LinearRegression

October 8, 2018

1 Linear Regression

1.1 1 - Description

Linear regression on p variables focusses on fitting a straight line in p-dimensions that passes as close as possible to the data points in order to reduce error.

- A supervised learning technique
- Useful for predicting a quantitative response
- Linear Regression attempts to fit a function to predict a response variable
  - The problem is reduced to a paramteric problem of finding a set of parameters
  - The function is limited to having a straight line form

1.2 2- Advertising Dataset

The Advertising dataset is obtained from http://www-bcf.usc.edu/~gareth/ISL/data.html and contains 200 datapoints of sales of a particular product, and TV, newspaper and radio advertising budgets (all figures are in units of $1,000s).

In [57]:
```
# Import modules
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import random
from numpy.random import RandomState
import math
%matplotlib inline
```

In [58]:
```
# Import Advertising dataset (http://www-bcf.usc.edu/~gareth/ISL/data.html)
advert = pd.read_csv("Advertising.csv").iloc[:,1:]
```

In [59]:
```
print("Number of observations (n) =",advert.shape[0])
print("Number of predictor variables (p) =",advert.shape[1]-1)
print()
print("Advertising.csv")
advert.head()
```

```
Number of observations (n) = 200
Number of predictor variables (p) = 3

Advertising.csv
```

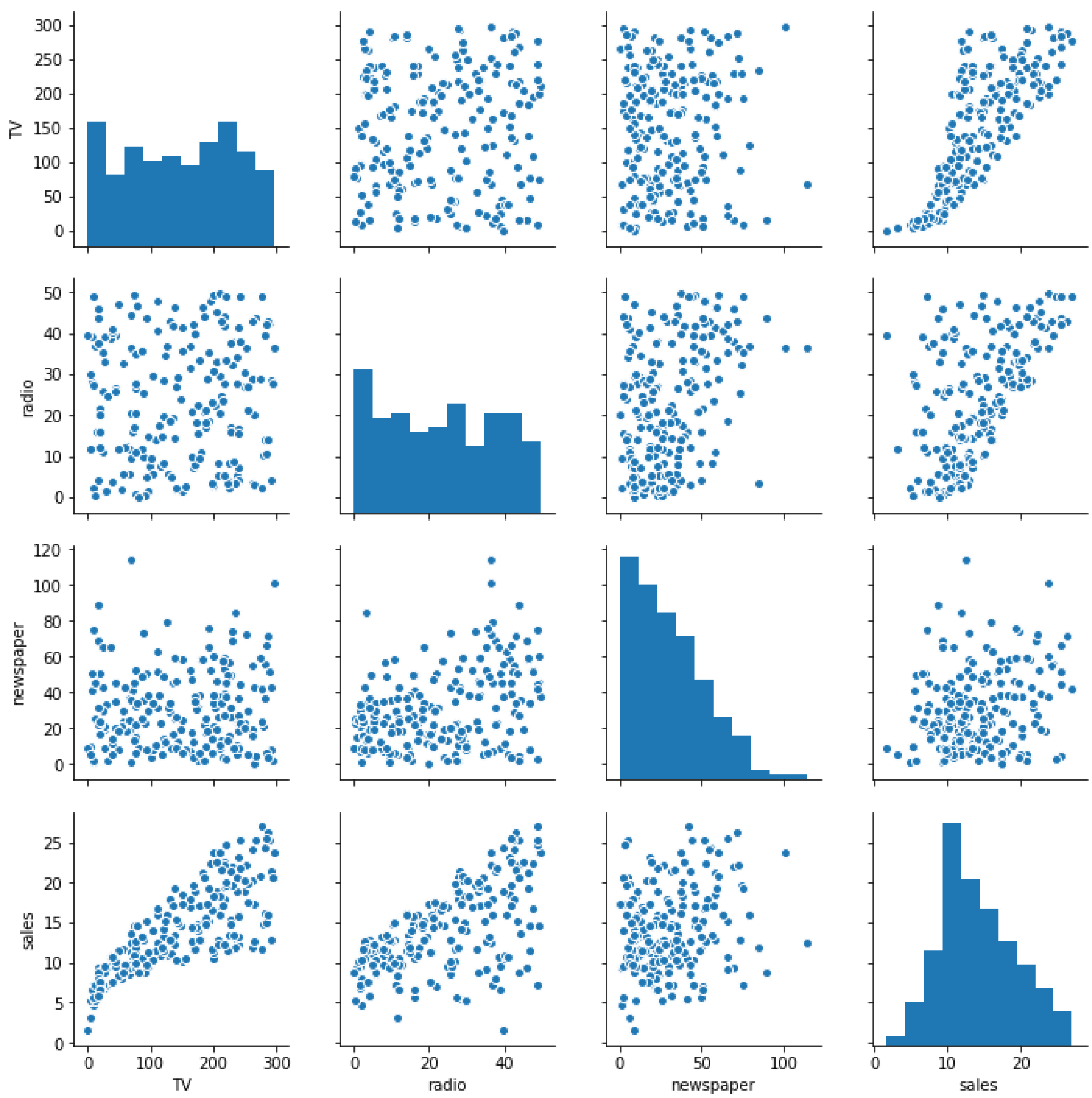
Out[59]:

	TV	radio	newspaper	sales
0	230.1	37.8	69.2	22.1
1	44.5	39.3	45.1	10.4
2	17.2	45.9	69.3	9.3
3	151.5	41.3	58.5	18.5
4	180.8	10.8	58.4	12.9

The response variable is "sales". The predictor variables are "TV", "radio" and "newspaper".

In [60]:
```
sns.pairplot(data=advert)
```

Out[60]: <seaborn.axisgrid.PairGrid at 0x29948a32be0>



By looking at a pairplot to see the simple relationships between the variables, we see a strong positive correlation between sales and TV. A similar relationship between sales and radio is also observed. Newspaper and radio seem to have a slight positive correlation also. We can see this in the correlation matrix below.

```
In [61]: advert.corr()
```

```
Out[61]:                  TV     radio  newspaper     sales
         TV         1.000000  0.054809   0.056648  0.782224
         radio      0.054809  1.000000   0.354104  0.576223
         newspaper  0.056648  0.354104   1.000000  0.228299
         sales      0.782224  0.576223   0.228299  1.000000
```

1.3 3- Linear Regression

The idea behind Linear Regression is that we reduce the problem of estimating the response variable, Y = sales, by assuming there is a linear function of the predictor variables, X_1 = TV, X_2 = radio and X_3 = newspaper which describes Y. This reduces the problem to that of solving for the parameters β_0, β_1, β_2 and β_3 in the equation:

$$Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \epsilon$$

where ϵ is the error term. After approximating the coefficients β_i as $\hat{\beta}_i$, we obtain an approximation, $\hat{Y}$ of Y. The coefficients $\hat{\beta}_i$ are obtained using the observed realisations of the random variables X_i. Namely, $X_i = (x_{1i}, x_{2i}, x_{3i}, ..., x_{ni})$ are n observations of X_i where $i = 1, 2, ..., p$.

We first limit the problem to $p = 1$. For example, we are looking to estimate the coefficients in the equation

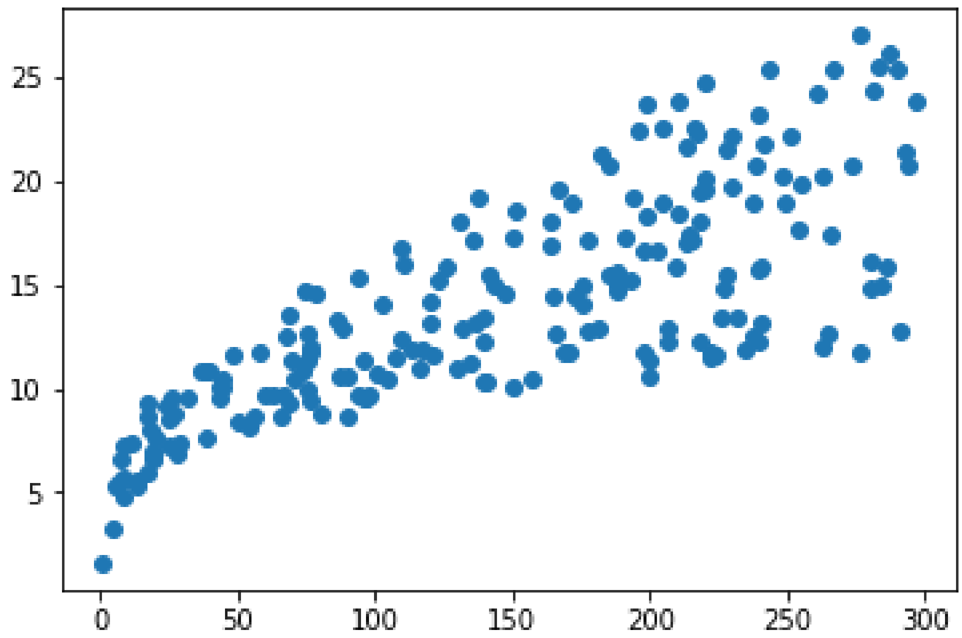
$$Y \approx \beta_0 + \beta_1 X_1 + \epsilon$$

using the n data points $(x_{11}, y_{11}), (x_{21}, y_{21}), ..., (x_{n1}, y_{n1})$. We can define the prediction discrepency of a particular prediction as the difference between the observed value and the predicted value. This is representated in mathematical notation for observation i as $y_i - \hat{y}_i$. Letting $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1$ we have $y_i - \hat{y}_i = \epsilon_i$. i.e. the error in the prediction of point observation i.

In summary, we are looking for a straight line to fit to the following data points as well as possible:

```
In [62]: plt.scatter(data=advert, x='TV', y='sales')

         #plt.plot([advert['TV'].min(),advert['TV'].max()], [advert['sales'].min(),advert['sal
```

```
Out[62]: <matplotlib.collections.PathCollection at 0x29946f95fd0>
```



In order to calculate appropriate values for parameters β_i, we would need a method of defining what it means for a line to be a good fit. A popular method is "Ordinary Least Squares". This method relies on minimising the Residual Sum of Squared errors (RSS). i.e. we are looking to minimise $RSS = \sum_{i=1}^{n} \epsilon_i^2$.

For the 1-parameter case we have that (the semi-colon below means the value of the parameters given the data we have observed)

$$RSS(\hat{\beta}_0, \hat{\beta}_1; X) = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

We would like to find the parameters (β_0, β_1) which minimise RSS. We first find the partial derivates:

$$\frac{\partial RSS}{\partial \hat{\beta}_0} = -2[\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \hat{\beta}_0 - \sum_{i=1}^{n} \hat{\beta}_1 x_i]$$

$$\frac{\partial RSS}{\partial \hat{\beta}_1} = -2[\sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} \hat{\beta}_0 x_i - \sum_{i=1}^{n} \hat{\beta}_1 x_i^2]$$

Then

$$\frac{\partial RSS}{\partial \hat{\beta}_0} = 0 \implies \hat{\beta}_0 = \frac{\sum_{i=1}^{n} y_i - \hat{\beta}_1 \sum_{i=1}^{n} y_i}{n} = \frac{n\bar{y} - \hat{\beta}_1 n\bar{x}}{n} = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\frac{\partial RSS}{\partial \hat{\beta}_1} = 0 \implies \sum_{i=1}^{n} y_i x_i - \hat{\beta}_0 \sum_{i=1}^{n} x_i - \hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = 0 \implies \hat{\beta}_1 = \frac{n\bar{y}\bar{x} - \sum_{i=1}^{n} y_i x_i}{n\bar{x}^2 - \sum_{i=1}^{n} x_i^2} = \frac{\sum_{i=1}^{n} y_i x_i - n\bar{y}\bar{x}}{\sum_{i=1}^{n} x_i^2 - n\bar{x}^2} = \frac{\sum_{i=1}^{n} y_i x_i - n\bar{y}}{\sum_{i=1}^{n} x_i^2 - n\bar{x}^2}$$

Where, in the penultimate line we completed the square and in the last equality we used the equality $n\bar{y}\bar{x} = \sum_{i=1}^{n} y_i\bar{x} = \sum_{i=1}^{n} x_i\bar{y}$ and $n\bar{x}^2 = n\bar{x}\bar{x} = \sum_{i=1}^{n} x_i\bar{x}$. Factorising

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

In the above, we have used the fact that $\hat{\mu} = \bar{x} = \frac{1}{n}\sum_{i=1}^{n}$ is an unbiased *Maximum Likelihood Estimator* (MLE) for the population mean μ (see Appendix).

We have now found the values of $(\hat{\beta}_0, \hat{\beta}_1)$ which corresponds to the extrema of RSS. We will still need to show that this is indeed a minima.

From Calculus, we know that if $\frac{\partial^2 RSS}{\partial \hat{\beta}_0^2}\frac{\partial^2 RSS}{\partial \hat{\beta}_1^2} - (\frac{\partial^2 RSS}{\partial \hat{\beta}_0 \partial \hat{\beta}_1})^2 > 0$, this is an extrema and not an inflexion point. Additionally, if $\frac{\partial^2 RSS}{\partial \hat{\beta}_0^2} > 0$ and $\frac{\partial^2 RSS}{\partial \hat{\beta}_1^2} > 0$ this is a minima.

We have that

$$\frac{\partial^2 RSS}{\partial \hat{\beta}_0^2} = 2n > 0$$
$$\frac{\partial^2 RSS}{\partial \hat{\beta}_1^2} = 2\sum_{i=1}^{n} x_i^2 > 0$$
$$\frac{\partial^2 RSS}{\partial \hat{\beta}_0 \partial \hat{\beta}_1} = 2\sum_{i=1}^{n} x_i$$

So,
$\frac{\partial^2 RSS}{\partial \hat{\beta}_0^2}\frac{\partial^2 RSS}{\partial \hat{\beta}_1^2} - (\frac{\partial^2 RSS}{\partial \hat{\beta}_0 \partial \hat{\beta}_1})^2 = (2n)(2\sum_{i=1}^{n} x_i^2) - (2\sum_{i=1}^{n} x_i)^2 > 0 \; \forall \; n > 1$ (see Appendix)
This means that this is indeed a minima (since we have satisfied the conditions stated above).
The equation

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1$$

then defines a straight line of best fit which minimises the expected value of the errors (residuals). From the form of this line, we can see that $\hat{\beta}_0$ corresponds to the value of $\hat{Y}$ if the independent variable X_1 is zero. $\hat{\beta}_1$ is then the gradient.

In the following we construct 3 functions dependent on a single independent variable and attach an error term and calculate the best fit. The three functions are chosen as:

1- $f_1(x) = 4.67 + 5.07 * x$
2- $f_2(x) = 4.67 + 5.07 * x^2$
3- $f_3(x) = 4.67 + 5.07 * sin(x)$

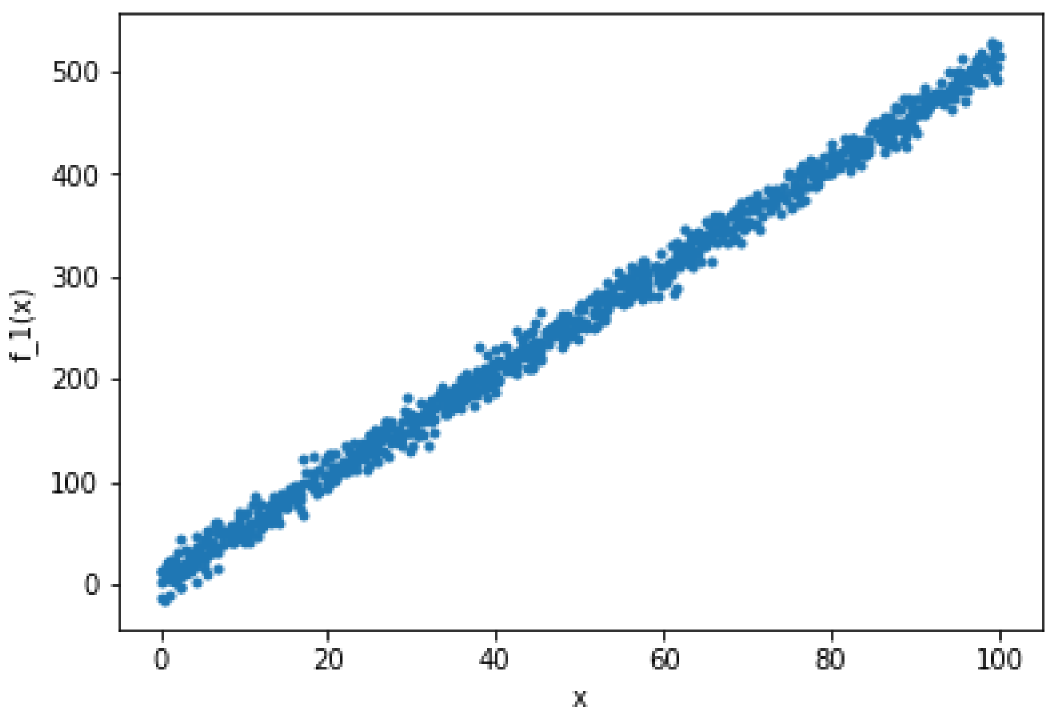
```
In [63]: #f_1(x)=4.67+5.07x
         def f_1(x):
             return 4.67 + 5.07*x

         #f_2(x)=4.67+5.07x2
         def f_2(x):
             return 4.67 + 5.07*x**2

         #f_3(x)=4.67+5.07sin(x/20)
         def f_3(x):
             return 4.67 + 5.07*math.sin(x/20)
```

In [64]:
```
r = np.random.RandomState(101)
X = 100*r.rand(1000)

#Error term with sigma = 10, mu = 0
E_1 = 10*r.randn(1000)

#Error term with sigma = 500, mu = 0
E_2 = 500*r.randn(1000)

#Error term with sigma = 19, mu = 0
E_3 = 1*r.randn(1000)

#Response variables
Y_1 = list(map(f_1,X))+E_1
Y_2 = list(map(f_2,X))+E_2
Y_3 = list(map(f_3,X))+E_3
```

First case 1- f_1

In [65]:
```
fig = plt.figure()
axes = fig.add_axes([0.1,0.1,0.8,0.8])
axes.plot(X,Y_1,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_1(x)')
```

Out[65]: Text(0,0.5,'f_1(x)')



Fit the model $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1$ to the data. We know that

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

and

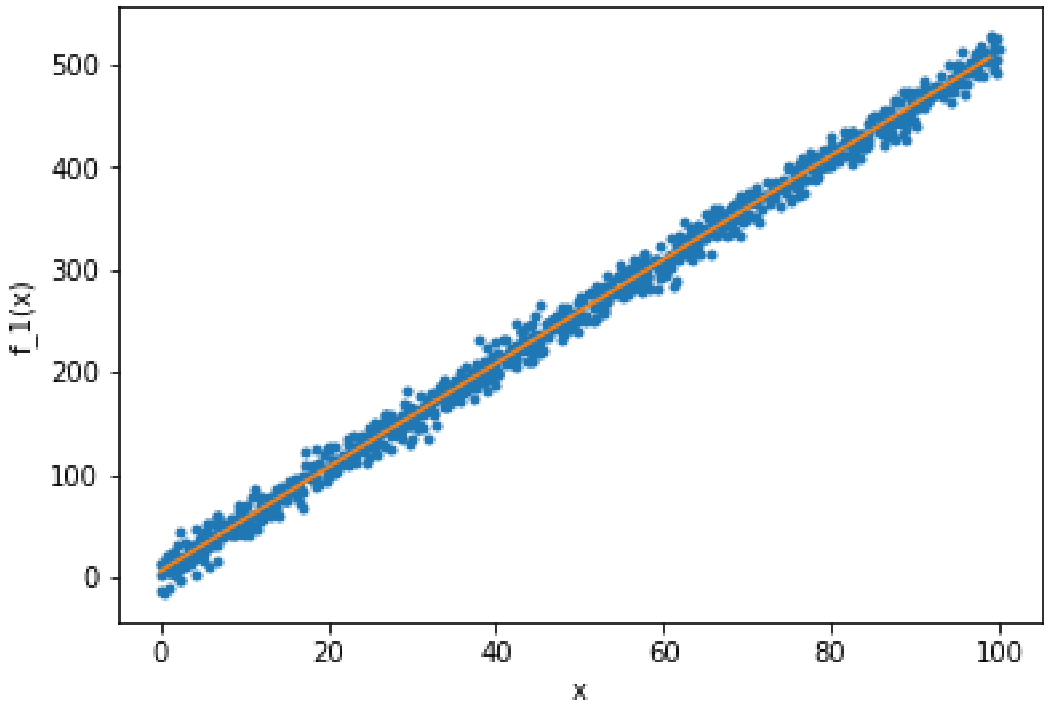
$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

In [305]:
```
#Find the mean of the data for f_1
x_bar1 = np.mean(X)
y_bar1 = np.mean(Y_1)

numerator = 0
denominator = 0

for i in range(len(Y_1)):
    numerator += (X[i] - x_bar1)*(Y_1[i] - y_bar1)
    denominator += (X[i] - x_bar1)**2

beta1_1 = numerator/denominator
beta1_0 = y_bar1 - beta1_1*x_bar1

print('Y = {beta_0} + {beta_1} * X'.format(beta_0 = beta1_0, beta_1 = beta1_1))
```

```
Y = 5.50124312485292 + 5.064254524922961 * X
```

In [306]:
```
x1 = np.linspace(0,99,1000) # 1000 linearly spaced numbers
y1 = beta1_0 + beta1_1 * x1

fig = plt.figure()
axes = fig.add_axes([0.1,0.1,0.8,0.8])
axes.plot(X,Y_1,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_1(x)')
axes.plot(x1,y1)
```

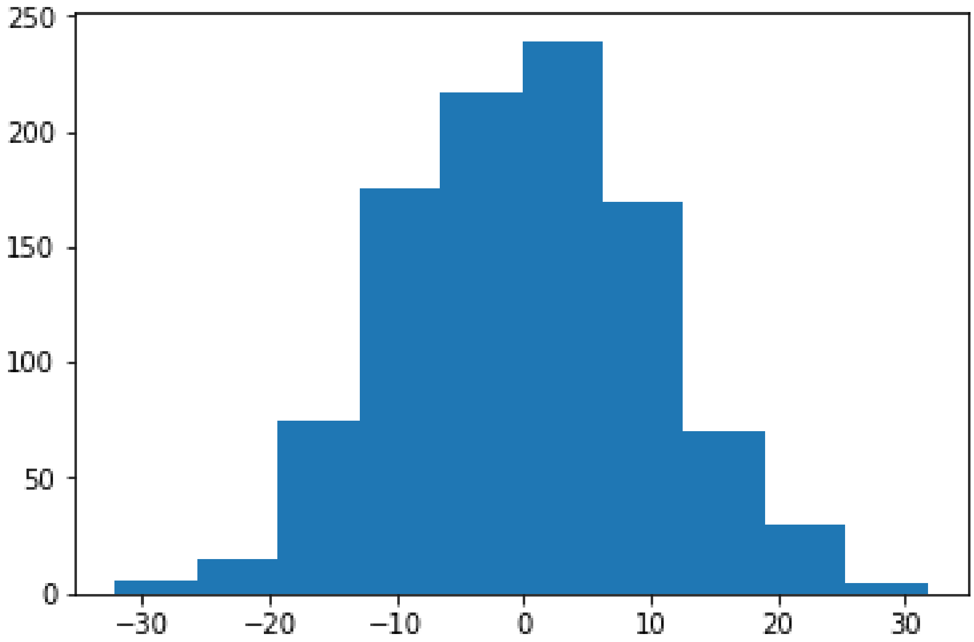
Out[306]:
```
[<matplotlib.lines.Line2D at 0x299527727b8>]
```



Let's see what the residuals look like by plotting them

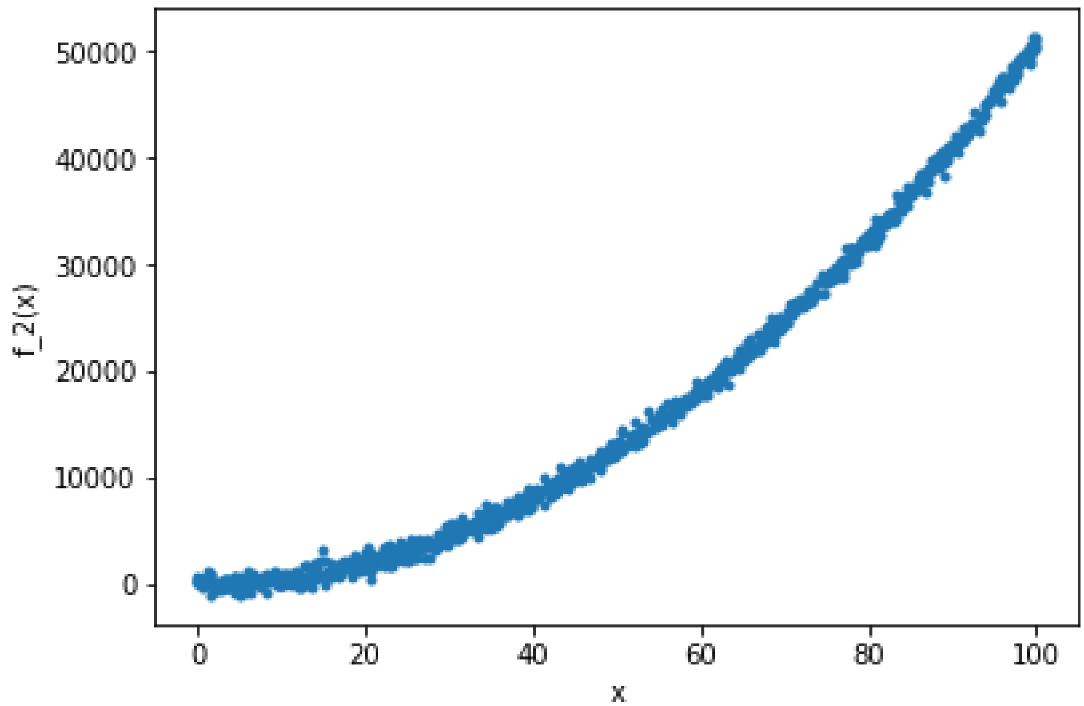
```
In [307]: y1_fitted = beta1_0 + beta1_1 * X
          Res_1 = y1_fitted - Y_1

          plt.hist(Res_1)

          print('This is roughly a normal distribution with mean {mean} and standard deviation
                .format(mean=np.mean(Res_1),std=np.std(Res_1)))
```

```
This is roughly a normal distribution with mean -1.2157386208855315e-14 and standard deviation
```



Since the residuals are roughly normally distributed, our model may be a good choice. Now let's do the same for f_2.

```
In [113]: fig = plt.figure()
          axes = fig.add_axes([0.1,0.1,0.8,0.8])
          axes.plot(X,Y_2,'.')
          axes.set_xlabel('x')
          axes.set_ylabel('f_2(x)')

Out[113]: Text(0,0.5,'f_2(x)')
```

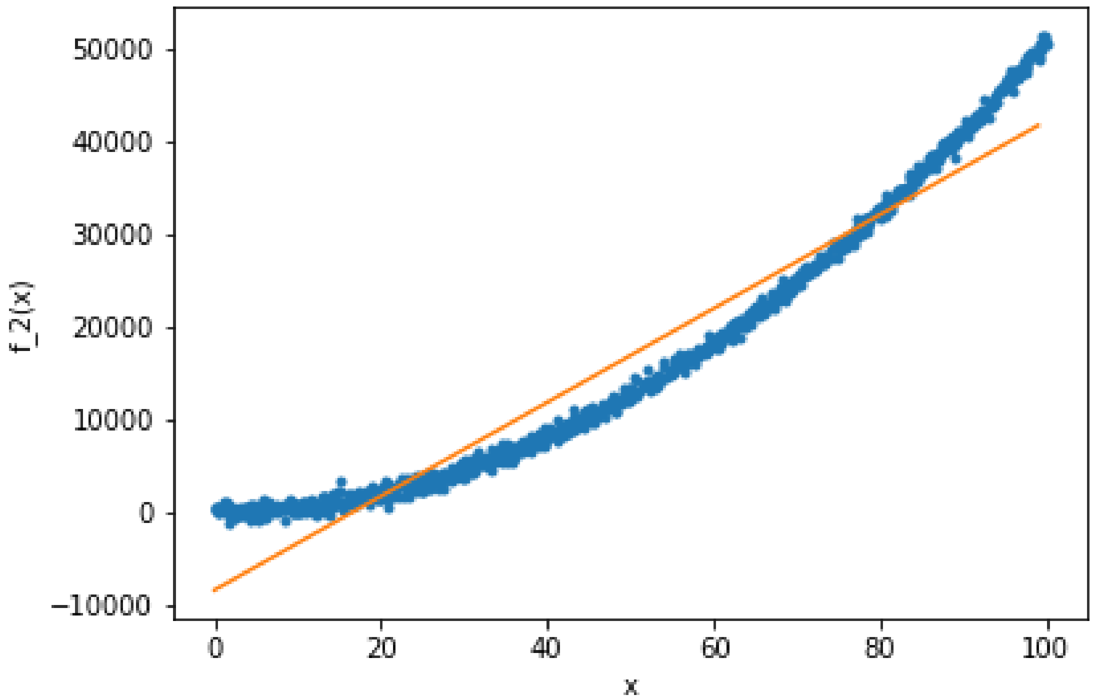



```
In [308]: #Find the mean of the data for f_2
          x_bar2 = np.mean(X)
          y_bar2 = np.mean(Y_2)

          numerator = 0
          denominator = 0

          for i in range(len(Y_2)):
              numerator += (X[i] - x_bar2)*(Y_2[i] - y_bar2)
              denominator += (X[i] - x_bar2)**2

          beta2_1 = numerator/denominator
          beta2_0 = y_bar2 - beta2_1*x_bar2

          print('Y = {beta_0} + {beta_1} * X'.format(beta_0 = beta2_0, beta_1 = beta2_1))

Y = -8445.98030682202 + 506.16066894401735 * X
```

```
In [309]: x2 = np.linspace(0,99,1000) # 1000 linearly spaced numbers
          y2 = beta2_0 + beta2_1 * x2

          fig = plt.figure()
          axes = fig.add_axes([0.1,0.1,0.8,0.8])
```

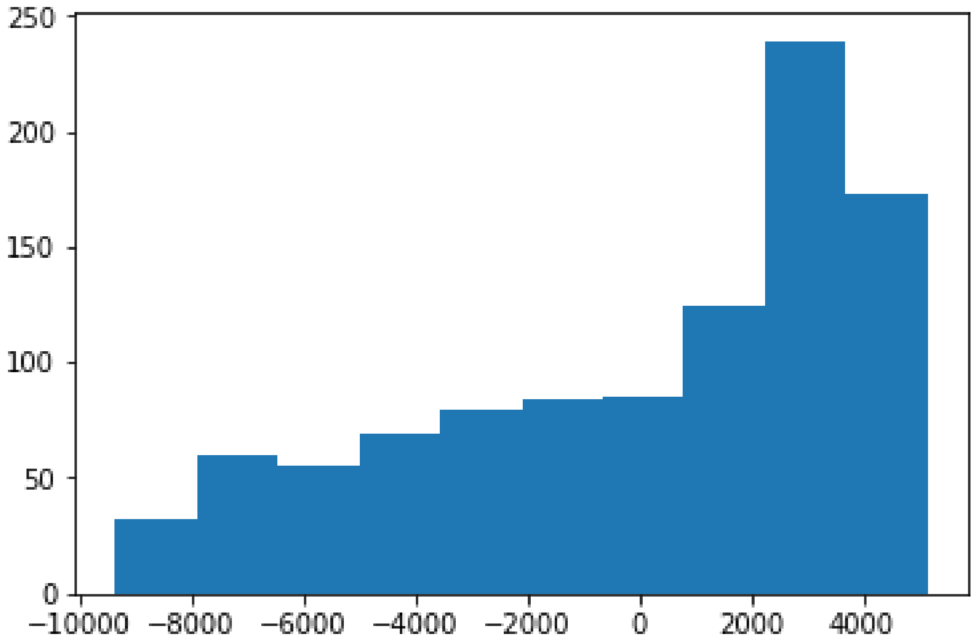
```
axes.plot(X,Y_2,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_2(x)')
axes.plot(x2,y2)
```

Out[309]: [<matplotlib.lines.Line2D at 0x29952992780>]




```
In [310]: y2_fitted = beta2_0 + beta2_1 * X
          Res_2 = y2_fitted - Y_2

          plt.hist(Res_2)

          print('The residuals are certainly not from a normal distribution')
```

The residuals are certainly not from a normal distribution



So let's try X^2 as a parameter instead of X in our linear model.

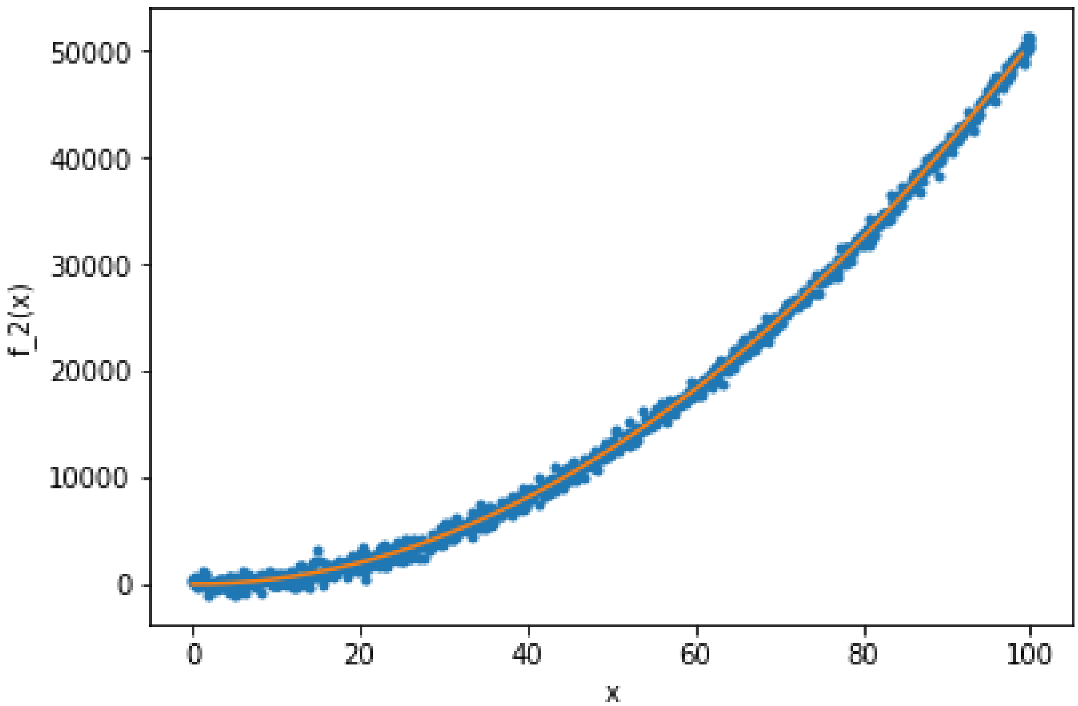
```
In [312]: X_2 = X**2

          #Find the mean of the data for f_3
          x_bar22 = np.mean(X_2)
          y_bar22 = np.mean(Y_2)

          numerator = 0
          denominator = 0

          for i in range(len(Y_2)):
              numerator += (X_2[i] - x_bar22)*(Y_2[i] - y_bar22)
              denominator += (X_2[i] - x_bar22)**2

          beta22_1 = numerator/denominator
          beta22_0 = y_bar22 - beta22_1*x_bar22

          print('Y = {beta_0} + {beta_1} * X^2'.format(beta_0 = beta22_0, beta_1 = beta22_1))
```

```
Y = 14.470063153316005 + 5.075020979320466 * X^2
```

```
In [313]: x22 = np.linspace(0,99,1000) # 1000 linearly spaced numbers
          y22 = beta22_0 + beta22_1 * ((x22)**2)

          fig = plt.figure()
```

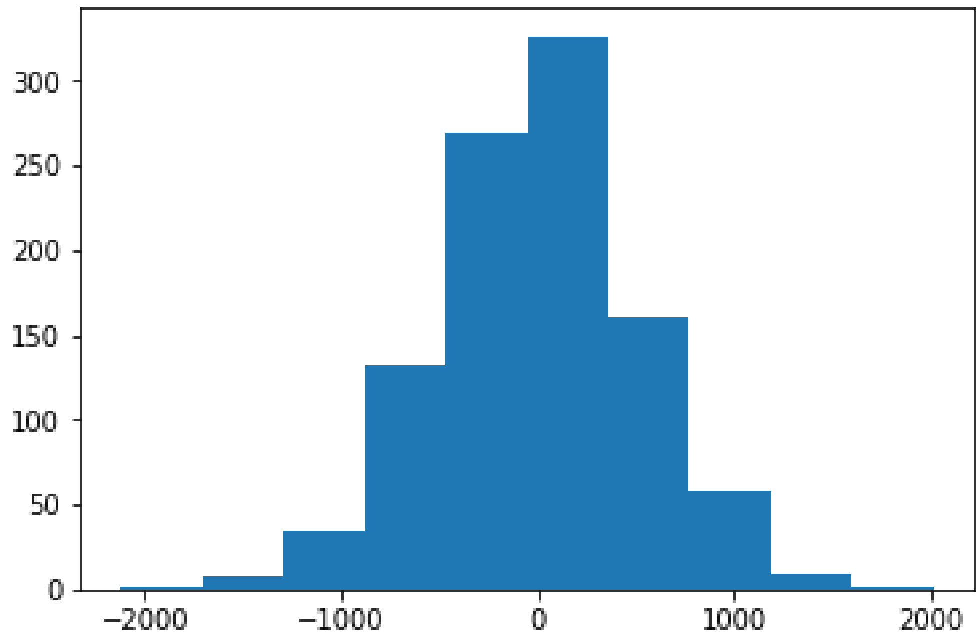
```
axes = fig.add_axes([0.1,0.1,0.8,0.8])
axes.plot(X,Y_2,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_2(x)')
axes.plot(x22,y22)
```

Out[313]: [<matplotlib.lines.Line2D at 0x29952b7d588>]



In [314]:
```
y22_fitted = beta22_0 + beta22_1 * X**2
Res_22 = y22_fitted - Y_2

plt.hist(Res_22)

print('This is roughly a normal distribution with mean {mean} and standard deviation
      .format(mean=np.mean(Res_22),std=np.std(Res_22)))
```

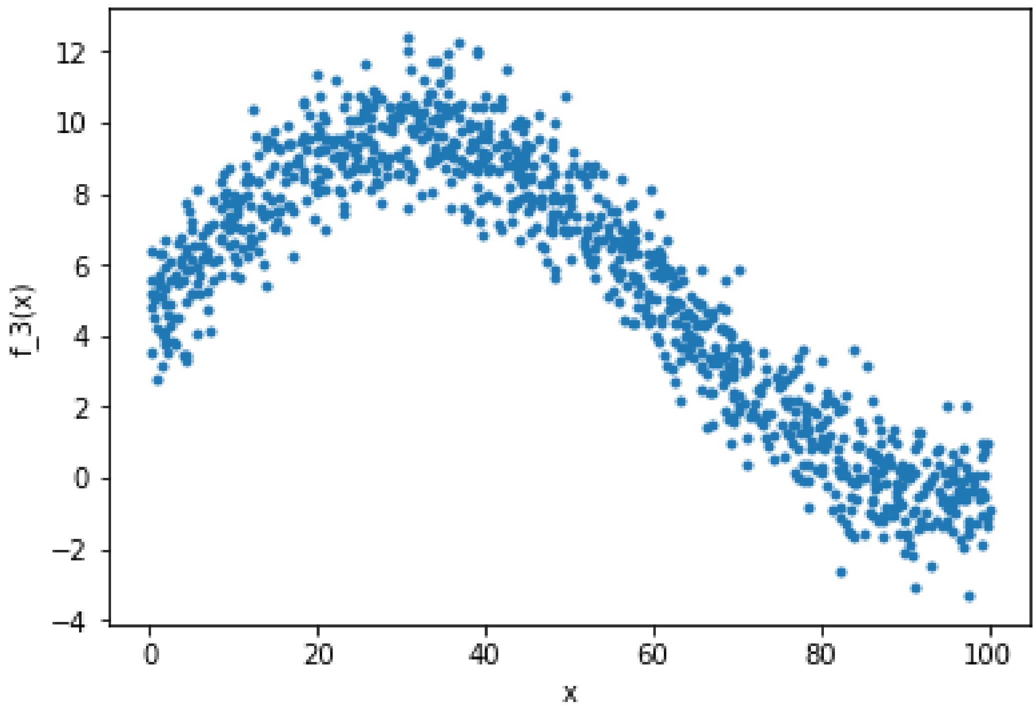
This is roughly a normal distribution with mean -1.1250449460931123e-12 and standard deviation



This shows that we can transform an independent variable and apply linear regression in order to regress the response variable onto the transformed Explanatory variable. This increases the power of linear regression techniques.

Now let's apply linear regression to f_3.

```
In [120]: fig = plt.figure()
          axes = fig.add_axes([0.1,0.1,0.8,0.8])
          axes.plot(X,Y_3,'.')
          axes.set_xlabel('x')
          axes.set_ylabel('f_3(x)')

Out[120]: Text(0,0.5,'f_3(x)')
```

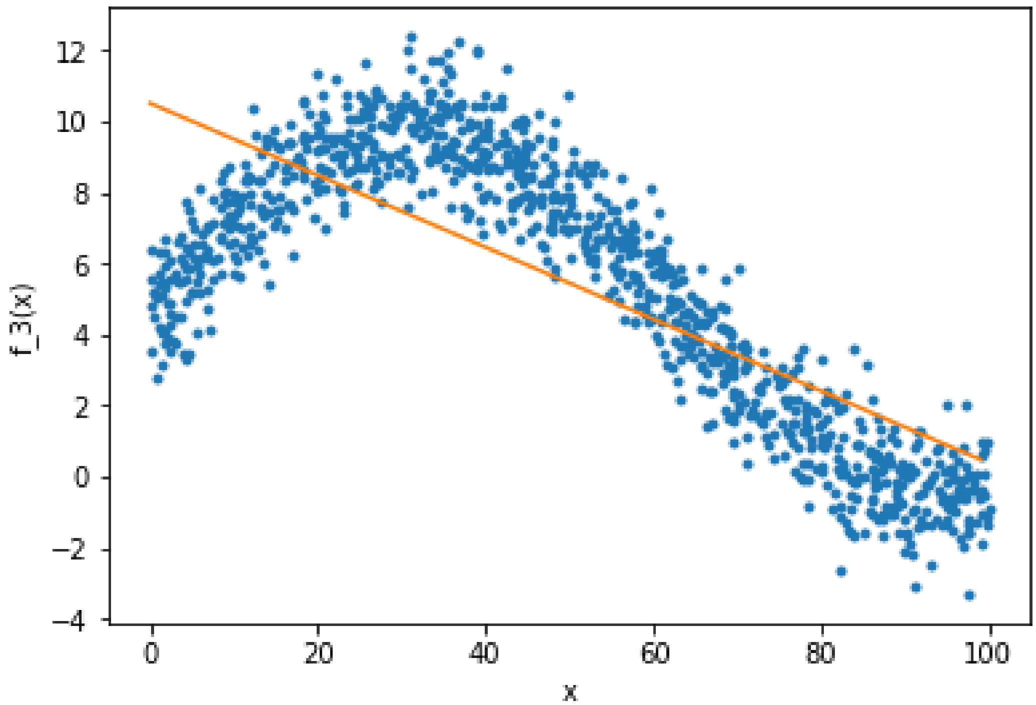



```
In [315]: #Find the mean of the data for f_2
          x_bar3 = np.mean(X)
          y_bar3 = np.mean(Y_3)

          numerator = 0
          denominator = 0

          for i in range(len(Y_3)):
              numerator += (X[i] - x_bar3)*(Y_3[i] - y_bar3)
              denominator += (X[i] - x_bar3)**2

          beta3_1 = numerator/denominator
          beta3_0 = y_bar3 - beta3_1*x_bar3

          print('Y = {beta_0} + {beta_1} * X'.format(beta_0 = beta3_0, beta_1 = beta3_1))

Y = 10.511143457700811 + -0.1011987818100197 * X
```

```
In [316]: x3 = np.linspace(0,99,1000) # 1000 linearly spaced numbers
          y3 = beta3_0 + beta3_1 * x3

          fig = plt.figure()
          axes = fig.add_axes([0.1,0.1,0.8,0.8])
```

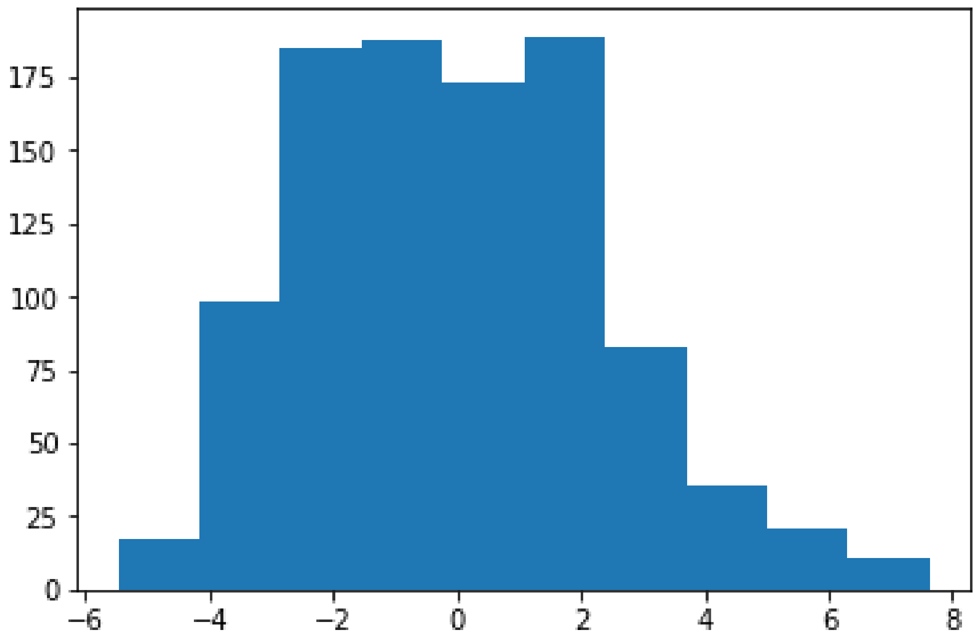
```
axes.plot(X,Y_3,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_3(x)')
axes.plot(x3,y3)
```

Out[316]: [<matplotlib.lines.Line2D at 0x29952c37d68>]



In [317]:
```
y3_fitted = beta3_0 + beta3_1 * X
Res_3 = y3_fitted - Y_3

plt.hist(Res_3)

print('This not a normal distribution but it is not that far off.')
```

```
This not a normal distribution but it is not that far off.
```



Even though a plot of the residuals does not show a clear divergence from a normal distribution, it is clear from the predicted-observed plot that this is not a good model and does not fit the data in a satisfactory manner. We therefore need more tools in order to asses the level of fit.

A metric we can use in order to assess the accuracy of the fit is the R-Squared (R^2) statistic. The R^2 statistic measures the percentage of variability of the response variable that is explained by the explanatory variable. This is mathematically:

$$R^2 = \frac{TSS - RSS}{TSS}$$

where $TSS = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the *total sum of squares* and $RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ is the *residual sum of squares*.

```
In [124]: TSS_3 = 0
          RSS_3 = 0

          for i in range(len(X)):
              TSS_3 += (Y_3[i] - y_bar3)**2
              RSS_3 += (Y_3[i] - y3_fitted[i])**2

          R_sq_3 = (TSS_3 - RSS_3)/TSS_3
          print('R^2 = {}'.format(R_sq_3))
```

```
R^2 = 0.5940625125965683
```

This means that roughly 59% of the variability in Y_3 is explained by X. Let's calculate the R^2 statistic for all the models above.

```
In [233]: def TSS_RSS(y_observed,y_fitted):
              TSS = 0
              RSS = 0

              y_bar = np.mean(y_observed)

              for i in range(len(X)):
                  TSS += (y_observed[i] - y_bar)**2
                  RSS += (y_observed[i] - y_fitted[i])**2

              return TSS,RSS
```

```
In [239]: TSS_1, RSS_1 = TSS_RSS(Y_1,y1_fitted)

          R_sq_1 = (TSS_1 - RSS_1)/TSS_1
          print('Model for Y_1: Explanatory variable X for Y_1 - R^2 = {}'.format(R_sq_1))



          TSS_2,RSS_2 = TSS_RSS(Y_2,y2_fitted)

          R_sq_2 = (TSS_2 - RSS_2)/TSS_2
          print('Model for Y_2: Explanatory variable X for Y_2 - R^2 = {}'.format(R_sq_2))



          TSS_22,RSS_22 = TSS_RSS(Y_2,y22_fitted)

          R_sq_22 = (TSS_22 - RSS_22)/TSS_22
          print('Model for Y_2: Explanatory variable X^2 for Y_2 - R^2 = {}'.format(R_sq_22))



          TSS_3,RSS_3 = TSS_RSS(Y_3,y3_fitted)

          R_sq_3 = (TSS_3 - RSS_3)/TSS_3
          print('Model for Y_3: Explanatory variable X for Y_3 - R^2 = {}'.format(R_sq_3))
```

```
Model for Y_1: Explanatory variable X for Y_1 - R^2 = 0.9951845734408926
Model for Y_2: Explanatory variable X for Y_2 - R^2 = 0.9336613222418227
Model for Y_2: Explanatory variable X^2 for Y_2 - R^2 = 0.99880452106502
Model for Y_3: Explanatory variable X for Y_3 - R^2 = 0.5940625125965683
```

From the above we can see that the model for Y_1 that is linear in X is satisfactory; The model for Y_2 that is non-linear exaplains more variability of the response variable than the linear model; The model for Y_3 shows that we are probably not fitting the correct form of the function, i.e. we have introduced bias in that the real function is not of the form $a + bX$ for constants a and b. We can try a conbination of cinear combinations of X, X^2, X^3 as well. We do this after we have introduced a much simpler way of obtaining the above fits using Scikit-Learn packages.

Below, we use sklearn.linear_model.LinearRegression() in order to fit and sklearn.metrics.r2_score() in order to calculate the R^2 statistic.

In [170]:
```python
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score

lm1 = LinearRegression()
lm1.fit(X.reshape(-1,1),Y_1.reshape(-1,1))
print('Model for Y_1: Explanatory variable X for Y_1')
print('beta_0 = {}'.format(lm1.intercept_[0]))
print('beta_1 = {}'.format(lm1.coef_[0][0]))
y1_fitted_sklearn = lm1.intercept_[0] + lm1.coef_[0][0]*X
print('R^2 = {}'.format(r2_score(Y_1,y1_fitted_sklearn)))

print()
print()

lm2 = LinearRegression()
lm2.fit(X.reshape(-1,1),Y_2.reshape(-1,1))
print('Model for Y_2: Explanatory variable X for Y_2')
print('beta_0 = {}'.format(lm2.intercept_[0]))
print('beta_1 = {}'.format(lm2.coef_[0][0]))
y2_fitted_sklearn = lm2.intercept_[0] + lm2.coef_[0][0]*X
print('R^2 = {}'.format(r2_score(Y_2,y2_fitted_sklearn)))

print()
print()

lm22 = LinearRegression()
lm22.fit((X**2).reshape(-1,1),Y_2.reshape(-1,1))
print('Model for Y_2: Explanatory variable X^2 for Y_2')
print('beta_0 = {}'.format(lm22.intercept_[0]))
print('beta_1 = {}'.format(lm22.coef_[0][0]))
y22_fitted_sklearn = lm22.intercept_[0] + lm22.coef_[0][0]*X**2
print('R^2 = {}'.format(r2_score(Y_2,y22_fitted_sklearn)))

print()
print()

lm3 = LinearRegression()
lm3.fit(X.reshape(-1,1),Y_3.reshape(-1,1))
print('Model for Y_3: Explanatory variable X for Y_3')
print('beta_0 = {}'.format(lm3.intercept_[0]))
print('beta_1 = {}'.format(lm3.coef_[0][0]))
y3_fitted_sklearn = lm3.intercept_[0] + lm3.coef_[0][0]*X
print('R^2 = {}'.format(r2_score(Y_3,y3_fitted_sklearn)))
```

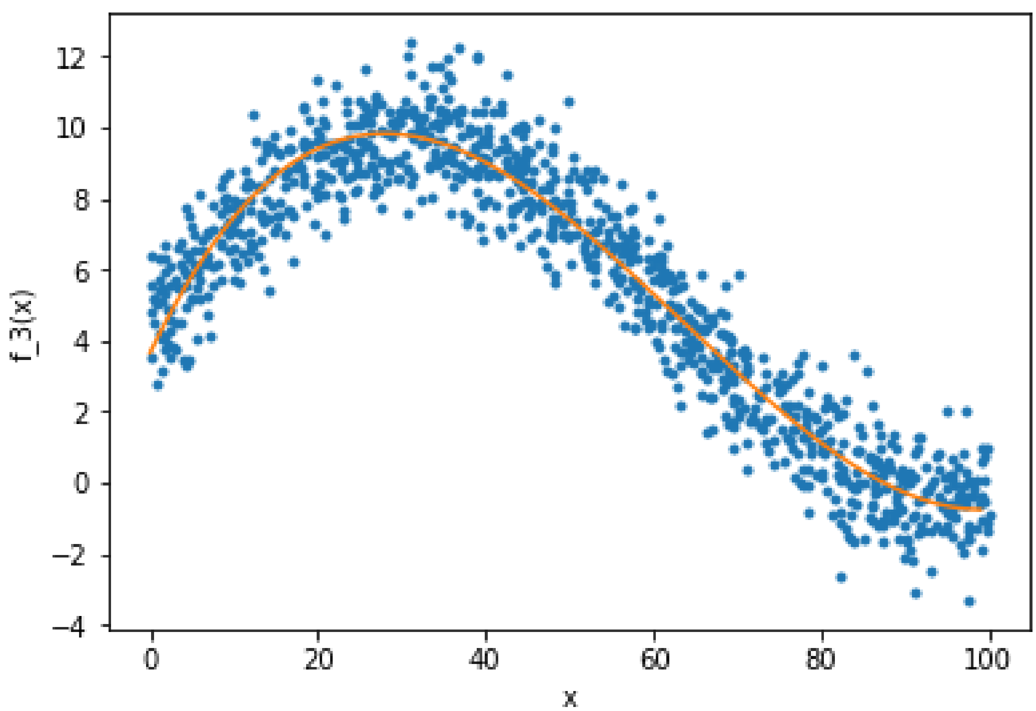
```
print()
print()

# Now we try adding the variables X,X^2 and X^3

#Create transformed variables
X2 = X**2
X3 = X**3

lm32 = LinearRegression()
X3_collection = pd.concat([pd.DataFrame(X,columns=['X']),pd.DataFrame(X**2,columns=[
lm32.fit(X3_collection,Y_3.reshape(-1,1))
print('Model for Y_3: Explanatory variables X,X^2,X^3 for Y_3')
print('beta_0 = {}'.format(lm32.intercept_[0]))
print('beta_1 = {}'.format(lm32.coef_[0][0]))
print('beta_2 = {}'.format(lm32.coef_[0][1]))
print('beta_3 = {}'.format(lm32.coef_[0][2]))
y32_fitted_sklearn = lm32.intercept_[0] + lm32.coef_[0][0]*X + lm32.coef_[0][1]*X**2
print('R^2 = {}'.format(r2_score(Y_3,y32_fitted_sklearn)))
```

```
Model for Y_1: Explanatory variable X for Y_1
beta_0 = 5.501243124853005
beta_1 = 5.064254524922959
R^2 = 0.9951845734408926


Model for Y_2: Explanatory variable X for Y_2
beta_0 = -8445.980306821977
beta_1 = 506.16066894401644
R^2 = 0.9336613222418227


Model for Y_2: Explanatory variable X^2 for Y_2
beta_0 = 14.470063153316005
beta_1 = 5.075020979320466
R^2 = 0.99880452106502


Model for Y_3: Explanatory variable X for Y_3
beta_0 = 10.511143457700808
beta_1 = -0.10119878181001966
R^2 = 0.5940625125965684


Model for Y_3: Explanatory variables X,X^2,X^3 for Y_3
beta_0 = 3.664431201636692
beta_1 = 0.48709842203796394
```

```
beta_2 = -0.0111793303584544434
beta_3 = 5.867605764948042e-05
R^2 = 0.9229011520420615
```

In the above, we fit using 3 explanatory variables, namely X, X^2, X^3 with coefficients β_1, β_2, $beta_3$ respectively. We can see that we have a much improved R^2 statistic meaning we have managed to explain much more of the data using the transformed variables we have created. We can plot the model to see how well it follows the response variable.

```
In [171]: x32 = np.linspace(0,99,1000) # 1000 linearly spaced numbers
          y32 = lm32.intercept_[0] + lm32.coef_[0][0]*x32 + lm32.coef_[0][1]*x32**2 + lm32.coe

          fig = plt.figure()
          axes = fig.add_axes([0.1,0.1,0.8,0.8])
          axes.plot(X,Y_3,'.')
          axes.set_xlabel('x')
          axes.set_ylabel('f_3(x)')
          axes.plot(x32,y32)

Out[171]: [<matplotlib.lines.Line2D at 0x2994c5926a0>]
```

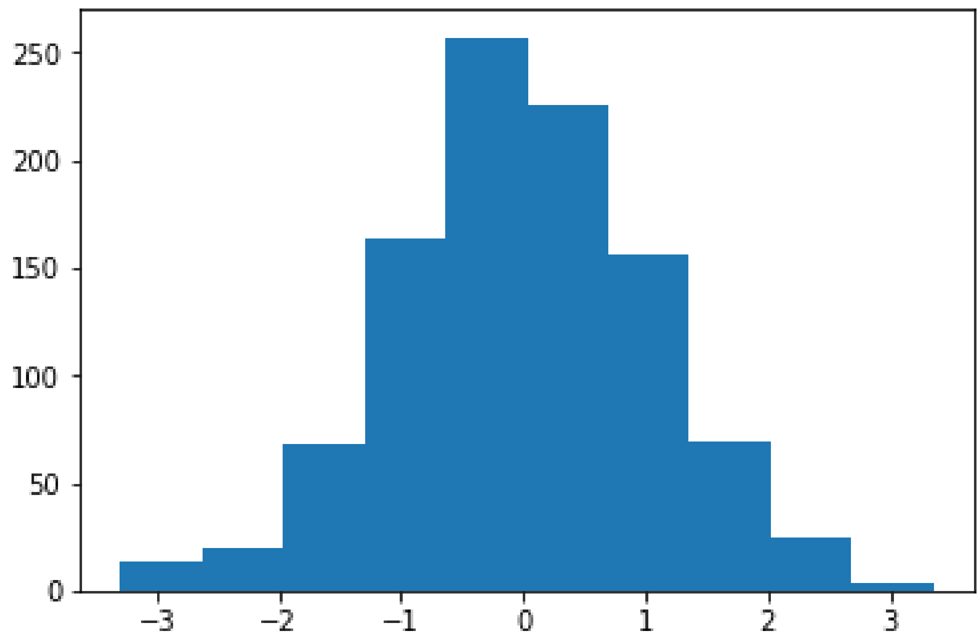


We can also check the residual plot

```
In [174]: y32_fitted_sklearn = lm32.intercept_[0] + lm32.coef_[0][0]*X + lm32.coef_[0][1]*X**2
          Res_32 = y32_fitted_sklearn - Y_3
```

```
plt.hist(Res_32)

print('This is roughly a normal distribution with mean {mean} and standard deviation
      .format(mean=np.mean(Res_32),std=np.std(Res_32)))
```

```
This is roughly a normal distribution with mean -1.7408297026122454e-15 and standard deviation
```



It is not a surprise that we were able to fit a function of the form $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$. Using taylor expansion, $f(x) = sin(x)$ estimated around the point $x = 0$ as

$$\begin{aligned} f(x=0) &= f(0) + f^{(1)}(0)x + f^{(2)}(0)x^2/(2!) + f^{(3)}(0)x^3/(3!) + O(x^4) \\ &= \sin(0) + \cos(0)x - \sin(0)x^2/(2!) - \cos(0)x^3/(3!) \\ &= x - x^3/(6) \end{aligned}$$

If we apply Taylor series expansion to $f(x) = 4.67 + 5.07sin(x/20)$ instead:

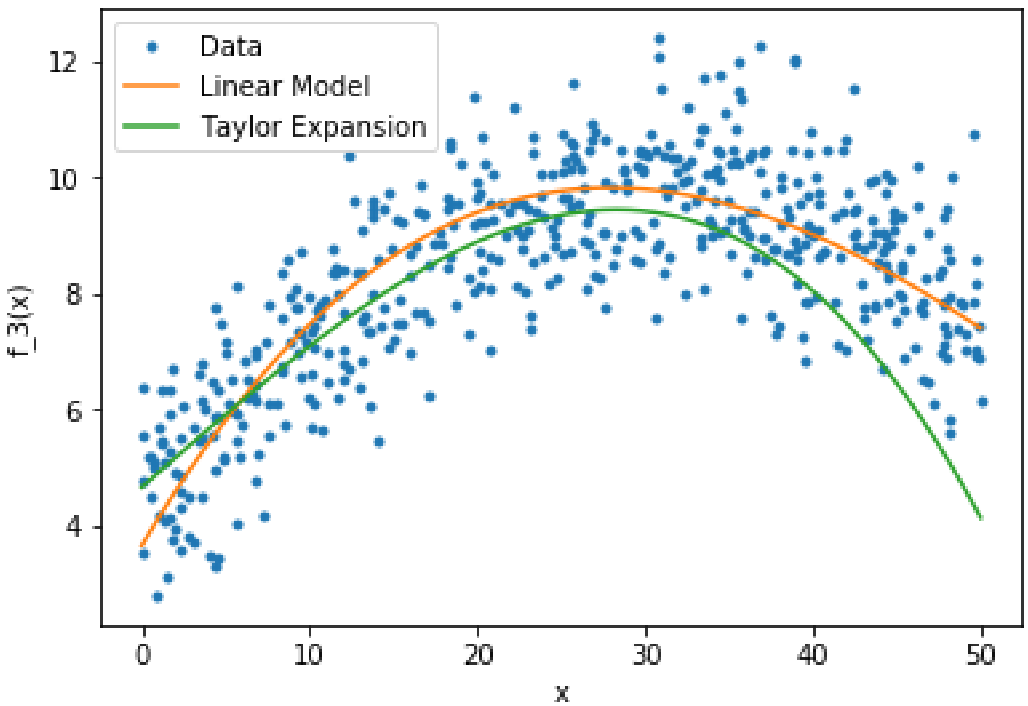
$$f(x=0) = 4.67 + \frac{5.07}{20}\cos(0)x - \frac{5.07}{20^3}\cos(0)x^3/(3!) = 4.67 + 0.25x - 1 \times 10^{-4}x^3$$

Let's plot this along with the above for smaller values of X for which this approximation of sin(x) is acceptable.

```
In [230]: x32 = np.linspace(0,50,1000) # 1000 linearly spaced numbers
          y32 = lm32.intercept_[0] + lm32.coef_[0][0]*x32 + lm32.coef_[0][1]*x32**2 + lm32.coe
          y_taylor_32 = 4.67 + (5.07/20)*x32 + 0*x32**2 - (5.07/(20**3 * 6))*x32**3
```

```
X_small = list(filter(lambda x: x < 50,X))
Y_small = Y_3[pd.concat([pd.DataFrame(X,columns=['X']),pd.DataFrame(Y_3,columns=['Y']

fig = plt.figure()
axes = fig.add_axes([0.1,0.1,0.8,0.8])
axes.plot(X_small,Y_small,'.',label='Data')
axes.set_xlabel('x')
axes.set_ylabel('f_3(x)')
axes.plot(x32,y32,label='Linear Model')
axes.plot(x32,y_taylor_32,label='Taylor Expansion')
axes.legend()
```

```
Out[230]: <matplotlib.legend.Legend at 0x2995179d320>
```



In addition to the R^2 statistic, it is useful to assess whether a variable is statistically significant. To do this for a variable X with coefficient β_1, we test the null hypothesis

$$H_O : \beta_1 = 0$$

against

$$H_A : \beta_1 \neq 0$$

For the first model we have the fitted model

```
In [246]: print('f(x) = {} + {} X'.format(lm1.intercept_[0],lm1.coef_[0][0]))
```

```
f(x) = 5.501243124853005 + 5.064254524922959 X
```

The standard errors of the estimators $\hat{\beta}_0$ and $\hat{\beta}_1$ for the coefficients have the form

$$SE(\beta_0) = \sqrt{\sigma^2[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}]} \approx RSE\sqrt{[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}]}$$

Where RSE is the *residual standard error* estimating the population $\sigma = \sqrt{Var(\epsilon)}$ and has the form $RSE = \sqrt{\frac{\sum_{i=1}^{n}\epsilon_i^2}{n-2}} = \sqrt{\frac{RSS}{n-2}}$.

$$SE(\beta_1) = \sqrt{\frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}} \approx RSE\sqrt{\frac{1}{\sum_{i=1}^{n}(x_i - \bar{x})^2}}$$

(PROOF of these equations?)

Using the standard errors, we can then conduct the hypothesis test above as a t-test. We have that

$$\frac{\hat{\beta}_0 - \beta_0^{(0)}}{SE(\beta_0)} \sim t_{n-2}$$

$$\frac{\hat{\beta}_1 - \beta_1^{(0)}}{SE(\beta_1)} \sim t_{n-2}$$

where $^{(0)}$ denotes the null value.

(PROOF that this is distributed as student t?)

```
In [332]: # we need the scipy.stats package for the t-distribution
          from scipy import stats

          # number of observations n
          n = len(X)

          # residual standard error
          RSE_1 = np.sqrt(RSS_1/(n-2))

          # variance of x = sum (x_i - x_bar)^2. Note that this is the population variance cal
          # so we would need to multiply by n
          varx_1 = np.var(X)

          # mean of x
          meanx_1 = np.mean(X)

          SE_beta_0 = RSE_1 * np.sqrt(1.0/n + meanx_1**2/(n*varx_1))
          SE_beta_1 = RSE_1 * np.sqrt(1.0/(n*varx_1))

          print('SE(beta_0) = {}, SE(beta_1) = {}'.format(SE_beta_0,SE_beta_1))

          # null hypothesis
```

```
betanull_0 = 0
betanull_1 = 0

tstatistic1_0 = (beta1_0 - betanull_0)/SE_beta_0
tstatistic1_1 = (beta1_1 - betanull_1)/SE_beta_1

print('beta_0 t-statistic = {}'.format(tstatistic1_0))
print('beta_1 t-statistic = {}'.format(tstatistic1_1))

# p-value
# the following function calculates the area under the student t pdf with 2 degrees
stats.t.cdf(-4.303,2)

# calculate the p-value using the tstatistic and degrees of freedom n-2
pval1_0 = stats.t.cdf(-tstatistic1_0,n-2)
pval1_1 = stats.t.cdf(-tstatistic1_1,n-2)

print('p-value for beta_0 = {}'.format(pval1_0))
print('p-value for beta_1 = {}'.format(pval1_1))
print('These are both statistically significant!')
```

```
SE(beta_0) = 0.6406034056188337, SE(beta_1) = 0.011151051418375258
beta_0 t-statistic = 8.587595814509644
beta_1 t-statistic = 454.150405635995
p-value for beta_0 = 1.685985282508196e-17
p-value for beta_1 = 0.0
These are both statistically significant!
```

```
In [350]: def calcpvalue(X,y_observed,y_fitted,beta_0,beta_1,betanull_0,betanull_1):
              '''
              A function to calculate whether the coefficients in a model with 1 variable is s
              X = a list for the data for the variable
              y_observed = the observed values for the response variable
              y_fitted = the predicted values of the model
              beta_0 = the intercept of the model
              beta_1 = the coefficient of the explanatory variable in the model
              betanull_0 = null hypothesis value for the intercept (usually 0)
              betanull_1 = null hypothesis value for the coefficient of the response variable
              '''
              # number of observations n
              n = len(X)

              # calculate RSS
              temp,RSS = TSS_RSS(y_observed,y_fitted)

              # residual standard error
              RSE = np.sqrt(RSS/(n-2))
```

```python
# variance of x = sum (x_i - x_bar)^2. Note that this is the population variance
# so we would need to multiply by n
varx = np.var(X)

# mean of x
meanx = np.mean(X)

SE_beta_0 = RSE * np.sqrt(1.0/n + meanx**2/(n*varx))
SE_beta_1 = RSE * np.sqrt(1.0/(n*varx))

print('SE(beta_0) = {}, SE(beta_1) = {}'.format(SE_beta_0,SE_beta_1))

# null hypothesis
betanull_0 = 0
betanull_1 = 0

tstatistic1_0 = (beta_0 - betanull_0)/SE_beta_0
tstatistic1_1 = (beta_1 - betanull_1)/SE_beta_1

print('beta_0 t-statistic = {}'.format(tstatistic1_0))
print('beta_1 t-statistic = {}'.format(tstatistic1_1))

# p-value

# calculate the p-value using the tstatistic and degrees of freedom n-2
if(tstatistic1_0 > 0):
    pval_0 = stats.t.cdf(-tstatistic1_0,n-2)
else:
    pval_0 = stats.t.cdf(tstatistic1_0,n-2)

if(tstatistic1_1 > 0):
    pval_1 = stats.t.cdf(-tstatistic1_1,n-2)
else:
    pval_1 = stats.t.cdf(tstatistic1_1,n-2)

print('p-value for beta_0 = {}'.format(pval_0))
print('p-value for beta_1 = {}'.format(pval_1))
if((pval_0 <= 0.05) and (pval_1 <=0.05)):
    print('These are both statistically significant!')
elif(pval_0 <= 0.05):
    print('Only beta_0 is statistically significant!')
elif(pval_1 <= 0.05):
    print('Only beta_1 is statistically significant!')
else:
    print('The parameters of this model are not statistically significant!')
```

We can do the same calculations for significance for all the models using this function

```
In [351]: print('Model for Y_1: Explanatory variable X for Y_1')
          calcpvalue(X,Y_1,y1_fitted,beta1_0,beta1_1,0,0)

          print()
          print()

          print('Model for Y_2: Explanatory variable X for Y_2')
          calcpvalue(X,Y_2,y2_fitted,beta2_0,beta2_1,0,0)

          print()
          print()

          print('Model for Y_2: Explanatory variable X^2 for Y_2')
          calcpvalue(X,Y_2,y22_fitted,beta22_0,beta22_1,0,0)

          print()
          print()

          print('Model for Y_3: Explanatory variable X for Y_3')
          calcpvalue(X,Y_3,y3_fitted,beta3_0,beta3_1,0,0)
```

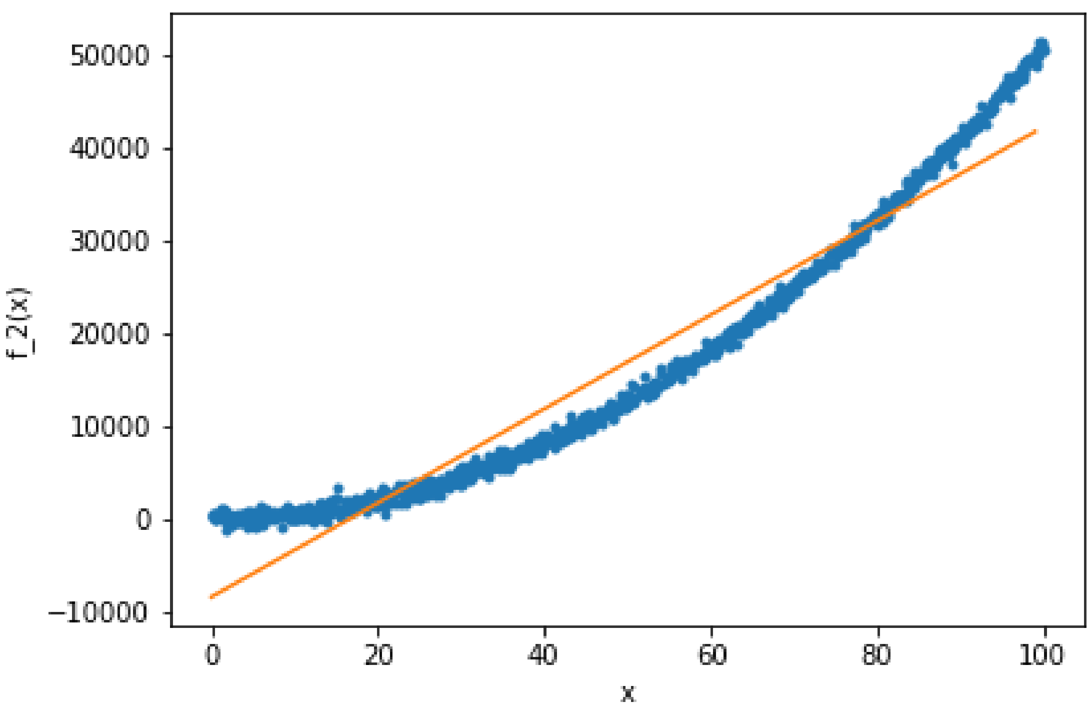
```
Model for Y_1: Explanatory variable X for Y_1
SE(beta_0) = 0.6406034056188337, SE(beta_1) = 0.011151051418375258
beta_0 t-statistic = 8.587595814509644
beta_1 t-statistic = 454.150405635995
p-value for beta_0 = 1.685985282508196e-17
p-value for beta_1 = 0.0
These are both statistically significant!


Model for Y_2: Explanatory variable X for Y_2
SE(beta_0) = 245.34955295438897, SE(beta_1) = 4.2708256878947495
beta_0 t-statistic = -34.424274285888536
beta_1 t-statistic = 118.51588098729522
p-value for beta_0 = 4.062734353712651e-172
p-value for beta_1 = 0.0
These are both statistically significant!


Model for Y_2: Explanatory variable X^2 for Y_2
SE(beta_0) = 32.936149817301605, SE(beta_1) = 0.5733230527884089
beta_0 t-statistic = 0.4393368148245055
beta_1 t-statistic = 8.851939503631746
p-value for beta_0 = 0.33025630512965964
p-value for beta_1 = 1.9265051090518403e-18
Only beta_1 is statistically significant!
```

```
Model for Y_3: Explanatory variable X for Y_3
SE(beta_0) = 0.15212372264589394, SE(beta_1) = 0.0026480337730023893
beta_0 t-statistic = 69.09601786545896
beta_1 t-statistic = -38.21657519695403
p-value for beta_0 = 0.0
p-value for beta_1 = 6.841386859358049e-198
These are both statistically significant!
```

If we look at the plot for the second model, we see that our linear model estimates an intercept close to -10000. This is clearly not true. Additionally, the shape of the data is not well modelled either. It is not a surprise that some coefficients are statistically insignificant. Similarly with the first model for Y_3

In [344]:
```
fig = plt.figure()
axes = fig.add_axes([0.1,0.1,0.8,0.8])
axes.plot(X,Y_2,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_2(x)')
axes.plot(x2,y2)
```

Out[344]: `[<matplotlib.lines.Line2D at 0x299542ec1d0>]`



We can use the statsmodels.api to verify our results

In [345]:
```
import statsmodels.api as sm
from scipy import stats
```

In [370]:
```
print('Model for Y_1: Explanatory variable X for Y_1')

# add a column of ones to X
X_new = sm.add_constant(X)

# ordinary least squares approach to optimisation
est = sm.OLS(Y_1, X_new)

# fit the data to the model using OLS
est2 = est.fit()

# print a summary of the model
print(est2.summary())

print()
print()

#re-run the above for all the models

print('Model for Y_2: Explanatory variable X for Y_2')
X_new = sm.add_constant(X)
est = sm.OLS(Y_2, X_new)
est2 = est.fit()
print(est2.summary())

print()
print()

print('Model for Y_2: Explanatory variable X^2 for Y_2')
X_new = sm.add_constant(X**2)
est = sm.OLS(Y_2, X_new)
est2 = est.fit()
print(est2.summary())

print()
print()

print('Model for Y_3: Explanatory variable X for Y_3')
X_new = sm.add_constant(X)
est = sm.OLS(Y_3, X_new)
est2 = est.fit()
print(est2.summary())

print()
print()
```

```python
print('Model for Y_3: Explanatory variables X,X^2,X^3 for Y_3')
# concatenate multiple variables
X_new = sm.add_constant(pd.concat([pd.DataFrame(X,columns=['X']),pd.DataFrame(X**2,co
est = sm.OLS(Y_3, X_new)
est2 = est.fit()
print(est2.summary())
```

```
Model for Y_1: Explanatory variable X for Y_1
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.995
Model:                            OLS   Adj. R-squared:                  0.995
Method:                 Least Squares   F-statistic:                 2.063e+05
Date:                Mon, 08 Oct 2018   Prob (F-statistic):               0.00
Time:                        13:05:18   Log-Likelihood:                -3730.1
No. Observations:                1000   AIC:                             7464.
Df Residuals:                     998   BIC:                             7474.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          5.5012      0.641      8.588      0.000       4.244       6.758
x1             5.0643      0.011    454.150      0.000       5.042       5.086
==============================================================================
Omnibus:                        0.350   Durbin-Watson:                   1.952
Prob(Omnibus):                  0.839   Jarque-Bera (JB):                0.376
Skew:                          -0.045   Prob(JB):                        0.828
Kurtosis:                       2.970   Cond. No.                         115.
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.


Model for Y_2: Explanatory variable X for Y_2
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.934
Model:                            OLS   Adj. R-squared:                  0.934
Method:                 Least Squares   F-statistic:                 1.405e+04
Date:                Mon, 08 Oct 2018   Prob (F-statistic):               0.00
Time:                        13:05:18   Log-Likelihood:                -9678.1
No. Observations:                1000   AIC:                         1.936e+04
Df Residuals:                     998   BIC:                         1.937e+04
Df Model:                           1
Covariance Type:            nonrobust
```

```
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const      -8445.9803    245.350    -34.424      0.000   -8927.440   -7964.520
x1           506.1607      4.271    118.516      0.000     497.780     514.541
==============================================================================
Omnibus:                      136.837   Durbin-Watson:                   1.872
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              102.303
Skew:                           0.681   Prob(JB):                     6.10e-23
Kurtosis:                       2.227   Cond. No.                         115.
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.


Model for Y_2: Explanatory variable X^2 for Y_2
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.999
Model:                            OLS   Adj. R-squared:                  0.999
Method:                 Least Squares   F-statistic:                 8.338e+05
Date:                Mon, 08 Oct 2018   Prob (F-statistic):               0.00
Time:                        13:05:18   Log-Likelihood:                -7670.0
No. Observations:                1000   AIC:                         1.534e+04
Df Residuals:                     998   BIC:                         1.535e+04
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         14.4701     24.615      0.588      0.557     -33.832      62.772
x1             5.0750      0.006    913.134      0.000       5.064       5.086
==============================================================================
Omnibus:                        5.725   Durbin-Watson:                   2.021
Prob(Omnibus):                  0.057   Jarque-Bera (JB):                7.275
Skew:                           0.018   Prob(JB):                       0.0263
Kurtosis:                       3.416   Cond. No.                     6.64e+03
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 6.64e+03. This might indicate that there are
strong multicollinearity or other numerical problems.


Model for Y_3: Explanatory variable X for Y_3
                            OLS Regression Results
```

```
==============================================================================
Dep. Variable:                      y   R-squared:                       0.594
Model:                            OLS   Adj. R-squared:                  0.594
Method:                 Least Squares   F-statistic:                     1461.
Date:                Mon, 08 Oct 2018   Prob (F-statistic):         1.37e-197
Time:                        13:05:18   Log-Likelihood:                -2292.4
No. Observations:                1000   AIC:                             4589.
Df Residuals:                     998   BIC:                             4599.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         10.5111      0.152     69.096      0.000      10.213      10.810
x1            -0.1012      0.003    -38.217      0.000      -0.106      -0.096
==============================================================================
Omnibus:                       26.494   Durbin-Watson:                   1.871
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               28.130
Skew:                          -0.405   Prob(JB):                     7.79e-07
Kurtosis:                       2.860   Cond. No.                         115.
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.


Model for Y_3: Explanatory variables X,X^2,X^3 for Y_3
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.923
Model:                            OLS   Adj. R-squared:                  0.923
Method:                 Least Squares   F-statistic:                     3974.
Date:                Mon, 08 Oct 2018   Prob (F-statistic):               0.00
Time:                        13:05:18   Log-Likelihood:                -1461.8
No. Observations:                1000   AIC:                             2932.
Df Residuals:                     996   BIC:                             2951.
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          3.6644      0.128     28.526      0.000       3.412       3.917
X              0.4871      0.011     43.605      0.000       0.465       0.509
X2            -0.0112      0.000    -42.571      0.000      -0.012      -0.011
X3          5.868e-05   1.74e-06     33.743      0.000    5.53e-05    6.21e-05
==============================================================================
Omnibus:                        0.415   Durbin-Watson:                   1.980
Prob(Omnibus):                  0.813   Jarque-Bera (JB):                0.368
```

```
Skew:                           0.046   Prob(JB):                        0.832
Kurtosis:                       3.019   Cond. No.                     1.46e+06
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.46e+06. This might indicate that there are
strong multicollinearity or other numerical problems.
```

It looks like the intercept for *Model for Y_2: Explanatory variable X^2 for Y_2* is not statistically significant. The intercept can then be omitted from the model and fitted again.

```
In [384]: print('Model for Y_2: Explanatory variable X^2 for Y_2')
          est = sm.OLS(Y_2, X**2)
          est2 = est.fit()
          print(est2.summary())
```

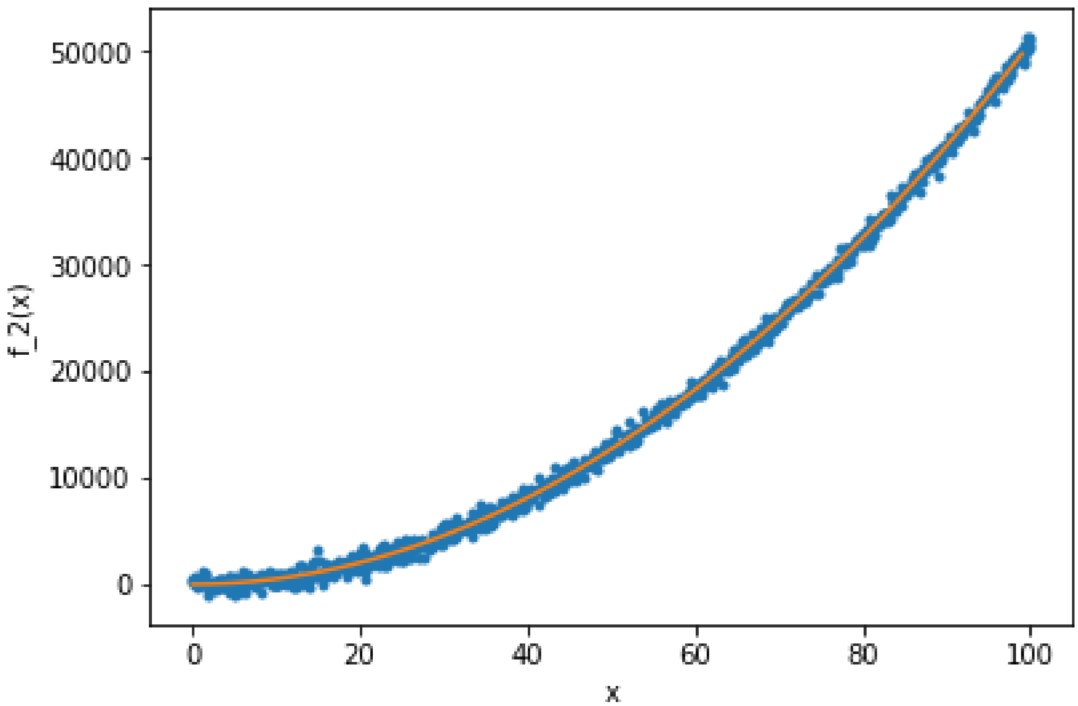
```
Model for Y_2: Explanatory variable X^2 for Y_2
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.999
Model:                            OLS   Adj. R-squared:                  0.999
Method:                 Least Squares   F-statistic:                 1.878e+06
Date:                Mon, 08 Oct 2018   Prob (F-statistic):               0.00
Time:                        13:18:54   Log-Likelihood:                -7670.2
No. Observations:                1000   AIC:                         1.534e+04
Df Residuals:                     999   BIC:                         1.535e+04
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
x1             5.0775      0.004   1370.392      0.000       5.070       5.085
==============================================================================
Omnibus:                        6.001   Durbin-Watson:                   2.020
Prob(Omnibus):                  0.050   Jarque-Bera (JB):                7.710
Skew:                           0.019   Prob(JB):                       0.0212
Kurtosis:                       3.428   Cond. No.                         1.00
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

This is a good fit also

```
In [385]: x23 = np.linspace(0,99,1000) # 1000 linearly spaced numbers
          y23 = est2.params[0] * x23**2
```

```
fig = plt.figure()
axes = fig.add_axes([0.1,0.1,0.8,0.8])
axes.plot(X,Y_2,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_2(x)')
axes.plot(x23,y23)
```

Out[385]: [<matplotlib.lines.Line2D at 0x29953b028d0>]



If we set $\beta_0 = 0$ in the derivation for $\hat{\beta_0}$ and $\hat{\beta_1}$ earlier in the article, we would have obtained the equation

$$\hat{\beta_1} = \frac{\sum_{i=1}^{n} y_i x_i}{\sum_{i=1}^{n} x_i^2}$$

Using this equation, we can reproduce the statsmodels solution above. Note that removing β_0 has changed β_1 slightly:

```
In [393]: # remember that we are fitting the variable X^2
          sum1 = np.sum(Y_2*X**2)
          sum2 = np.sum(X**4)

          beta23_1 = sum1/sum2

          print('Y ~ {} X^2'.format(beta23_1))
```

```
Y ~ 5.077455649665152 X^2
```

F-Statistic The F-Statistic answers the question 'Is there evidence that at least one of the explanatory variables is related to the response variable?'. This corresponds to a hypothesis test with:

$$H_O : \beta_0, \beta_1, ..., \beta_p = 0$$
$$H_A : \text{at least one of } \beta_i \text{ is non-zero}$$

The F-Statistic has the form:

$$F = \frac{(TSS - RSS)/p}{RSS/(n-p-1)}$$

where p is the number of explanatory variables/parameters.
(DERIVATION of this equation?)
If H_O is not true, the numerator in the above equation becomes larger, i.e. F > 1. If H_0 is true, then the F-Statistic is close to 1.
(PROOF of this - take expectation of numerator and denominator and these are both equal to Var(ϵ). If H_A is true then the numerator > Var(ϵ))
We can use this to calculate the F-Statistics of the above models:

```
In [420]: def FStat(n,p,TSS,RSS):
              F = ((TSS-RSS)/p)/(RSS/(n-p-1))
              print('The F-Statistic is {}'.format(F))
```

```
In [421]: # we didn't calculate the last model ourselves, we used sklearn so we retrieve the c
          beta32_0 = lm32.intercept_[0]
          beta32_1 = lm32.coef_[0][0]
          beta32_2 = lm32.coef_[0][1]
          beta32_3 = lm32.coef_[0][2]
```

```
In [423]: print('Model for Y_1: Explanatory variable X for Y_1')
          FStat(len(X),1,TSS_1,RSS_1)

          print()
          print()

          #re-run the above for all the models

          print('Model for Y_2: Explanatory variable X for Y_2')
          FStat(len(X),1,TSS_2,RSS_2)

          print()
          print()

          print('Model for Y_2: Explanatory variable X^2 for Y_2')
          FStat(len(X),1,TSS_22,RSS_22)
```

```
        print()
        print()

        print('Model for Y_3: Explanatory variable X for Y_3')
        FStat(len(X),1,TSS_3,RSS_3)

        print()
        print()

        TSS_32,RSS_32 = TSS_RSS(Y_3,y32_fitted_sklearn)

        print('Model for Y_3: Explanatory variables X,X^2,X^3 for Y_3')
        # now we have 3 explanatory variables
        FStat(len(X),3,TSS_32,RSS_32)
```

```
Model for Y_1: Explanatory variable X for Y_1
The F-Statistic is 206252.59093933867


Model for Y_2: Explanatory variable X for Y_2
The F-Statistic is 14046.014046194661


Model for Y_2: Explanatory variable X^2 for Y_2
The F-Statistic is 833813.8656032282


Model for Y_3: Explanatory variable X for Y_3
The F-Statistic is 1460.506619784441


Model for Y_3: Explanatory variables X,X^2,X^3 for Y_3
The F-Statistic is 3974.1603226694533
```

These match the *statsmodels* outputs. We can also find the p-value of a coefficient/intercept using the F-Statistic. The F-Statistic formula becomes:

$$F = \frac{(RSS_0 - RSS)/q}{RSS/(n-p-1)}$$

where RSS_0 is the residual sum of squares for the model with q removed parameters. The corresponding hypothesis test is then

$$H_0 : \beta_i = 0 \text{ where i is one of the q removed parameters}$$
$$H_A : \text{at least one of those q parameters is non-zero}$$

Above, we ran a model for Y_2 which had an intercept, coefficient of X^2 and RSS of:

```
In [479]: beta22_0, beta22_1, RSS_22
```

Out[479]: (14.470063153316005, 5.075020979320466, 268902718.6114595)

We then attempted to fit a model to Y_2 but this time without the intercept. The Coefficient of Xˆ2 and RSS for that model was calculated to be

```
In [481]: TSS_23,RSS_23 = TSS_RSS(Y_2,beta23_1 * X**2)
          beta23_1,RSS_23
```

Out[481]: (5.077455649665152, 268995834.0780044)

```
In [482]: def FStatCompare(n,p,q,RSS0,RSS):
              '''
              A function to calculate the F-Statistic when we are comparing models with differ
              RSS0 is a sub-model of RSS
              '''
              F = ((RSS0-RSS)/q)/(RSS/(n-p-1))
              print('The F-Statistic is {}'.format(F))
```

```
In [497]: Y23_fitted = beta23_1 * X**2
          TSS_2_test,RSS_2_test = TSS_RSS(Y_2,Y23_fitted)
          FStatCompare(len(X),0,1,RSS_23,RSS_22)

          # the following function calculated the area underneath the cdf F-distribution with
          #dfn(degrees of freedom in the numerator)=1,
          #dfd(degrees of freedom in the denominator)=len(X)-2 less than 0.5
          stats.f.cdf(0.5,1,len(X)-2)

          print('The p-value of the intercept is {}'.format(1-stats.f.cdf(0.3459331001141355,1
```

```
The F-Statistic is 0.3459331001141355
The p-value of the intercept is 0.5565574505496756
```

1.4 Appendix

1.4.1 A1 - $(2n)(2\sum_{i=1}^n x_i^2) - (2\sum_{i=1}^n x_i)^2 > 0$

Statement: $(2n)(2\sum_{i=1}^n x_i^2) - (2\sum_{i=1}^n x_i)^2 > 0 \; \forall \; n > 1$

Proof: We prove this by induction on n. If n = 1, we have $(2n)(2\sum_{i=1}^n x_i^2) - (2\sum_{i=1}^n x_i)^2 = 0$, but this is not what we want.

Let n = 2 > 1. Then

$$(2n)(2\sum_{i=1}^n x_i^2) - (2\sum_{i=1}^n x_i)^2 = 2x_1^2 + 2x_2^2 - (x_1 + x_2)^2 = 2x_1^2 + 2x_2^2 - x_1^2 - x_2^2 - 2x_1x_2 = x_1^2 + x_2^2 - 2x_1x_2 = (x_1 - x_2)^2 >$$

So we have proved the assertion for n = 2.

Let us prove the statement for n+1 assuming it is true for n.

i.e. Assume $n\sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2 > 0$

Then

$$(n+1)\sum_{i=1}^{n+1} x_i^2 - (\sum_{i=1}^{n+1} x_i)^2 = (n+1)[\sum_{i=1}^{n} x_i^2 + x_{n+1}^2] - (\sum_{i=1}^{n} x_i + x_{n+1})^2 = [n\sum_{i=1}^{n} x_i^2 + \sum_{i=1}^{n} x_i^2 + (n+1)x_{n+1}^2] - (\sum_{i=1}^{n} x_i)^2 - x$$

$$= n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2 + \sum_{i=1}^{n} x_i^2 + (n+1)x_{n+1}^2 - x_{n+1}^2 + 2x_{n+1}\sum_{i=1}^{n} x_i$$

by the assumption for n we have

$$> \sum_{i=1}^{n} x_i^2 + (n+1)x_{n+1}^2 - x_{n+1}^2 + 2x_{n+1}\sum_{i=1}^{n} x_i$$

by the assumption for n that $\sum_{i=1}^{n} x_i^2 > \frac{1}{n}(\sum_{i=1}^{n} x_i)^2$ we have

$$> \frac{1}{n}(\sum_{i=1}^{n} x_i)^2 + (n+1)x_{n+1}^2 - x_{n+1}^2 + 2x_{n+1}\sum_{i=1}^{n} x_i = \frac{1}{n}(\sum_{i=1}^{n} x_i)^2 + nx_{n+1}^2 + 2x_{n+1}\sum_{i=1}^{n} x_i = \frac{1}{n}[(\sum_{i=1}^{n} x_i)^2 + n^2x_{n+1}^2 + 2nx_{n+}$$

$$= \frac{1}{n}[(\sum_{i=1}^{n} x_i)^2 + n^2x_{n+1}^2 + 2nx_{n+1}\sum_{i=1}^{n} x_i] = \frac{1}{n}[(\sum_{i=1}^{n} x_i + nx_{n+1})^2] > 0$$