LinearRegression

October 3, 2018

1 Linear Regression

1.1 1 - Description

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

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

1.2 2- Advertising Dataset

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

```
In [3]: # Import modules
        import pandas as pd
        import numpy as np
        import matplotlib.pyplot as plt
        import seaborn as sns
        import random
        from numpy.random import RandomState
        import math
        %matplotlib inline
```

```
In [4]: # Import Advertising dataset (http://www-bcf.usc.edu/~gareth/ISL/data.html)
        advert = pd.read_csv("Advertising.csv").iloc[:,1:]
```

```
In [5]: print("Number of observations (n) =",advert.shape[0])
        print("Number of predictor variables (p) =",advert.shape[1]-1)
        print()
        print("Advertising.csv")
        advert.head()
```

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

Advertising.csv
```

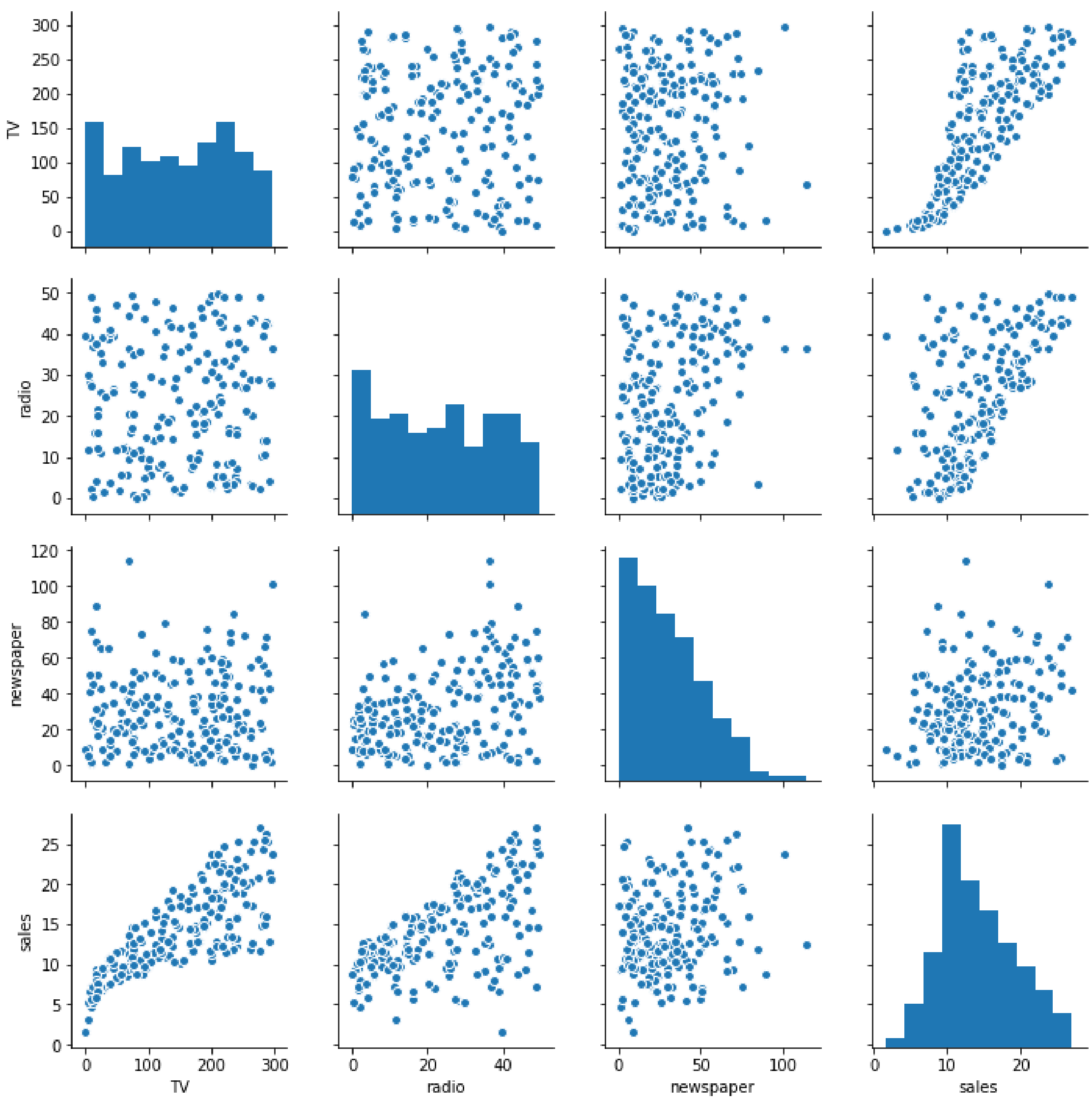
Out[5]:

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

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

In [6]:
```
sns.pairplot(data=advert)
```

Out[6]: <seaborn.axisgrid.PairGrid at 0x1f68d783198>



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

```
In [7]: advert.corr()
```

```
Out[7]:                   TV     radio  newspaper     sales
        TV          1.000000  0.054809   0.056648  0.782224
        radio       0.054809  1.000000   0.354104  0.576223
        newspaper   0.056648  0.354104   1.000000  0.228299
        sales       0.782224  0.576223   0.228299  1.000000
```

1.3 3- Linear Regression

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

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

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

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

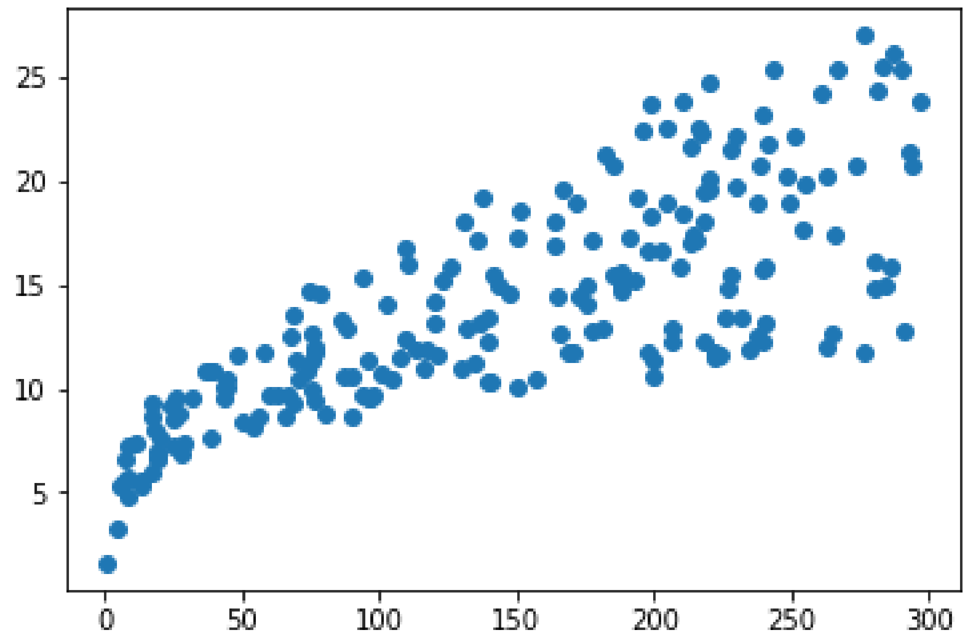
$$Y \approx \beta_0 + \beta_1 X_1 + \epsilon$$

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

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

```
In [8]: plt.scatter(data=advert, x='TV', y='sales')

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

```
Out[8]: <matplotlib.collections.PathCollection at 0x1f690bdadd8>
```



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

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

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

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

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

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

Then

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

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

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

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

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

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

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

We have that

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

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

The equation

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

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

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

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

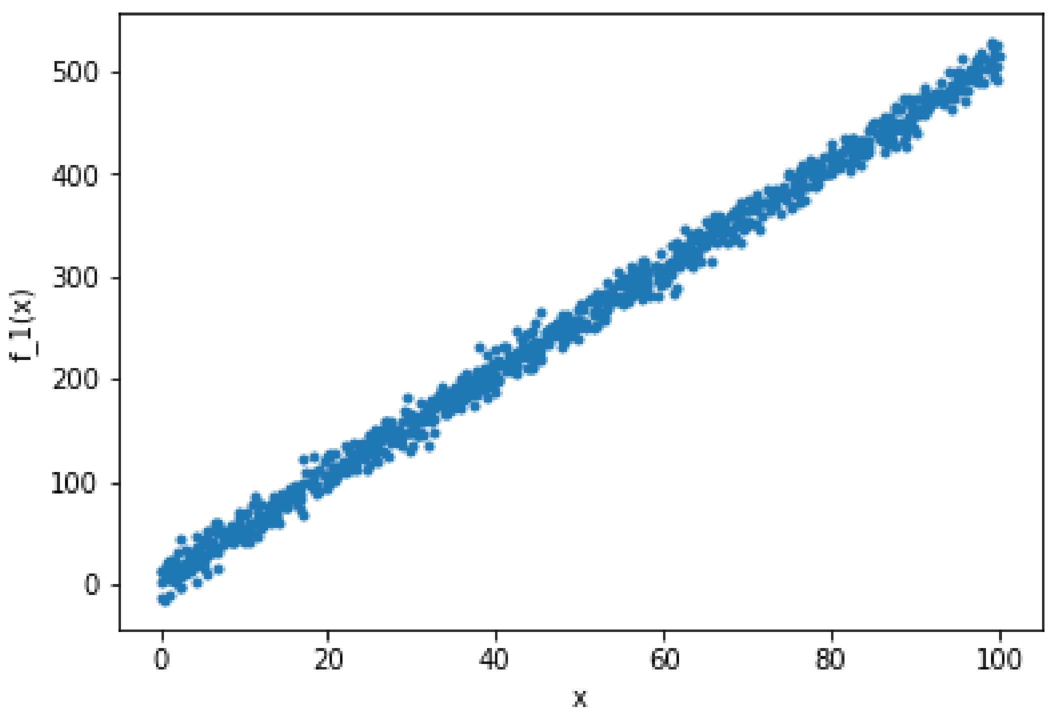
In [9]:
```
#f_1(x)=4.67+5.07x
def f_1(x):
    return 4.67 + 5.07*x

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

In [10]:
```
r = np.random.RandomState(101)
X = 100*r.rand(1000)

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

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

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

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

First case 1- f_1

In [11]:
```
fig = plt.figure()
axes = fig.add_axes([0.1,0.1,0.8,0.8])
axes.plot(X,Y_1,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_1(x)')
```

Out[11]:
```
Text(0,0.5,'f_1(x)')
```



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

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

and

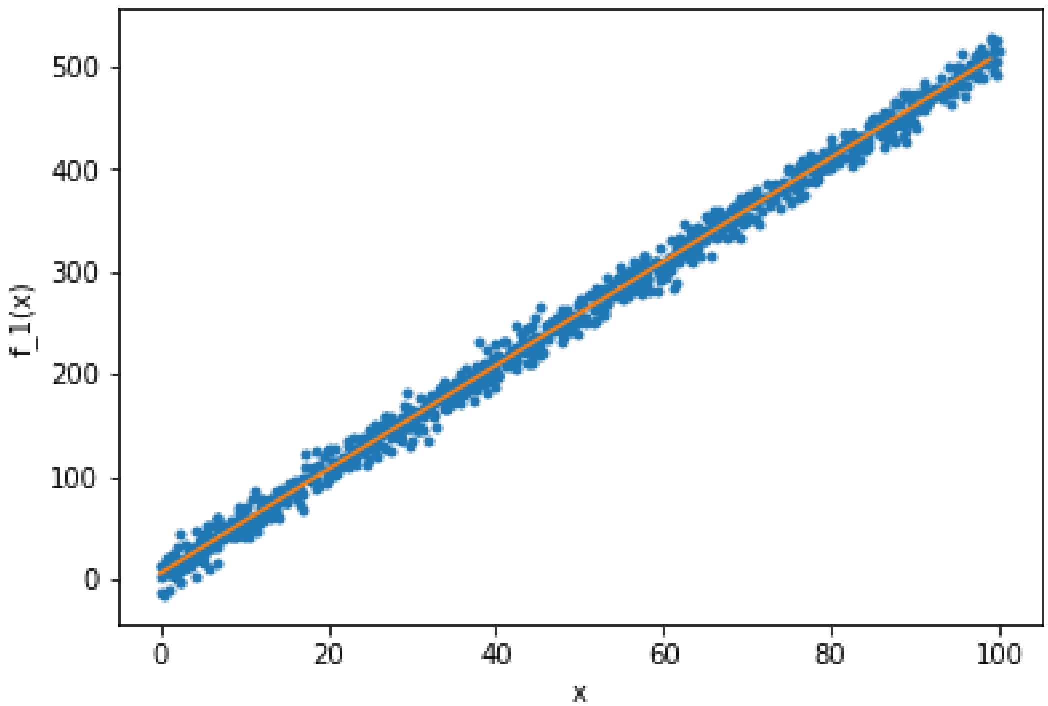
$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

In [12]:
```
#Find the mean of the data for f_1
x_bar1 = np.mean(X)
y_bar1 = np.mean(Y_1)

numerator = 0
denominator = 0

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

beta_1 = numerator/denominator
beta_0 = y_bar1 - beta_1*x_bar1

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

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

In [13]:
```
x = np.linspace(0,99,1000) # 1000 linearly spaced numbers
y = beta_0 + beta_1 * x

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

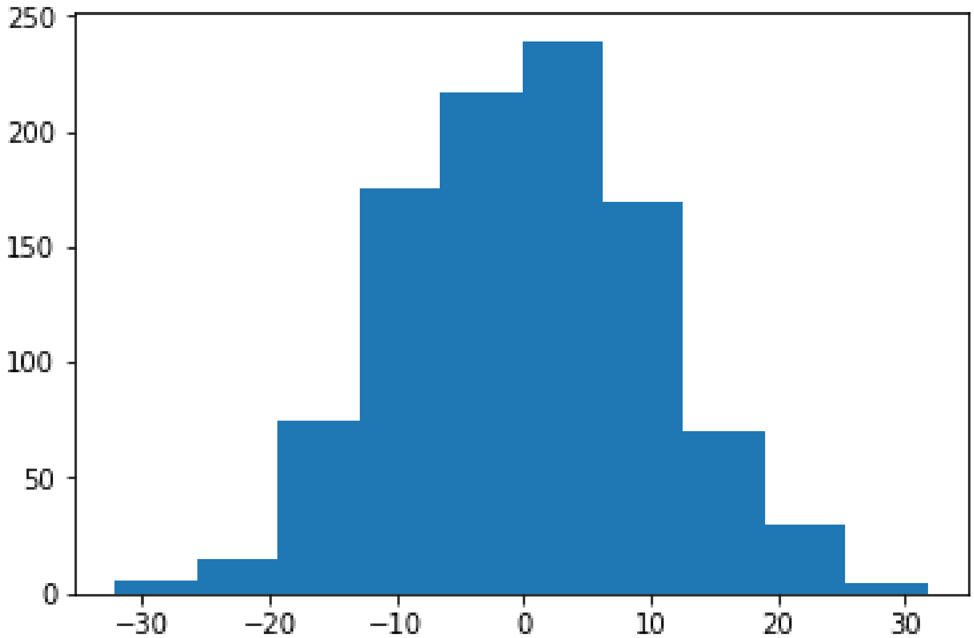
Out[13]:
```
[<matplotlib.lines.Line2D at 0x1f690ea8390>]
```



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

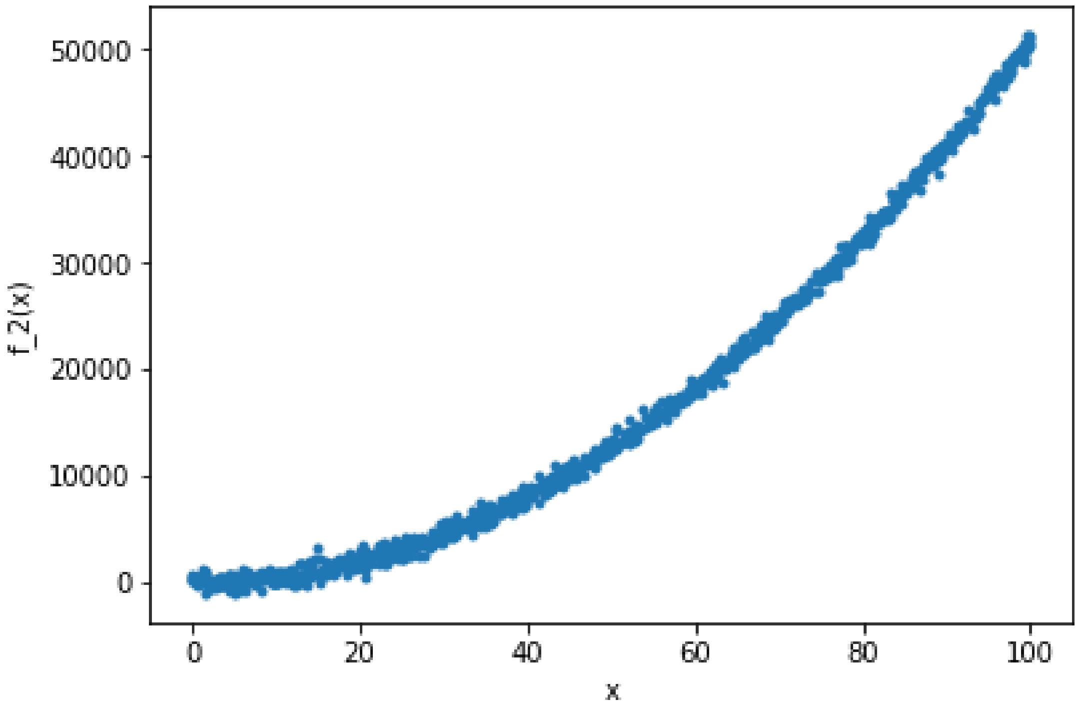
```
In [14]: y_fitted = beta_0 + beta_1 * X
         Res_1 = y_fitted - Y_1

         plt.hist(Res_1)

         print('This is roughly a normal distribution with mean {mean} and {std}'.format(mean=n
```

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



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

```
In [15]: fig = plt.figure()
         axes = fig.add_axes([0.1,0.1,0.8,0.8])
         axes.plot(X,Y_2,'.')
         axes.set_xlabel('x')
         axes.set_ylabel('f_2(x)')

Out[15]: Text(0,0.5,'f_2(x)')
```



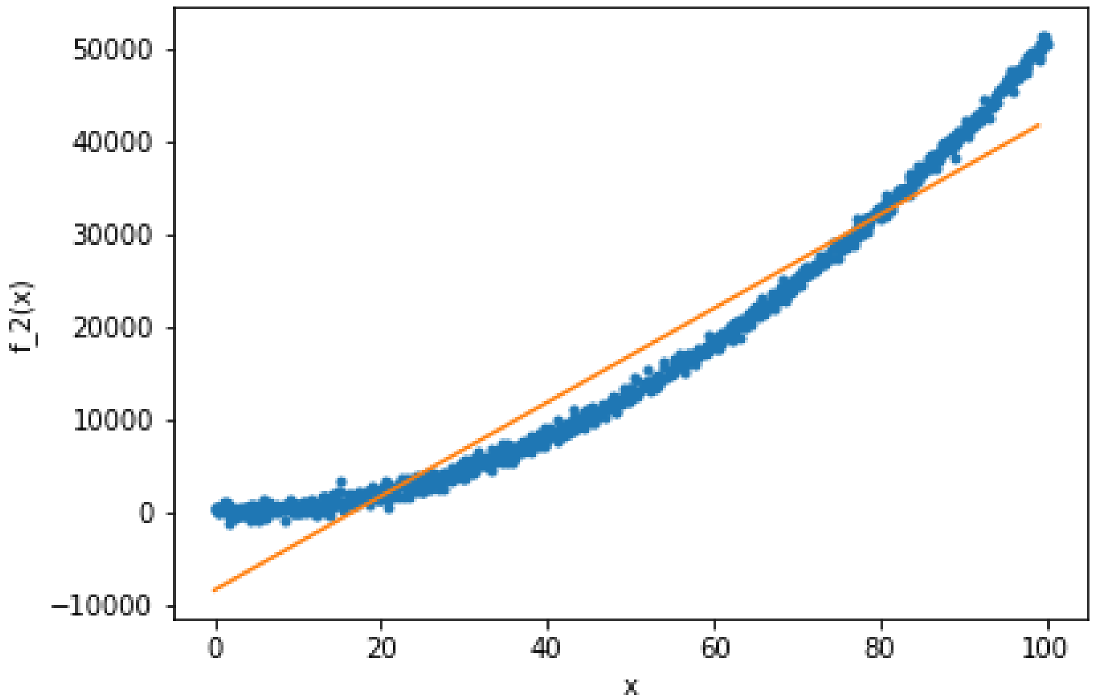
In [16]:
```
#Find the mean of the data for f_1
x_bar2 = np.mean(X)
y_bar2 = np.mean(Y_2)

numerator = 0
denominator = 0

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

beta_1 = numerator/denominator
beta_0 = y_bar2 - beta_1*x_bar2

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

```
Y = -8445.98030682202 + 506.16066894401735 * X
```

In [17]:
```
x = np.linspace(0,99,1000) # 1000 linearly spaced numbers
y = beta_0 + beta_1 * x

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

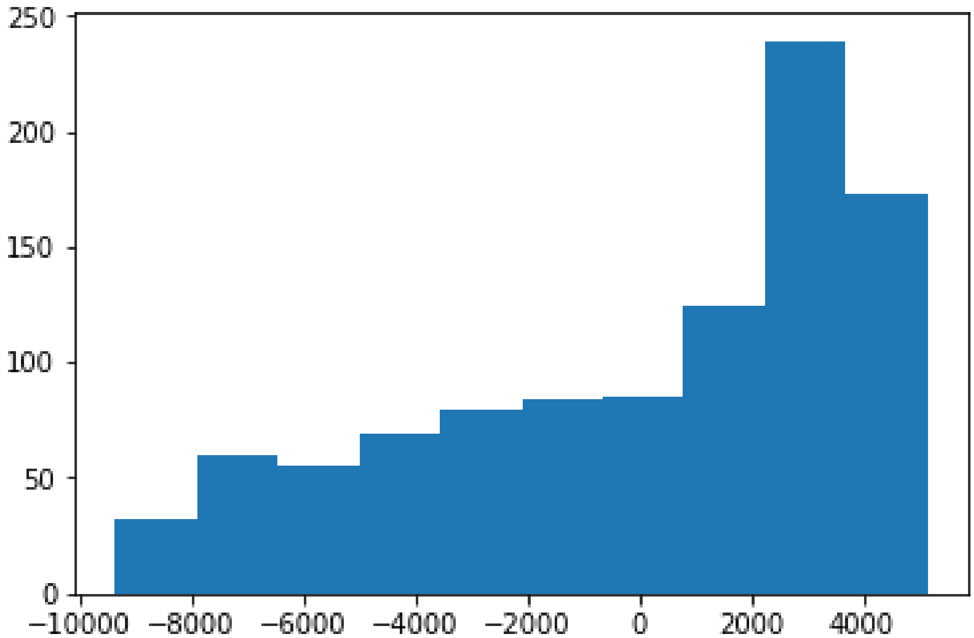
```
axes.plot(X,Y_2,'.')
axes.set_xlabel('x')
axes.set_ylabel('f_2(x)')
axes.plot(x,y)
```

Out[17]: [<matplotlib.lines.Line2D at 0x1f690fdc1d0>]



In [18]:
```
y_fitted = beta_0 + beta_1 * X
Res_2 = y_fitted - Y_2

plt.hist(Res_2)

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

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



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

```
In [19]: from sklearn.linear_model import LinearRegression
```

```
In [33]: lm = LinearRegression()
         lm.fit(X.reshape(-1,1),Y_1.reshape(-1,1))
         print('beta_0 = {}'.format(lm.intercept_))
         print('beta_1 = {}'.format(lm.coef_))
```

```
beta_0 = [5.50124312]
beta_1 = [[5.06425452]]
```

1.4 Appendix

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

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

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

Let n = 2 > 1. Then

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

So we have proved the assertion for n = 2.

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

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

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

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

by the assumption for n we have

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

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

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

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