LinearRegression

April 13, 2020

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 cover 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 examines the relationaship between a dependent variable and one or more independent variables. Linear regression with p independent variables focusses on fitting a straight line in $p+1$-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 parametric problem of finding a set of parameters
- The function shape is limited (as a function of the parameters)

1.2 2- Advertising and Housing Datasets

Here we will use two datasets in order to get a feel of what Linear Regression is capable of.

First we use the Advertising dataset which 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). We will predict sales of a product given its advertising budgets.

Then we use the HousePrice dataset which is obtained from https://www.kaggle.com/c/house-prices-advanced-regression-techniques/data and contains 1460 houses along with many properties (only quantitative properties) including their sales prices. We will preduct the sale price of a property given certain parameters that characterise it.

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

import statsmodels.api as sm
from scipy import stats

from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score
from sklearn.model_selection import train_test_split
from sklearn.metrics import r2_score,mean_squared_error
from sklearn.model_selection import cross_val_score
from sklearn.metrics import mean_squared_error
from sklearn.linear_model import Ridge

import random
```

Then we import the datasets

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

        # Import House Prices dataset - Only quantitative fields and cleaned (https://www.kagg
        housePrice = pd.read_csv("HousePrice.csv").iloc[:,1:]

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

```
Number of observations (n) in advertising file = 200
Number of predictor variables (p) in advertising file = 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

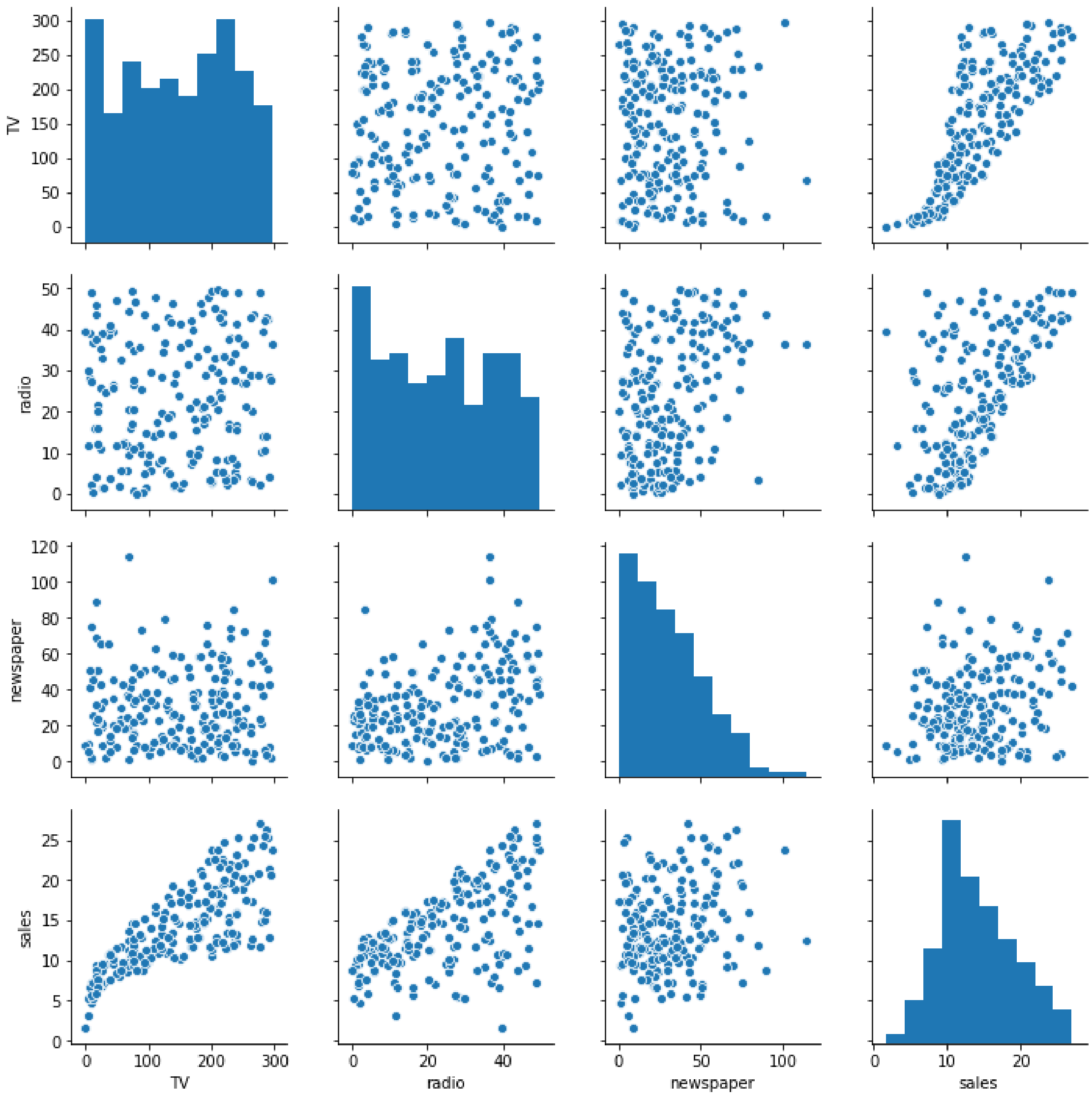
```
In [4]: print("Number of observations (n) in house-prices file =",housePrice.shape[0])
        print("Number of predictor variables (p) in house-prices file =",housePrice.shape[1]-1
        print()
        print("HousePrice.csv")
        display(housePrice.head())
```

```
Number of observations (n) in house-prices file = 1460
Number of predictor variables (p) in house-prices file = 34

HousePrice.csv
```

```
   LotArea  OverallQual  OverallCond  YearBuilt  YearRemodAdd  MasVnrArea  \
0     8450            7            5       2003          2003       196.0
1     9600            6            8       1976          1976         0.0
2    11250            7            5       2001          2002       162.0
3     9550            7            5       1915          1970         0.0
4    14260            8            5       2000          2000       350.0

   BsmtFinSF1  BsmtFinSF2  BsmtUnfSF  TotalBsmtSF  ...  WoodDeckSF  \
0         706           0        150          856  ...           0
1         978           0        284         1262  ...         298
2         486           0        434          920  ...           0
3         216           0        540          756  ...           0
4         655           0        490         1145  ...         192

   OpenPorchSF  EnclosedPorch  3SsnPorch  ScreenPorch  PoolArea  MiscVal  \
0           61              0          0            0         0        0
1            0              0          0            0         0        0
2           42              0          0            0         0        0
3           35            272          0            0         0        0
4           84              0          0            0         0        0

   MoSold  YrSold  SalePrice
0       2    2008     208500
1       5    2007     181500
2       9    2008     223500
3       2    2006     140000
4      12    2008     250000

[5 rows x 35 columns]
```

For the Advertising dataset the response variable is “sales”. The predictor variables are “TV”, “radio” and “newspaper”. It’s useful to visually inspect the data and see how each variable relates to the others. Using seaborn we can produce a pairplot of the data seen below:

```
In [5]: 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 use the Pearson correlation given by:

$$corr = \frac{Cov(X, Y)}{\sigma_X \sigma_Y}$$

where X and Y are random variables, $Cov(X, Y)$ is the Covariance of X and Y and σ_X is the standard deviation of X. This allows us to examine the correlations between the parameters as seen in the correlation matrix below.

```
In [6]: advert.corr()
```

```
Out[6]:                   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 $i = 1, 2, ..., p$.

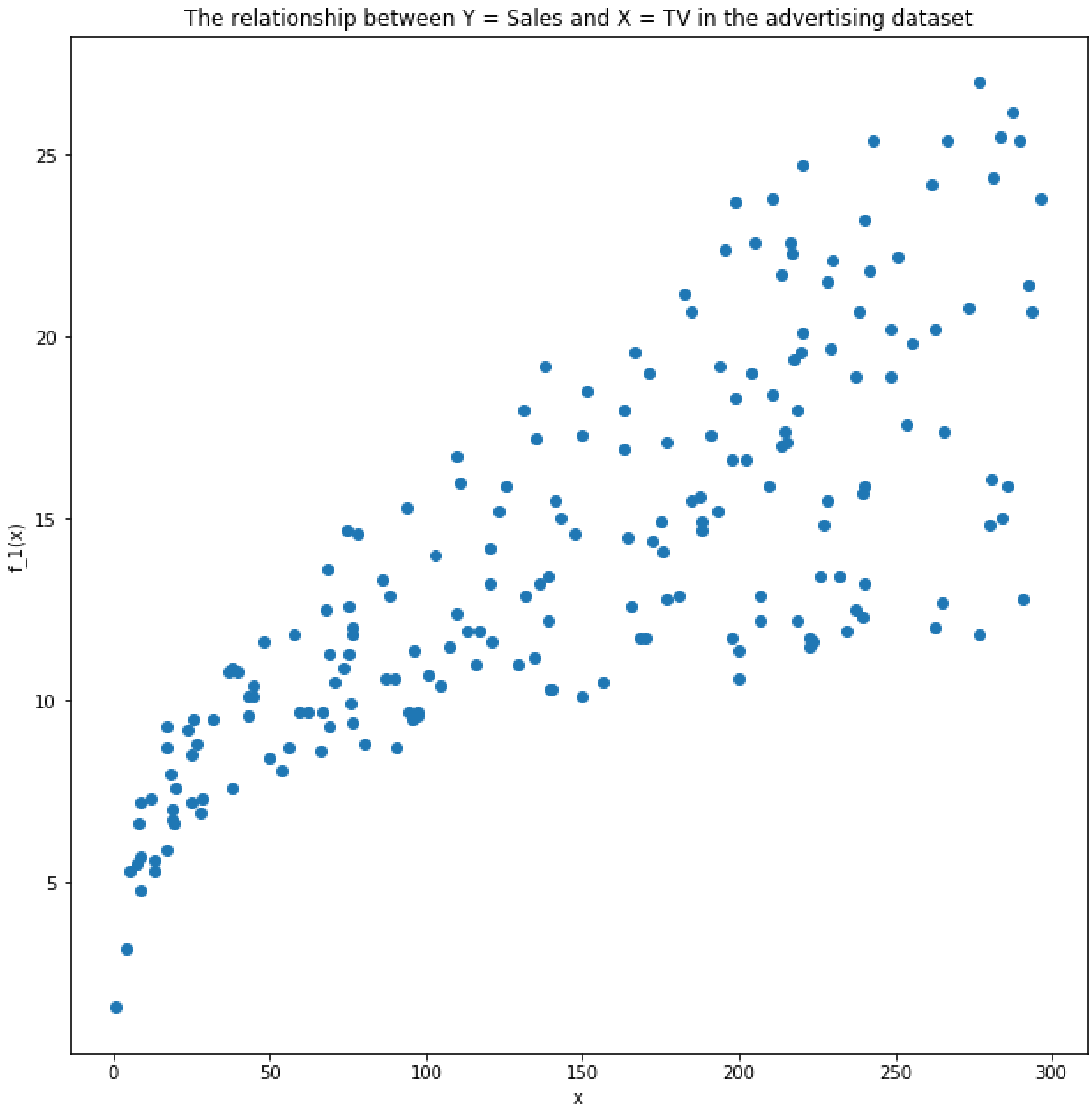
We first limit the problem to $p = 1$. For example, we are looking to estimate the coefficients in the equation

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

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 [7]: # 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 $RSS = \sum_{i=1}^{n} \epsilon_i^2$. While this intuitively makes sense, this can also be arrived at using a *Maximum Likelihood Estimation* (MLE) approach (see Appendix A2).

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 setting these to zero and solving

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

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

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

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

where 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

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

Additionally, we can show that the point $(\bar{x}, \bar{y})$ lies on the regression line (see Appendix A3).

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 A1).
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- $f_3(x) = 4.67 + 5.07 * sin(x/20)$

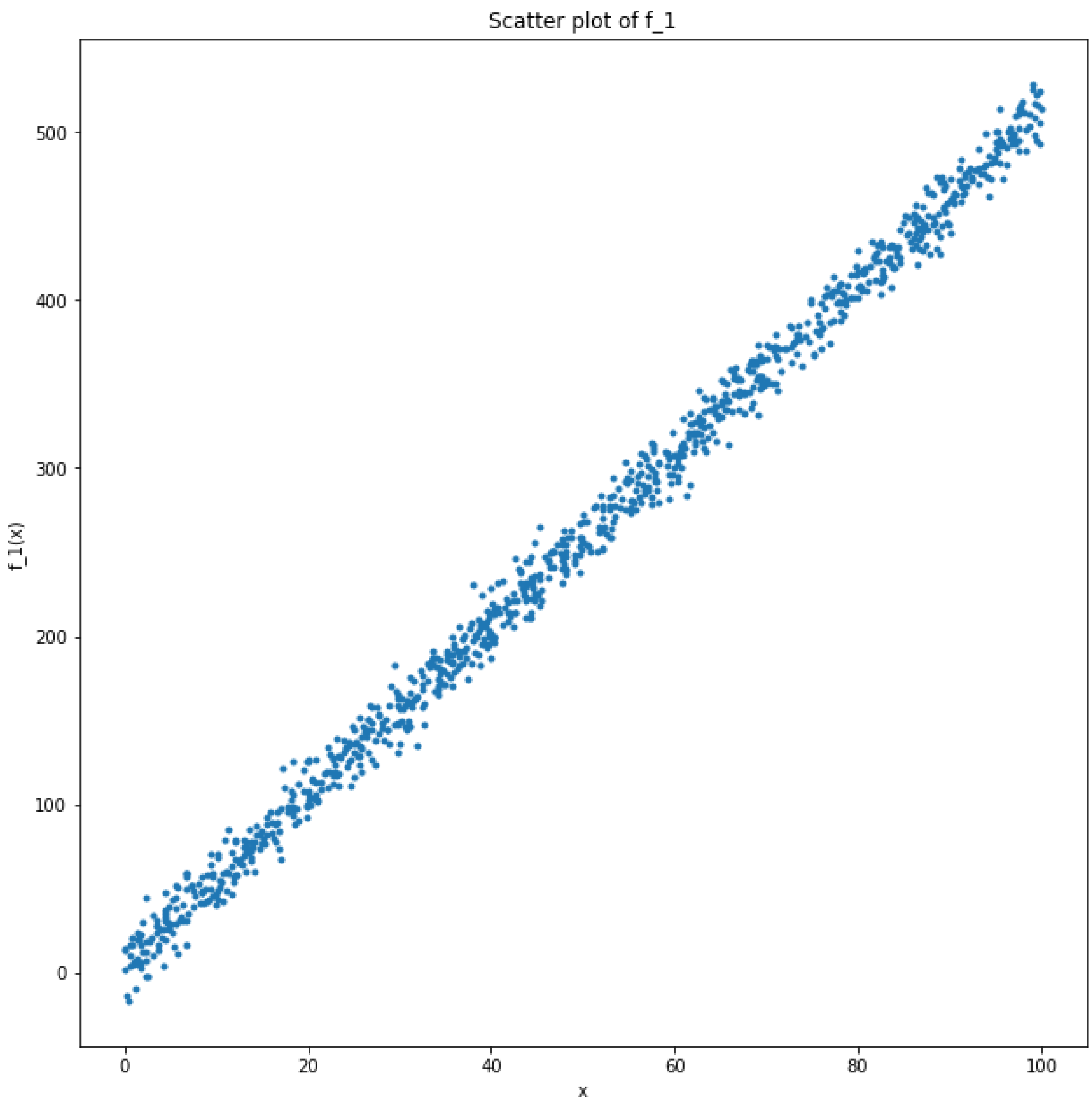
In [8]:
```
#f_1(x)=4.67+5.07x
def f_1(x):
    return 4.67 + 5.07*x

#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 [9]:
```
# 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, randn samples from the standard normal distributi
E_1 = 10*r.randn(1000)

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

#Error term with sigma = 1, 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
```

In the above, $s \times$ *r.randn(n)* samples n points from the $N(0, s^2)$ distribution. First we look at what f_1 looks like

In [10]:
```
# 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
axes.set_xlabel('x')
axes.set_ylabel('f_1(x)')
```

```python
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

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

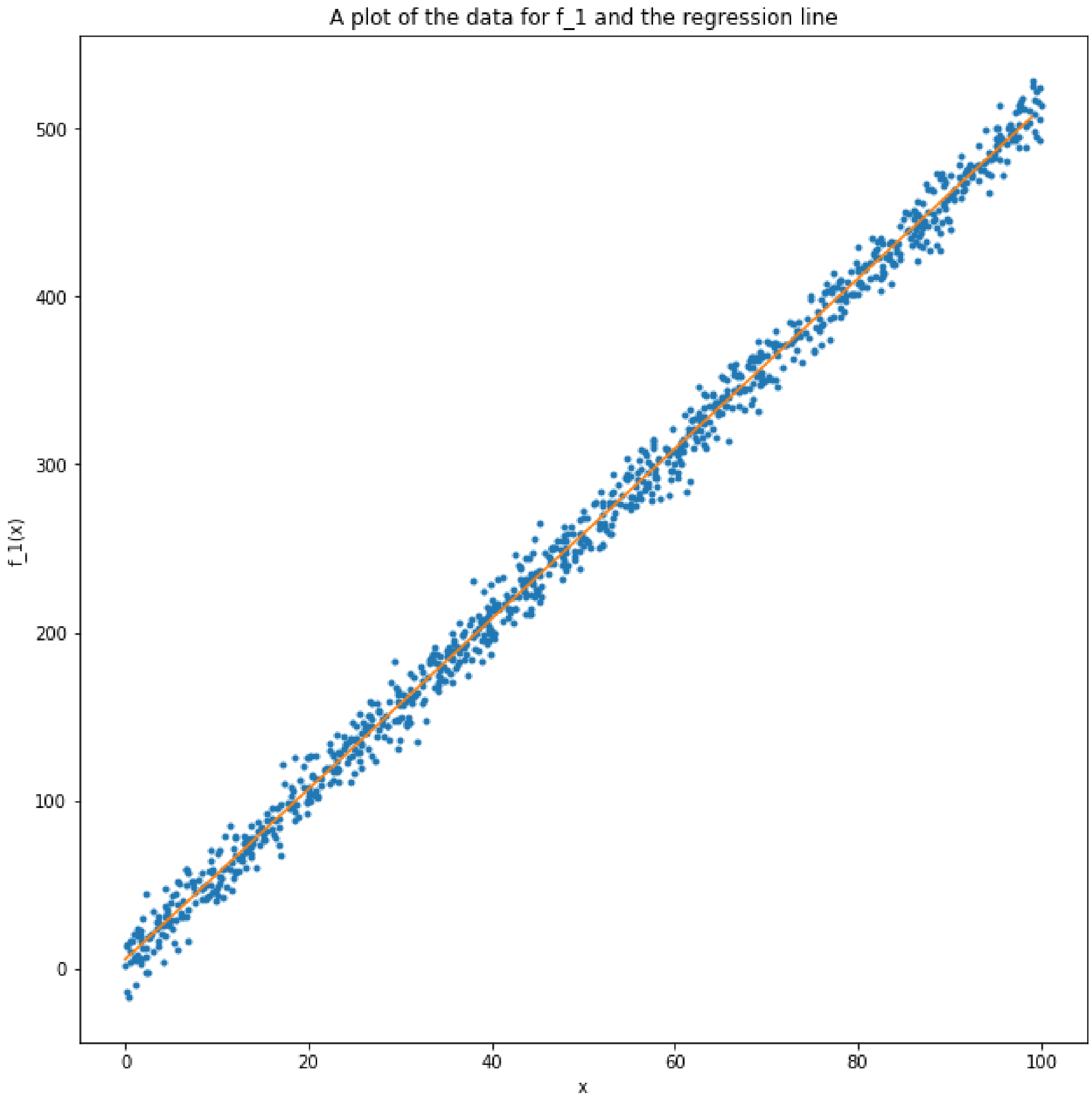
We can calculate these as below

```
In [11]: #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

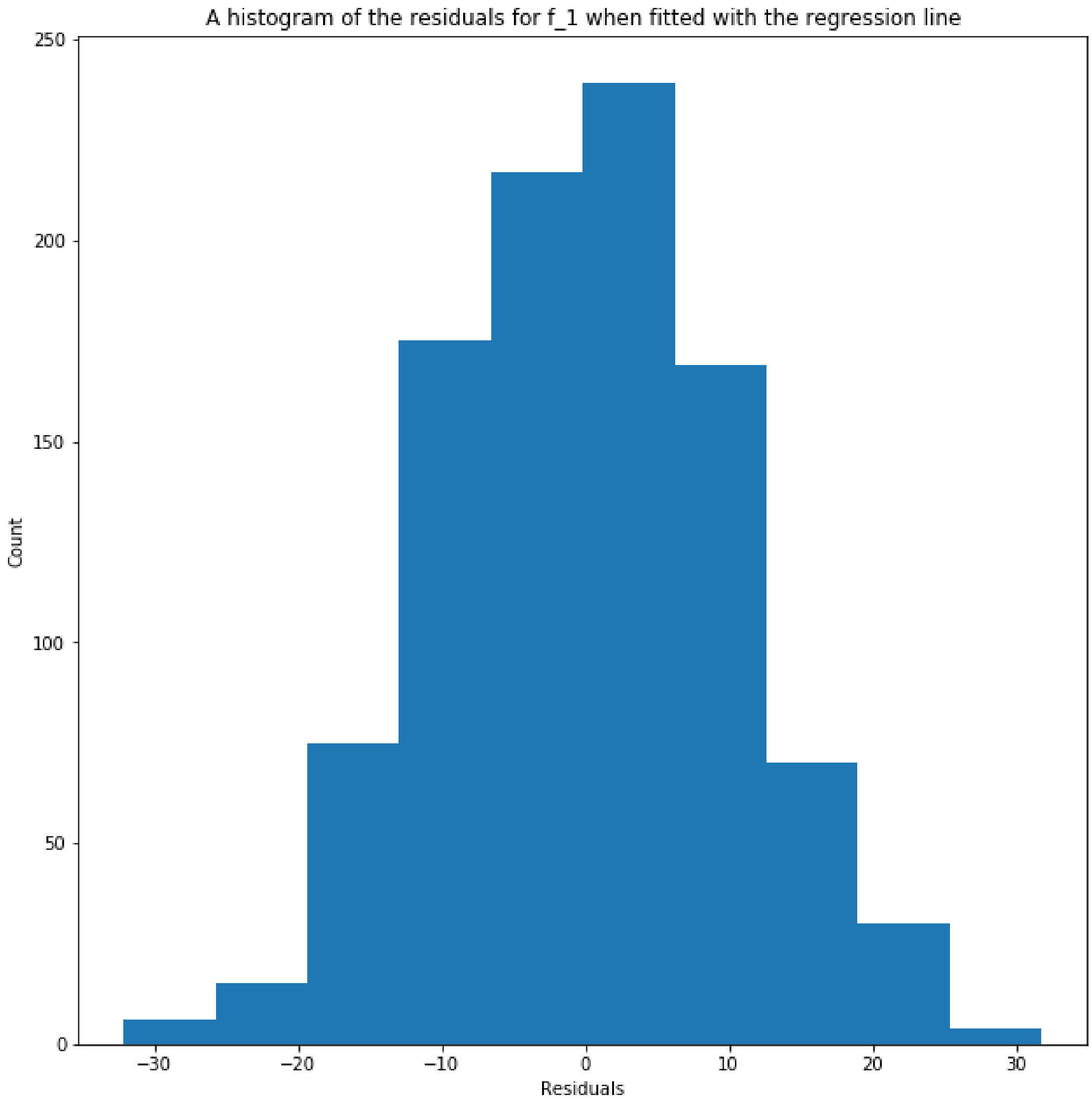
```
In [12]: # 1000 linearly spaced numbers
         x1 = np.linspace(0,99,1000)

         # 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 residuals require the knowledge of the actual response variables so that we can compare them with the predicted 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 [13]:
```
# 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))
```

```
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)))
```



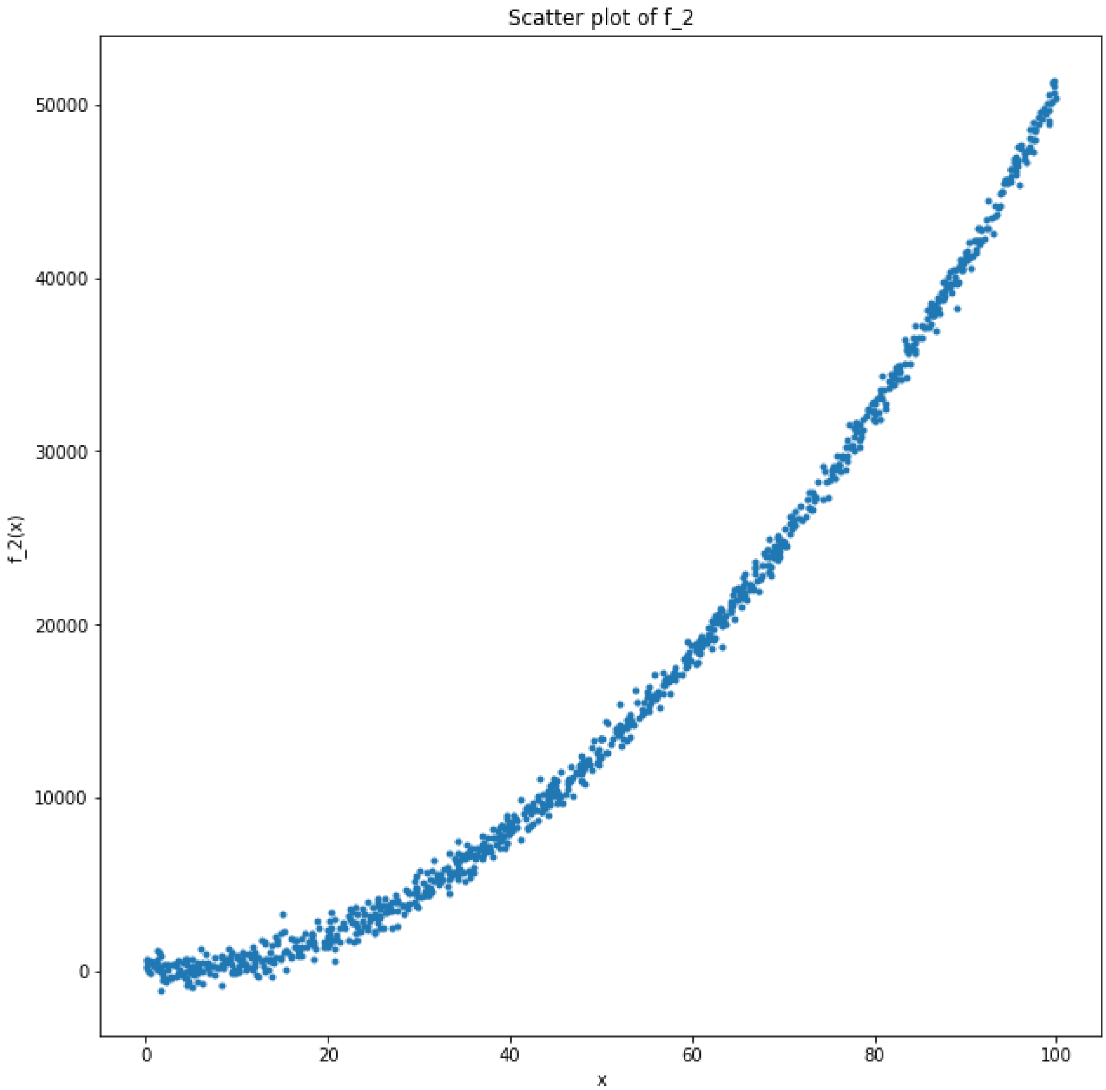
```
This is roughly a normal distribution with mean -1.2157386208855315e-14
and standard deviation 10.08588495757817
```

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 (this is the reducible error), and * error due to random noise (this is the irreducible error). We can see here that the residuals are from irreducible error.

Above we fitted a linear model to our 'designed' linear data. The error terms we expect to get are irreducible and a result of the error term E1 added above.

Now let's do the same for f_2.

```
In [14]: # 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[14]: Text(0.5,1,'Scatter plot of f_2')
```



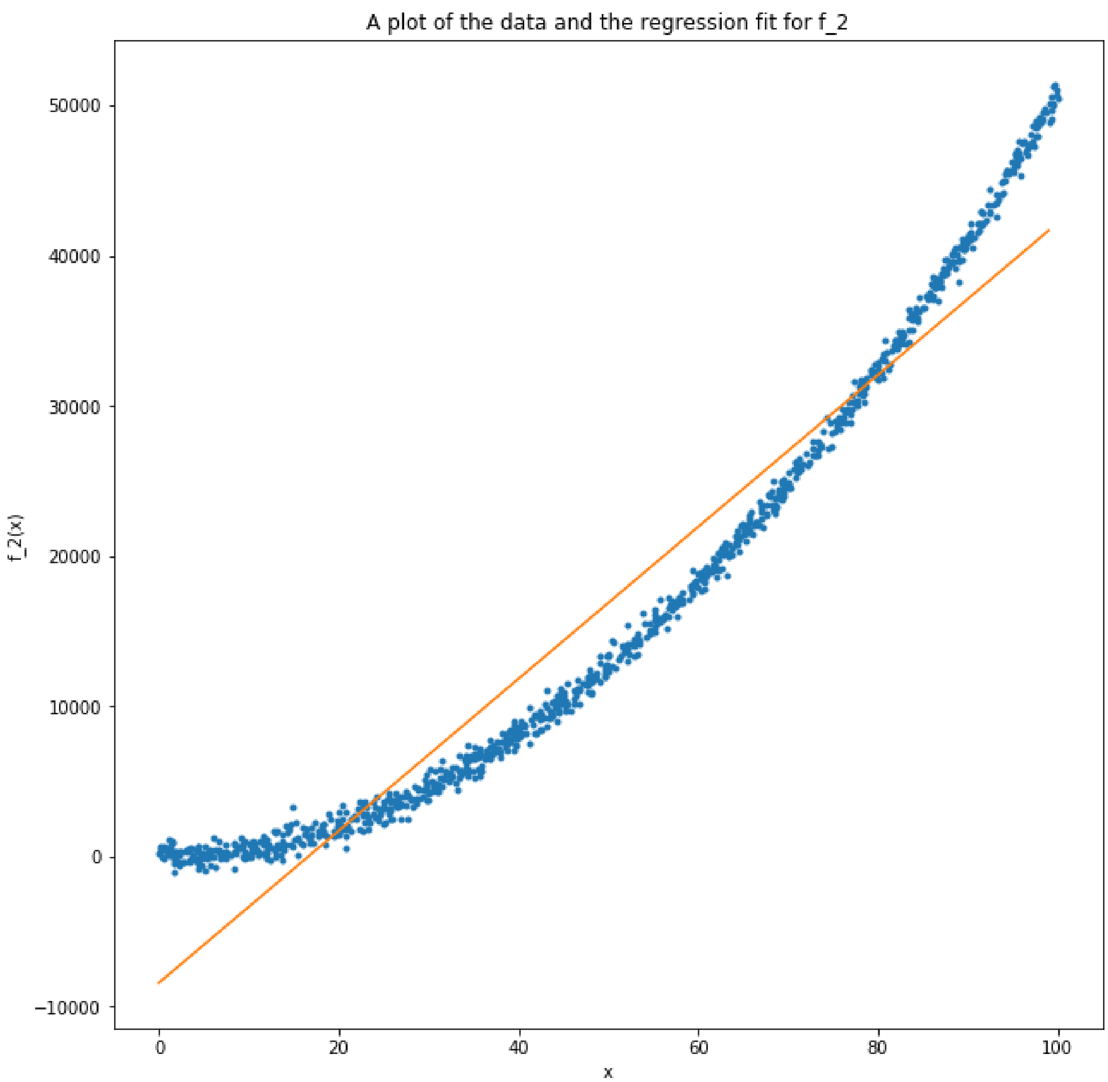
In [15]:
```
#Find the mean of the data for f_2
x_bar2 = np.mean(X)
y_bar2 = np.mean(Y_2)

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

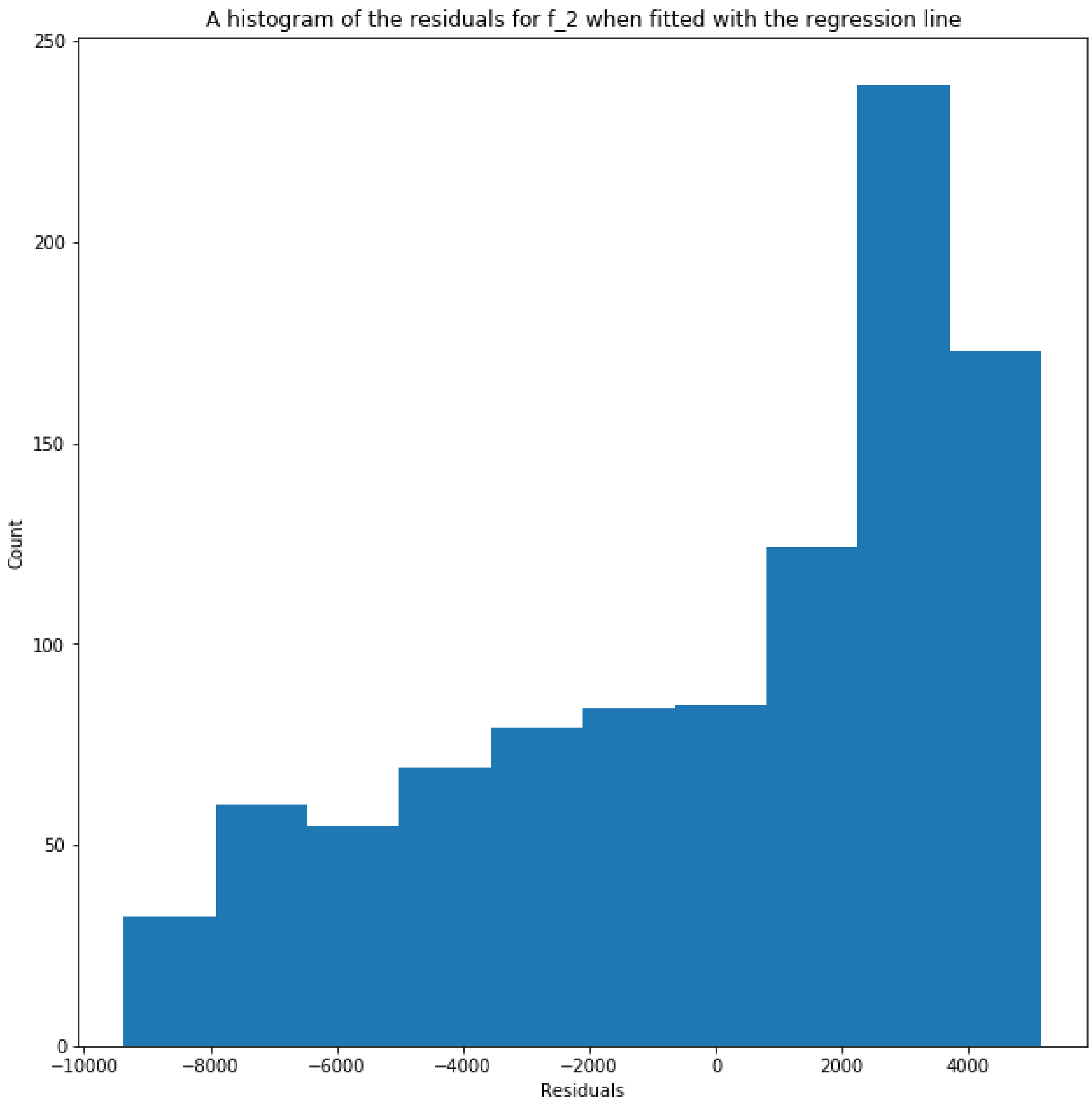
In [16]:
```
# 1000 linearly spaced numbers
x2 = np.linspace(0,99,1000)

# 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()
```



We can then look at the residuals plot as we did before

```
In [17]: # 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
```

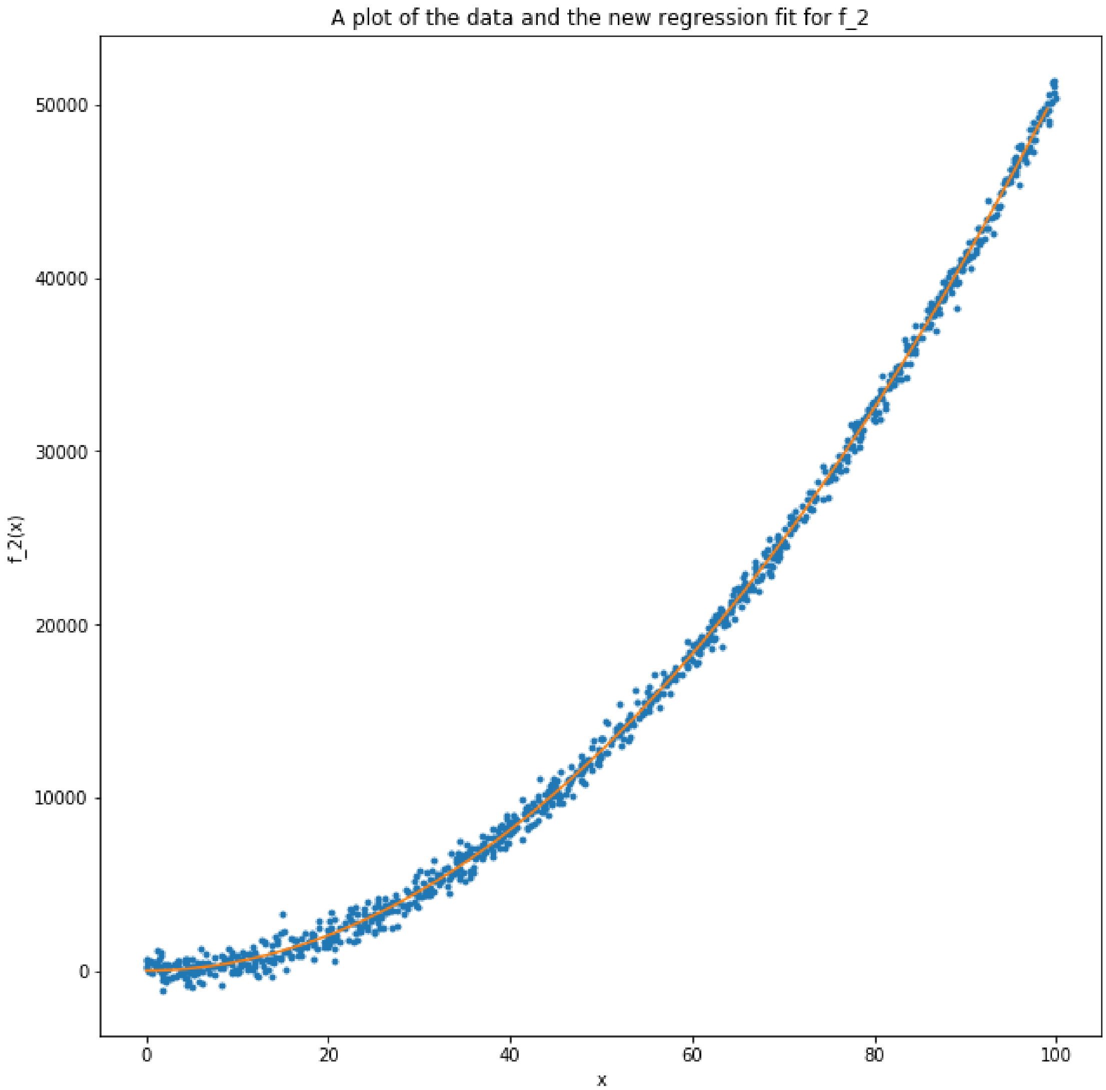
This shows that the linear model we have chosen may not be a good choice. We can try X^2 as a parameter instead of X in our linear model. This way, we are transforming an existing parameter to form a new parameter.

```
In [18]: # 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

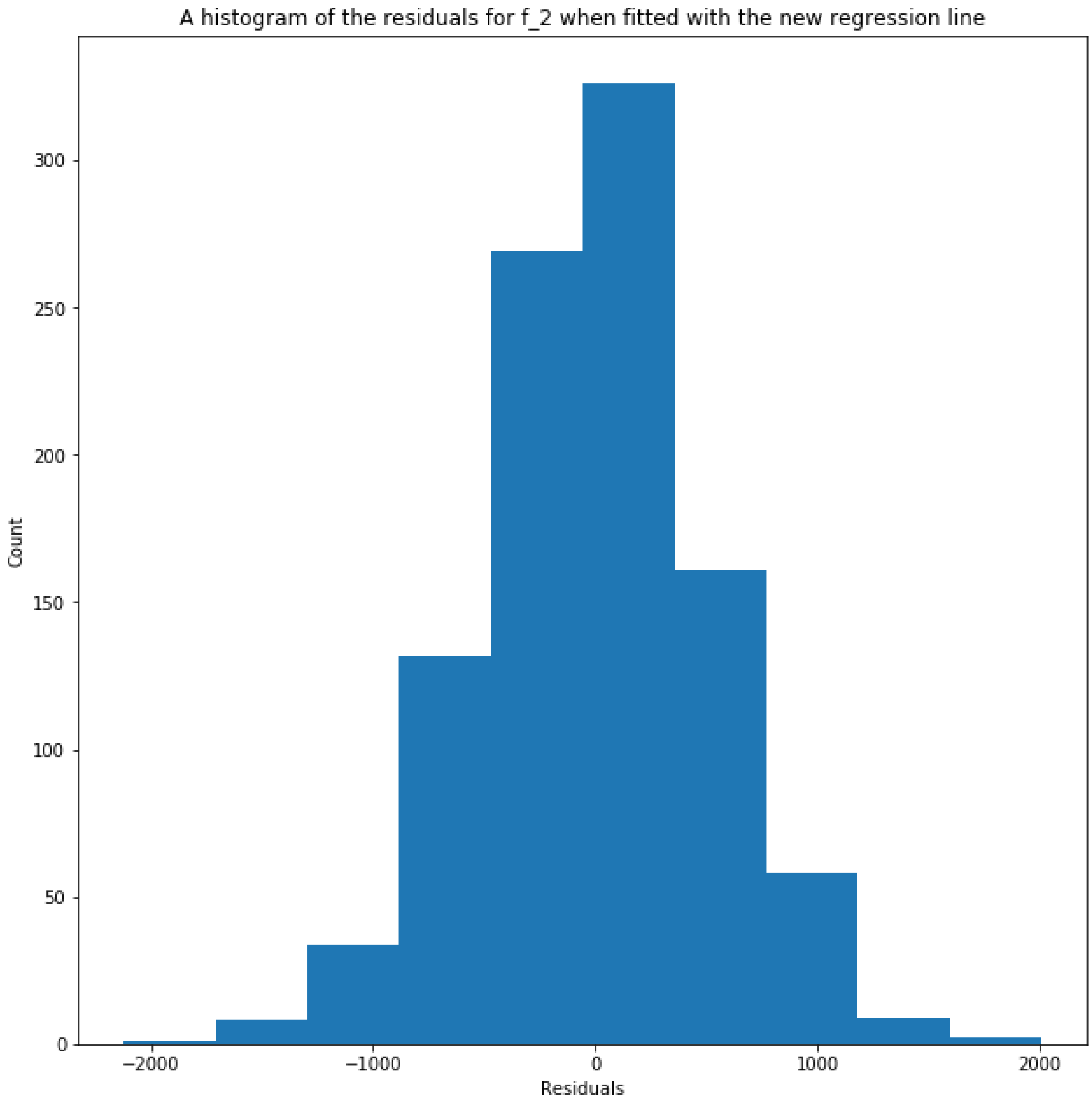
```
In [19]: # 1000 linearly spaced numbers
         x22 = np.linspace(0,99,1000)

         # 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()
```



We see a much better fit. 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 as has been assumed by the model architecture

```
In [20]: # 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)))
```

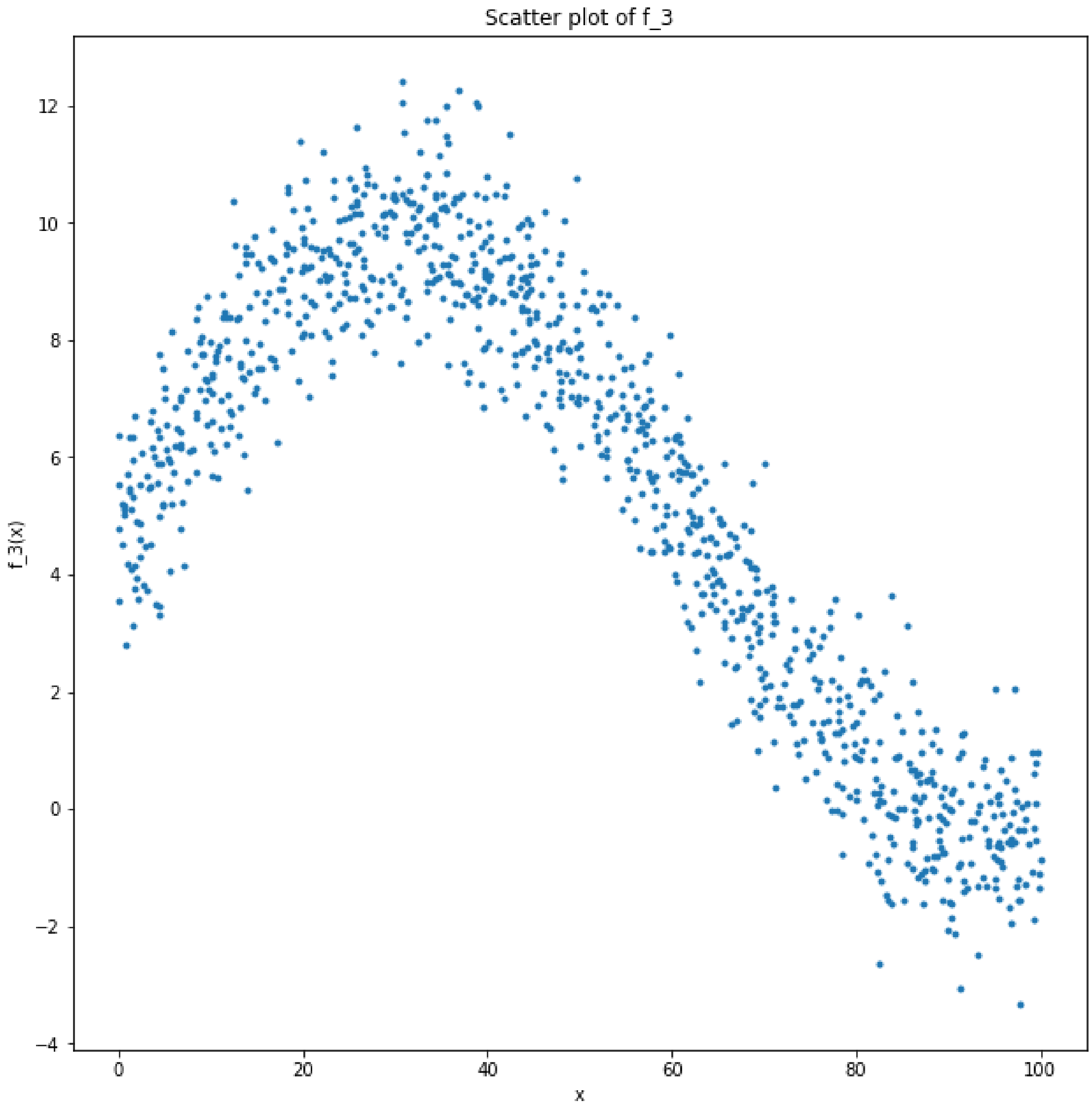



```
This is roughly a normal distribution with mean -1.1250449460931123e-12 and standard deviation
```

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 [21]:
```
# 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

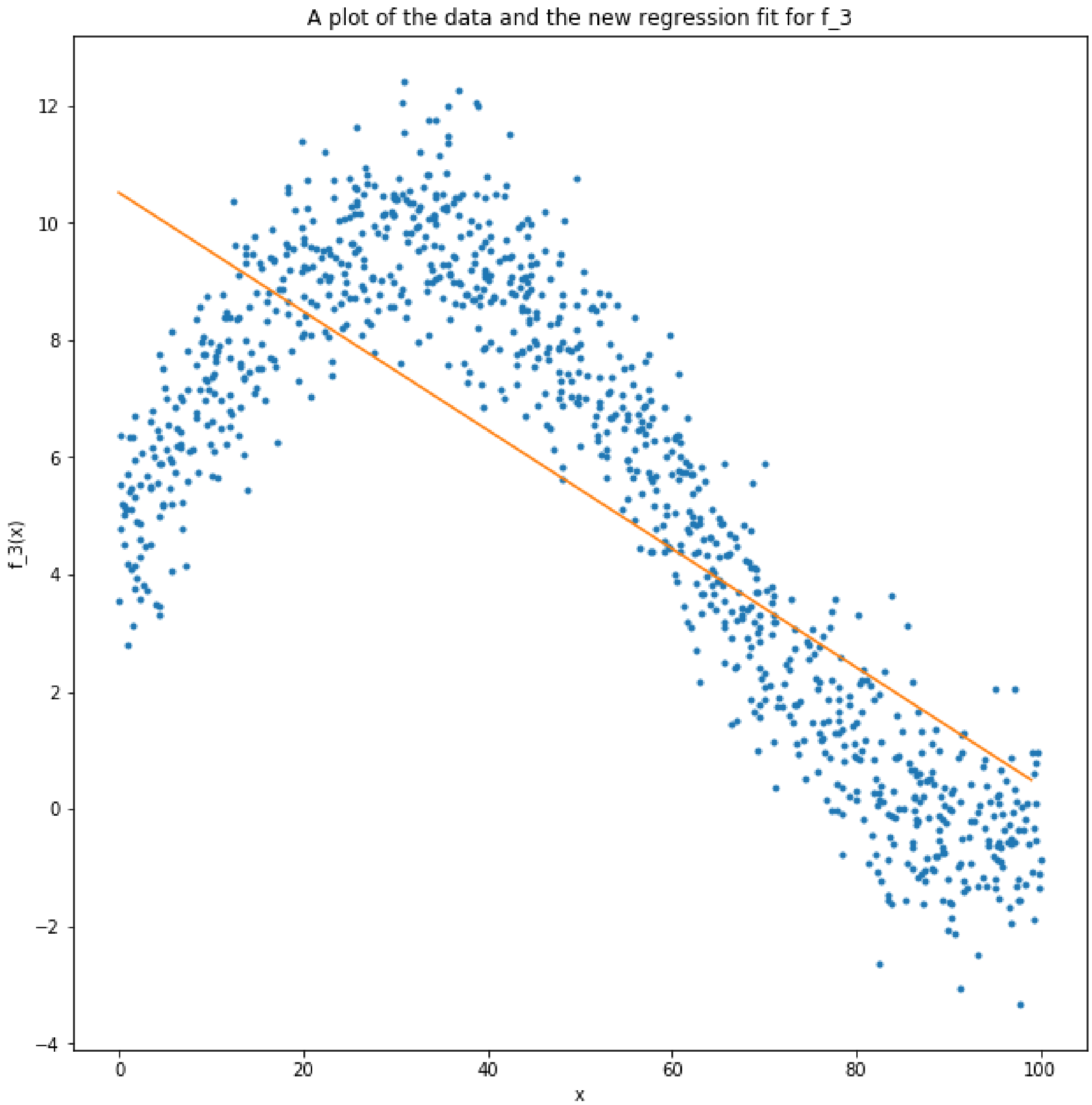
In [22]:
```
#Find the mean of the data for f_3
x_bar3 = np.mean(X)
y_bar3 = np.mean(Y_3)

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

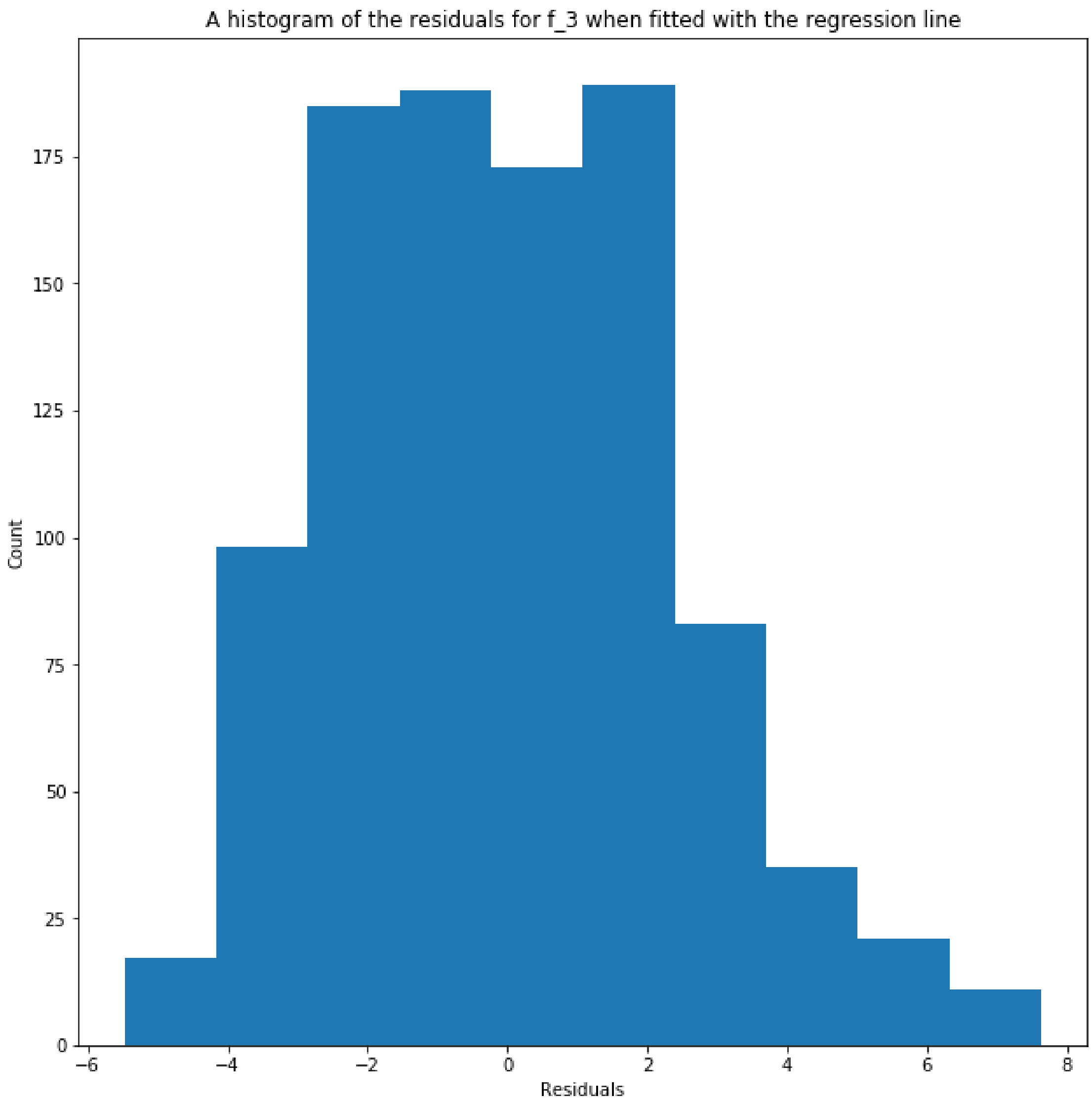
```
In [23]: # 1000 linearly spaced numbers
         x3 = np.linspace(0,99,1000)

         # 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 [24]: # 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.
```

1.3.1 Alternative View

Often in Machine Learning, we pose a hypothesis ($h_\theta(X)$) and a cost function ($J(\theta)$) and proceed to minimise this cost function. Here, X is the data and θ is a vector of parameters (such as the β in the Linear Regression models above).

For Linear Regression as stated above, the hypothesis function is that there is a straight line passing through all the data points:

$$h_\theta(X) = \theta_0 + \theta_1 X_1 + \theta_2 X_2 + \theta_3 X_3 + ... = X\theta$$

The Cost function is the least squares sum residuals (eventually written in index notation):

$$J(\theta) = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (h_\theta(X^{(i)}) - Y^{(i)})^2 = (X\theta - Y)^T(X\theta - Y) = (X\theta)^T X\theta - 2(X\theta)^T Y + Y^T Y = \theta_j x_{ji} x_{ij} \theta_j - 2\theta_j x_{ji} y_i$$

where the superscript $^{(i)}$ refers to the ith observation. Taking the derivative of the cost function:

$$\frac{\partial J(\theta)}{\partial \theta_k} = 2x_{ki}x_{ik}\theta_k - 2x_{ki}y_i$$

Setting this to zero for all k and solving:

$$\theta = (X^T X)^{-1} X^T Y$$

Let's test this out with the sine curve above by considering X,X^2 and X^3 as predictor variables.

In [25]:
```python
# Calculate x^2
X2 = X**2

# Calculate X^3
X3 = X**3

# Combine into a single array (n X 3)
X_full = np.concatenate((X.reshape(-1,1),X2.reshape(-1,1),X3.reshape(-1,1)),axis=1)

# Create transpose (3 X n)
X_fullT = X_full.transpose()

# Calculate X^T X
XTX = X_fullT.dot(X_full)

# calculate inverse of XTX
XTX_inv = np.linalg.inv(XTX)

# Calculate theta
theta = XTX_inv.dot(X_fullT.dot(Y_3))

print('Y_3 = {} * X + {} * X^2 + {} * X^3'.format(theta[0],theta[1],theta[2]))
```

```
Y_3 = 0.7593137639575493 * X + -0.01661989155701321 * X^2 + 9.044569969888496e-05 * X^3
```

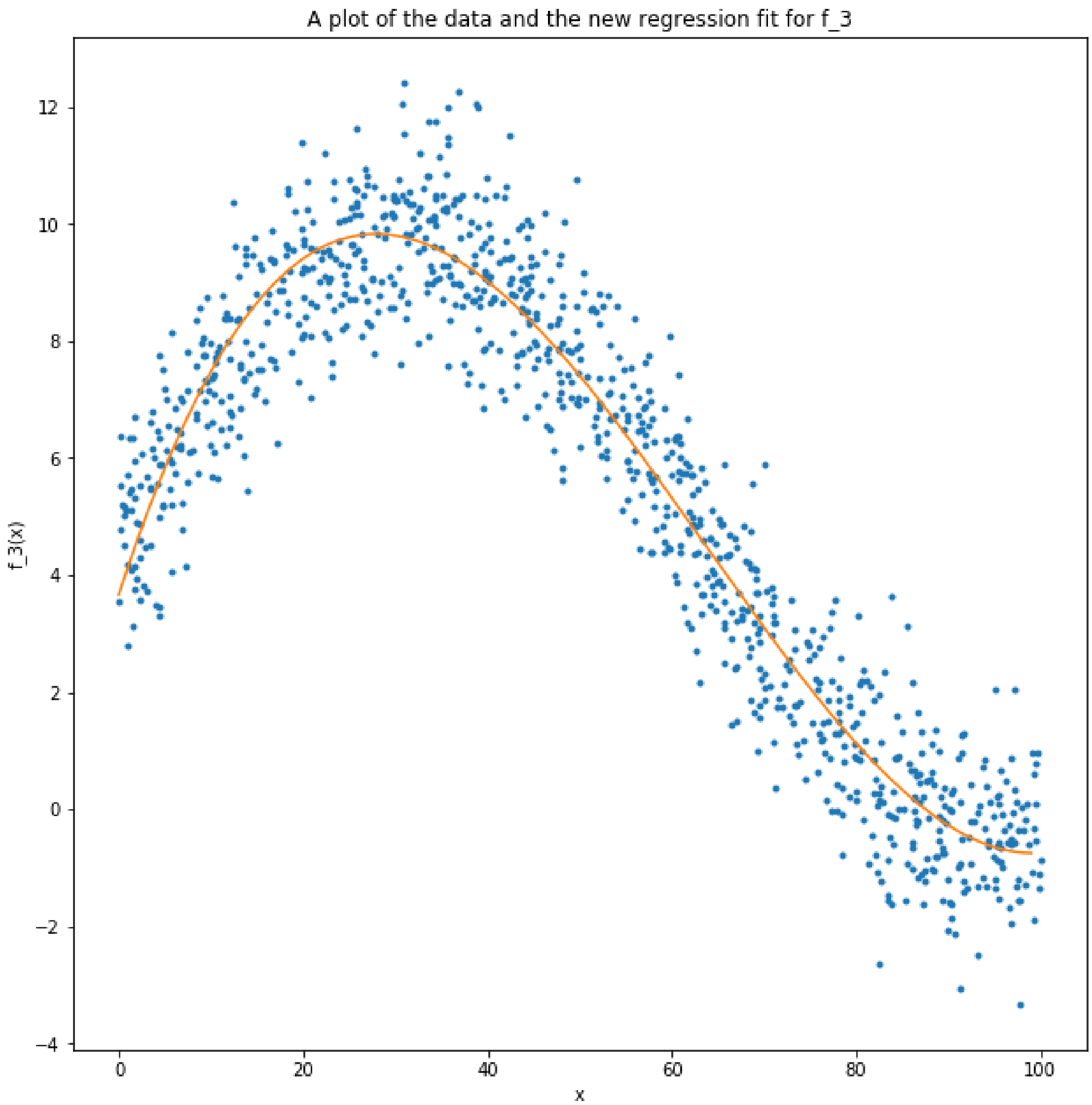
We can add a constant to the above by create an extra predictor full of ones

```
In [26]: # Calculate x^2
         X2 = X**2

         # Calculate X^3
         X3 = X**3

         # Combine into a single array (n X 4)
         X_full = np.concatenate((np.ones((Y_3.shape[0],1)),X.reshape(-1,1),X2.reshape(-1,1),X3

         # Create transpose (4 X n)
         X_fullT = X_full.transpose()

         # Calculate X^T X (4 X 4)
         XTX = X_fullT.dot(X_full)

         # calculate inverse of XTX (4 X 4)
         XTX_inv = np.linalg.inv(XTX)

         # Calculate theta
         theta = XTX_inv.dot(X_fullT.dot(Y_3))

         print('Y_3 = {} + {} * X + {} * X^2 + {} * X^3'.format(theta[0],theta[1],theta[2],the

Y_3 = 3.664431201640241 + 0.48709842203752807 * X + -0.011179330358443984 * X^2 + 5.86760576494
```

We plot the original data along with this solution to the parameters to see how well it fits the data.

```
In [27]: # 1000 linearly spaced numbers
         x3 = np.linspace(0,99,1000)
         x3_2 = x3**2
         x3_3 = x3**3

         # Predict the response for those numbers
         y3 = theta[0] + theta[1] * x3 + theta[2] * x3_2 + theta[3] * x3_3

         # 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()
```



R^2**-Statistic** Even though a plot of the residuals above 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 goodness 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*.

Note: Another way to assess the lack of fit is through the *Residual Squared Error* $RSE = \sqrt{\frac{RSS}{n-2}}$.

R^2, as the form above suggests, is the proportion of variance that is explained. For a simple linear regression with 1 parameter (see Appendix A4):

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

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 [28]: # 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 [29]: 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 list
             y_fitted := Fitted data as a list
             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(y_observed)):
        TSS += (y_observed[i] - y_bar)**2
        RSS += (y_observed[i] - y_fitted[i])**2

    return TSS,RSS
```

Then we apply this function to the three fitted models

```
In [30]: # 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 explains 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 [31]: # 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')
```

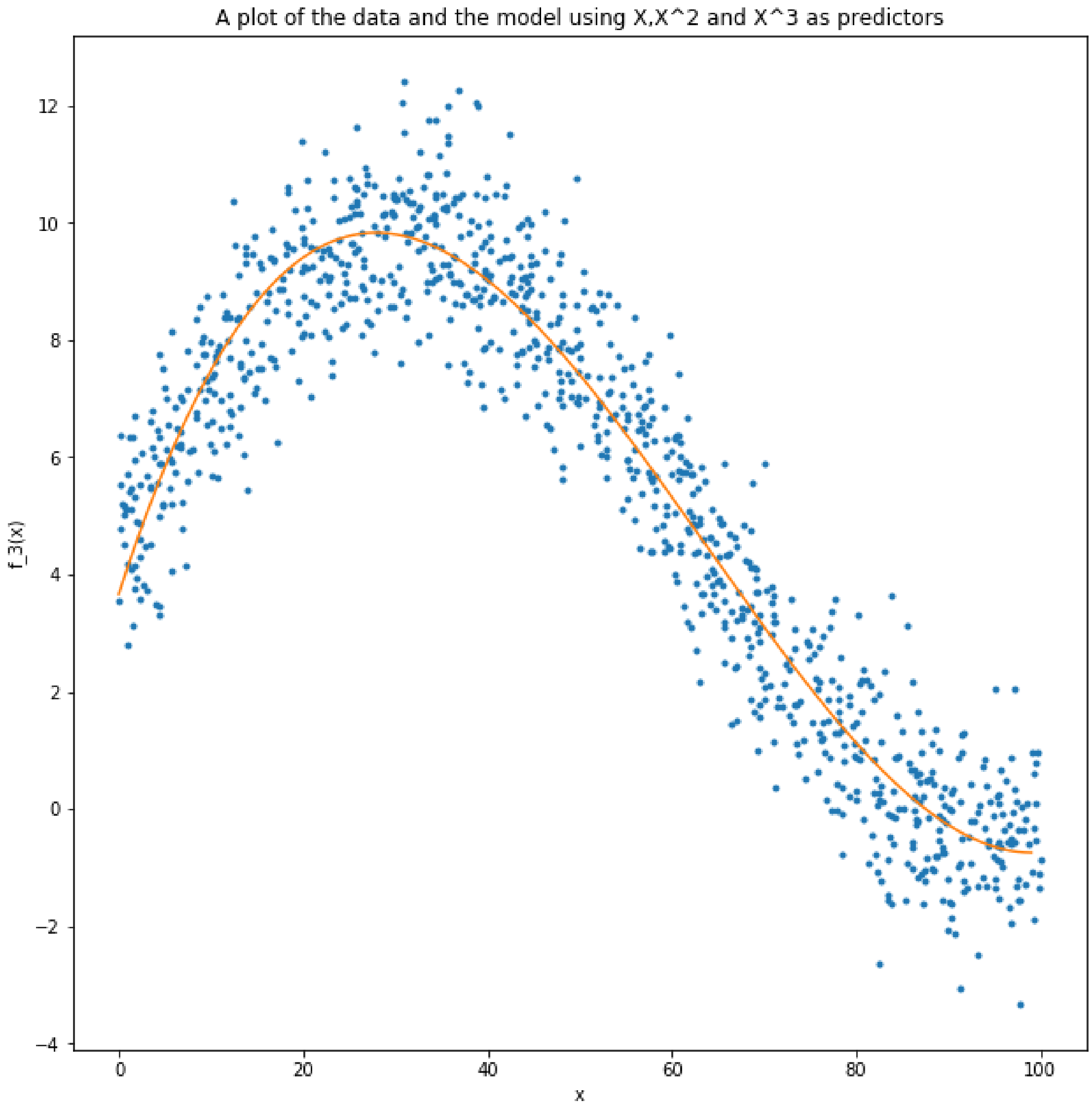
```python
print('beta_0 = {}'.format(lm22.intercept_[0]))
print('beta_1 = {}'.format(lm22.coef_[0][0]))
y22_fitted_sklearn = lm22.intercept_[0] + lm22.coef_[0][0]*X**2
print('R^2 = {}'.format(r2_score(Y_2,y22_fitted_sklearn)))

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 = -8445.980306821988
beta_1 = 506.16066894401666
```

```
R^2 = 0.9336613222418227


Model for Y_2: Explanatory variable X^2 for Y_2
beta_0 = 14.470063153308729
beta_1 = 5.075020979320469
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 = 3.6644312016355887
beta_1 = 0.48709842203796766
beta_2 = -0.011179330358454217
beta_3 = 5.8676057649481236e-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.

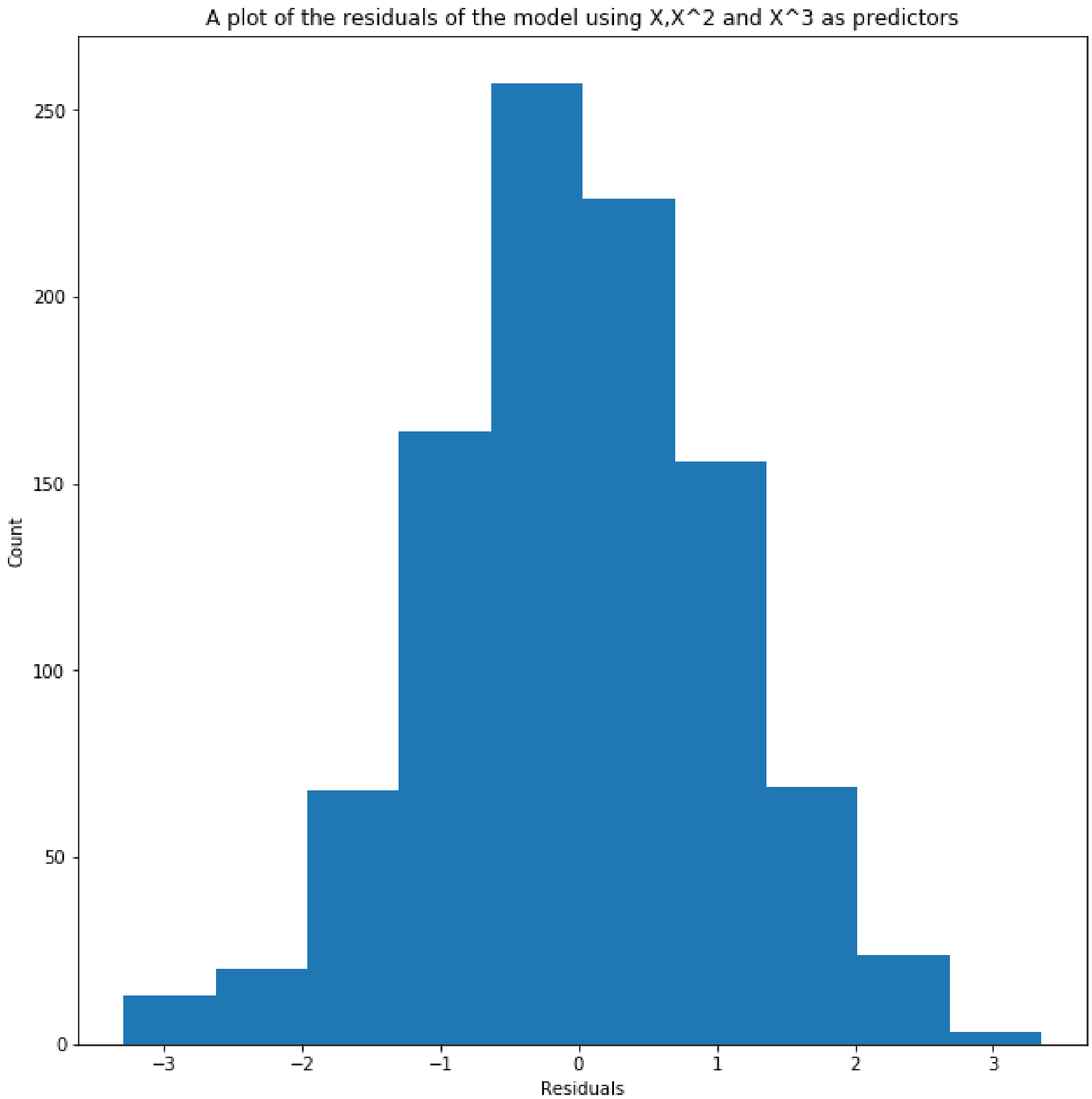
In [32]:
```
# 1000 linearly spaced numbers
x32 = np.linspace(0,99,1000)
y32 = lm32.intercept_[0] + lm32.coef_[0][0]*x32 + lm32.coef_[0][1]*x32**2\
    + lm32.coef_[0][2]*x32**3

# 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 [33]: # 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)
```

```python
# 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 \
standard deviation {std}'.format(mean=np.mean(Res_32),std=np.std(Res_32)))
```




```
This is roughly a normal distribution with mean -4.387601393318619e-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 $x = 0$ is

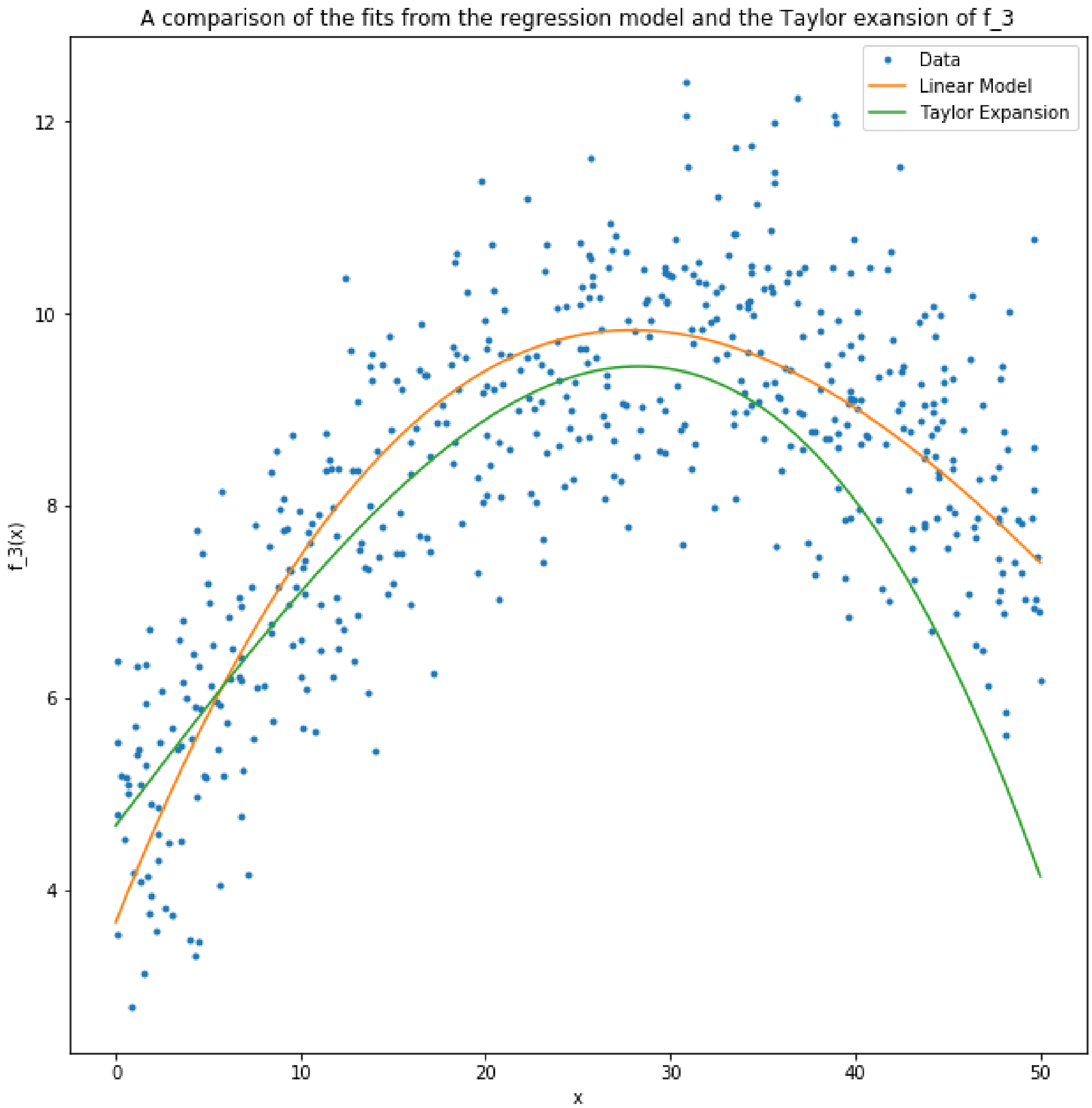
$$
\begin{aligned}
f(x=0) &= f(0) + f^{(1)}(0)x + f^{(2)}(0)x^2/(2!) + f^{(3)}(0)x^3/(3!) + O(x^4) \\
&= \sin(0) + \cos(0)x - \sin(0)x^2/(2!) - \cos(0)x^3/(3!) \\
&= x - x^3/(6)
\end{aligned}
$$

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 [34]: # 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[list(map(lambda x: x < 50,X))]

         # 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()
```



Statistical significance of regression coefficients 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 [35]: 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 (See Appendix A5):

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

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

In addition we can show that:

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

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 (the null hypothesis above sets both $\beta_0^{(0)} = 0$ and $\beta_1^{(0)} = 0$).

```
In [36]: # 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!
```

We can put this into a function

```
In [37]: 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
```

```python
temp,RSS = TSS_RSS(y_observed,y_fitted)

# 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!')
            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 [38]: 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!
```

We can use the statsmodels.api to verify our results

```
In [39]: 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)
```

```python
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:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:22:13   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:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:22:13   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:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:22:13   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:                Sat, 27 Jul 2019   Prob (F-statistic):          1.37e-197
Time:                        18:22:13   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:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:22:13   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.


C:\Users\HVAD\Anaconda3\lib\site-packages\numpy\core\fromnumeric.py:52: FutureWarning: Method
  return getattr(obj, method)(*args, **kwds)
```

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 [40]: 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())
```

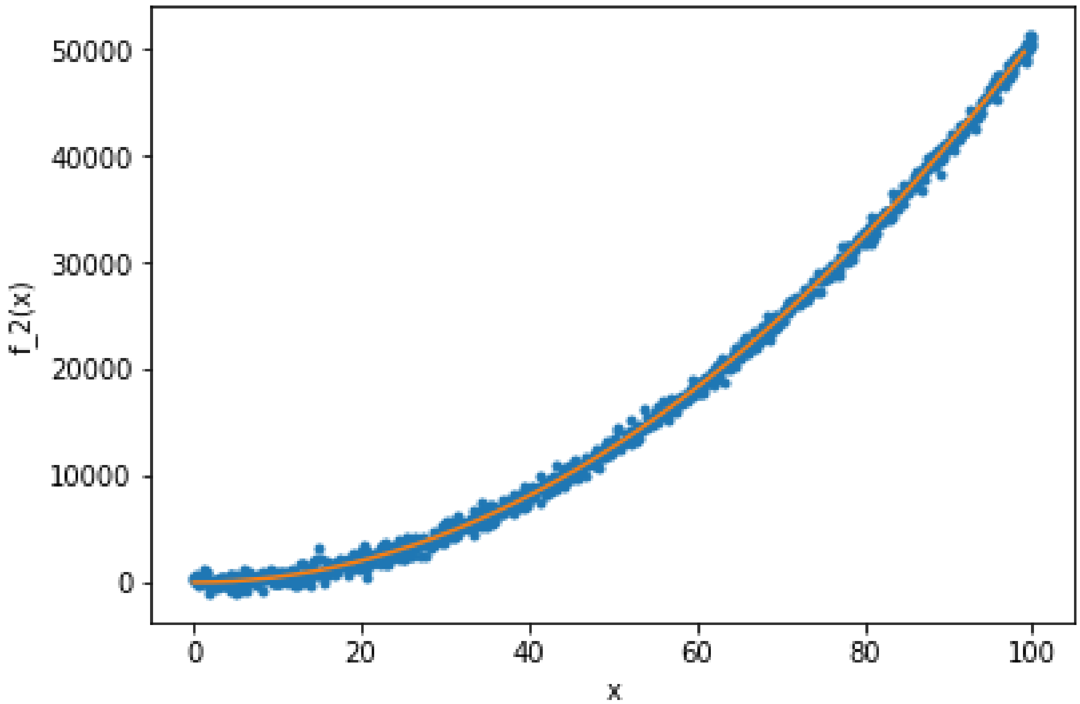
```
Model for Y_2: Explanatory variable X^2 for Y_2
                                 OLS Regression Results
=======================================================================================
Dep. Variable:                      y   R-squared (uncentered):                   0.999
Model:                            OLS   Adj. R-squared (uncentered):              0.999
Method:                 Least Squares   F-statistic:                          1.878e+06
Date:                Sat, 27 Jul 2019   Prob (F-statistic):                        0.00
Time:                        18:22:14   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 [41]:
```
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[41]:
```
[<matplotlib.lines.Line2D at 0x1b551a9aa58>]
```



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 [42]: # 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.

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

```
In [44]: # 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 [45]: 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 3974.16032266946
```

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

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

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

```
In [46]: beta22_0, beta22_1, RSS_22
```

```
Out[46]: (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 [47]: 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 [48]: 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 [49]: # 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 [50]: 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 [51]: 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 [52]: # 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
```

1.3.2 Synergy Effect

Suppose we have the following function

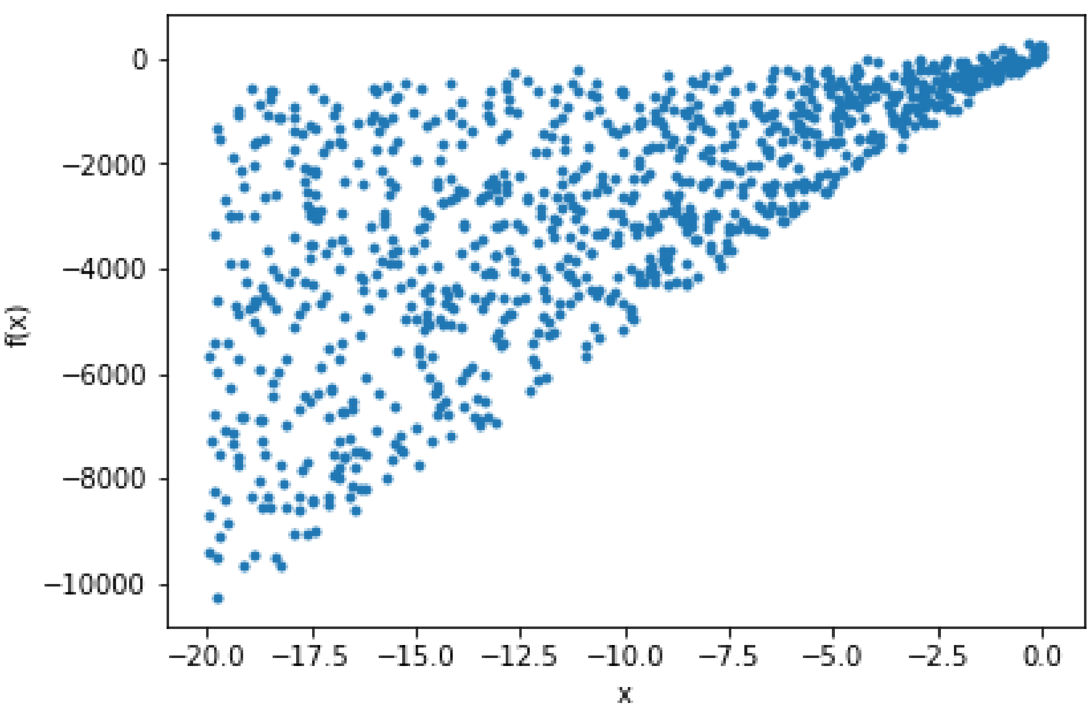
$$f(x) = 4.67 + 2 * X_1 + 3 * X_2 + 5.07X_1 * X_2$$

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 [53]: # We will need to plot in 3D
         from mpl_toolkits.mplot3d import Axes3D

         #f(x)=4.67+2*X_1+30*X_2+5.07X_1*X_2
         def f(x1,x2):
```

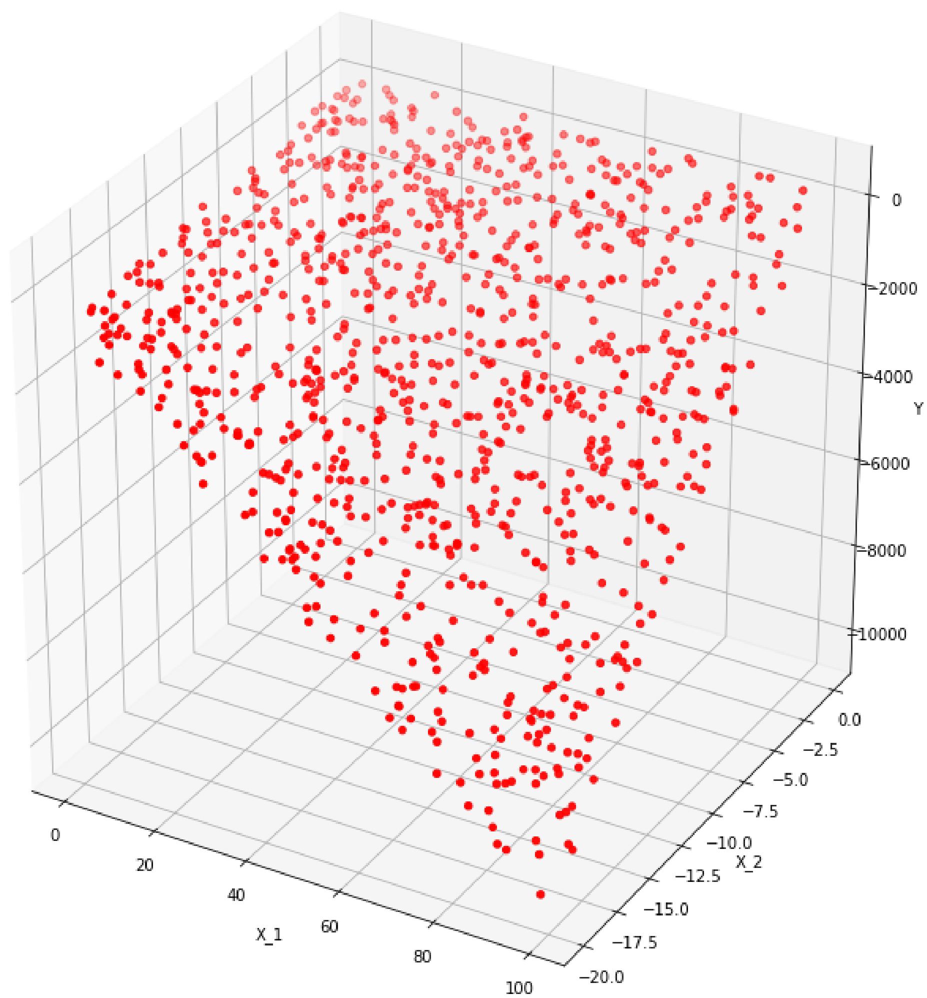
```
    return 4.67+2*x1+30*x2+5.07*x1*x2
# Set the seed
r = np.random.RandomState(101)
X_1 = 100*r.rand(1000)
X_2 = -20*r.rand(1000)

#Error term with sigma = 10, mu = 0
E = 100*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[53]: Text(0,0.5,'f(x)')



In [54]:
```
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()
```



Suppose we continued to fit a linear regression model with parameters X_1 and X_2 with the assumption that there is no synergy effect.

```
In [55]: print('Model for Y: Explanatory variable X_1 and X_2 for Y')
         X_new = sm.add_constant(pd.concat([pd.DataFrame(X_1,columns=['X_1']),\
                                            pd.DataFrame(X_2,columns=['X_2'])],axis=1))
         est = sm.OLS(Y, X_new)
```

```
est2 = est.fit()
print(est2.summary())
```

```
Model for Y: Explanatory variable X_1 and X_2 for Y
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.864
Model:                            OLS   Adj. R-squared:                  0.864
Method:                 Least Squares   F-statistic:                     3169.
Date:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:22:16   Log-Likelihood:                -8160.3
No. Observations:                1000   AIC:                         1.633e+04
Df Residuals:                     997   BIC:                         1.634e+04
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const       2562.3530     71.652     35.761      0.000    2421.746    2702.960
X_1          -49.6977      0.937    -53.063      0.000     -51.536     -47.860
X_2          279.5368      4.683     59.693      0.000     270.347     288.726
==============================================================================
Omnibus:                        3.561   Durbin-Watson:                   1.909
Prob(Omnibus):                  0.169   Jarque-Bera (JB):                4.035
Skew:                          -0.022   Prob(JB):                        0.133
Kurtosis:                       3.308   Cond. No.                         155.
==============================================================================

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


C:\Users\HVAD\Anaconda3\lib\site-packages\numpy\core\fromnumeric.py:52: FutureWarning: Method
  return getattr(obj, method)(*args, **kwds)
```

The above output shows that the R^2 is almost 87% with both X_1 and X_2 being statistically significant. Below, we show that including the synergy term $X_1 X_2$ into the model as well greatly improves the R^2 metric.

```
In [56]: print('Model for f: Explanatory variables X_1, X_2 and X_1 * 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 f: Explanatory variables X_1, X_2 and X_1 * X_2 for Y_2
                            OLS Regression Results
```

```
==============================================================================
Dep. Variable:                      y   R-squared:                       0.998
Model:                            OLS   Adj. R-squared:                  0.998
Method:                 Least Squares   F-statistic:                 1.651e+05
Date:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:22:16   Log-Likelihood:                -6052.5
No. Observations:                1000   AIC:                         1.211e+04
Df Residuals:                     996   BIC:                         1.213e+04
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         17.9262     13.164      1.362      0.174      -7.907      43.759
X_1            2.0906      0.231      9.054      0.000       1.637       2.544
X_2           30.3293      1.122     27.035      0.000      28.128      32.531
X_12           5.0841      0.020    257.798      0.000       5.045       5.123
==============================================================================
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.


C:\Users\HVAD\Anaconda3\lib\site-packages\numpy\core\fromnumeric.py:52: FutureWarning: Method
  return getattr(obj, method)(*args, **kwds)
```

We have seen above that adding a term X_1X_2 significantly increased the R^2 statistic. Instead of adding this joint term, what would be the effect on R^2 if we added random noise? We see the effect below.

```
In [57]: # Set the seed
         r = np.random.RandomState(11)

         #Error term with sigma = 10, mu = 0
         noise = 100*r.randn(1000)

         print('Model for Y: Explanatory variable X_1 and X_2 for Y')
         X_new = sm.add_constant(pd.concat([pd.DataFrame(X_1,columns=['X_1']),\
                                            pd.DataFrame(X_2,columns=['X_2']),\
                                           pd.DataFrame(noise,columns=['Noise'])],axis=1))
```

```python
est = sm.OLS(Y, X_new)
est2 = est.fit()
print(est2.summary())
```

```
Model for Y: Explanatory variable X_1 and X_2 for Y
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.865
Model:                            OLS   Adj. R-squared:                  0.864
Method:                 Least Squares   F-statistic:                     2123.
Date:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:22:16   Log-Likelihood:                -8157.8
No. Observations:                1000   AIC:                         1.632e+04
Df Residuals:                     996   BIC:                         1.634e+04
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const       2548.0238     71.812     35.482      0.000    2407.103    2688.945
X_1          -49.6148      0.936    -53.033      0.000     -51.451     -47.779
X_2          278.5613      4.695     59.331      0.000     269.348     287.775
Noise         -0.5863      0.267     -2.196      0.028      -1.110      -0.062
==============================================================================
Omnibus:                        3.763   Durbin-Watson:                   1.906
Prob(Omnibus):                  0.152   Jarque-Bera (JB):                4.348
Skew:                          -0.006   Prob(JB):                        0.114
Kurtosis:                       3.323   Cond. No.                         271.
==============================================================================

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


C:\Users\HVAD\Anaconda3\lib\site-packages\numpy\core\fromnumeric.py:52: FutureWarning: Method
  return getattr(obj, method)(*args, **kwds)
```

Including an unrelated, random noise term to the model increases the R^2 statistic. This makes sense since when fitting the model to the training data, in the worst case, the model could choose a predictor's coefficient to be zero. This means that the R^2 statistic for the training data should never decrease as a function of the number of predictors. The main reason for introducing such a metric is to gauge how well the model describes the population from which our data originates from. However, if it never decreases then how can it be determined whether the added parameter is useful or not?

In order to cater for this, the Adjusted R^2 metric can be used. This metric applies a penalty to the usual R^2 the more predictors that are used. This way, it is not possible that the Adjusted R^2 can increase indefinitely. At some point, the contribution to the R^2 of adding a new predictor will be overcome by the penalty attributed to adding that new parameter. The Adjusted R^2 is as follows:

$$\text{Adjusted } R^2 = 1 - \frac{RSS/(n-p-1)}{TSS/(n-1)}$$

where p is the number of predictors. It can be seen in the above model that the Adjusted R^2 did not increase with the addition of another predictor.

Another approach we can apply to take into account that the test R^2 will always be smaller than the training R^2, is to divide the data we have into a training set and a testing set. We can then train the model on the training set and test it on the unseen testing set in order to determine how well it has performed.

We tackle this in the next section.

1.3.3 Cross Validation

Cross Validation is a technique to estimate how well a model will perform on unseen data. As mentioned in the previous section, the entire data set available can be divided into two: a training set and a testing set. The question then becomes, 'what portion of the dataset should be the training set?'. This question can be expressed as follows:

- Let the number of observations be n, then the trainnig set is $n - k$ where $k \in [1, n-1]$

The reason this question is important is that the choice of k greatly influences the bias in our cross validation. If $k = \lfloor n/2 \rfloor$ then the test error will be greatly overestimated since the final model will be trained on n observations, not $\lfloor n/2 \rfloor$ observations. On the other hand, if $k = 1$, the variance of our test error will be very large since the technique will depend greatly on which observation we chose as the test observation.

Going further, we can divide the entire dataset into roughly n/k subsets. We can then run n/k different cross validations leaving a different subset as the test set at each iteration. The test error (or R^2) can then be approximated as the average of the different subset test errors. This immediately means that if n is large, choosing to assess the model performance using cross validation with $k = 1$ could be computationally intense. Therefore, a value for k somewhere in the range $(1, \lfloor n/2 \rfloor)$ may be wiser.

To start things off, let's fit a linear regression model to the house prices dataset and test it on a portion of the data.

```
In [58]: housePrice.columns
```

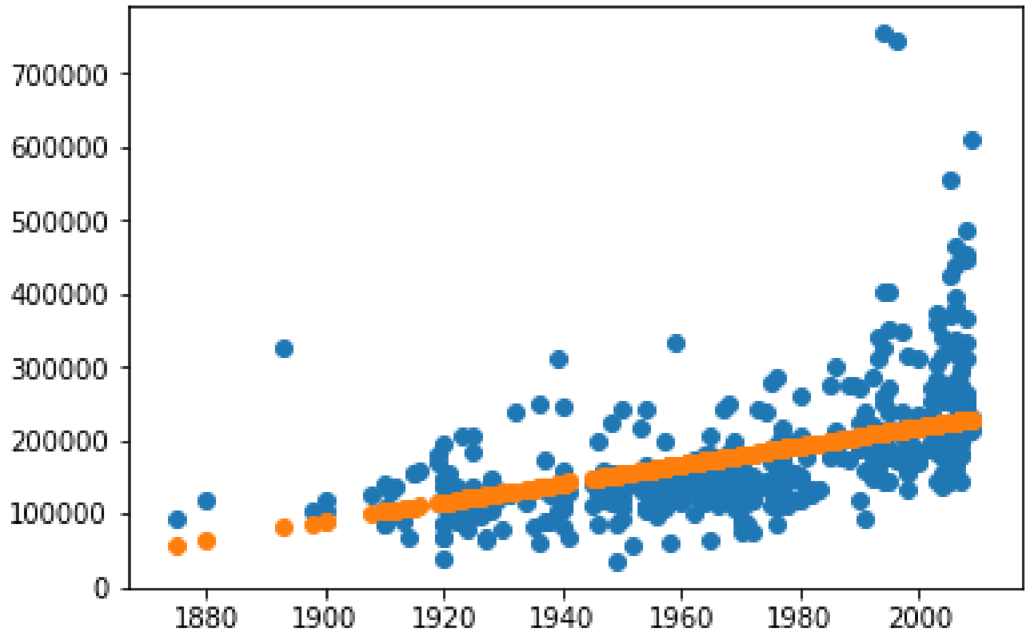
```
Out[58]: Index(['LotArea', 'OverallQual', 'OverallCond', 'YearBuilt', 'YearRemodAdd',
                'MasVnrArea', 'BsmtFinSF1', 'BsmtFinSF2', 'BsmtUnfSF', 'TotalBsmtSF',
                '1stFlrSF', '2ndFlrSF', 'LowQualFinSF', 'GrLivArea', 'BsmtFullBath',
                'BsmtHalfBath', 'FullBath', 'HalfBath', 'BedroomAbvGr', 'KitchenAbvGr',
                'TotRmsAbvGrd', 'Fireplaces', 'GarageYrBlt', 'GarageCars', 'GarageArea',
                'WoodDeckSF', 'OpenPorchSF', 'EnclosedPorch', '3SsnPorch',
                'ScreenPorch', 'PoolArea', 'MiscVal', 'MoSold', 'YrSold', 'SalePrice'],
               dtype='object')
```

We use train test split (using 33% of the dataset as a test set) to calculate the MSE on the test set

In [59]:
```python
# The predictor and response
X = housePrice['YearBuilt'].values.reshape(-1,1)
y = housePrice['SalePrice'].values.reshape(-1,1)

# Make 33% of this dataset a test set
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, random_stat

# Linear Regression model object
model = LinearRegression()

# Fit this model using the training data
model.fit(X_train,y_train)

# Predict
predictions = model.predict(X_test)

# Get the RSS
tss,rss = TSS_RSS(y_test,predictions)

# The MSE is RSS/n_test
MSE = rss/len(y_test)

print('The MSE is {}'.format(MSE))

# Plot the predictions
plt.scatter(X_test,y_test)
plt.scatter(X_test,predictions)
```

```
The MSE is [5.29577792e+09]
```

Out[59]:
```
<matplotlib.collections.PathCollection at 0x1b551e20b70>
```



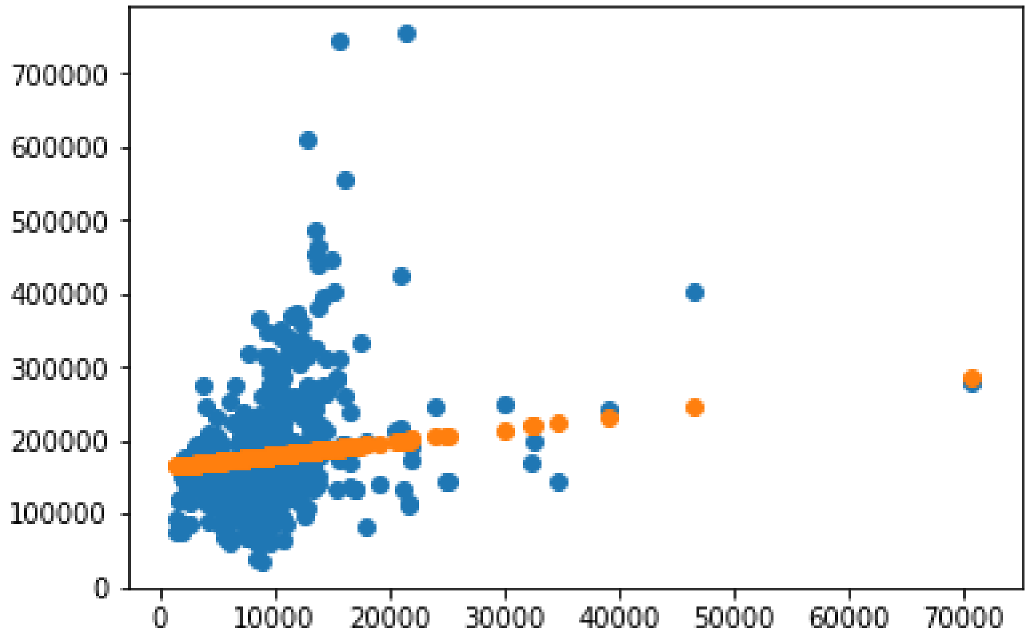
Let's see what the MSE is when we use the 'LotArea' predictor to predict 'SalePrice'.

```
In [60]: # The predictor and response
         X = housePrice['LotArea'].values.reshape(-1,1)
         y = housePrice['SalePrice'].values.reshape(-1,1)

         # Make 33% of this dataset a test set
         X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, random_stat

         # Linear Regression model object
         model = LinearRegression()

         # Fit this model using the training data
         model.fit(X_train,y_train)

         # Predict
         predictions = model.predict(X_test)

         # Get the RSS
         tss,rss = TSS_RSS(y_test,predictions)

         # The MSE is RSS/n_test
         MSE = rss/len(y_test)

         print('The MSE is {}'.format(MSE))
```

```
# Plot the predictions
plt.scatter(X_test,y_test)
plt.scatter(X_test,predictions)
```

```
The MSE is [6.89081973e+09]
```

Out[60]: <matplotlib.collections.PathCollection at 0x1b551ea96a0>



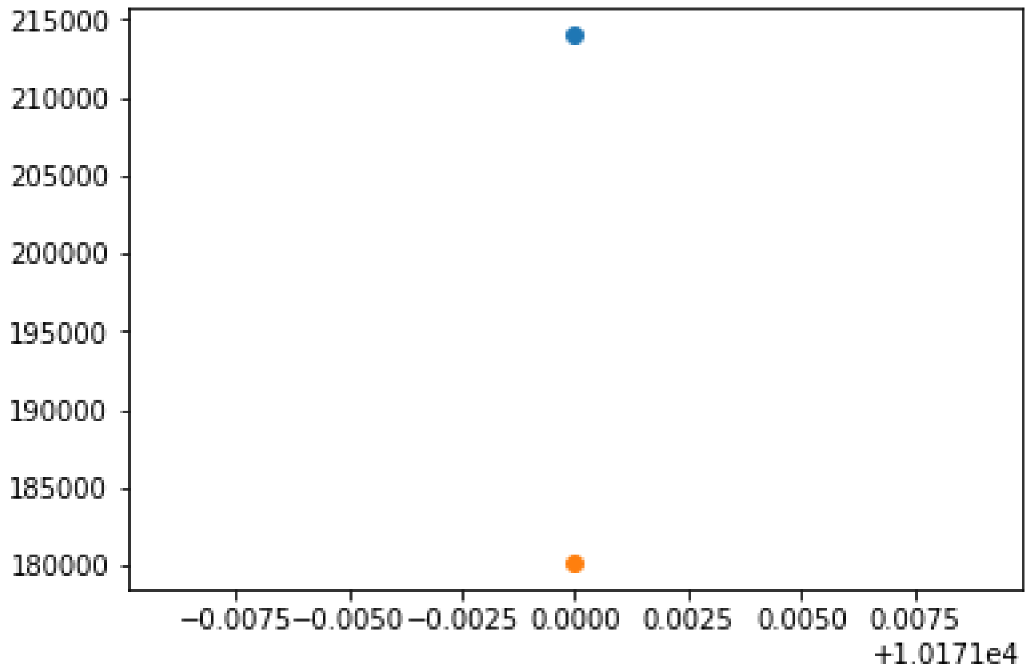
An important point to note in the above MSE calculations is that these MSE results are highly biased. We used a train - test split of 33%. However, in reality, we have the full dataset to train our model on. This means that the above is overestimating the test MSE of the model. In other words, by using only a subset of our dataset to train our model, we are not making use of the full power of the data we have. We can go to the other extreme and select one single observation from our data set of n observations as a test set and the remaining n-1 observations as a training set. This is called Leave One Out Cross Validation (LOOCV). We do that below.

In [61]:
```
# The predictor and response
X = housePrice['LotArea']
y = housePrice['SalePrice']

# Select a random element to be the test set
r = random.SystemRandom()
testint = r.randint(0,len(X))

# The train set
X_train = X.copy().values.reshape(-1,1)
```

```python
    y_train = y.copy().values.reshape(-1,1)

    # The test set is that one observation
    X_test = X_train[testint]
    X_test = X_test.reshape(1,-1)

    # The train set is all observations except that one observation
    np.delete(X_train,testint)

    # The test set consist of one response
    y_test = y_train[testint]
    np.delete(y_train,testint)

    # The Linear Regression model object
    model = LinearRegression()

    # Fit the model
    model.fit(X_train,y_train)

    # Predict
    predictions = model.predict(X_test)

    # Get the MSE. MSE = RSS/n
    tss,rss = TSS_RSS(y_test,predictions)
    MSE = rss/len(y)
    print('MSE = {}'.format(MSE))

    # Plot
    plt.scatter(X_test,y_test)
    plt.scatter(X_test,predictions)
```

```
MSE = [782726.22053338]
```

```
Out[61]: <matplotlib.collections.PathCollection at 0x1b552591860>
```



Each time we run the above code, we get a completely different test MSE. This is because the test MSE depends on which observation we chose to test the model on. So this reduces the bias to a minimum but has a large variance. We can iterate over all the cases where for each iteration we leave a different observation as a test observation. Then we calculate the average MSE over all these Cross Validations.

First for 'YearBuilt' as a predictor variable then the 'LotArea' as a predictor variable.

```
In [62]: # The predictor and response
         X = housePrice['YearBuilt']
         y = housePrice['SalePrice']

         # The MSE array. Each element is the MSE of a particular Cross Validation
         MSE = []

         # Perform LOOCV on the data using Linear Regression
         for i in range(len(X)):
             # The training set
             X_train = X.copy().values.reshape(-1,1)
             y_train = y.copy().values.reshape(-1,1)

             # The test set is a single observation
             X_test = X_train[i]
             X_test = X_test.reshape(1,-1)
             X_train = np.delete(X_train,i)

             # The test set is a single observation
```

```
        y_test = y_train[i]
        y_test = y_test.reshape(1,-1)
        y_train = np.delete(y_train,i)

        # Train the model
        model = LinearRegression()

        # Fit
        model.fit(X_train.reshape(-1,1),y_train.reshape(-1,1))

        # Predict
        predictions = model.predict(X_test)

        # Calculate the MSE. MSE = RSS/n_test
        tss,rss = TSS_RSS(y_test,predictions)
        MSE.append(rss[0])

    # Print the mean MSE value
    print(np.mean(MSE))
```

```
4597328547.297892
```

```
In [63]: X = housePrice['LotArea']
    y = housePrice['SalePrice']

    MSE = []

    for i in range(len(X)):
        X_train = X.copy().values.reshape(-1,1)
        y_train = y.copy().values.reshape(-1,1)

        X_test = X_train[i]
        X_test = X_test.reshape(1,-1)
        X_train = np.delete(X_train,i)

        y_test = y_train[i]
        y_test = y_test.reshape(1,-1)
        y_train = np.delete(y_train,i)

        # Train
        model = LinearRegression()

        # Fit
        model.fit(X_train.reshape(-1,1),y_train.reshape(-1,1))

        # Predict
        predictions = model.predict(X_test)
```

```
        # MSE
        tss,rss = TSS_RSS(y_test,predictions)
        MSE.append(rss[0])

    print(np.mean(MSE))
```

```
5954196196.345753
```

We can leverage the cross_val_score method to do the above cross validation for us

```
In [64]: X = housePrice['LotArea']
         y = housePrice['SalePrice']

         linregCVScores = cross_val_score(LinearRegression(),X.values.reshape(-1,1),y.values.re
         -linregCVScores.mean()
```

```
Out[64]: 5954196196.345753
```

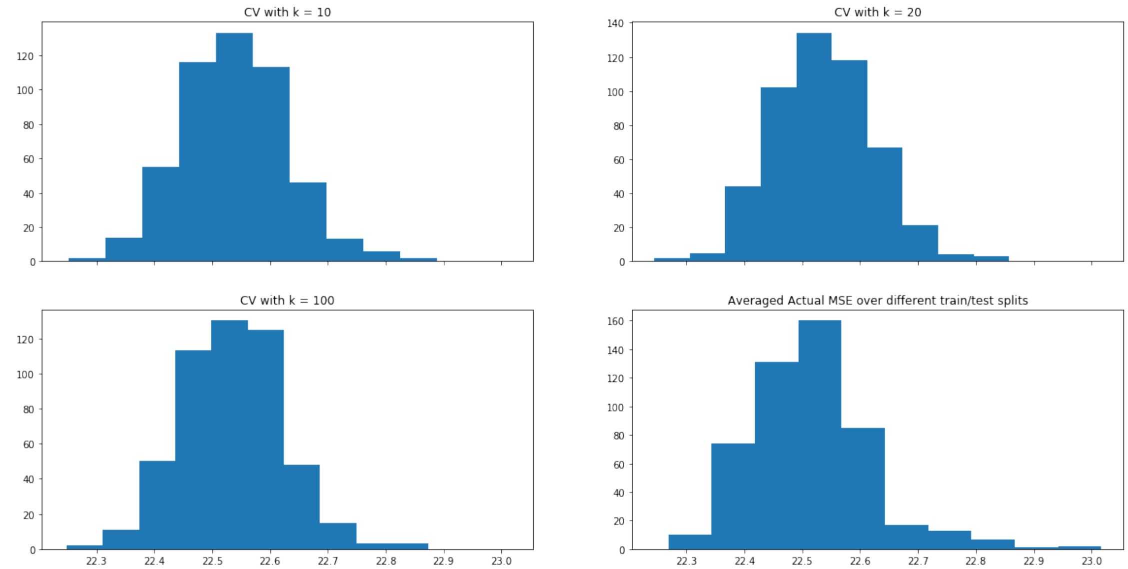
Let's observe now which approach (value of k in k-fold cross validation) predicts the test MSE best. We split our train and test data. Then estimate the test MSE using the training data.

```
In [65]: datasetMSEEstimatek_10 = []
         datasetMSEEstimatek_20 = []
         datasetMSEEstimatek_100 = []
         datasetMSEActual = []

         # The predictor and response
         X = housePrice['LotArea'].values.reshape(-1,1)
         y = housePrice['SalePrice'].values.reshape(-1,1)


         for j in range(500):
             X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5, random_s

             linregCVScores = cross_val_score(LinearRegression(),X_train.reshape(-1,1),y_train
             datasetMSEEstimatek_10.append(-linregCVScores.mean())

             linregCVScores = cross_val_score(LinearRegression(),X_train.reshape(-1,1),y_train
             datasetMSEEstimatek_20.append(-linregCVScores.mean())

             linregCVScores = cross_val_score(LinearRegression(),X_train.reshape(-1,1),y_train
             datasetMSEEstimatek_100.append(-linregCVScores.mean())


             model = LinearRegression()
             model.fit(X_train,y_train)
             predictions = model.predict(X_test)
```

```
            datasetMSEActual.append(mean_squared_error(y_test,predictions))

            if j%50 == 0:
                print('Step = {}'.format(j))

        print('The mean MSE Estimation using K-fold CV with k = 10 is : {}'.format(np.mean(da
        print('The mean MSE Estimation using K-fold CV with k = 20 is : {}'.format(np.mean(da
        print('The mean MSE Estimation using K-fold CV with k = 100 is : {}'.format(np.mean(d
        print('The actual MSE on this data set is : {}'.format(np.mean(datasetMSEActual)))

        fig,axes = plt.subplots(nrows = 2,ncols = 2,sharex=True)
        fig.set_size_inches(20,10)

        axes[0][0].hist(list(map(math.log,datasetMSEEstimatek_10)))
        axes[0][0].set_title('CV with k = 10')

        axes[0][1].hist(list(map(math.log,datasetMSEEstimatek_20)))
        axes[0][1].set_title('CV with k = 20')

        axes[1][0].hist(list(map(math.log,datasetMSEEstimatek_100)))
        axes[1][0].set_title('CV with k = 100')

        axes[1][1].hist(list(map(math.log,datasetMSEActual)))
        axes[1][1].set_title('Averaged Actual MSE over different train/test splits')
```

```
Step = 0
Step = 50
Step = 100
Step = 150
Step = 200
Step = 250
Step = 300
Step = 350
Step = 400
Step = 450
The mean MSE Estimation using K-fold CV with k = 10 is : 6170090398.833329
The mean MSE Estimation using K-fold CV with k = 20 is : 6161875851.874799
The mean MSE Estimation using K-fold CV with k = 100 is : 6146620803.335432
The actual MSE on this data set is : 6046571007.118181
```

```
Out[65]: Text(0.5,1,'Averaged Actual MSE over different train/test splits')
```

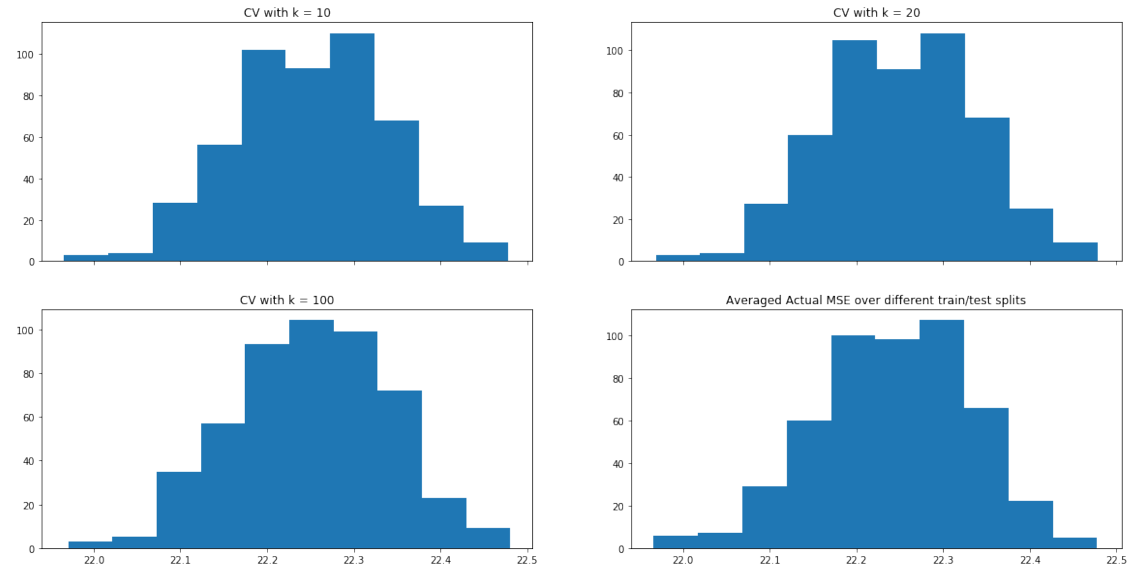


In [66]:
```
datasetMSEEstimatek_10 = []
datasetMSEEstimatek_20 = []
datasetMSEEstimatek_100 = []
datasetMSEActual = []

# The predictor and response
X = housePrice['YearBuilt'].values.reshape(-1,1)
y = housePrice['SalePrice'].values.reshape(-1,1)


for j in range(500):
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5, random_s

    linregCVScores = cross_val_score(LinearRegression(),X_train.reshape(-1,1),y_train
    datasetMSEEstimatek_10.append(-linregCVScores.mean())

    linregCVScores = cross_val_score(LinearRegression(),X_train.reshape(-1,1),y_train
    datasetMSEEstimatek_20.append(-linregCVScores.mean())

    linregCVScores = cross_val_score(LinearRegression(),X_train.reshape(-1,1),y_train
    datasetMSEEstimatek_100.append(-linregCVScores.mean())


    model = LinearRegression()
    model.fit(X_train,y_train)
    predictions = model.predict(X_test)
    datasetMSEActual.append(mean_squared_error(y_test,predictions))
```

```python
            if j%50 == 0:
                print('Step = {}'.format(j))

        print('The mean MSE Estimation using K-fold CV with k = 10 is : {}'.format(np.mean(da
        print('The mean MSE Estimation using K-fold CV with k = 20 is : {}'.format(np.mean(da
        print('The mean MSE Estimation using K-fold CV with k = 100 is : {}'.format(np.mean(d
        print('The actual MSE on this data set is : {}'.format(np.mean(datasetMSEActual)))

        fig,axes = plt.subplots(nrows = 2,ncols = 2,sharex=True)
        fig.set_size_inches(20,10)

        axes[0][0].hist(list(map(math.log,datasetMSEEstimatek_10)))
        axes[0][0].set_title('CV with k = 10')

        axes[0][1].hist(list(map(math.log,datasetMSEEstimatek_20)))
        axes[0][1].set_title('CV with k = 20')

        axes[1][0].hist(list(map(math.log,datasetMSEEstimatek_100)))
        axes[1][0].set_title('CV with k = 100')

        axes[1][1].hist(list(map(math.log,datasetMSEActual)))
        axes[1][1].set_title('Averaged Actual MSE over different train/test splits')
```

```
Step = 0
Step = 50
Step = 100
Step = 150
Step = 200
Step = 250
Step = 300
Step = 350
Step = 400
Step = 450
The mean MSE Estimation using K-fold CV with k = 10 is : 4622083078.925203
The mean MSE Estimation using K-fold CV with k = 20 is : 4621267854.562423
The mean MSE Estimation using K-fold CV with k = 100 is : 4620965999.249676
The actual MSE on this data set is : 4587675012.9899845
```

```
Out[66]: Text(0.5,1,'Averaged Actual MSE over different train/test splits')
```



We can see above that the MSE when we choose the 'LotArea' predictor is not as good as using 'YearBuilt'. So in this case we choose 'YearBuilt' over 'LotArea' to include in our linear regression model.

It can be seen that there is a general pattern in the above when comparing the MSE estimates from varying blocks (k) in Cross Validation. Namely, the larger k is, the more blocks we use to split the data up and the less portion of the data there is for the test set and the more iteration that is required per Cross Validation. For example, suppose n = 1000, when k = 10 we have 10 blocks with 100 observations per block. So we fit the model 10 times, each time leaving out a different k block when training. When comparing this with the case where k = 100, we have 100 blocks each with 10 observations. This means that the training set for each of these model fits is a lot closer to reality in that we will be using the entire dataset to fit the model. However, this comes at a computational cost, in this case we would need to run a model to fit and predict 100 times instead of 10.

Depending on the computational cost of the model used, we may choose a smaller value of k = 10 when comparing the same model but with different parameters.

We can try out all the predictors and choose the one that minimises the mean squared errors. This can be done by using a loop as below.

```
In [67]: # Run through each model in the correct order and run CV on it and save the best CV s
         bestMeanCV = -1
         bestMeanCVModel = []

         X = housePrice.drop('SalePrice',axis=1)

         # y is the response variable
         y = housePrice['SalePrice']

         for i in X.columns:
             # First set X to be the full set of remaining parameters
```

```
X = housePrice.loc[:,i]

linregCVScores = cross_val_score(LinearRegression(),X.values.reshape(-1,1),y,scor

if bestMeanCV > -linregCVScores.mean():
    bestMeanCV = -linregCVScores.mean()
    bestMeanCVModel = i
elif bestMeanCV == -1:
    bestMeanCV = -linregCVScores.mean()
    bestMeanCVModel = i

print('The final best model is {} and its TEST MSE is {}'.format(bestMeanCVModel,bestM
```

```
The final best model is OverallQual and its TEST MSE is 2371260934.069026
```

We can then iterate through the predictors adding it to the model each time in order to improve the test MSE of the model. For instance, in the above, we have selected as the first predictor in our model, the predictor 'OverallQual'. Next, we cycle through all the remaining predictors to include in our model along with 'OverallQual' and repeat. The final result will be a list of all predictors in the order they were added. Once we get to a point where adding another predictor to the model does not improve the test MSE, then we stop there.

```
In [112]: # Run through each model in the correct order and run CV on it and save the best CV
          bestMeanCV = None
          bestMeanCVModel = []
          oldArraySize = 0

          X = housePrice.drop('SalePrice',axis=1)

          columnsArray = X.columns

          # y is the response variable
          y = housePrice['SalePrice']

          while oldArraySize != len(X):
              bestPredictor = ''
              oldArraySize = len(X.columns)
              for i in columnsArray:
                  thisModel = bestMeanCVModel.copy()
                  thisModel.append(i)
                  # First set X to be the full set of remaining parameters
                  x = X.loc[:,thisModel]

                  if len(x.columns) == 1:
                      linregCVScores = cross_val_score(LinearRegression(),x.values.reshape(-1,1
                  else:
                      linregCVScores = cross_val_score(LinearRegression(),x,y,scoring='neg_mean
```

```
                if not bestMeanCV:
                    bestMeanCV = linregCVScores.mean()
                    bestPredictor = i
                elif bestMeanCV < linregCVScores.mean():
                    bestMeanCV = linregCVScores.mean()
                    bestPredictor = i

            if bestPredictor not in columnsArray:
                break

            columnsArray.drop(bestPredictor)
            bestMeanCVModel.append(bestPredictor)
            print('{} was added with test MSE {}'.format(bestMeanCVModel[-1],bestMeanCV))


        print('The final best model is {} and its TEST MSE is {}'.format(bestMeanCVModel,bes
```

```
OverallQual was added with test MSE -2371260934.069026
GrLivArea was added with test MSE -1821343747.2253425
BsmtFinSF1 was added with test MSE -1653396814.3900447
GarageCars was added with test MSE -1522575852.80887
YearRemodAdd was added with test MSE -1477506784.3227758
LotArea was added with test MSE -1445259871.69055
MasVnrArea was added with test MSE -1418244120.600768
KitchenAbvGr was added with test MSE -1399446462.6115127
1stFlrSF was added with test MSE -1376812086.0548759
YearBuilt was added with test MSE -1366762325.3833966
OverallCond was added with test MSE -1352021476.9079351
ScreenPorch was added with test MSE -1346347855.653913
WoodDeckSF was added with test MSE -1339278365.3061535
TotRmsAbvGrd was added with test MSE -1334799185.148554
BedroomAbvGr was added with test MSE -1315922220.78058
EnclosedPorch was added with test MSE -1315305925.9789593
PoolArea was added with test MSE -1314438332.6507847
GrLivArea was added with test MSE -1314438332.6507568
LotArea was added with test MSE -1314414828.8009648
OverallQual was added with test MSE -1313300135.6850371
WoodDeckSF was added with test MSE -1313028916.9084868
The final best model is ['OverallQual', 'GrLivArea', 'BsmtFinSF1', 'GarageCars', 'YearRemodAdd
```

Our final model is now contained in bestMeanCVModel.

1.3.4 Ridge Regression

Ridge Regression adds a twist to Linear Regression with the aim of reducing the variance of the model and managing multicollinearity.

We begin with the normal equation as we did for Linear Regression and arrive at a method of calculating the parameters of the regression formula.

As before, we pose a hypothesis ($h_\theta(X)$) and a cost function ($J(\theta)$) and proceed to minimise this cost function. Here, X is the data and θ is a vector of parameters (such as the β in the Linear Regression models above).

For Linear Regression as stated above, the hypothesis function is that there is a straight line passing through all the data points:

$$h_\theta(X) = \theta_0 + \theta_1 X_1 + \theta_2 X_2 + \theta_3 X_3 + ... = X\theta$$

The Cost function is the least squares sum residuals (eventually written in index notation):

$$J(\theta) = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (h_\theta(X^{(i)}) - Y^{(i)})^2 = (X\theta - Y)^T(X\theta - Y) = (X\theta)^T X\theta - 2(X\theta)^T Y + Y^T Y = \theta_j x_{ji} x_{ij} \theta_j - 2\theta_j x_{ji} y_i$$

where the superscript $^{(i)}$ refers to the ith observation. The extra step we will be taking here is to add an additional term in this equation which is the L2 norm $\lambda||\theta||^2 = \lambda \sum_{i=1}^{n} \theta_i^2 = \lambda\theta'^T\theta' = \lambda\theta'_j\theta'_j$, where θ' is the parameter vector θ but with the first term corresponding to the coefficient of the constant term set to zero and λ is a scaling factor or shrinkage factor:

$$J(\theta) = \theta_j x_{ji} x_{ij} \theta_j - 2\theta_j x_{ji} y_i + \lambda\theta'_j\theta'_j$$

Taking the derivative of the cost function:

$$\frac{\partial J(\theta)}{\partial \theta_k} = 2x_{ki}x_{ik}\theta_k - 2x_{ki}y_i + 2\lambda\theta'_k$$

where $\theta'_k = 0$ for $k = 0$.

Setting this to zero for all k and solving:

$$\theta = (X^T X + \lambda I')^{-1} X^T Y$$

where we have used the fact that $\theta' I = \theta I'$ with I the identity matrix and I' the identity matrix where element $I_{11} = 0$ (i.e. we are transfering effect of the first element of θ being zero to the identity matrix).

In summary, this additional regularisation term serves to attach a penalty to large coefficients in the minimisation process. It should be added that if we set $\lambda = 0$, no additional constraint is performed and we just get the Linear Regression solution.

Let's test this out the sklearn module:

$\lambda||\theta||^2 = \lambda \sum_{i=1}^{n} \theta_i^2 = \lambda\theta'^T\theta' = \lambda\theta'_j\theta'_j$

In [115]:
```
L = 0.2
normalize = False

# X is the predictor variable
X = housePrice.drop('SalePrice',axis=1)[['LotArea','YearBuilt']]

# y is the response variable
y = housePrice['SalePrice']
```

```
# Convert the predictor dataframe and the response dataframe to arrays to be consist
X = np.concatenate((np.ones((X.shape[0],1)),np.array(X)),axis=1)
y = np.array(y)

ncols = X.shape[1]

if normalize:
    # standardise X if required
    for i in range(1,ncols):
        X[:,i] = (X[:,i] - np.mean(X[:,i]))/np.std(X[:,i])

    # standardise y if required
    y = (y - np.mean(y))/np.std(y)

# Create transpose (3 X n)
X_T = X.transpose()

# Calculate X^T X (3 X 3)
XTX = X_T.dot(X)

# Create I'
Id = np.eye(XTX.shape[0])
Id[0,0] = 0

# Add the shrinkage factor part
XTX = XTX + L*Id

# calculate inverse of XTX + lambda I' (3 X 3)
XTX_inv = np.linalg.inv(XTX)

# Calculate theta
theta = XTX_inv.dot(X_T.dot(y))

print('Y_3 = {} + {} * LotArea + {} * YearBuilt'.format(theta[0],theta[1],theta[2]))
```

```
Y_3 = -2532855.620003462 + 2.041172157436325 * LotArea + 1365.7759478454827 * YearBuilt
```

We can run this using the package and we see the exact same results

```
In [116]: # X is the predictor variable
          X = housePrice.drop('SalePrice',axis=1)[['LotArea','YearBuilt']]

          # y is the response variable
          y = housePrice['SalePrice']

          ridgeModel = Ridge(alpha=0.2, normalize=False)
```

```
ridgeModel.fit(X,y)

ridgeModel.intercept_,ridgeModel.coef_
```

Out[116]: (-2532855.620003232, array([2.04117216, 1365.77594785]))

Let's see how different this performs compared to the usual Linear Regression model. We would like to test if we can reduce the MSE on unseen test data if we use a non-zero shrinkage factor. This will demonstrate that the solution to the Ridge Regression line is less effected by a change in the data.

First Linear Regression

In [118]:
```
# Run through each model in the correct order and run CV on it and save the best CV
bestMeanCV = None
bestMeanCVModel = []
oldArraySize = 0

X = housePrice.drop('SalePrice',axis=1)

columnsArray = X.columns.copy()

# y is the response variable
y = housePrice['SalePrice']

while oldArraySize != len(X):
    bestPredictor = ''
    oldArraySize = len(X.columns)
    for i in columnsArray:
        thisModel = bestMeanCVModel.copy()
        thisModel.append(i)
        # First set X to be the full set of remaining parameters
        x = X.loc[:,thisModel]

        if len(x.columns) == 1:
            linregCVScores = cross_val_score(Ridge(alpha=0.0001),x.values.reshape(-1
        else:
            linregCVScores = cross_val_score(Ridge(alpha=0.0001),x,y,scoring='neg_mea

        if not bestMeanCV:
            bestMeanCV = linregCVScores.mean()
            bestPredictor = i
        elif bestMeanCV < linregCVScores.mean():
            bestMeanCV = linregCVScores.mean()
            bestPredictor = i

    if bestPredictor not in columnsArray:
        break
```

```
        columnsArray = columnsArray.drop(bestPredictor)
        bestMeanCVModel.append(bestPredictor)
        print('{} was added with test MSE {}'.format(bestMeanCVModel[-1],bestMeanCV))


    print('The final best model is {} and its TEST MSE is {}'.format(bestMeanCVModel,bes
```

```
OverallQual was added with test MSE -2371260933.576952
GrLivArea was added with test MSE -1821343747.2524974
BsmtFinSF1 was added with test MSE -1653396815.643581
GarageCars was added with test MSE -1522575854.1067336
YearRemodAdd was added with test MSE -1477506784.5675159
LotArea was added with test MSE -1445259871.8107793
MasVnrArea was added with test MSE -1418244120.7510715
KitchenAbvGr was added with test MSE -1399446459.9374409
1stFlrSF was added with test MSE -1376812080.8984106
YearBuilt was added with test MSE -1366762319.9338892
OverallCond was added with test MSE -1352021471.1023602
ScreenPorch was added with test MSE -1346347849.9059243
WoodDeckSF was added with test MSE -1339278358.4927483
TotRmsAbvGrd was added with test MSE -1334799178.888196
BedroomAbvGr was added with test MSE -1315922213.1356974
EnclosedPorch was added with test MSE -1315305918.2179291
PoolArea was added with test MSE -1314438325.8843122
The final best model is ['OverallQual', 'GrLivArea', 'BsmtFinSF1', 'GarageCars', 'YearRemodAdd
```

Now with a larger λ

```
In [119]: # Run through each model in the correct order and run CV on it and save the best CV
          bestMeanCV = None
          bestMeanCVModel = []
          oldArraySize = 0

          X = housePrice.drop('SalePrice',axis=1)

          columnsArray = X.columns.copy()

          # y is the response variable
          y = housePrice['SalePrice']

          while oldArraySize != len(X):
              bestPredictor = ''
              oldArraySize = len(X.columns)
              for i in columnsArray:
                  thisModel = bestMeanCVModel.copy()
                  thisModel.append(i)
                  # First set X to be the full set of remaining parameters
```

```
                x = X.loc[:,thisModel]

                if len(x.columns) == 1:
                    linregCVScores = cross_val_score(Ridge(alpha=6),x.values.reshape(-1,1),y
                else:
                    linregCVScores = cross_val_score(Ridge(alpha=6),x,y,scoring='neg_mean_sq

                if not bestMeanCV:
                    bestMeanCV = linregCVScores.mean()
                    bestPredictor = i
                elif bestMeanCV < linregCVScores.mean():
                    bestMeanCV = linregCVScores.mean()
                    bestPredictor = i

            if bestPredictor not in columnsArray:
                break

            columnsArray = columnsArray.drop(bestPredictor)
            bestMeanCVModel.append(bestPredictor)
            print('{} was added with test MSE {}'.format(bestMeanCVModel[-1],bestMeanCV))


        print('The final best model is {} and its TEST MSE is {}'.format(bestMeanCVModel,bes
```

```
OverallQual was added with test MSE -2371254029.0760694
GrLivArea was added with test MSE -1821363518.5244935
BsmtFinSF1 was added with test MSE -1653488270.7651806
GarageCars was added with test MSE -1522674235.152098
YearRemodAdd was added with test MSE -1477543064.7221112
LotArea was added with test MSE -1445288001.4210088
MasVnrArea was added with test MSE -1418272851.0154374
KitchenAbvGr was added with test MSE -1399503544.1065402
1stFlrSF was added with test MSE -1376798534.1186767
YearBuilt was added with test MSE -1366723443.0781755
OverallCond was added with test MSE -1351925127.2305455
ScreenPorch was added with test MSE -1346240217.2577364
WoodDeckSF was added with test MSE -1339095696.4405167
TotRmsAbvGrd was added with test MSE -1334732891.2793584
BedroomAbvGr was added with test MSE -1315808790.2185073
EnclosedPorch was added with test MSE -1315182547.8506525
PoolArea was added with test MSE -1314370013.4542491
Fireplaces was added with test MSE -1314248045.3630013
The final best model is ['OverallQual', 'GrLivArea', 'BsmtFinSF1', 'GarageCars', 'YearRemodAdd
```

A small improvement in the test MSE. Running Ridge Regression with the identified features gives us the coefficients:

```
In [120]: X = housePrice.drop('SalePrice',axis=1)[bestMeanCVModel]
```

```
# y is the response variable
y = housePrice['SalePrice']

rm = Ridge(alpha=6)
rm.fit(X,y)

s = 'SalePrice = {}'.format(round(rm.intercept_,2))

for i,j in zip(rm.coef_,bestMeanCVModel):
    s = s + ' + {}*{}'.format(round(i,2),j)

s
```

```
Out[120]: 'SalePrice = -1114268.8 + 17481.52*OverallQual + 39.74*GrLivArea + 16.75*BsmtFinSF1 +
```

1.3.5 Reproducing P-Values

First we will use statsmodels to give us the p-values of the coefficients. Then we will show that we can calculate these ourselves using linear algebra. Then we will use our method to calculate the p-values for the Ridge Regression model.

```
In [121]: X = housePrice.drop('SalePrice',axis=1)[bestMeanCVModel]

          # y is the response variable
          y = housePrice['SalePrice']

          X_new = sm.add_constant(X)
          est = sm.OLS(y, X_new)
          est2 = est.fit()
          print(est2.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:              SalePrice   R-squared:                       0.804
Model:                            OLS   Adj. R-squared:                  0.802
Method:                 Least Squares   F-statistic:                     329.2
Date:                Sat, 27 Jul 2019   Prob (F-statistic):               0.00
Time:                        18:37:58   Log-Likelihood:                -17353.
No. Observations:                1460   AIC:                         3.474e+04
Df Residuals:                    1441   BIC:                         3.484e+04
Df Model:                          18
Covariance Type:            nonrobust
=================================================================================
                    coef    std err          t      P>|t|      [0.025      0.975]
---------------------------------------------------------------------------------
const           -1.1e+06   1.22e+05     -9.011      0.000   -1.34e+06    -8.6e+05
OverallQual    1.745e+04   1156.715     15.082      0.000    1.52e+04    1.97e+04
GrLivArea        39.4748      4.039      9.774      0.000      31.552      47.398
```

```
BsmtFinSF1        16.7307      2.424      6.903      0.000      11.976      21.485
GarageCars      1.151e+04   1714.064      6.716      0.000    8148.780    1.49e+04
YearRemodAdd     190.8258     65.700      2.905      0.004      61.948     319.703
LotArea            0.4987      0.101      4.932      0.000       0.300       0.697
MasVnrArea        28.8277      5.961      4.836      0.000      17.135      40.521
KitchenAbvGr   -2.381e+04   4777.891     -4.983      0.000   -3.32e+04   -1.44e+04
1stFlrSF          18.4213      3.377      5.456      0.000      11.798      25.045
YearBuilt        334.5033     56.393      5.932      0.000     223.882     445.124
OverallCond     4361.6048   1020.554      4.274      0.000    2359.674    6363.535
ScreenPorch       54.3900     17.323      3.140      0.002      20.408      88.372
WoodDeckSF        26.3639      8.007      3.293      0.001      10.658      42.070
TotRmsAbvGrd    5850.6359   1243.198      4.706      0.000    3411.964    8289.308
BedroomAbvGr   -8433.9916   1674.575     -5.036      0.000   -1.17e+04   -5149.126
EnclosedPorch     18.4944     16.992      1.088      0.277     -14.838      51.827
PoolArea         -37.1000     23.830     -1.557      0.120     -83.846       9.646
Fireplaces      2986.9485   1761.315      1.696      0.090    -468.067    6441.964
==============================================================================
Omnibus:                      627.897   Durbin-Watson:                   1.962
Prob(Omnibus):                  0.000   Jarque-Bera (JB):           106807.567
Skew:                          -0.886   Prob(JB):                         0.00
Kurtosis:                      44.864   Cond. No.                     1.94e+06
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.94e+06. This might indicate that there are
strong multicollinearity or other numerical problems.


C:\Users\HVAD\Anaconda3\lib\site-packages\numpy\core\fromnumeric.py:52: FutureWarning: Method
  return getattr(obj, method)(*args, **kwds)
```

Let $\hat{\theta}$ be an unbiased estimator of θ and $\hat{Y}$ be the fitted values for Y. i.e. we expect that $E[\hat{\theta}] = \theta$ and $E[\hat{Y}] = Y$.

Then the variance of the estimator can be calculated as follows:

$$\sigma^2_{\hat{\theta}} = E[(\hat{\theta} - E[\hat{\theta}])(\hat{\theta} - E[\hat{\theta}])^T] = E[(\hat{\theta} - \theta)(\hat{\theta} - \theta)^T] = E[((X^TX)^{-1}X^T(\hat{Y} - Y))((X^TX)^{-1}X^T(\hat{Y} - Y))^T] = (X^TX)^{-1}$$

where $\hat{Y} - Y = e$ are the residuals and $MSE = \frac{\sum_{i=1}^{n}(\hat{Y}^{(i)} - Y^{(i)})^2}{n-p}$ is the Mean Squared Error with p predictors.

```
In [122]: # Get the coefficient solutions from the model
          coefs = np.append(est2.params[0],est2.params[1:])

          # Get the predictions (X_new includes the constant term)
          predictions = est2.predict(X_new)
```

```
# Calculate the MSE
MSE = (sum((y-predictions)**2))/(len(X_new)-len(X_new.columns))

# Calculate the variance
var = MSE*(np.linalg.inv(np.dot(X_new.T,X_new)).diagonal())

# Calculate the standard deviation
sd = np.sqrt(var)

# Calculate the t-statistics
t = coefs/ sd

# Calculate the p-values using the t-statistics and the t-distribution (2 is two-sid
p_values =[2*(1-stats.t.cdf(np.abs(i),(len(X_new)-1))) for i in t]

# 3 decimal places to match statsmodels output
var = np.round(var,3)
t = np.round(t,3)
p_values = np.round(p_values,3)

# 4 decimal places to match statsmodels
coefs = np.round(coefs,4)

summary_df = pd.DataFrame()
summary_df["Features"],summary_df["coef"],summary_df["std err"],summary_df["t"],summa
    X_new.columns,coefs,sd,t,p_values]
print(summary_df)
```

```
         Features          coef        std err       t  P > |t|
0           const -1.099679e+06  122041.446311  -9.011    0.000
1     OverallQual  1.744563e+04    1156.714726  15.082    0.000
2       GrLivArea  3.947480e+01       4.038924   9.774    0.000
3      BsmtFinSF1  1.673070e+01       2.423746   6.903    0.000
4      GarageCars  1.151111e+04    1714.064086   6.716    0.000
5    YearRemodAdd  1.908258e+02      65.699730   2.905    0.004
6         LotArea  4.987000e-01       0.101129   4.932    0.000
7      MasVnrArea  2.882770e+01       5.960942   4.836    0.000
8    KitchenAbvGr -2.380787e+04    4777.891291  -4.983    0.000
9        1stFlrSF  1.842130e+01       3.376628   5.456    0.000
10      YearBuilt  3.345033e+02      56.393014   5.932    0.000
11    OverallCond  4.361605e+03    1020.553865   4.274    0.000
12    ScreenPorch  5.439000e+01      17.323448   3.140    0.002
13     WoodDeckSF  2.636390e+01       8.006592   3.293    0.001
14   TotRmsAbvGrd  5.850636e+03    1243.198150   4.706    0.000
15   BedroomAbvGr -8.433992e+03    1674.574959  -5.036    0.000
16  EnclosedPorch  1.849440e+01      16.992309   1.088    0.277
17       PoolArea -3.710000e+01      23.830194  -1.557    0.120
```

```
18     Fireplaces  2.986948e+03    1761.314694   1.696    0.090
```

```
In [123]: def fitAndPValues(model,X,y):
              # Get the coefficient solutions from the model
              coefs = []
              if 'params' in dir(model):
                  coefs = np.append(model.params[0],model.params[1:])
              else:
                  coefs = np.append(model.intercept_,model.coef_)

              # Get the predictions (X_new includes the constant term)
              predictions = model.predict(X)

              if len(X.columns) < len(coefs):
                  X = X.copy()
                  X.insert(0,'Const',1)

              # Calculate the MSE
              MSE = (sum((y-predictions)**2))/(len(X)-len(X.columns))

              # Calculate the variance
              var = MSE*(np.linalg.inv(np.dot(X.T,X)).diagonal())

              # Calculate the standard deviation
              sd = np.sqrt(var)

              # Calculate the t-statistics
              t = coefs/ sd

              # Calculate the p-values using the t-statistics and the t-distribution (2 is two
              p_values =[2*(1-stats.t.cdf(np.abs(i),(len(X)-1))) for i in t]

              # 3 decimal places to match statsmodels output
              var = np.round(var,3)
              t = np.round(t,3)
              p_values = np.round(p_values,3)

              # 4 decimal places to match statsmodels
              coefs = np.round(coefs,4)

              summary_df = pd.DataFrame()
              summary_df["Features"],summary_df["coef"],summary_df["std err"],summary_df["t"],s

              print(summary_df)
```

Let's make sure our Ridge Regression p-values match the statsmodels outputs when we set the shrinkage term to 0 (i.e. Linear Regression without the L2 norm term)

```
In [124]: X = housePrice.drop('SalePrice',axis=1)[bestMeanCVModel]

          # y is the response variable
          y = housePrice['SalePrice']

          rm = Ridge(alpha=0)
          rm.fit(X,y)

          fitAndPValues(rm,X,y)
```

```
        Features          coef        std err       t  P > |t|
0          Const -1.099679e+06  122041.446311  -9.011    0.000
1    OverallQual  1.744563e+04    1156.714726  15.082    0.000
2      GrLivArea  3.947480e+01       4.038924   9.774    0.000
3     BsmtFinSF1  1.673070e+01       2.423746   6.903    0.000
4     GarageCars  1.151111e+04    1714.064086   6.716    0.000
5   YearRemodAdd  1.908258e+02      65.699730   2.905    0.004
6        LotArea  4.987000e-01       0.101129   4.932    0.000
7     MasVnrArea  2.882770e+01       5.960942   4.836    0.000
8   KitchenAbvGr -2.380787e+04    4777.891291  -4.983    0.000
9       1stFlrSF  1.842130e+01       3.376628   5.456    0.000
10     YearBuilt  3.345033e+02      56.393014   5.932    0.000
11   OverallCond  4.361605e+03    1020.553865   4.274    0.000
12   ScreenPorch  5.439000e+01      17.323448   3.140    0.002
13    WoodDeckSF  2.636390e+01       8.006592   3.293    0.001
14  TotRmsAbvGrd  5.850636e+03    1243.198150   4.706    0.000
15  BedroomAbvGr -8.433992e+03    1674.574959  -5.036    0.000
16 EnclosedPorch  1.849440e+01      16.992309   1.088    0.277
17      PoolArea -3.710000e+01      23.830194  -1.557    0.120
18    Fireplaces  2.986948e+03    1761.314694   1.696    0.090
```

Now we are able to return p-values for Ridge Regression for our model with shrinkage term 6

```
In [125]: X = housePrice.drop('SalePrice',axis=1)[bestMeanCVModel]

          # y is the response variable
          y = housePrice['SalePrice']

          rm = Ridge(alpha=6)
          rm.fit(X,y)

          fitAndPValues(rm,X,y)
```

```
        Features          coef        std err       t  P > |t|
0          Const -1.114269e+06  122052.144169  -9.129    0.000
1    OverallQual  1.748152e+04    1156.816121  15.112    0.000
2      GrLivArea  3.974460e+01       4.039278   9.840    0.000
3     BsmtFinSF1  1.674920e+01       2.423958   6.910    0.000
```

4	GarageCars	1.137126e+04	1714.214337	6.634	0.000
5	YearRemodAdd	1.936712e+02	65.705489	2.948	0.003
6	LotArea	5.009000e-01	0.101138	4.953	0.000
7	MasVnrArea	2.895370e+01	5.961464	4.857	0.000
8	KitchenAbvGr	-2.149685e+04	4778.310109	-4.499	0.000
9	1stFlrSF	1.827980e+01	3.376924	5.413	0.000
10	YearBuilt	3.380716e+02	56.397957	5.994	0.000
11	OverallCond	4.390405e+03	1020.643324	4.302	0.000
12	ScreenPorch	5.493510e+01	17.324966	3.171	0.002
13	WoodDeckSF	2.665780e+01	8.007293	3.329	0.001
14	TotRmsAbvGrd	5.626965e+03	1243.307126	4.526	0.000
15	BedroomAbvGr	-8.289604e+03	1674.721749	-4.950	0.000
16	EnclosedPorch	1.892600e+01	16.993798	1.114	0.266
17	PoolArea	-3.721990e+01	23.832283	-1.562	0.119
18	Fireplaces	3.096515e+03	1761.469087	1.758	0.079

1.3.6 Module for Ridge Regression

In [150]:
```python
class RidgeRegression(Ridge):
    '''
    This class inherits from the Ridge class in the sklearn package. It extends that
    adding the capability to produce p-values, run feature selection and find the be
    which minimises the MSE
    '''

    def summary(self,X,y):
        '''
        This method produces a summary similar to the one produced by statsmodels.ap
        It includes the coefficients and their p-values in a summary table
        :param X: features array
        :param y: response array
        '''

        # This will store the coefficients of the model that has already been run
        coefs = []

        # If the model was fit with an intercept
        if 'intercept_' in dir(self):
            coefs = np.append(self.intercept_,self.coef_)
        else:
            coefs = self.coef_

        # Get the predictions
        predictions = self.predict(X)

        # If a constant column needs to be added (determine this dynamically)
        if len(X.columns) < len(coefs):
```

```python
        X = X.copy()
        X.insert(0,'Const',1)

    # Calculate the MSE
    MSE = (sum((y-predictions)**2))/(len(X)-len(X.columns))

    # Calculate the variance
    var = MSE*(np.linalg.inv(np.dot(X.T,X)).diagonal())

    # Calculate the standard deviation
    sd = np.sqrt(var)

    # Calculate the t-statistics
    t = coefs/ sd

    # Calculate the p-values using the t-statistics and the t-distribution (2 is
    p_values =[2*(1-stats.t.cdf(np.abs(i),(len(X)-1))) for i in t]

    # 3 decimal places to match statsmodels output
    var = np.round(var,3)
    t = np.round(t,3)
    p_values = np.round(p_values,3)

    # 4 decimal places to match statsmodels
    coefs = np.round(coefs,4)

    # Summary dataframe
    summary_df = pd.DataFrame()
    summary_df["Features"],summary_df["coef"],summary_df["std err"],summary_df["

    print(summary_df)

def findBestAlpha(self,X,y,silent=True):
    '''
    This method keeps changing alpha until the MSE is reduced as much as it can
    alpha selection depends on input datasets
    :param X: features array
    :param y: response array
    :param silent: if True, then progress is omitted
    '''

    silent = True
    alpha = 1
    prevAlpha = None
    bestMSE = None
    tol = 0.000001
    doublingMode = True
```

```
# Here, we start by continuously doubling alpha until we get to a point where
# Then, at this point, we switch to incrementing (or decrementing) by smalle
while True:
    # Calculate the MSE using this alpha
    thisMSE = np.mean(cross_val_score(RidgeRegression(alpha=alpha),X,y,scorin

    if not silent:
        print('alpha = {}\nbestMSE = {}\nthisMSE = {}\n############'.format

    # if doubling mode
    if doublingMode:
        # update bestMSE
        if (not bestMSE) or (bestMSE < thisMSE):
            bestMSE = thisMSE
        else:
            if not silent:
                print('Doubling Finished!!!!')

            # switch the mode and roll back alpha to the previous one
            doublingMode = False
            tempAlpha = prevAlpha
            prevAlpha = alpha
            alpha = tempAlpha
            continue

        # update alpha
        prevAlpha = alpha
        alpha = (alpha + 0.001)*2
    else:
        # update alpha to |alpha-prevAlpha|/2 away from where it currently i
        ghostPoint = alpha + (alpha - prevAlpha)
        nextAlpha1 = (prevAlpha + alpha)/2
        nextAlpha2 = (alpha + ghostPoint)/2

        # The Ridge class has numerical issues when alpha is close to zero
        if(nextAlpha1 < 0.0001):
            nextAlpha1 = 0.0001
        if(nextAlpha2 < 0.0001):
            nextAlpha2 = 0.0001

        # Calculate the MSE on either side of alpha
        MSE1 = np.mean(cross_val_score(RidgeRegression(alpha=nextAlpha1),X,y
        MSE2 = np.mean(cross_val_score(RidgeRegression(alpha=nextAlpha2),X,y

        # Choose the MSE and the corresponding alpha of the one that is bett
        if (MSE1 > MSE2) and (MSE1 > bestMSE) and (np.abs(prevAlpha - alpha)
            prevAlpha = alpha
            alpha = nextAlpha1
```

```python
                bestMSE = MSE1
            elif (MSE2 > MSE1) and (MSE2 > bestMSE) and (np.abs(prevAlpha - alpha
                prevAlpha = alpha
                alpha = nextAlpha2
                bestMSE = MSE2
            else:
                if (np.abs(prevAlpha - alpha) > tol):
                    # pull prevAlpha closer to alpha
                    prevAlpha = (prevAlpha + alpha)/2
                else:
                    alpha = prevAlpha
                    break

        self.alpha = alpha
        print('Ridge Regression MSE = {}, best alpha = {}'.format(bestMSE,alpha))

    def featureSelection(self,X,y):
        '''
        This method iterates and adds a new feature to the features list in the
        order of best improvement of MSE
        :param X: features array
        :param y: response array
        '''

        # Run through each model in the correct order and run CV on it and save the
        bestMeanCV = None
        bestMeanCVModel = []
        oldArraySize = 0

        columnsArray = X.columns.copy()

        while oldArraySize != len(X):
            bestPredictor = ''
            oldArraySize = len(X.columns)
            for i in columnsArray:
                thisModel = bestMeanCVModel.copy()
                thisModel.append(i)
                # First set X to be the full set of remaining parameters
                x = X.loc[:,thisModel]

                if len(x.columns) == 1:
                    linregCVScores = cross_val_score(Ridge(alpha=self.alpha),x.value
                else:
                    linregCVScores = cross_val_score(Ridge(alpha=self.alpha),x,y,sco

            if not bestMeanCV:
                bestMeanCV = linregCVScores.mean()
                bestPredictor = i
```

```
                elif bestMeanCV < linregCVScores.mean():
                    bestMeanCV = linregCVScores.mean()
                    bestPredictor = i

                if bestPredictor not in columnsArray:
                    break

                columnsArray = columnsArray.drop(bestPredictor)
                bestMeanCVModel.append(bestPredictor)
                print('{} was added with test MSE {}'.format(bestMeanCVModel[-1],bestMea


            self.bestMeanCVModel = bestMeanCVModel
            self.bestMeanCV = bestMeanCV
            print('The final best model is {} and its TEST MSE is {}'.format(bestMeanCVM
```

```
In [151]: X = housePrice.drop('SalePrice',axis=1)[bestMeanCVModel]

          # y is the response variable
          y = housePrice['SalePrice']

          rm = RidgeRegression(alpha=6)
          rm.fit(X,y)
          rm.summary(X,y)
```

	Features	coef	std err	t	P > |t|
0	Const	-1.114269e+06	122052.144169	-9.129	0.000
1	OverallQual	1.748152e+04	1156.816121	15.112	0.000
2	GrLivArea	3.974460e+01	4.039278	9.840	0.000
3	BsmtFinSF1	1.674920e+01	2.423958	6.910	0.000
4	GarageCars	1.137126e+04	1714.214337	6.634	0.000
5	YearRemodAdd	1.936712e+02	65.705489	2.948	0.003
6	LotArea	5.009000e-01	0.101138	4.953	0.000
7	MasVnrArea	2.895370e+01	5.961464	4.857	0.000
8	KitchenAbvGr	-2.149685e+04	4778.310109	-4.499	0.000
9	1stFlrSF	1.827980e+01	3.376924	5.413	0.000
10	YearBuilt	3.380716e+02	56.397957	5.994	0.000
11	OverallCond	4.390405e+03	1020.643324	4.302	0.000
12	ScreenPorch	5.493510e+01	17.324966	3.171	0.002
13	WoodDeckSF	2.665780e+01	8.007293	3.329	0.001
14	TotRmsAbvGrd	5.626965e+03	1243.307126	4.526	0.000
15	BedroomAbvGr	-8.289604e+03	1674.721749	-4.950	0.000
16	EnclosedPorch	1.892600e+01	16.993798	1.114	0.266
17	PoolArea	-3.721990e+01	23.832283	-1.562	0.119
18	Fireplaces	3.096515e+03	1761.469087	1.758	0.079

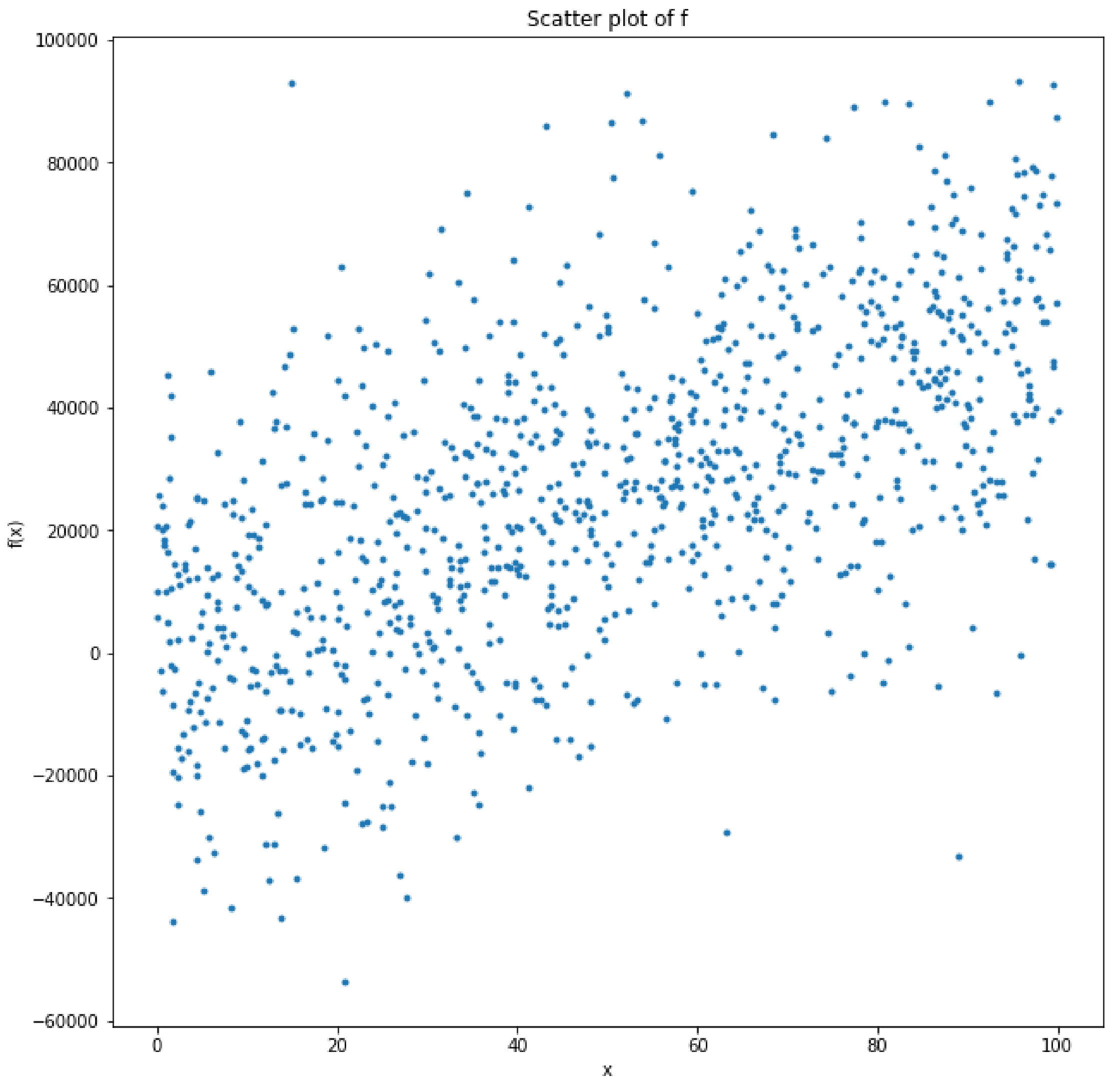
1.3.7 Ridge Regression and Multicollinearity

Steps:
Create data and 2 variables to create a multicollinear problem
Split the data into train and test
Show using statsmodels.api that we have multicollinearity
Linear Regression
Show cross-validated mean squared error
Train on training dataset and show mean squared error on test dataset
Ridge Regression
Show cross-validated mean squared error
Find the value of alpha in Ridge Regression which minimises MSE. This should better than Linear Regression
Compare coefficients between Linear Regression and Ridge Regression
Compare summary outputs between Ridge Regression and Linear Regression
Predict a new set of points and find MSE for Linear Regression and Ridge Regression
Confirm that the standard deviation of predictions is smaller for Ridge Regression than for Linear Regression
Apply Ridge Regression and Linear Regression to the housing dataset and confirm that the MSE and prediction standard deviation are smaller for Ridge Regression

In [152]:
```
# Create data and 2 variables to create a multicollinear problem

def f(x):
    return 4.67 + 507*x

# Set the seed
r = np.random.RandomState(101)

# Choose 1000 random observations for x between 0 and 100
X1 = 100*r.rand(1000)

# Create a correlated variable
X2 = X1 + 100 + 1*r.randn(1000)

#Error term with sigma = 100, mu = 0, randn samples from the standard normal distrib
E = 20000*r.randn(1000)

#Response variables
Y = list(map(f,X1))+E
```

In [153]:
```
# Plot
fig = plt.figure(figsize=(8,8))
axes = fig.add_axes([0.1,0.1,1,1])
axes.plot(X1,Y,'.')

# Set labels and title
axes.set_xlabel('x')
axes.set_ylabel('f(x)')
```

```
axes.set_title('Scatter plot of f')

plt.show()
```



In [154]:
```
# Split the data into train test

X = pd.concat([pd.DataFrame(X1,columns=['X1']),pd.DataFrame(X2,columns=['X2'])],axis=
X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=0.33, random_sta
```

In [155]:
```
# Show correlation
X_train.corr()
```

Out[155]:

	X1	X2
X1	1.000000	0.999391
X2	0.999391	1.000000

In [156]:
```
# Show using statsmodels.api that we have multicollinearity

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

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

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

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

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.365
Model:                            OLS   Adj. R-squared:                  0.363
Method:                 Least Squares   F-statistic:                     191.9
Date:                Sat, 27 Jul 2019   Prob (F-statistic):           1.43e-66
Time:                        18:49:08   Log-Likelihood:                -7616.5
No. Observations:                 670   AIC:                         1.524e+04
Df Residuals:                     667   BIC:                         1.525e+04
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const      -3.352e+04    8.1e+04     -0.414      0.679   -1.93e+05    1.26e+05
X1           215.3056    808.737      0.266      0.790   -1372.672    1803.283
X2           337.7488    808.747      0.418      0.676   -1250.248    1925.746
==============================================================================
Omnibus:                        6.860   Durbin-Watson:                   1.933
Prob(Omnibus):                  0.032   Jarque-Bera (JB):                9.425
Skew:                           0.051   Prob(JB):                      0.00898
Kurtosis:                       3.572   Cond. No.                     1.63e+04
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.63e+04. This might indicate that there are
strong multicollinearity or other numerical problems.


C:\Users\HVAD\Anaconda3\lib\site-packages\numpy\core\fromnumeric.py:52: FutureWarning: Method
  return getattr(obj, method)(*args, **kwds)
```

In [157]:
```
# LINEAR REGRESSION
```

```
# Show cross-validated mean squared error

np.mean(cross_val_score(LinearRegression(),X_train,y_train,scoring='neg_mean_squared_
```

Out[157]: -443116270.3419094

In [158]:
```
# Train on training set and show mean squared error on test set

lm = LinearRegression()
lm.fit(X_train,y_train)
(lm.predict(X_test) - y_test).dot(lm.predict(X_test) - y_test)
```

Out[158]: 139251509589.51065

In [159]:
```
# RIDGE REGRESSION
# Show cross-validated mean squared error

np.mean(cross_val_score(RidgeRegression(alpha=1000),X_train,y_train,scoring='neg_mean
```

Out[159]: -441532513.0246685

In [160]:
```
# Find the value of alpha in Ridge Regression which minimises MSE
rmtest = RidgeRegression()
rmtest.findBestAlpha(X_train,y_train)
```

```
Ridge Regression MSE = -441146916.2805335, best alpha = 11468.420305810927
```

In [161]:
```
bestAlpha = rmtest.alpha
bestAlpha
```

Out[161]: 11468.420305810927

This is an improvement over Linear Regression. Let's look at the differences in the parameter estimations of the two models

In [162]:
```
# Compare coefficients between Linear Regression and Ridge Regression
lm = LinearRegression()
lm.fit(X_train,y_train)
print('Parameters of the linear regression model = {}'.format([lm.intercept_,lm.coef_

rm = RidgeRegression(alpha=bestAlpha)
rm.fit(X_train,y_train)
print('Parameters of the linear regression model = {}'.format([rm.intercept_,rm.coef_
```

```
Parameters of the linear regression model = [-33517.19098806189, array([215.30558151, 337.7488
Parameters of the linear regression model = [-26991.170068539966, array([271.94186319, 275.4289
```

Now let's look at the standard deviations of the parameters of the Ridge Regression model and compare them to the Linear Regression output from the statsmodels.api output

```
In [163]: # Compare summary outputs between Ridge Regression and Linear Regression
          print('RIDGE REGRESSION SUMMARY')
          rm.summary(X_train,y_train)

          print('\n\nLINEAR REGRESSION SUMMARY')
          rmlm = RidgeRegression(alpha=0)
          rmlm.fit(X_train,y_train)
          print('Parameters of the linear regression model = {}'.format([rmlm.intercept_,rmlm.
          rmlm.summary(X_train,y_train)
```

```
RIDGE REGRESSION SUMMARY
  Features        coef       std err      t  P > |t|
0    Const -26991.1701  80996.557139 -0.333    0.739
1       X1    271.9419    808.765278  0.336    0.737
2       X2    275.4290    808.775094  0.341    0.734



LINEAR REGRESSION SUMMARY
Parameters of the linear regression model = [-33517.19098807497, array([215.30558151, 337.7488
  Features        coef       std err      t  P > |t|
0    Const -33517.1910  80993.767760 -0.414    0.679
1       X1    215.3056    808.737425  0.266    0.790
2       X2    337.7488    808.747241  0.418    0.676
```

```
In [164]: # Predict a new set of points and find MSE for Linear Regression and Ridge Regressio

          print('Linear Regression MSE = {}'.format((rmlm.predict(X_test) - y_test).dot(rmlm.pr
          print('Ridge Regression MSE = {}'.format((rm.predict(X_test) - y_test).dot(rm.predic
```

```
Linear Regression MSE = 139251509589.5106
Ridge Regression MSE = 139075651590.56067
```

And how much do the predictions vary

```
In [165]: # Confirm that the standard deviation of predictions is smaller for Ridge Regression

          rmpredictions = []
          for i,j in list(zip(list(X_test.values),list(y_test))):
              rmpredictions.append(rm.predict(i.reshape(1,-1)))

          rmlmpredictions = []
          for i,j in list(zip(list(X_test.values),list(y_test))):
              rmlmpredictions.append(rmlm.predict(i.reshape(1,-1)))

          print('Standard deviation of Linear Regression predictions = {}'.format(np.std(rmlmp
          print('Standard deviation of Ridge Regression predictions = {}'.format(np.std(rmpred
```

```
Standard deviation of Linear Regression predictions = 15687.352084606513
Standard deviation of Ridge Regression predictions = 15526.206678003531
```

1.3.8 Summary steps

```
In [167]: # The local module containing our custom RidgeRegression class
          import Regression

          # Predictor variables
          X = housePrice.drop('SalePrice',axis=1)

          # Response variable
          y = housePrice['SalePrice']

          # Create a RidgeRegression object
          rm = Regression.RidgeRegression()

          # Run the feature selection method as above to limit to the most important variables
          # Stores the order of variables to the object
          rm.featureSelection(X,y)

          # Find the value of alpha minimising MSE for these features
          rm.findBestAlpha(X[rm.bestMeanCVModel],y)

          # Print the alpha
          print('Alpha = {}'.format(rm.alpha))

          # Fit the model with the best features and the alpha
          rm.fit(X[rm.bestMeanCVModel],y)

          # Display a summary including p-values
          rm.summary(X[rm.bestMeanCVModel],y)
```

```
OverallQual was added with test neg_mean_squared_error -2371256644.090804
GrLivArea was added with test neg_mean_squared_error -1821344525.7839134
BsmtFinSF1 was added with test neg_mean_squared_error -1653409803.8064983
GarageCars was added with test neg_mean_squared_error -1522589407.420225
YearRemodAdd was added with test neg_mean_squared_error -1477509838.9287422
LotArea was added with test neg_mean_squared_error -1445261661.6914485
MasVnrArea was added with test neg_mean_squared_error -1418246177.6939814
KitchenAbvGr was added with test neg_mean_squared_error -1399426759.141863
1stFlrSF was added with test neg_mean_squared_error -1376770121.511752
YearBuilt was added with test neg_mean_squared_error -1366717179.473287
OverallCond was added with test neg_mean_squared_error -1351971584.6744504
ScreenPorch was added with test neg_mean_squared_error -1346298056.478502
WoodDeckSF was added with test neg_mean_squared_error -1339217526.5940492
TotRmsAbvGrd was added with test neg_mean_squared_error -1334746769.416609
```

```
BedroomAbvGr was added with test neg_mean_squared_error -1315857153.2608094
EnclosedPorch was added with test neg_mean_squared_error -1315239600.5930305
PoolArea was added with test neg_mean_squared_error -1314381817.375801
Fireplaces was added with test neg_mean_squared_error -1314367411.2780588
The final best model is ['OverallQual', 'GrLivArea', 'BsmtFinSF1', 'GarageCars', 'YearRemodAdd
Ridge Regression neg_mean_squared_error = -1314242814.4290702, best alpha = 5.0823069858551015
Alpha = 5.0823069858551015
         Features          coef        std err       t  P > |t|
0           Const -1.112135e+06  122049.345972  -9.112    0.000
1     OverallQual  1.747749e+04    1156.789600  15.109    0.000
2       GrLivArea  3.970460e+01       4.039186   9.830    0.000
3      BsmtFinSF1  1.674660e+01       2.423903   6.909    0.000
4      GarageCars  1.139215e+04    1714.175037   6.646    0.000
5    YearRemodAdd  1.932458e+02      65.703982   2.941    0.003
6         LotArea  5.006000e-01       0.101136   4.950    0.000
7      MasVnrArea  2.893470e+01       5.961328   4.854    0.000
8    KitchenAbvGr -2.181997e+04    4778.200560  -4.567    0.000
9        1stFlrSF  1.829860e+01       3.376846   5.419    0.000
10      YearBuilt  3.375494e+02      56.396664   5.985    0.000
11    OverallCond  4.386581e+03    1020.619925   4.298    0.000
12    ScreenPorch  5.485660e+01      17.324569   3.166    0.002
13     WoodDeckSF  2.661620e+01       8.007110   3.324    0.001
14   TotRmsAbvGrd  5.658864e+03    1243.278622   4.552    0.000
15   BedroomAbvGr -8.310760e+03    1674.683354  -4.963    0.000
16  EnclosedPorch  1.886360e+01      16.993409   1.110    0.267
17       PoolArea -3.720020e+01      23.831736  -1.561    0.119
18     Fireplaces  3.081496e+03    1761.428703   1.749    0.080
```

In [168]:
```python
# The local module containing our custom RidgeRegression class
from model_arena import RidgeRegression

# Predictor variables
X = housePrice.drop('SalePrice',axis=1)

# Response variable
y = housePrice['SalePrice']

# Create a RidgeRegression object
rm = RidgeRegression()

# Run the feature selection method as above to limit to the most important variables
# Stores the order of variables to the object
rm.featureSelection(X,y)

# Find the value of alpha minimising MSE for these features
rm.findBestAlpha(X[rm.bestMeanCVModel],y)
```

```python
# Print the alpha
print('Alpha = {}'.format(rm.alpha))

# Fit the model with the best features and the alpha
rm.fit(X[rm.bestMeanCVModel],y)

# Display a summary including p-values
rm.summary(X[rm.bestMeanCVModel],y)
```

```
OverallQual was added with test MSE 2371254029.0760694
GrLivArea was added with test MSE 1821363518.5244935
BsmtFinSF1 was added with test MSE 1653488270.7651806
GarageCars was added with test MSE 1522674235.152098
YearRemodAdd was added with test MSE 1477543064.7221112
LotArea was added with test MSE 1445288001.4210088
MasVnrArea was added with test MSE 1418272851.0154374
KitchenAbvGr was added with test MSE 1399503544.1065402
1stFlrSF was added with test MSE 1376798534.1186767
YearBuilt was added with test MSE 1366723443.0781755
OverallCond was added with test MSE 1351925127.2305455
ScreenPorch was added with test MSE 1346240217.2577364
WoodDeckSF was added with test MSE 1339095696.4405167
TotRmsAbvGrd was added with test MSE 1334732891.2793584
BedroomAbvGr was added with test MSE 1315808790.2185073
EnclosedPorch was added with test MSE 1315182547.8506525
PoolArea was added with test MSE 1314370013.4542491
Fireplaces was added with test MSE 1314248045.3630013
The final best model is ['OverallQual', 'GrLivArea', 'BsmtFinSF1', 'GarageCars', 'YearRemodAdd
Ridge Regression MSE = -1314242814.4290702, best alpha = 5.0823069858551015
Alpha = 5.0823069858551015
         Features          coef        std err       t  P > |t|
0           Const -1.112135e+06  122049.345972  -9.112    0.000
1     OverallQual  1.747749e+04    1156.789600  15.109    0.000
2       GrLivArea  3.970460e+01       4.039186   9.830    0.000
3      BsmtFinSF1  1.674660e+01       2.423903   6.909    0.000
4      GarageCars  1.139215e+04    1714.175037   6.646    0.000
5    YearRemodAdd  1.932458e+02      65.703982   2.941    0.003
6         LotArea  5.006000e-01       0.101136   4.950    0.000
7      MasVnrArea  2.893470e+01       5.961328   4.854    0.000
8    KitchenAbvGr -2.181997e+04    4778.200560  -4.567    0.000
9        1stFlrSF  1.829860e+01       3.376846   5.419    0.000
10      YearBuilt  3.375494e+02      56.396664   5.985    0.000
11    OverallCond  4.386581e+03    1020.619925   4.298    0.000
12    ScreenPorch  5.485660e+01      17.324569   3.166    0.002
13     WoodDeckSF  2.661620e+01       8.007110   3.324    0.001
14   TotRmsAbvGrd  5.658864e+03    1243.278622   4.552    0.000
15   BedroomAbvGr -8.310760e+03    1674.683354  -4.963    0.000
16  EnclosedPorch  1.886360e+01      16.993409   1.110    0.267
```

```
17        PoolArea -3.720020e+01       23.831736  -1.561    0.119
18      Fireplaces  3.081496e+03    1761.428703   1.749    0.080
```

1.4 Appendix

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

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

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

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

$$= \frac{1}{n}\left(\sum_{i=1}^{n} x_i + nx_{n+1}\right)^2 > 0$$

This proves the statement. This assumes that at least one X_i is non-zero.

1.4.2 A2 - Maximum Likelihood Estimation (MLE)

Let's assume that there is a linear relationship between the response and predictor variables and that any discrepency is due to random noise, this is expressed as

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

where the errors are normally distributed, $\epsilon \sim N(0, \sigma^2)$. Then, the response variable given the data are normally distributed

$$Y_i | X_i \sim N(\beta_0 + \beta_1 X_i, \sigma^2)$$

where the mean or expectation is

$$E\left[Y_i | X_i\right] = E[\beta_0 + \beta_1 X_i + \epsilon_i] = E[\beta_0] + E[\beta_1 X_i] + E[\epsilon_i] = \beta_0 + \beta_1 X_i$$

The probability density function for Y_i is then

$$P(Y_i = y_i | X_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}[y_i - (\beta_0 + \beta_1 x_i)]^2\right)$$

Then, if the Y_i observations are independent of each other, we have that the likelihood of $\beta = (\beta_0, \beta_1)$ (the probability of observing this data given these parameters) is

$$L(\beta) = P(Y|\beta, X) = P(Y_1 = y_1, Y_2 = y_2, ..., Y_n = y_n | \beta, X) = P(Y_1 = y_1 | \beta, X_1) P(Y_2 = y_2 | \beta, X_2) ..., P(Y_n = y_n | \beta, X_n)$$

where the last equality is due to the independence of each observation and that Y_i is only dependent on β and X_i. Using the probability density function above, this becomes

$$L(\beta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}[y_i - (\beta_0 + \beta_1 x_i)]^2\right) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}[y_i - (\beta_0 + \beta_1 x_i)]^2\right)$$

Therefore, maximising this function with respect to β, corresponds to finding values for β which maximises the probability of obtaining this response data given the predictor data. Instead of working with this equation as it stands, we note that the right hand side of the above equation is positive for all values of β and x_i. This means that we can apply a handy trick in that since the log function is a monotonically increasing function, maximising $\log(L(\beta))$ is the same as maximising $L(\beta)$. Due to the existence of exp in $L(\beta)$, we may choose the natural logarithm so that the exponential disappears (we will still denote this as log).

$$l(\beta) = \log(L(\beta)) = \log\left(\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n\right) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}[y_i - (\beta_0 + \beta_1 x_i)]^2$$

Since the first term on the right-hand side is indifferent to the choice of β, maximising $l(\beta)$ corresponds to maximising the last term on the right-hand side

$$\max_{\beta} l(\beta) = \max_{\beta}\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}[y_i - (\beta_0 + \beta_1 x_i)]^2\right)$$

which is equivalent to

$$\max_{\beta} l(\beta) = \min_{\beta} \left(\sum_{i=1}^{n} [y_i - (\beta_0 + \beta_1 x_i)]^2 \right) = \min_{\beta} RSS$$

where $RSS = \sum_{i=1}^{n} \epsilon_i^2$. Note that for multiple predictors (p predictors), the above becomes

$$\max_{\beta} l(\beta) = \min_{\beta} \left(\sum_{i=1}^{n} \left[y_i - \left(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij} \right) \right]^2 \right) = \min_{\beta} RSS$$

where x_{ij} is the j^{th} predictor for observation i.

1.4.3 A3 - The mean point ($\bar{X}$,$\bar{Y}$) lies on the linear regression line

Let's assume that the random variable that represents the response be assumed to be linearly dependent on the predictors:

$$Y = \beta_0 + \beta_1 X + \epsilon$$

We approximate the coefficients using the data we have observed:

$$\hat{Y} = \hat{\beta_0} + \hat{\beta_1} X$$

Note that it is assumed that β_i and $\hat{\beta_i}$ are constant and determined such that they satisfy the line of best fit. Taking the expectation of both sides of the above equations:

$$\mu_Y = E[Y] = E[\beta_0 + \beta_1 X + \epsilon] = E[\beta_0] + E[\beta_1 X] + E[\epsilon] = \beta_0 + \beta_1 E[X] + 0 = \beta_0 + \beta_1 \mu_X$$

$$\mu_{\hat{Y}} = E[\hat{Y}] = E[\hat{\beta_0} + \hat{\beta_1} X] = E[\hat{\beta_0}] + E[\hat{\beta_1} X] = \hat{\beta_0} + \hat{\beta_1} E[X] + 0 = \hat{\beta_0} + \hat{\beta_1} \mu_{\hat{X}}$$

The first equation above says that if we assume the linear model, then the population means (μ_X, μ_Y) must be a solution to this model. The second equation says that the point $(\mu_{\hat{X}}, \mu_{\hat{Y}})$ must lie on any linear model we fit to the data regardless of the coefficients we have chosen. Now the sample means are easily obtained and have the exact equality below:

$$\mu_{\hat{Y}} = \bar{Y}$$
$$\mu_{\hat{X}} = \bar{X}$$

This result also holds when $\boldsymbol{X}$ is a vector of predictors.

1.4.4 A4 - For a single predictor, $R^2 = Cor(X, Y)^2$

We start with the definition of R^2:

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

Using $TSS = \sum_{i=1}^{n} (y_i - \bar{y})^2$ and $RSS = \sum_{i=1}^{n} (y_i - \hat{y})^2$

$$R^2 = \frac{\sum_{i=1}^{n} (y_i - \bar{y})^2 - \sum_{i=1}^{n} (y_i - \hat{y})^2}{\sum_{i=1}^{n} (y_i - \hat{y})^2} = \frac{\sum_{i=1}^{n} [(y_i - \bar{y}) - (y_i - \hat{y})][(y_i - \bar{y}) + (y_i - \hat{y})]}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

$$= \frac{\sum_{i=1}^{n}[(y_i - \bar{y}) - (y_i - \hat{y})][(y_i - \bar{y}) + (y_i - \hat{y})]}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

Using $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1\bar{x}$ and $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i = \bar{y} - \hat{\beta}_1\bar{x} + \hat{\beta}_1 x_i = \bar{y} - \hat{\beta}_1(\bar{x} - x_i)$

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

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

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

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

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

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

$$= \frac{\left[\sum_{i=1}^{n}(\bar{x} - x_i)(y_i - \bar{y})\right]^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$= \frac{\left[\sum_{i=1}^{n}(\bar{x} - x_i)(y_i - \bar{y})\right]^2}{\left[\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2\sum_{i=1}^{n}(x_i - \bar{x})^2}\right]^2}$$

$$= corr(X, Y)^2$$

1.4.5 A5 - Variance of β_0 and β_1

First, note that y is a dependent variable on x. This means that any linear model and subsequently the calculations of β_0 and β_1 are susceptible to a variation of y for a given x value. Hence in the derivation of the variance of those parameters x values are treated as a constant.

We start with the definition of β_1:

$$\beta_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

The variance of β_1 is therefore given by:

$$Var(\beta_1) = Var\left[\frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right] = \frac{1}{\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^2}Var\left[\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})\right] = \frac{1}{\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^2}Var\left[\sum_{i=1}^{n}(x\right.$$

As each observation is indepedent from another (y_i are independent of each other) we have:

$$Var(\beta_1) = \frac{1}{\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^2}\sum_{i=1}^{n}Var(x_i y_i - \bar{x}y_i) = \frac{1}{\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^2}\sum_{i=1}^{n}(x_i - \bar{x})^2 Var(y_i) = \frac{1}{\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right)^2}\sum_{i=1}^{n}(x_i -$$

However since $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$ and ϵ_i is the only random variable on the right hand side, we have:

$$Var(y_i) = Var(\epsilon_i) = \sigma^2$$

.

Then our expression above becomes:

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

Since $\beta_0 = \bar{y} - \beta_1 \bar{x}$ we have:

$$\begin{aligned}
E(\beta_0) &= E[\bar{y}] + \bar{x}E[\beta_1] \\
&= E[\frac{1}{n}\sum_{i=1}^{n} y_i] + \bar{x}\frac{1}{\sum_{k=1}^{n}(x_i - \bar{x})^2} E[\sum_{i=1}^{n} x_i y_i - n\bar{x}\bar{y}] \\
&= \mu_Y + \bar{x}\frac{1}{\sum_{k=1}^{n}(x_i - \bar{x})^2}[\sum_{i=1}^{n} x_i E[y_i] - n\bar{x}E[\bar{y}]] \\
&= \mu_Y + \bar{x}\frac{1}{\sum_{k=1}^{n}(x_i - \bar{x})^2}[\mu_Y \sum_{i=1}^{n} x_i - n\bar{x}\mu_Y] \\
&= \mu_Y
\end{aligned} \tag{1}$$

and

$$\begin{aligned}
E(\beta_0^2) &= E[\bar{y}^2 + 2\beta_1\bar{x}\bar{y} + \beta_1^2\bar{x}^2] \\
&= E[\bar{y}^2] + 2\bar{x}E[\beta_1\bar{y}] + \bar{x}^2 E[\beta_1^2] \\
&= Var(\bar{y}) + E[\bar{y}]^2 + \bar{x}^2\left[Var(\beta_1) + E[\beta_1]^2\right] \\
&= Var(\bar{y}) + \mu_Y^2 + \bar{x}^2\left[Var(\beta_1)\right] \\
&= \frac{\sigma^2}{n} + \mu_Y^2 + \frac{\bar{x}^2\sigma^2}{\sum_{k=1}^{n}(x_k - \bar{x})}
\end{aligned} \tag{2}$$

finally

$$\begin{aligned}
Var(\beta_0) &= E[\beta_0^2] - E[\beta_0]^2 \\
&= \sigma^2\left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right]
\end{aligned} \tag{3}$$

Note that, with a bit of algebraic manipulation $\left(\text{hint: } \sum(x_i - \bar{x})^2 = \sum x_i^2 - n\bar{x}^2)\right)$, this is also equal to:

$$Var(\beta_0) = \frac{\sigma^2 \sum_{i=1}^{n} x_i^2}{n\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}$$