LinearRegression

November 5, 2018

1 Linear Regression

Linear Regression is one of the simplest yet fundamental statistical learning techniques. It is a great initial step towards more advanced and computationally demanding methods.

This article aims to form a statistically sound approach to Linear Regression and its inferences while tying these to popular statistical packages and reproducing the results.

We first begin with a brief description of Linear Regression and move on to investigate it in light of a dataset.

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.

General Characteristics: - 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 shape is limited (as a function of the parameters)

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).

First we import the required libraries

```
In [1]: # 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
```

Then we import the dataset

```
In [2]: # Import Advertising dataset (http://www-bcf.usc.edu/~gareth/ISL/data.html)
        advert = pd.read_csv("Advertising.csv").iloc[:,1:]
```

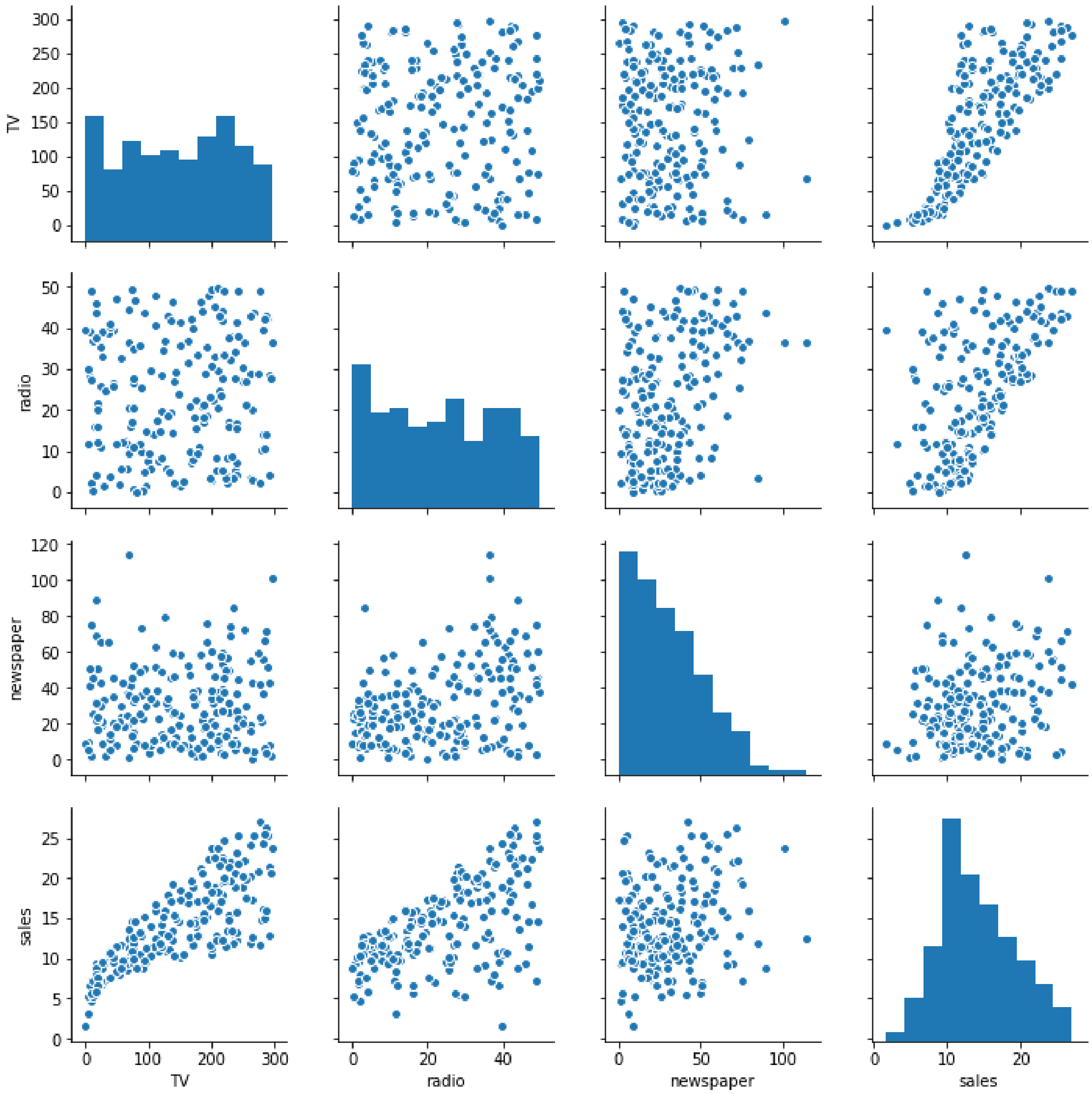
```
In [3]: print("Number of observations (n) =",advert.shape[0])
        print("Number of predictor variables (p) =",advert.shape[1]-1)
        print()
        print("Advertising.csv")
        display(advert.head())
```

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

Advertising.csv
```

	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". We can produce a pairplot of the data below.

```
In [4]: ax = sns.pairplot(data=advert)
```



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 [5]: advert.corr()
```

Out[5]:

	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

We may want to fit a line to this data which is as close as possible. We describe the Linear Regression model next and then apply it to this data.

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 an 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 $i = 1, 2, ..., p$.

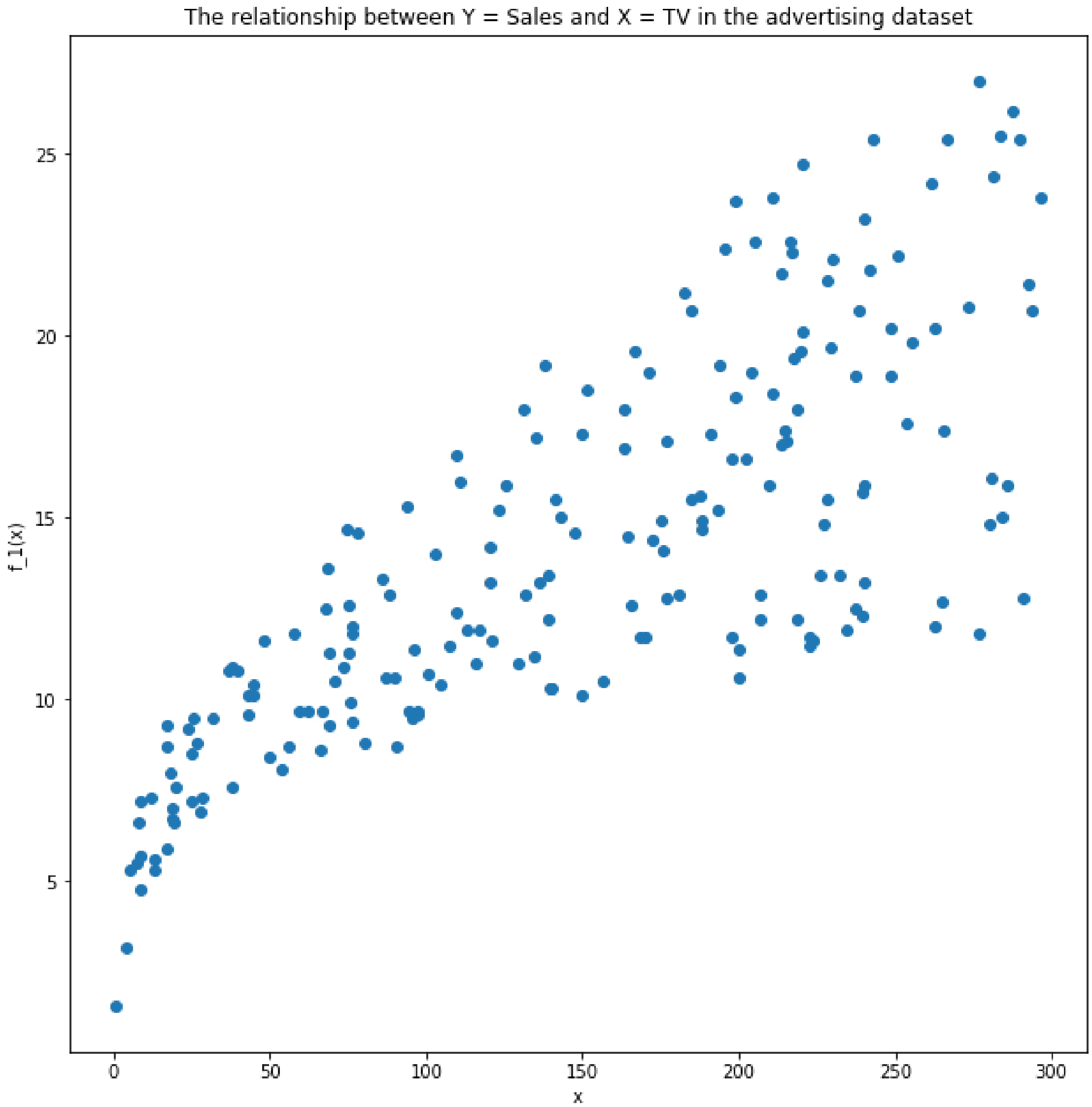
We first limit the problem to $p = 1$. For example, we are looking to estimate the coefficients in the equation

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

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 (also called the ith *residual*).

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

In [6]:
```
# plt.scatter(data=advert, x='TV', y='sales')
# plt.show()

# Get the figure handle and set figure size
fig = plt.figure(figsize=(8,8))

# Get the axis
axes = fig.add_axes([0.1,0.1,1,1])

# Plot onto the axis
axes.scatter(data=advert, x='TV', y='sales')

# Set the labels and title
axes.set_xlabel('x')
axes.set_ylabel('f_1(x)')
axes.set_title('The relationship between Y = Sales and X = TV in \
the advertising dataset')
plt.show()
```



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

$$\frac{\partial RSS}{\partial \hat{\beta_0}} = 0 \implies \hat{\beta}_0 = \frac{\sum_{i=1}^{n} y_i - \hat{\beta}_1 \sum_{i=1}^{n} y_i}{n} = \frac{n\bar{y} - \hat{\beta}_1 n\bar{x}}{n} = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\frac{\partial RSS}{\partial \hat{\beta_1}} = 0 \implies \sum_{i=1}^{n} y_i x_i - \hat{\beta}_0 \sum_{i=1}^{n} x_i - \hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = 0$$

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

$$= \frac{\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} y_i \bar{x} - \sum_{i=1}^{n} x_i \bar{y} + \sum_{i=1}^{n} \bar{y}\bar{x}}{\sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} x_i \bar{x} - \sum_{i=1}^{n} x_i \bar{x} + \sum_{i=1}^{n} \bar{x}^2}$$

Where, in the penultimate line we completed the square and in the last equality we used $n\bar{y}\bar{x} = \sum_{i=1}^{n} y_i \bar{x} = \sum_{i=1}^{n} x_i \bar{y}$ 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, $\hat{\mu} = \bar{x} = \frac{1}{n}\sum_{i=1}^{n}$ 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- $f_3(x) = 4.67 + 5.07 * sin(x)$

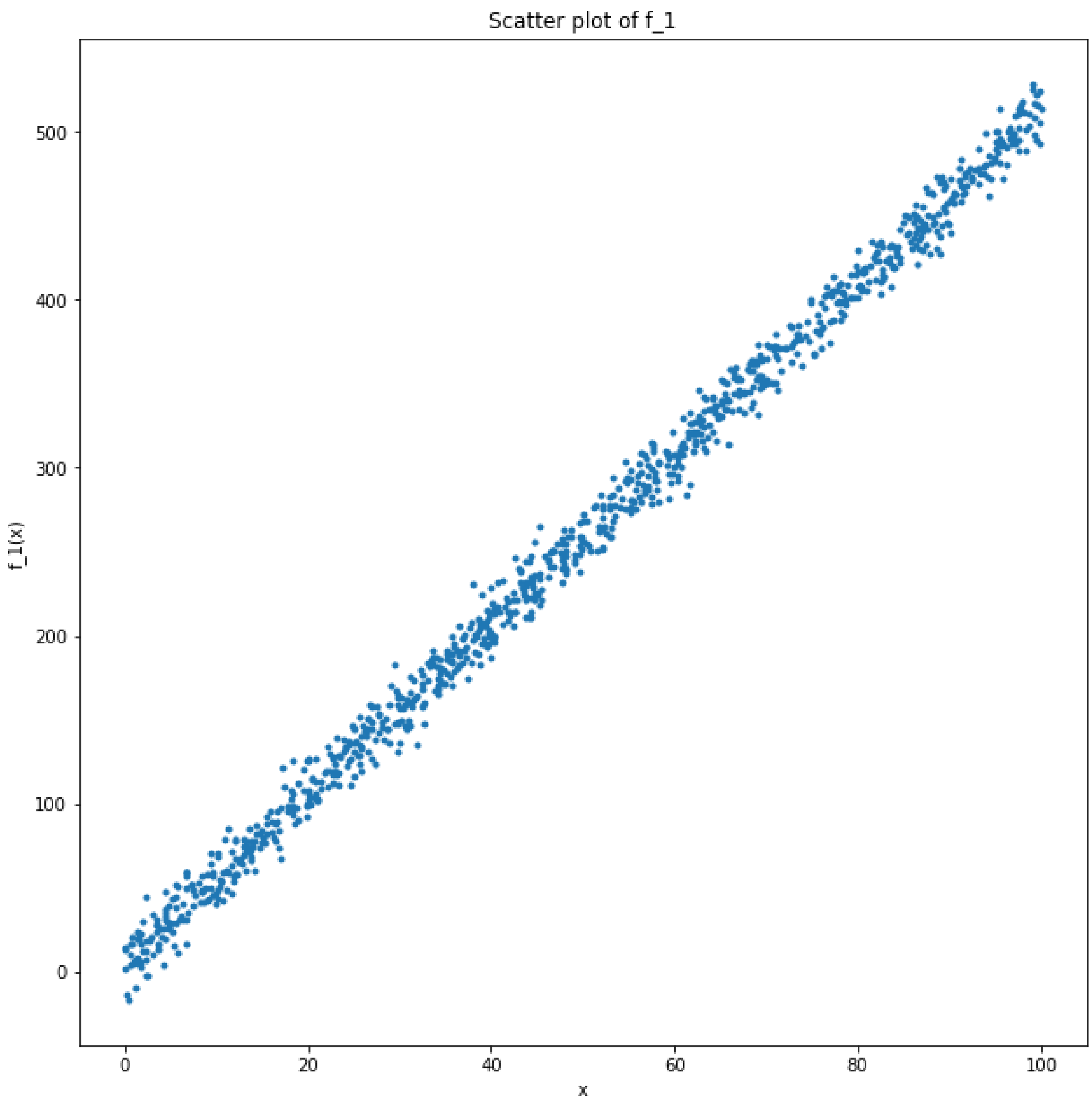
In [7]:
```
#f_1(x)=4.67+5.07x
def f_1(x):
    return 4.67 + 5.07*x

#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 [8]:
```
# Set the seed
r = np.random.RandomState(101)

# Choose 1000 random observations for x between 0 and 100
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 we look at what f_1 looks like

In [9]:
```
# Plot
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.plot(X,Y_1,'.')

# Set labels and title
```

```python
axes.set_xlabel('x')
axes.set_ylabel('f_1(x)')
axes.set_title('Scatter plot of f_1')

plt.show()
```



The task is to 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

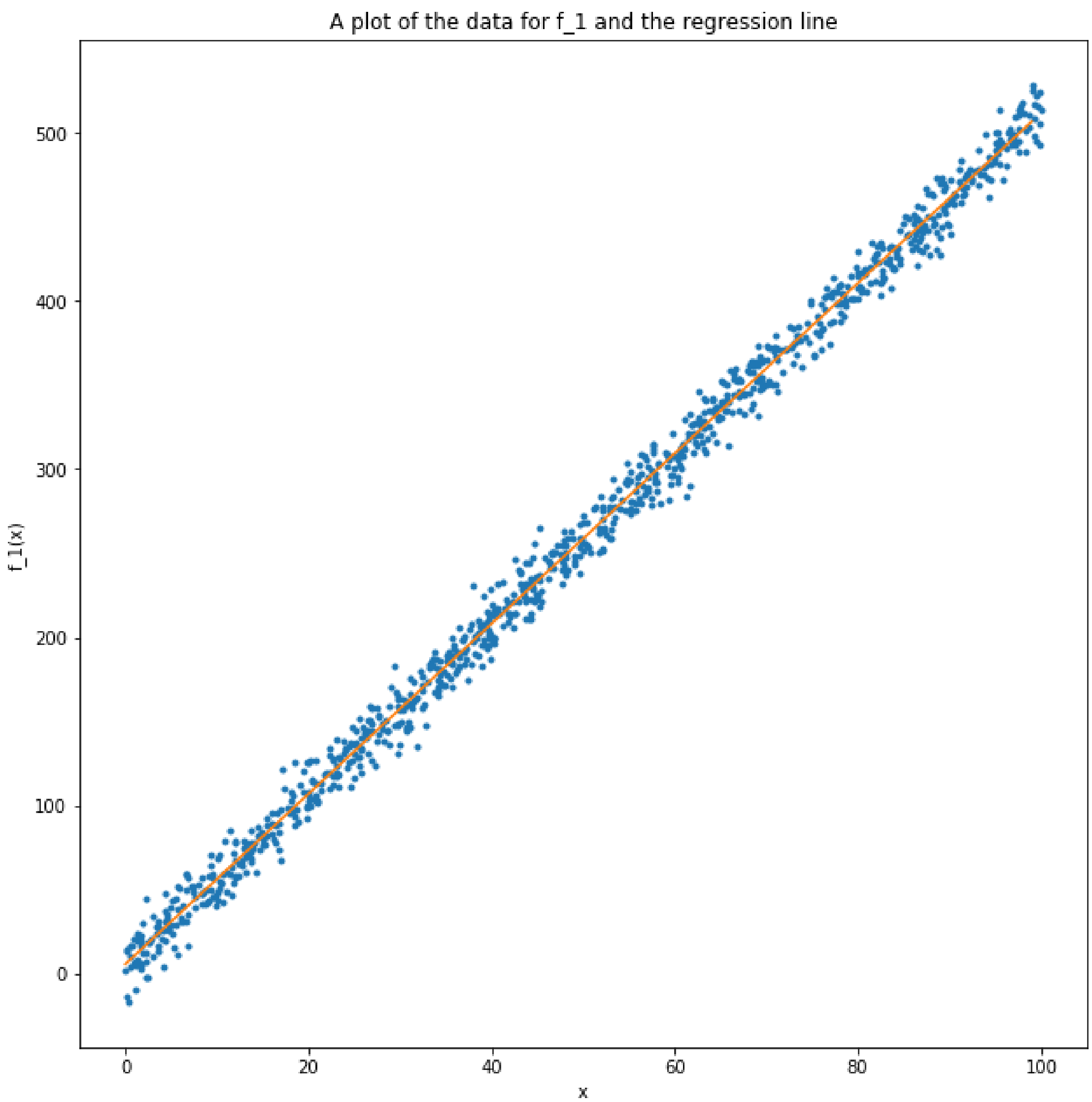
$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

```
In [10]: #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)):
             # Add to the numerator for beta_1
             numerator += (X[i] - x_bar1)*(Y_1[i] - y_bar1)

             # Add to the denominator for beta_1
             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
```

Below, we see how the line defined by the equation above fits the data for f_1

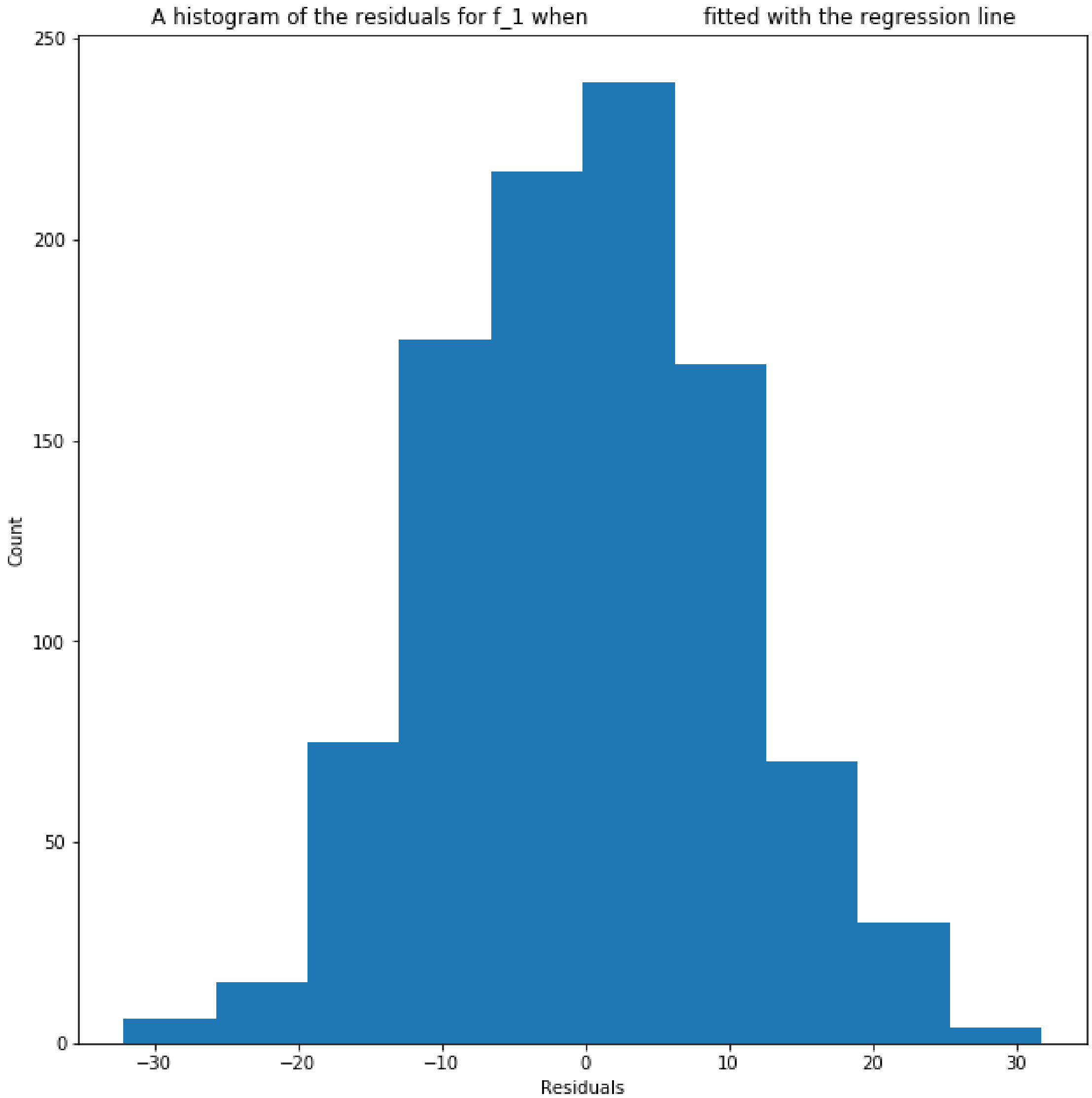
```
In [11]: # 1000 linearly spaced numbers
         x1 = np.linspace(0,99,1000)

         # The equation using the betas above
         y1 = beta1_0 + beta1_1 * x1

         # Plot the observed data
         fig = plt.figure(figsize=(8,8))
         axes = fig.add_axes([0.1,0.1,1,1])
         axes.plot(X,Y_1,'.')

         # Plot the regression line
         axes.plot(x1,y1)

         # Set labels and title
         axes.set_xlabel('x')
         axes.set_ylabel('f_1(x)')
         axes.set_title('A plot of the data for f_1 and the regression line')

         plt.show()
```



Let's see what the residuals look like by plotting them. The residual require the knowledge of the actual response variables. So we use the regression line above to predict the response variable using the observed predictor variables. Then we plot them using a histogram to gain some insight into their distribution

In [12]:
```
# The fitted values are the predicted values given the observed values
y1_fitted = beta1_0 + beta1_1 * X

# The residuals are the differences between our predicted values and
# the observed responses
Res_1 = y1_fitted - Y_1

# Plot the residuals
fig = plt.figure(figsize=(8,8))
```

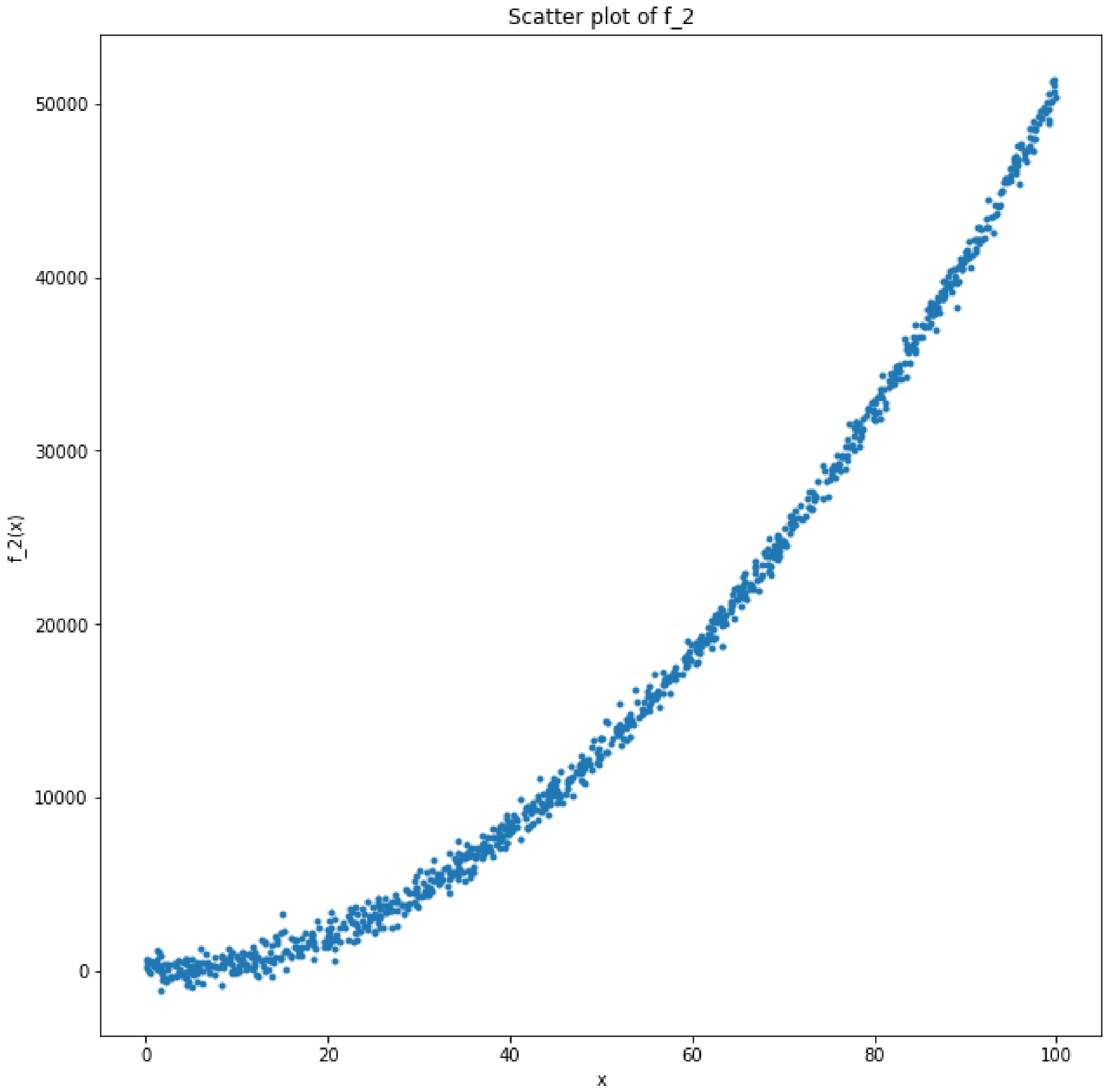
```python
axes = fig.add_axes([0.1,0.1,1,1])
axes.hist(Res_1)

# Set labels and title
axes.set_xlabel('Residuals')
axes.set_ylabel('Count')
axes.set_title('A histogram of the residuals for f_1 when \
                fitted with the regression line')

plt.show()

print('This is roughly a normal distribution with mean {mean} \n\
and standard deviation {std}'.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 10.08588495757817
```

Since the residuals are roughly normally distributed, our model may be a good choice. In fact, the standard deviation for the residuals was roughly equal to the standard deviation for the error term when we constructed the function f_1. A model may suffer from two types of error: error due to a discrepancy between the chosen function shape (here a linear model) and the true function shape (reducible); error due to random noise (irreducible). We can see here that the residuals are from irreducible error. Now let's do the same for f_2.

```
In [13]: # Get figure handle
         fig = plt.figure(figsize=(8,8))

         # Get axis handle and specify size
         axes = fig.add_axes([0.1,0.1,1,1])

         # Plot onto this axis
         axes.plot(X,Y_2,'.')

         # Set the axis labels
         axes.set_xlabel('x')
         axes.set_ylabel('f_2(x)')
         axes.set_title('Scatter plot of f_2')

Out[13]: Text(0.5,1,'Scatter plot of f_2')
```



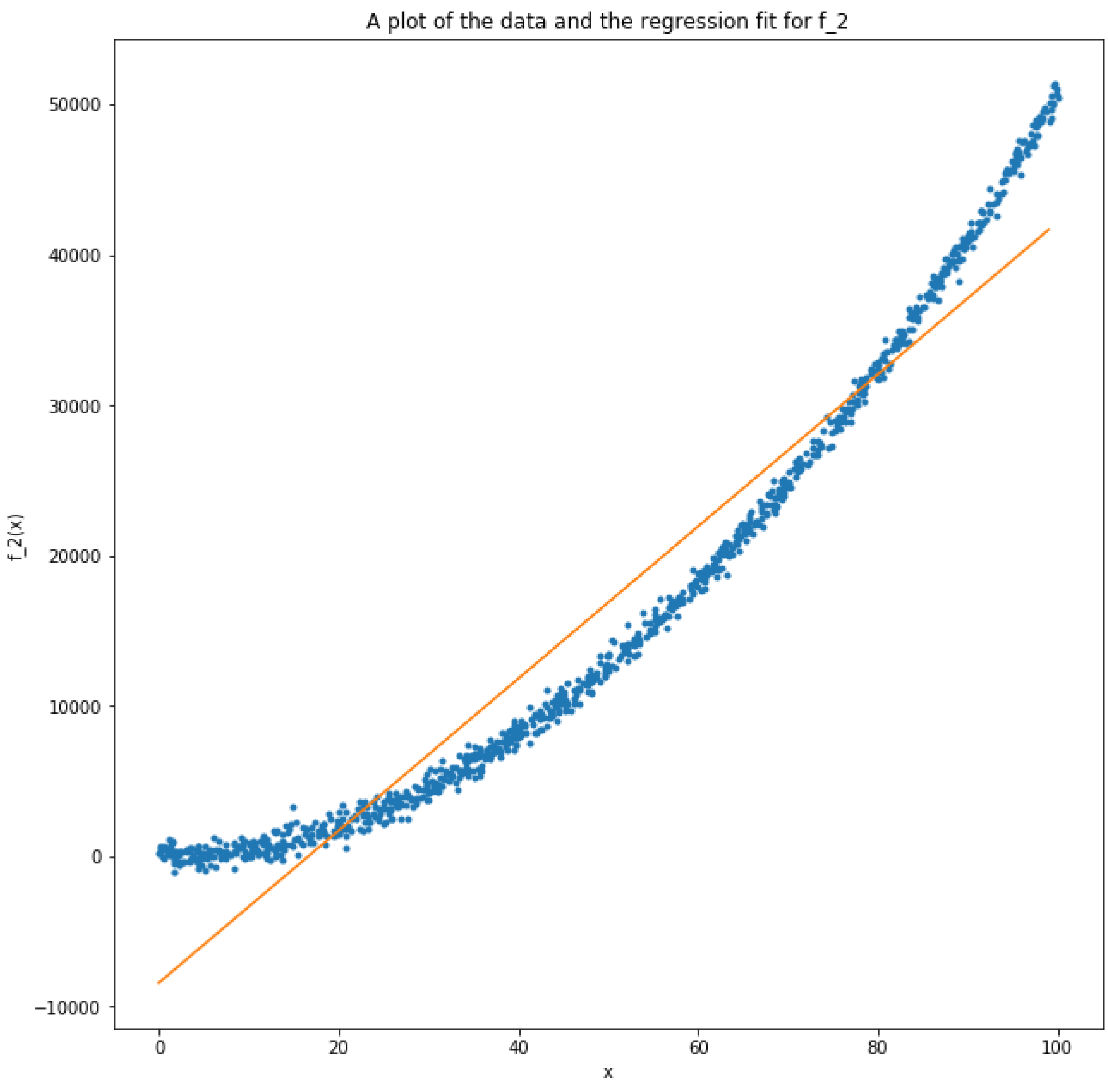
In [14]:
```
#Find the mean of the data for f_2
x_bar2 = np.mean(X)
y_bar2 = np.mean(Y_2)

numerator = 0
denominator = 0

for i in range(len(Y_2)):
    # Add to the numerator for beta_1
    numerator += (X[i] - x_bar2)*(Y_2[i] - y_bar2)

    # Add to the denominator for beta_1
    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
```

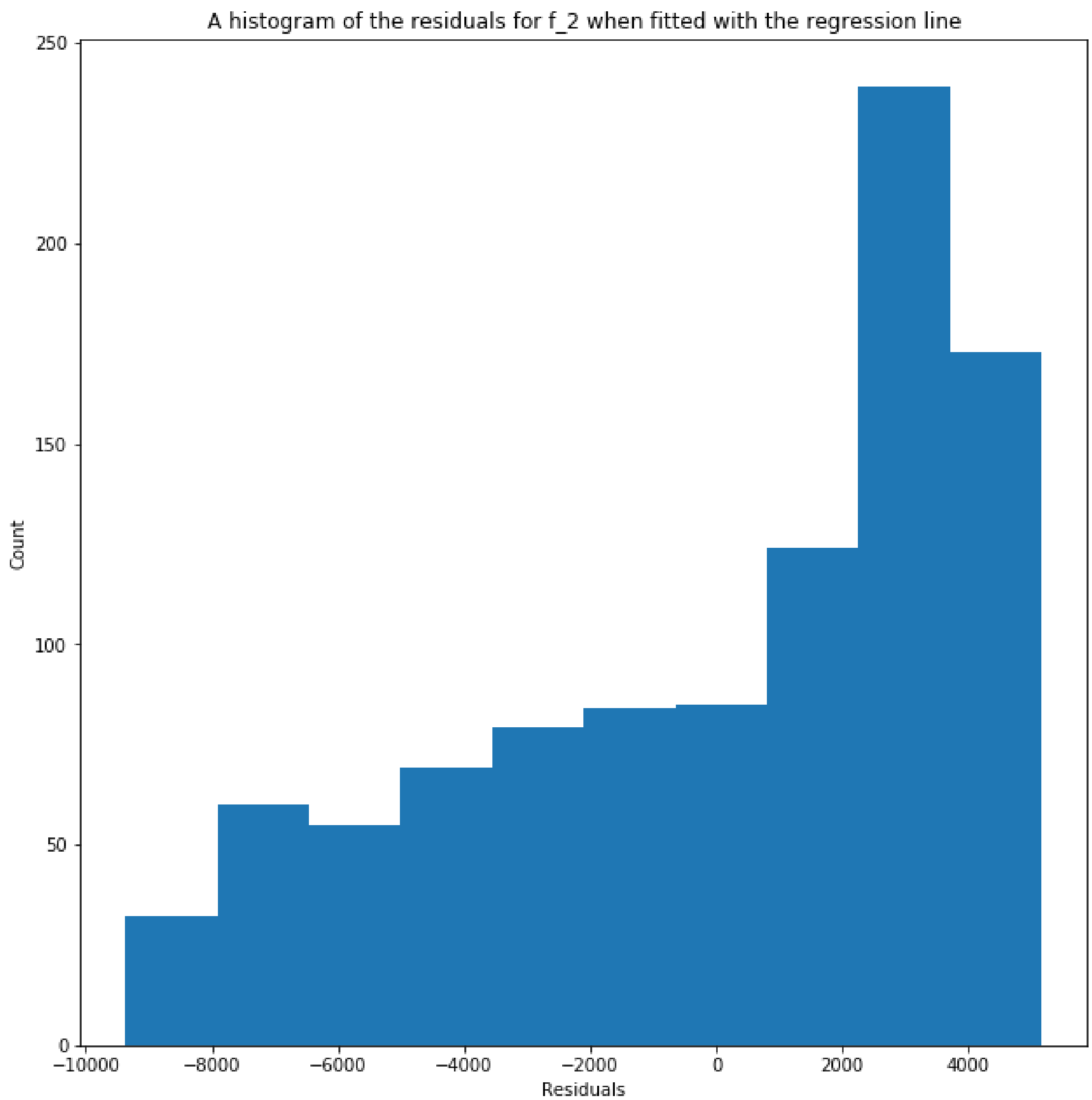
Below, we see how the line defined by the equation above fits the data for f_2

In [15]:
```
# 1000 linearly spaced numbers
x2 = np.linspace(0,99,1000)

# The predicted responses of these 1000 numbers
y2 = beta2_0 + beta2_1 * x2

# Plot
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.plot(X,Y_2,'.')
axes.plot(x2,y2)

# Set labels and title
axes.set_xlabel('x')
axes.set_ylabel('f_2(x)')
axes.set_title('A plot of the data and the regression fit for f_2')

plt.show()
```




```
In [16]: # The fitted values are the predicted values given the observed values
         y2_fitted = beta2_0 + beta2_1 * X

         # The residuals are the differences between our predicted values and
         # the observed responses
         Res_2 = y2_fitted - Y_2


         # Plot the residuals
         fig = plt.figure(figsize=(8,8))
         axes = fig.add_axes([0.1,0.1,1,1])
         axes.hist(Res_2)

         # Set labels and title
```

```
axes.set_xlabel('Residuals')
axes.set_ylabel('Count')
axes.set_title('A histogram of the residuals for f_2 when fitted with the regression l

plt.show()

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




```
The residuals are certainly not from a normal distribution
```

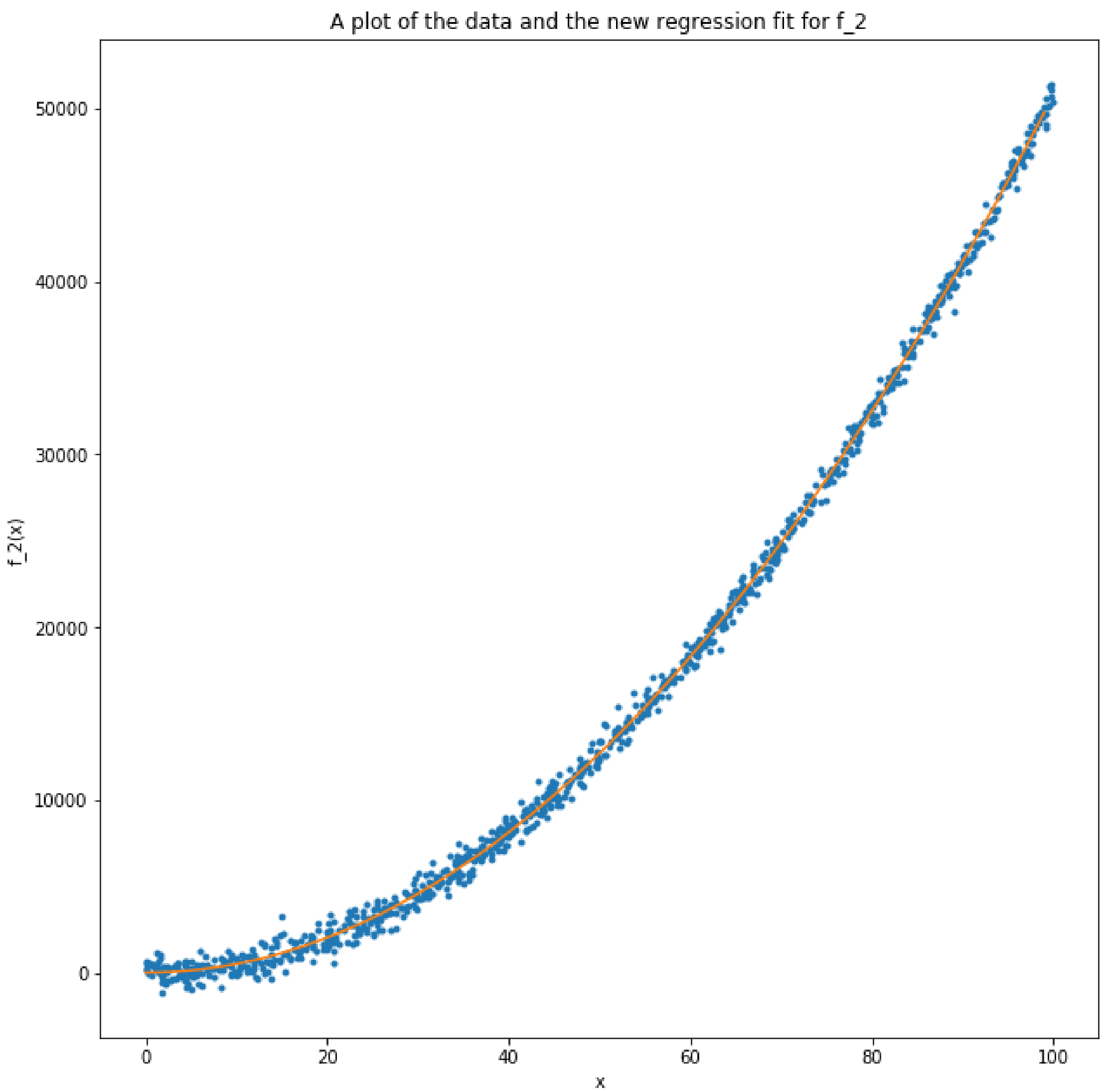
So let's try X^2 as a parameter instead of X in our linear model

In [17]:
```
# Create X^2 parameter
X_2 = X**2

#Find the mean of the data for f_2
x_bar22 = np.mean(X_2)
y_bar22 = np.mean(Y_2)

numerator = 0
denominator = 0

for i in range(len(Y_2)):
    # Calculate the numerator for beta_1
    numerator += (X_2[i] - x_bar22)*(Y_2[i] - y_bar22)

    # Calculate the denominator for beta_1
    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
```

Below, we see how the new line defined by the equation above fits the data for f_2

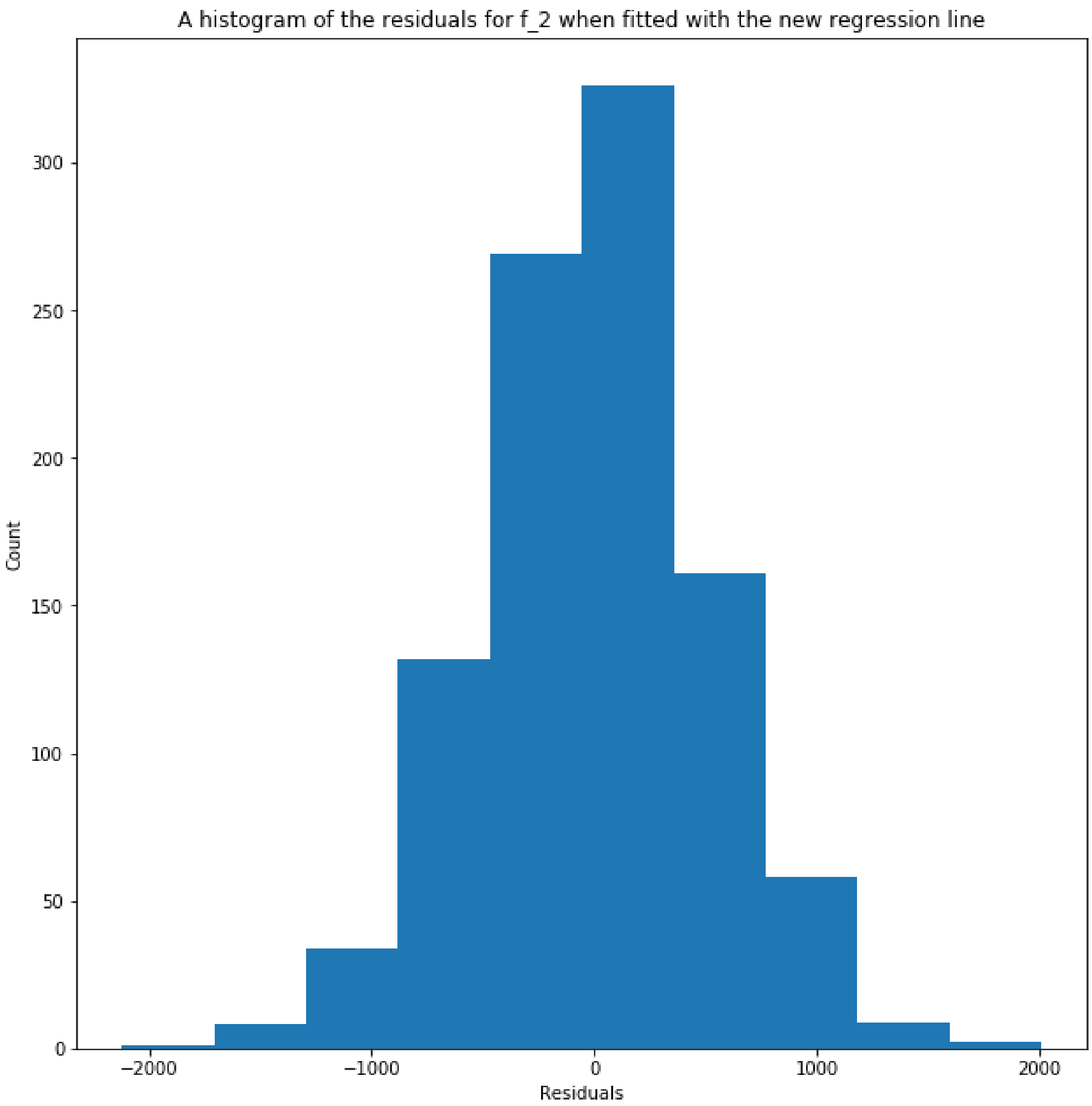
In [18]:
```
# 1000 linearly spaced numbers
x22 = np.linspace(0,99,1000)

# Predicted responses to the 1000 numbers
y22 = beta22_0 + beta22_1 * ((x22)**2)

# Plot this regression line and the data
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.plot(X,Y_2,'.')
axes.plot(x22,y22)

# Set labels and title
axes.set_xlabel('x')
axes.set_ylabel('f_2(x)')
axes.set_title('A plot of the data and the new regression fit for f_2')
plt.show()
```



Now we investigate the residuals to see if the new regression fit using X^2 as a parameter yields residuals that look more normally distributed

In [19]:
```
# The fitted values are the predicted values given the observed values
y22_fitted = beta22_0 + beta22_1 * X**2

# The residuals are the differences between our predicted values and
# the observed responses
Res_22 = y22_fitted - Y_2

# Plot the residuals
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.hist(Res_22)
```

```
# Set labels and title
axes.set_xlabel('Residuals')
axes.set_ylabel('Count')
axes.set_title('A histogram of the residuals for f_2 when fitted with the new regress

plt.show()

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

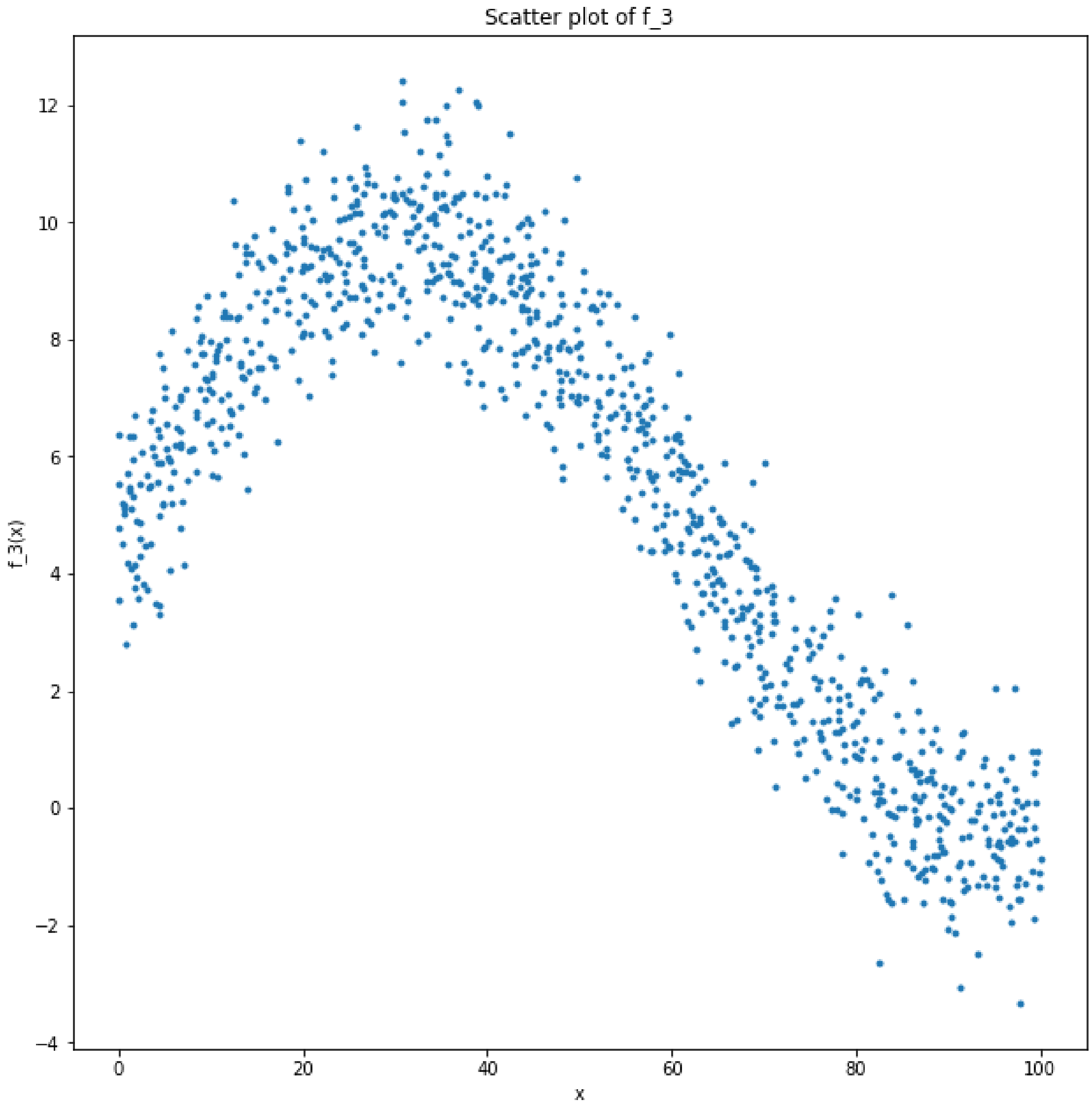



```
This is roughly a normal distribution with mean -1.1250449460931123e-12 and standard deviation
```

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. Note also that the standard deviation from the residual distribution is close to the 500 for the errors when the function was created.

Now let's apply linear regression to f_3 in a similar manner

```
In [20]: # Get figure handle
         fig = plt.figure(figsize=(8,8))

         # Get axis handle and specify size
         axes = fig.add_axes([0.1,0.1,1,1])

         # Plot onto this axis
         axes.plot(X,Y_3,'.')

         # Set the axis labels
         axes.set_xlabel('x')
         axes.set_ylabel('f_3(x)')
         axes.set_title('Scatter plot of f_3')

         plt.show()
```



It is very clear from the above scatter plot that we will not be able to get away with fitting a linear line to the data. This is a hint that we should use transformed variables. But let's carry out a linear fit to show that the results can be misleading when we only consider the residuals plot to assess the quality of fit

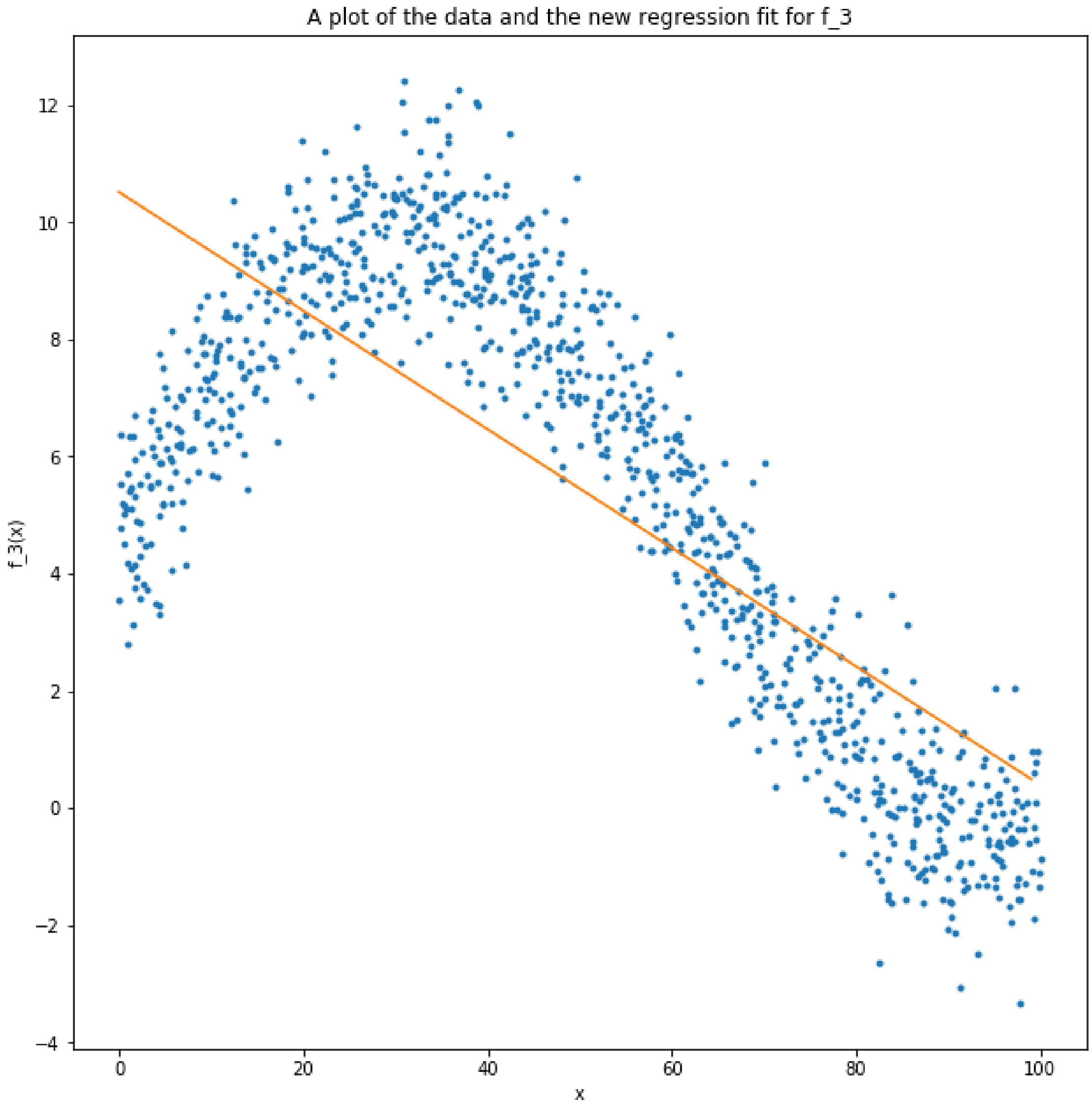
In [21]:
```
#Find the mean of the data for f_3
x_bar3 = np.mean(X)
y_bar3 = np.mean(Y_3)

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
```

Below, we see how the line defined by the equation above fits the data for f_3

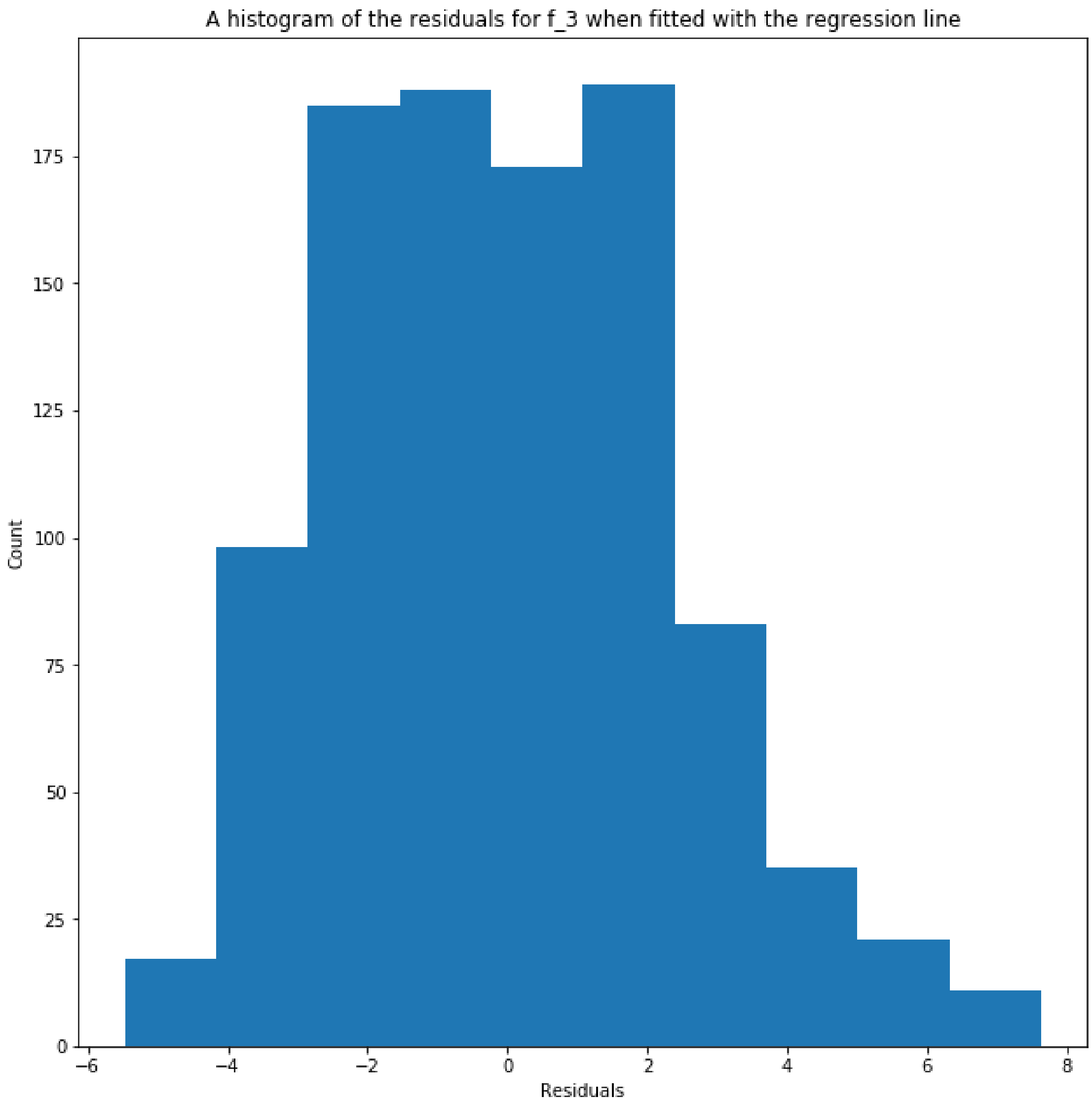
```
In [22]: # 1000 linearly spaced numbers
         x3 = np.linspace(0,99,1000)

         # Predict the response for those numbers
         y3 = beta3_0 + beta3_1 * x3

         # Plot both the data and the fit
         fig = plt.figure(figsize=(8,8))
         axes = fig.add_axes([0.1,0.1,1,1])
         axes.plot(X,Y_3,'.')
         axes.plot(x3,y3)

         # Set the labels and title
         axes.set_xlabel('x')
         axes.set_ylabel('f_3(x)')
         axes.set_title('A plot of the data and the new regression fit for f_3')

         plt.show()
```



We now assess the residuals

In [23]:
```
# The fitted values are the predicted values given the observed values
y3_fitted = beta3_0 + beta3_1 * X

# The residuals are the differences between our predicted values and
# the observed responses
Res_3 = y3_fitted - Y_3

# Plot the residuals
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.hist(Res_3)
```

```
# Set labels and title
axes.set_xlabel('Residuals')
axes.set_ylabel('Count')
axes.set_title('A histogram of the residuals for f_3 when fitted with the regression l

plt.show()

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 additional 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 expressed as:

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

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*.

STATEMENT: The *Residual Squared Error* $RSE = \sqrt{\frac{RSS}{n-2}}$ is a measure of lack of fit. R^2, as the form above suggests, is the proportion of variance that is explained. For a simple linear regression with 1 parameters (see Appendix):

$$R^2 = Cor(X,Y)^2 = \left(\frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \right)^2$$

However, for multiple linear regression this does not hold. It is not clear how to adapt the Correlation in order to explain the fit of a multiple regression model. R^2 however, is a clearly defined metric which is easily extended to multiple regression.

Below, we calculate this metric for f_3

```
In [24]: # TSS
         TSS_3 = 0

         # RSS
         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^2 for f_3
         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. To do this, we create a function that accepts observed and fitted values and returns the TSS and RSS of the fit

```
In [25]: def TSS_RSS(y_observed,y_fitted):
             '''
             A function that calculates the TSS and RSS of a fit given observed
                 and fitted values
             y_observed := Observed data as a series object
             y_fitted := Fitted data as a series object
```

```
    output := A (TSS,RSS) tuple of floats
    '''

    # TSS
    TSS = 0

    # RSS
    RSS = 0

    # Get the mean of the observed values
    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 [26]:
```
# Calculate the TSS and RSS for the fitted regression line to f_1
TSS_1, RSS_1 = TSS_RSS(Y_1,y1_fitted)

# Calculate the R^2 for the fit to f_1
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))


# Calculate the TSS and RSS for the fitted regression line to f_2
TSS_2,RSS_2 = TSS_RSS(Y_2,y2_fitted)

# Calculate the R^2 for the fit to f_2
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))


# Calculate the TSS and RSS for the new fitted regression line to f_2
TSS_22,RSS_22 = TSS_RSS(Y_2,y22_fitted)

# Calculate the R^2 for the new fit to f_2
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))


# Calculate the TSS and RSS for the fitted regression line to f_3
TSS_3,RSS_3 = TSS_RSS(Y_3,y3_fitted)
```

```
# Calculate the R^2 for the fit to f_3
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 (note that in this case, the R^2 metric alone wouldn't tell us whether the fit linear in X was terrible. But along with the residual plot we would arrive at the correct conclusion); 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 and that applying a model non-linear in X may provide a boost to the explained variance. We can try 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. We will see that the results match the manual results above

In [27]:
```
# Import the linear model and the metric we'll be using
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score

# Create the model object
lm1 = LinearRegression()

# Fit this model to the data for f_1
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]))

# Get the fitted values and print it
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=['X2']),\
                pd.DataFrame(X**3,columns=['X3'])],axis=1)
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 + lm32.coef_[0][2]*X**3
```

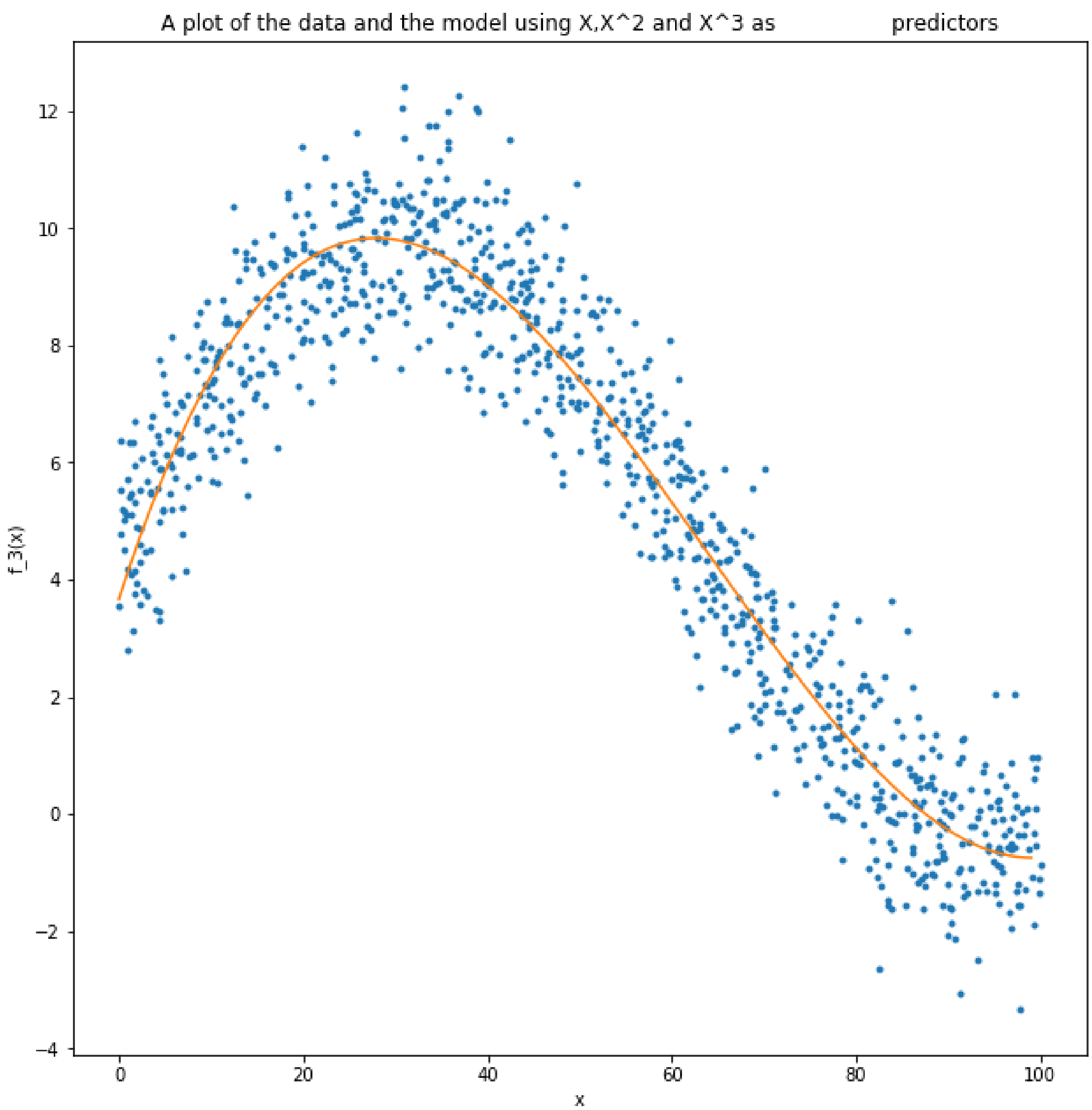
```
print('R^2 = {}'.format(r2_score(Y_3,y32_fitted_sklearn)))
```

```
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 = -0.011179330358454434
beta_3 = 5.867605764948042e-05
R^2 = 0.9229011520420615
```

In the above, we fit a model using 3 explanatory variables, namely X, X^2, X^3 with coefficients β_1, β_2, β_3 respectively. We can see that we have a much improved R^2 statistic for the fitted model to f_3 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 [28]: # 1000 linearly spaced numbers
         x32 = np.linspace(0,99,1000)
         y32 = lm32.intercept_[0] + lm32.coef_[0][0]*x32 + lm32.coef_[0][1]*x32**2\
             + lm32.coef_[0][2]*x32**3

         # Plot the data and the fit
         fig = plt.figure(figsize=(8,8))
         axes = fig.add_axes([0.1,0.1,1,1])
         axes.plot(X,Y_3,'.')
```

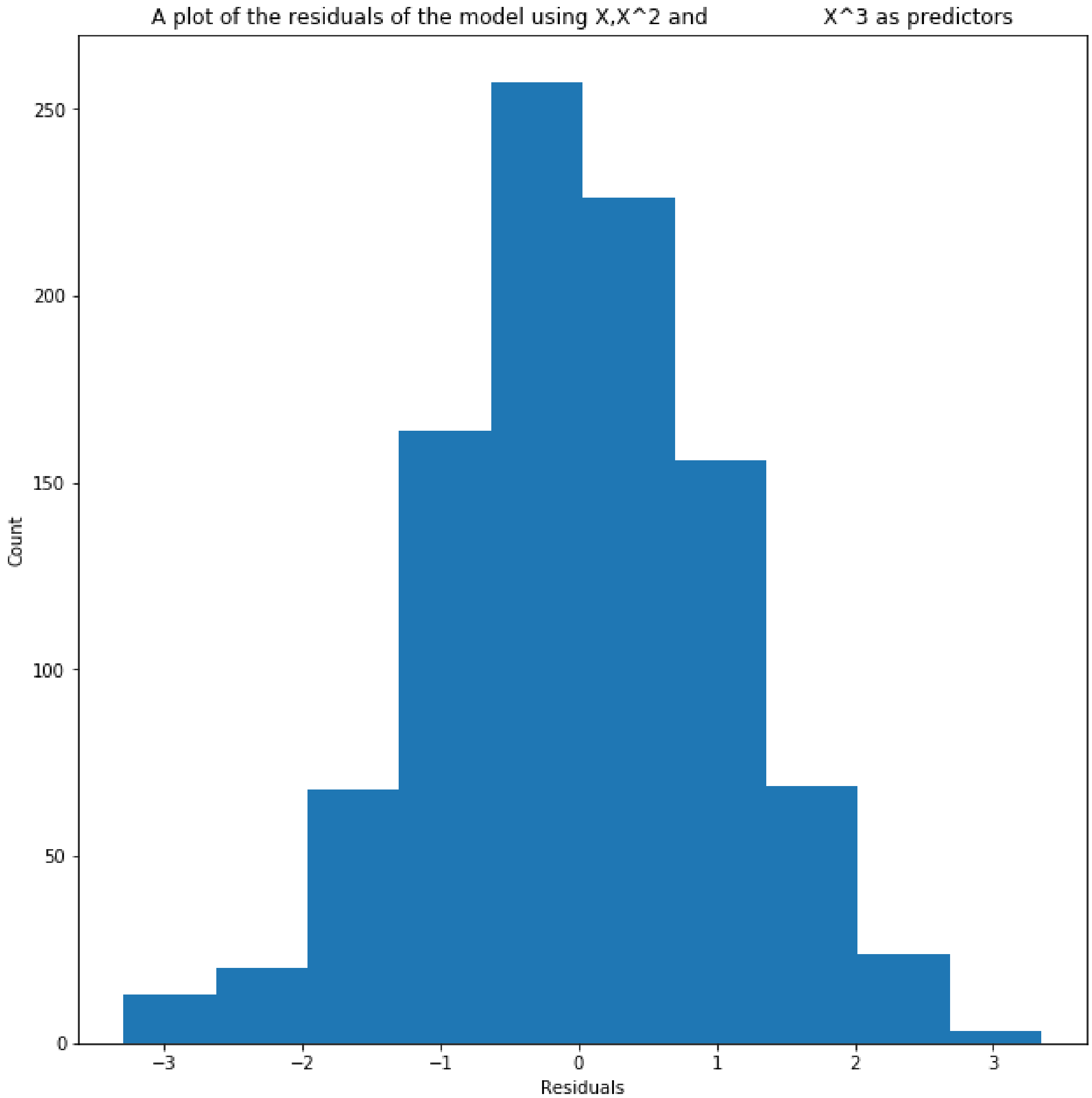
```
axes.plot(x32,y32)

# Set the lables and title
axes.set_xlabel('x')
axes.set_ylabel('f_3(x)')
axes.set_title('A plot of the data and the model using X,X^2 and X^3 as \
                predictors')

plt.show()
```



We can also check the residuals plot

In [29]:
```
# Calculate the fitted values using the observed values
y32_fitted_sklearn = lm32.intercept_[0] + lm32.coef_[0][0]*X + \
```

```
                    lm32.coef_[0][1]*X**2 + lm32.coef_[0][2]*X**3

# Calculate the residuals
Res_32 = y32_fitted_sklearn - Y_3

# Plot the residuals
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.hist(Res_32)

# Set the lables and title
axes.set_xlabel('Residuals')
axes.set_ylabel('Count')
axes.set_title('A plot of the residuals of the model using X,X^2 and \
                X^3 as predictors')

plt.show()

print('This is roughly a normal distribution with mean {mean} and\n \
    standard deviation {std}'.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 1.043797076853439
```

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

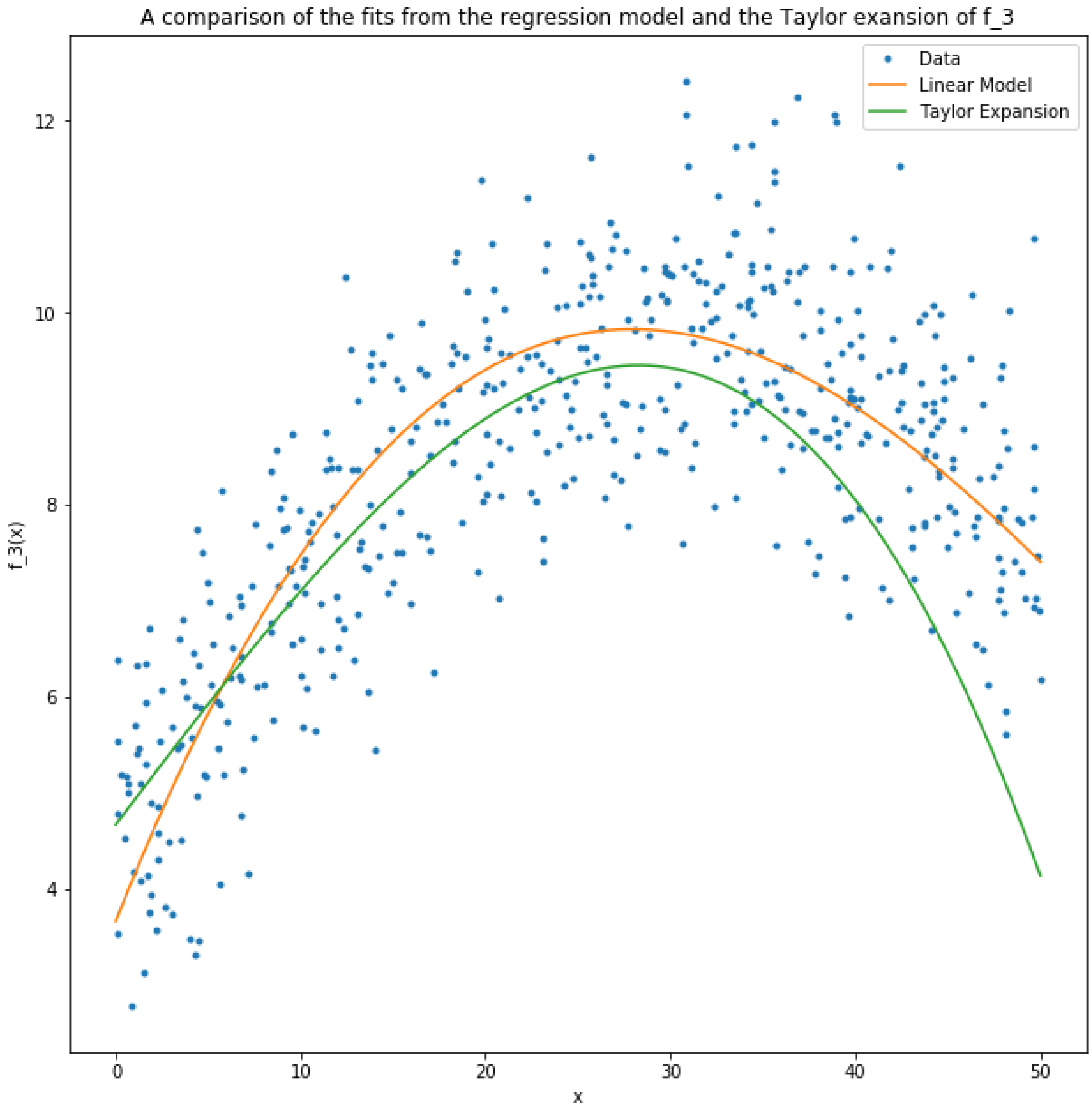
$$
\begin{aligned}
f(x=0) &= f(0) + f^{(1)}(0)x + f^{(2)}(0)x^2/(2!) + f^{(3)}(0)x^3/(3!) + O(x^4) \\
&= \sin(0) + \cos(0)x - \sin(0)x^2/(2!) - \cos(0)x^3/(3!) \\
&= x - x^3/(6)
\end{aligned}
$$

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 [30]:
```
# 1000 linearly spaced numbers
x32 = np.linspace(0,50,1000)

# Predictions
y32 = lm32.intercept_[0] + lm32.coef_[0][0]*x32 + lm32.coef_[0][1]*x32**2\
    + lm32.coef_[0][2]*x32**3

# Prediction using Taylor expansion
y_taylor_32 = 4.67 + (5.07/20)*x32 + 0*x32**2 - (5.07/(20**3 * 6))*x32**3

# Only get the observed predictors and response where the predictors are less
# than 50
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'])],axis=1).\
              apply(lambda x: x[0]<50,axis=1)]

# Plot the data, the fitted model and the taylor expansion
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.plot(X_small,Y_small,'.',label='Data')
axes.plot(x32,y32,label='Linear Model')
axes.plot(x32,y_taylor_32,label='Taylor Expansion')

# Set the labels and title
axes.set_xlabel('x')
axes.set_ylabel('f_3(x)')
axes.set_title('A comparison of the fits from the regression model and the \
Taylor exansion of f_3')

# Add the legend
axes.legend()

plt.show()
```



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 [31]: 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 [32]:
```
# 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 calculation
# 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 of freedom that is less than -4.303
    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 [33]: 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 statistically significant.
             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 (usually 0)
             '''
             # number of observations n
             n = len(X)

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

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

# variance of x = sum (x_i - x_bar)^2. Note that this is the population
# variance calculation
# 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
# Multiply by 2 since it's a 2 tailed test
if(tstatistic1_0 > 0):
    pval_0 = stats.t.cdf(-tstatistic1_0,n-2)*2
else:
    pval_0 = stats.t.cdf(tstatistic1_0,n-2)*2

if(tstatistic1_1 > 0):
    pval_1 = stats.t.cdf(-tstatistic1_1,n-2)*2
else:
    pval_1 = stats.t.cdf(tstatistic1_1,n-2)*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!')
```

```python
        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

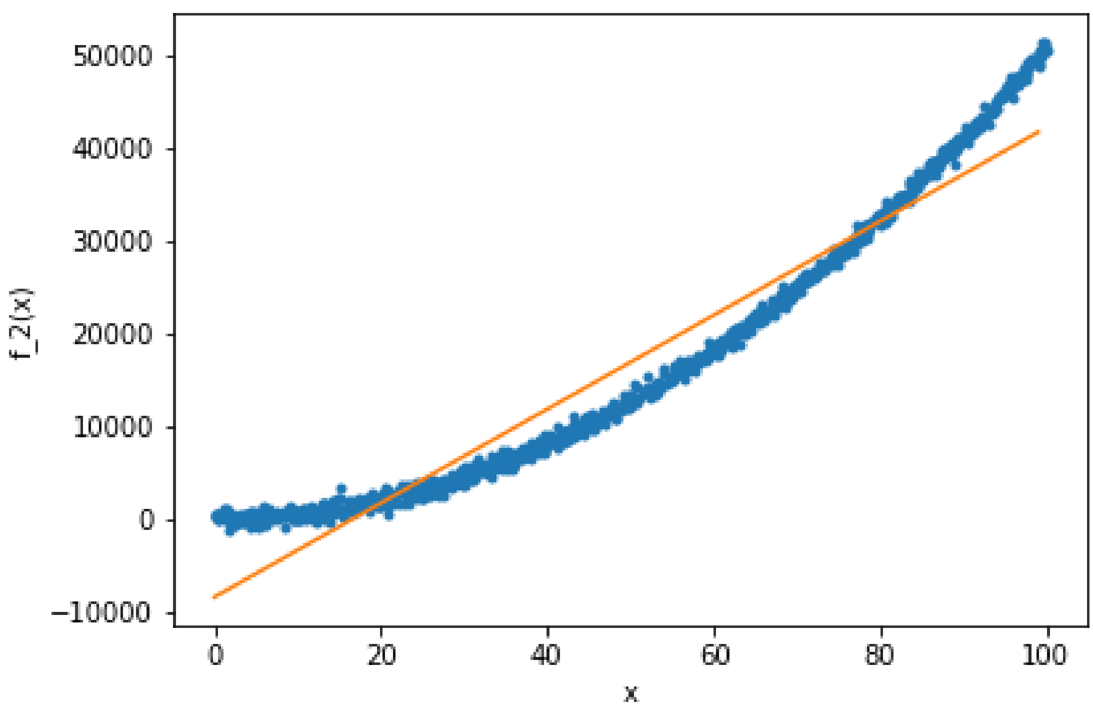
```python
In [34]: print('Model for Y_1: Explanatory variable X for Y_1')
         calcpvalue(X,Y_1,y1_fitted,beta1_0,beta1_1,0,0)

         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**2,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 = 3.371970565016392e-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 = 8.125468707425302e-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) = 24.614546607361707, SE(beta_1) = 0.005557804748590844
beta_0 t-statistic = 0.5878663289694033
beta_1 t-statistic = 913.1340896074505
```

```
p-value for beta_0 = 0.5567550098751695
p-value for beta_1 = 0.0
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 = 1.3682773718716098e-197
These are both statistically significant!
```

```
In [35]: 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[35]: [<matplotlib.lines.Line2D at 0x2bc3f93ae10>]
```



We can use the statsmodels.api to verify our results

In [36]:
```
import statsmodels.api as sm
from scipy import stats
```

```
C:\Users\HVAD\Anaconda3\lib\site-packages\statsmodels\compat\pandas.py:56: FutureWarning: The p
  from pandas.core import datetools
```

In [37]:
```
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()

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,columns=['X2']),\
                                   pd.DataFrame(X**3,columns=['X3'])],axis=1))
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, 05 Nov 2018   Prob (F-statistic):               0.00
Time:                        20:19:10   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, 05 Nov 2018   Prob (F-statistic):               0.00
Time:                        20:19:10   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, 05 Nov 2018   Prob (F-statistic):               0.00
Time:                        20:19:10   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, 05 Nov 2018   Prob (F-statistic):         1.37e-197
Time:                        20:19:10   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, 05 Nov 2018   Prob (F-statistic):               0.00
Time:                        20:19:10   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 [38]: 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())
```

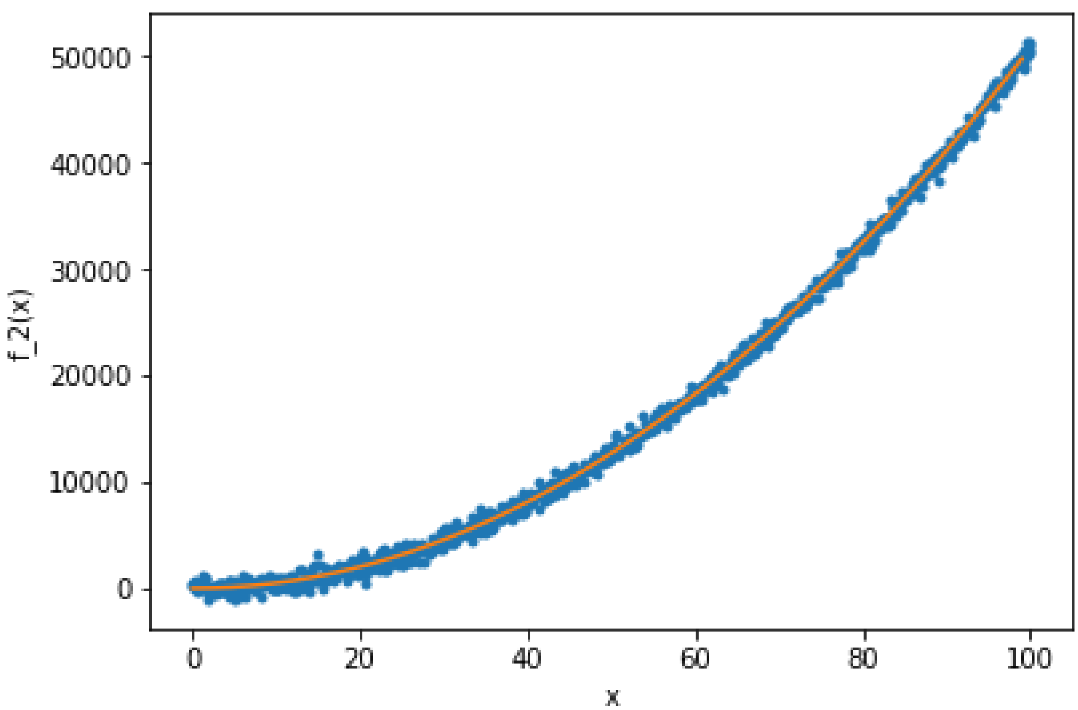
```
Model for Y_2: Explanatory variable X^2 for Y_2
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.999
Model:                            OLS   Adj. R-squared:                  0.999
Method:                 Least Squares   F-statistic:                 1.878e+06
Date:                Mon, 05 Nov 2018   Prob (F-statistic):               0.00
Time:                        20:19:10   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 [39]: 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[39]: [<matplotlib.lines.Line2D at 0x2bc40877908>]
```



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 [40]: # 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 [41]: def FStat(n,p,TSS,RSS):
             F = ((TSS-RSS)/p)/(RSS/(n-p-1))
             print('The F-Statistic is {}'.format(F))

In [42]: # we didn't calculate the last model ourselves, we used sklearn
         # so we retrieve the coefficients
         beta32_0 = lm32.intercept_[0]
         beta32_1 = lm32.coef_[0][0]
         beta32_2 = lm32.coef_[0][1]
         beta32_3 = lm32.coef_[0][2]

In [43]: 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 [44]: beta22_0, beta22_1, RSS_22

Out[44]: (14.470063153316005, 5.075020979320466, 268902718.6114595)
```

Here, we are going to calculate the p-value of the intercept for Y_2 when we try to fit an intercept as well as X^2. We do this by first fitting the full model including the intercept and getting the RSS value, then we fit the model without the intercept and get the RSS value. The Coefficient of X^2 and RSS for the model without the intercept was calculated to be

```
In [45]: TSS_23,RSS_23 = TSS_RSS(Y_2,beta23_1 * X**2)
         print('beta_1 = {}, RSS_0 = {}'.format(beta23_1,RSS_23))

beta_1 = 5.077455649665152, RSS_0 = 268995834.0780044
```

We now create a function to apply the formula shown above for calculating the F-Statistic for comparing models

```
In [46]: def FStatCompare(n,p,q,RSS0,RSS):
             '''
             A function to calculate the F-Statistic when we are comparing models
                 with different number of parameters.
             RSS0 is a sub-model of RSS
             '''
             F = ((RSS0-RSS)/q)/(RSS/(n-p-1))
             print('The F-Statistic is {}'.format(F))
             return F
```

Now we can confirm the p-value for the intercept

```
In [47]: # This is the fitted values for the model with no intercept
         Y23_fitted = beta23_1 * X**2

         # These are the TSS and RSS for this model with no intercept
         TSS_2_test,RSS_2_test = TSS_RSS(Y_2,Y23_fitted)

         # RSS_22 is the RSS for the model with the intercept. RSS_23 is the RSS
         # for the model without the intercept. We have p = 0 and q = 1 (i.e. we have
         # removed 1 parameter but there was only 1 parameter to begin with)
         F = FStatCompare(len(X),0,1,RSS_23,RSS_22)
```

```
# the following function calculates 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(F,1,len(X)-2)))
```

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

Note that above, we removed the intercept and used the F-Statistic to calculate the p-value for the intercept. We can also remove the coefficient of X^2 and calculate the p-value of this coefficient using the same procedure as above. First fit the model as we have done before

```
In [48]: lmOnlyIntercept = LinearRegression()
         lmOnlyIntercept.fit((X*0).reshape(-1,1),Y_2.reshape(-1,1))
         print('Model for Y_2: No explanatory variable for Y_2')
         print('beta_0 = {}'.format(lmOnlyIntercept.intercept_[0]))
         yOnlyIntercept_fitted_sklearn = lmOnlyIntercept.intercept_[0] + X*0
         print('R^2 = {}'.format(r2_score(Y_2,yOnlyIntercept_fitted_sklearn)))
```

```
Model for Y_2: No explanatory variable for Y_2
beta_0 = 16763.308428792458
R^2 = 0.0
```

Next, calculate the RSS for this model we have just fitted

```
In [49]: TSS_OnlyIntercept,RSS_OnlyIntercept = TSS_RSS(Y_2,yOnlyIntercept_fitted_sklearn)
         print('beta_0 = {}, RSS_0 = {}'.format(lmOnlyIntercept.intercept_[0],\
                                                RSS_OnlyIntercept))
```

```
beta_0 = 16763.308428792458, RSS_0 = 224933046282.3772
```

And now we calculate the p-value of the coefficient of X^2

```
In [50]: # These are the TSS and RSS for this model with only intercept
         TSS_2_test,RSS_2_test = TSS_RSS(Y_2,yOnlyIntercept_fitted_sklearn)

         # RSS_22 is the RSS for the model with the intercept. RSS_23 is the RSS
         # for the model without the intercept. We have p = 0 and q = 1 (i.e. we have
         # removed 1 parameter but there was only 1 parameter to begin with)
         F = FStatCompare(len(X),0,1,RSS_2_test,RSS_22)

         # the following function calculates 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 X^2 coefficient is {}'\
      .format(1-stats.f.cdf(F,1,len(X)-2)))
```

```
The F-Statistic is 834649.3504385022
The p-value of the X^2 coefficient is 1.1102230246251565e-16
```

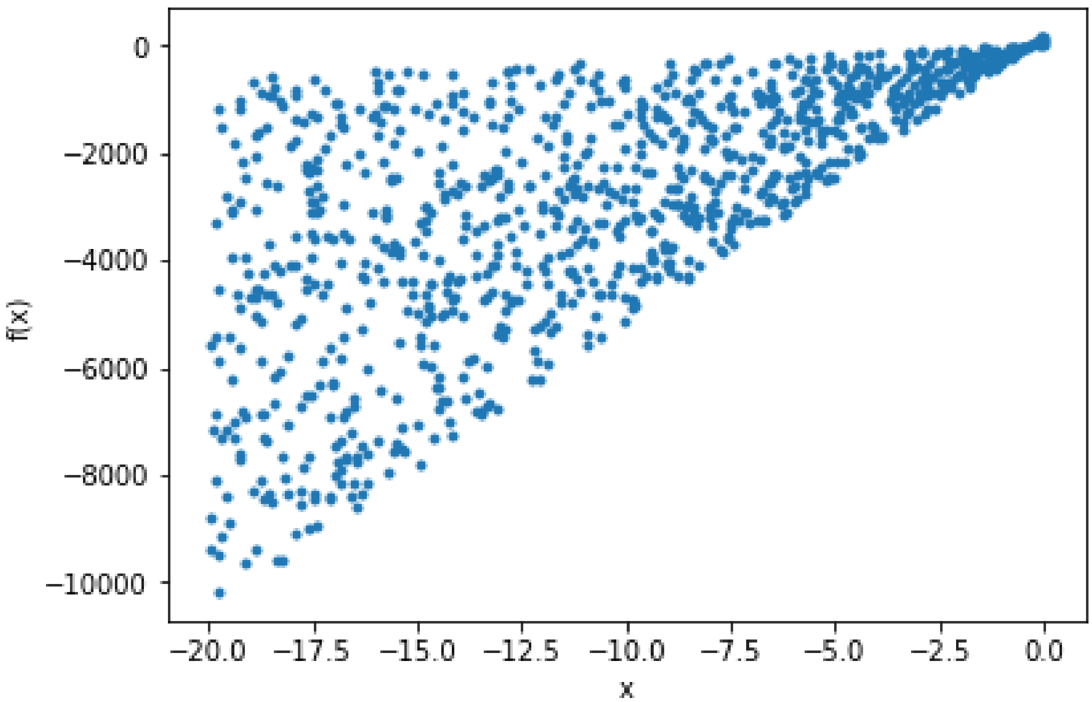
1.3.1 Synergy Effect

Suppose we have the following function

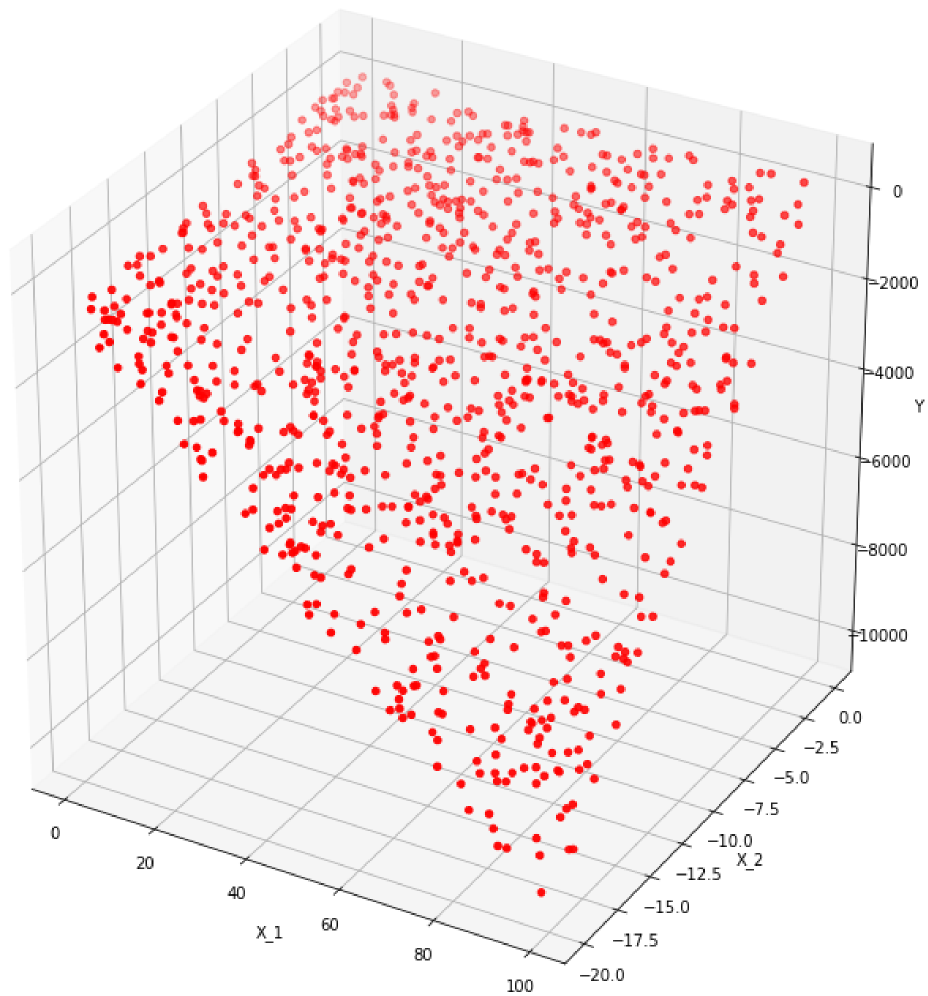
$$f(x) = 4.67 + 2 * X_1 + 3 * X_2 + 5.07X_1 * X_2$$

We can see that there is a mixed term $'X_1X_2'$. This is called a synergy effect.
Let's define this function and plot it

```
In [51]: from mpl_toolkits.mplot3d import Axes3D

         #f(x)=4.67+2*X_1+3*X_2+5.07X_1*X_2
         def f(x1,x2):
             return 4.67+2*x1+30*x2+5.07*x1*x2
         # Set the seed
         r = np.random.RandomState(101)
         X_1 = 100*r.rand(1000)
         X_2 = -20*r.rand(1000)

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

         #Response variables
         Y = list(map(f,X_1,X_2))+E

         fig = plt.figure()
         axes = fig.add_axes([0.1,0.1,0.8,0.8])
         axes.plot(X_2,Y,'.')
         axes.set_xlabel('x')
         axes.set_ylabel('f(x)')

Out[51]: Text(0,0.5,'f(x)')
```



In [52]:
```
fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(111, projection='3d')

ax.scatter(X_1, X_2, Y, c='r', marker='o')

ax.set_xlabel('X_1')
ax.set_ylabel('X_2')
ax.set_zlabel('Y')

plt.tight_layout()
```




```
In [53]: print('Model for Y_2: Explanatory variable X^2 for Y_2')
         X_new = sm.add_constant(pd.concat([pd.DataFrame(X_1,columns=['X_1']),\
                                    pd.DataFrame(X_2,columns=['X_2']),\
                                    pd.DataFrame(X_1*X_2,columns=['X_12'])],axis=1))
         est = sm.OLS(Y, X_new)
         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:                       1.000
Model:                            OLS   Adj. R-squared:                  1.000
```

```
Method:                     Least Squares   F-statistic:                  1.644e+07
Date:                    Mon, 05 Nov 2018   Prob (F-statistic):                0.00
Time:                            20:19:12   Log-Likelihood:                 -3749.9
No. Observations:                    1000   AIC:                              7508.
Df Residuals:                         996   BIC:                              7527.
Df Model:                               3
Covariance Type:                nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          5.9956      1.316      4.554      0.000       3.412       8.579
X_1            2.0091      0.023     87.005      0.000       1.964       2.054
X_2           30.0329      0.112    267.704      0.000      29.813      30.253
X_12           5.0714      0.002   2571.540      0.000       5.068       5.075
==============================================================================
Omnibus:                        8.045   Durbin-Watson:                   2.015
Prob(Omnibus):                  0.018   Jarque-Bera (JB):               11.082
Skew:                           0.035   Prob(JB):                      0.00392
Kurtosis:                       3.511   Cond. No.                     2.69e+03
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 2.69e+03. This might indicate that there are
strong multicollinearity or other numerical problems.
```

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

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

$$= 2x_1^2 + 2x_2^2 - x_1^2 - x_2^2 - 2x_1x_2 = x_1^2 + x_2^2 - 2x_1x_2 = (x_1 - x_2)^2 > 0$$

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

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

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

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

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

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

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

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