize (7)

$$f(y_1, \dots, y_n) \Rightarrow \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n e^{-\frac{1}{2\sigma^2} (\text{Minimized Mean square error})}$$

$$f(y_1, \dots, y_n) = \left(\frac{1}{\sqrt{2\pi}\sigma} \right)^n e^{-\frac{1}{2\sigma^2} \min(\text{MSE})} \Rightarrow \text{leads to maximizing } f(y_1, \dots, y_n)$$

\Rightarrow leads to maximizing MLE
hence proved

```

%matplotlib notebook
from typing import List
from typing import Tuple
from typing import Union

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
import statsmodels.formula.api as smf

from tqdm import tqdm

sns.set(font_scale=1.5)
sns.set_style("whitegrid", {'grid.linestyle':'--'})

from google.colab import drive
drive.mount('/content/drive')

data = pd.read_csv("/content/drive/MyDrive/simple_linear_regression.csv")
data.head()

%matplotlib inline
# distribution of the dependent variable
plt.scatter(x="x", y='y', data = data)
plt.tight_layout()
plt.show()

# correlations
continuous_variables = [
    "x",
]

for variable in continuous_variables:
    plt.figure()
    sns.scatterplot(x=variable, y="y", data=data)
    plt.tight_layout()

y = data["y"]
x = data["x"]

def simple_linear_regression(
    x: Union[List, np.ndarray, pd.Series],
    y: Union[List, np.ndarray, pd.Series]) -> Tuple[float, float]:
    """Return the intercept and slope of a simple linear regression."""
    beta_1 = np.cov(x, y)[0][1] / np.cov(x, x)[0][1]
    beta_0 = np.mean(y) - beta_1 * np.mean(x)

    return beta_0, beta_1

beta_0, beta_1 = simple_linear_regression(x=x, y=y)

# calculate R^2
y_pred = beta_0 + beta_1 * x
SST = np.sum(np.square(y - np.mean(y)))
residual = y - y_pred
SSE = np.sum(np.square(residual))
r2 = 1 - SSE / SST

print(f"beta_0 is: {beta_0:5.4f}")
print(f"beta_1 is: {beta_1:5.4f}")
print(f"R-square is: {r2:5.4f}")

plt.figure()
x_range = np.linspace(start=np.min(x), stop=np.max(x), num=100)
sns.scatterplot(x="x", y="y", data=data)
sns.lineplot(x=x_range, y=(beta_0 + beta_1 * x_range), color="red")
plt.tight_layout()

# confidence intervals
SE_beta_0 = (np.var(residual, ddof=2) * (1. / len(x) + (np.mean(x))**2 / np.sum((x - np.mean(x))**2)))**0.5
SE_beta_1 = (np.var(residual) / np.sum((x - np.mean(x))**2))**0.5

print(f"The standard error for beta_0 is: {SE_beta_0:5.4f}")

```

```

print(f"The standard error for beta_1 is: {SE_beta_1:5.4f}")

# simple linear regression with the `statsmodels` library
model_1 = smf.ols(formula='y ~ x', data=data)
result_1 = model_1.fit()
print(result_1.summary())

p2 = np.polyfit(x,y,2)
print(p2)
plt.plot(x,y,'ro',label='Measured (y)')
plt.plot(x,np.polyval(p2,x),'b-',label='Predicted (y)')
plt.legend(); plt.show()

from sklearn.metrics import r2_score
r2_score(y, y_pred)

import statsmodels.api as sm
xc = np.vstack((x**2,x,np.ones(n))).T
model = sm.OLS(y,xc).fit()
predictions = model.predict(xc)
model.summary()

```

Fig 1: Scatter Plot

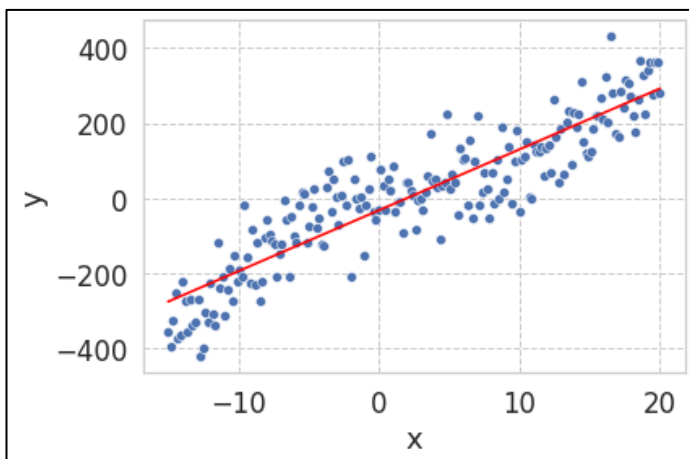
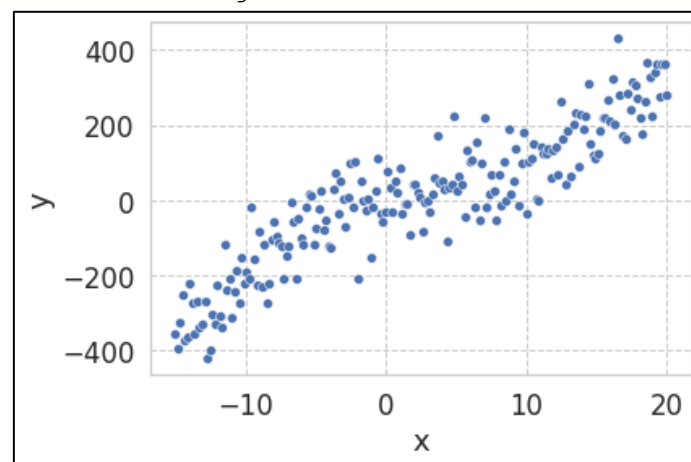


Fig 2 : Question 1 Linear Regression

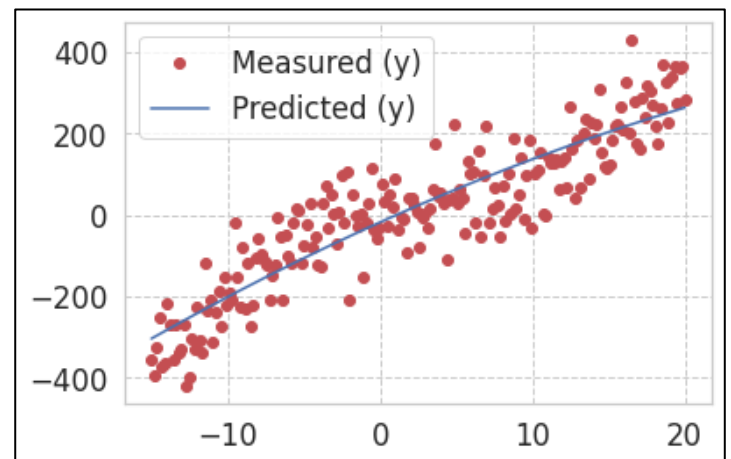


Fig 3 : Question 2 Linear Regression