$Multivariate\ \ Linear\ \ Regression$

Defintion and Usage

This is the same as **Univariate Linear Regression** with the only change is instead of one independent variable, we will use **multiple** independent variables (input).

Notation

$x_j^{(i)} =$ value of feature j^{th} in the i^{th} training example.

$x^{(i)} =$ the input (features) of the i^{th} training example.
$m =$ the number of training examples.
$n =$ the number of features.

For example:

$$\begin{matrix} x_1 & x_2 & x_3 \end{matrix}$$
$$\begin{bmatrix} 1 & 2 & 1 \\ 3 & 0 & 1 \\ 0 & 2 & 4 \end{bmatrix}$$

With the matrix above, the rows indicate the number of training examples, the columns indicate the number of features.

If we say $x^{(2)}$, that means we are taking a row vector $\begin{bmatrix} 3 & 0 & 1 \end{bmatrix}$ which is the input of the second training example.

If we take $x_2^{(3)}$ that means we are referring to third row, second column which is 2.

General form of Multivariate Linear Regression

$$f_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

Using linear algebra notation:

$$f_\theta(x) = \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 & \ldots & \theta_n \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \ldots \\ x_n \end{bmatrix} = \theta^T x$$

$x_0^{(i)} = 1$ for $(i \in 1, \dots, m)$

Gradient Descent for Multiple Variables

This is the same as with one variable. But now we have a set of features.

$$\theta_j = \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_j)$$

$$\theta_j = \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} [(h_\theta(x^{(i)}) - y^{(i)}) \phi_j(x^{(i)})]$$

(simutaneously update θ_j for $j = 0, 1, 2, \dots, m$)

Feature Scaling

We can speed up gradient descent by having each of our input values in roughly the same range. This is because θ will descend quickly on small ranges and slowly on large ranges, and so will oscillate inefficiently down to the optimum when the variables are very uneven.

The way to prevent this is to modify the ranges of our input variables so that they are all roughly the same. Ideally:

$$-1 \leqslant x_i \leqslant 1$$

or

$$-0.5 \leqslant x_i \leqslant 0.5$$

The goal is to get all input variables into roughly one of these ranges. This is called **Feature scaling**. In data processing, it is also known as **Data normalization** and is generally performed during the **data processing** step.

There are two techniques to achieve this:

1. **Max - Min normalization**.
2. **Mean normalization**.

The general formula for Standardization is:

$$x_i = \frac{x - \mu_i}{\sigma}$$

- μ_i is the average of all the values for feature i^{th}
- σ is the standard deviation (which can be found here), or the range between Max - Min value.

Max - Min normalization

Max - Min normalization involves dividing the input values by the ranges of the input variable, resulting in a new range around 1 .
General Formula for a Min - Max of $[0, 1]$ is given as:

$$x_i = \frac{x_i - x_{min}}{\sigma} = \frac{x_i - x_{min}}{x_{max} - x_{min}}$$

To rescale between an arbitrary set of values $[a, b]$, the formula becomes:

$$x_i = a + \frac{(x_i - x_{min})(b - a)}{\sigma} = a + \frac{(x_i - x_{min})(b - a)}{x_{max} - x_{min}}$$

Mean normalization

Mean normalization involves subtracting the average value for an input variable from the values for that input variable resulting in a new average value for the input variable of just zero.
General Formula:

$$x_i = \frac{x_i - \mu_i}{\sigma} = \frac{x_i - \mu_i}{x_{max} - x_{min}}$$

Choosing Learning rate α

The strategy to choose the most optimal learning rate is by choosing a random value then decrease/increase it accordingly. For example, we first choose the value of $\alpha = 0.01$. By evaluating the performance of Gradient Descent, we can either increase it by 3 times (0.03) or decrease it by 3 times (0.0003), and so on until the performance is optimal.

There are two ways to identify the correct learning rate α :

- **Debugging gradient descent**.
- **Automatic convergence test**.

Debugging gradient descent

By plotting cost function $J(\theta)$ against number of iterations, we can evaluate whether we chose the sufficient α or not. There are three possible kinds of plot:

1. Rises or oscillate back and forth (this happens when α is too large, making it may not converge).
2. Drops gradually (when the α is small but too small, which leads to the convergence process is slow).
3. Sharp decline (this when the α is sufficiently small, this is the optimal value for learning rate).

Automatic convergence test

Declare convergence if $J(\theta)$ decreases by less than E in one iteration, where E is some small value such as 10^{-3}. However in practice it's difficult to choose this threshold value.

Special case: Polynomial Regression

Polynomial Regression uses a hypothesis with an n-degree function:

$$f(\theta) = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_n x^n$$

By considering each $\phi(x)$ as an independent variable, we can see that Polynomial Regression can be treated as a Multivariate Linear Regression with every $x^{(i)} = \phi_i(x)$.
Note: With higher degree functions, we should use feature scaling to reduce the range of each input.

Normal Equation

The normal equation can be used to substitute for Gradient Descent when the number of features are small. The result of this equation is the optimized θ :

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

Pros and cons

Gradient Descent:

- Time complexity: $O(kn^2)$
- Pros:
  - Works well even if n is large ($n \geqslant 10^6$).
- Cons:
  - Needs to choose the sufficient learning rate α .
  - Needs many iterations.
  - Can suffer from vanishing gradient.
  - Have to use feature scaling in some cases.

Normal Equation:

- Time complexity: $O(n^3)$
- Pros:
  - No need to choose α .
  - No need to iterate.
  - No need to use feature scaling.
- Cons:
  - Needs to calculate the inverse of $X^T X$. If it cannot be inverted then we cannot use normal equation.
  - Slow if n is very large.

Exception handling

When $X^T X$ is **noninvertible**, the common causes might be having:

- Redundant features, where 2 features are closely related. (i.e. They are linearly dependent).
- Too many features (e.g. $m \leqslant n$). In this case, delete some features or use "regularization" technique.

Solutions to the above problems include deleting a feature that is linearly dependent with

another or deleting one or more features when there are too many features.

Summary

In practice, if the number of features is smaller than $10,000$ then normal function is the way to go. Else we should use Gradient Descent for better performance.

Demo Model

Data preprocessing

Read input, build DataFrame and plot data points

In [ ]:
```
import numpy as np
from matplotlib import cm
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import pandas as pd

plt.rcParams["figure.figsize"] = (10,8)

header_list = ['Area', 'Number of Bedrooms', 'Price']

df = pd.read_csv("/Users/danielnguyen/Repo/AI/Training_set/house_pricing.csv

m = len(df)

df.tail()
```

Out[ ]:

	Area	Number of Bedrooms	Price
42	2567	4	314000
43	1200	3	299000
44	852	2	179900
45	1852	4	299900
46	1203	3	239500

Now we set X equals to a matrix contains [Area, Number of Bedrooms] and y contains the price as a column vector.

In [ ]:
```
X = np.array(df.iloc[:, 0:2])
y = np.array(df.iloc[:, [-1]])

print(X[:5])
print(y[:5])
```

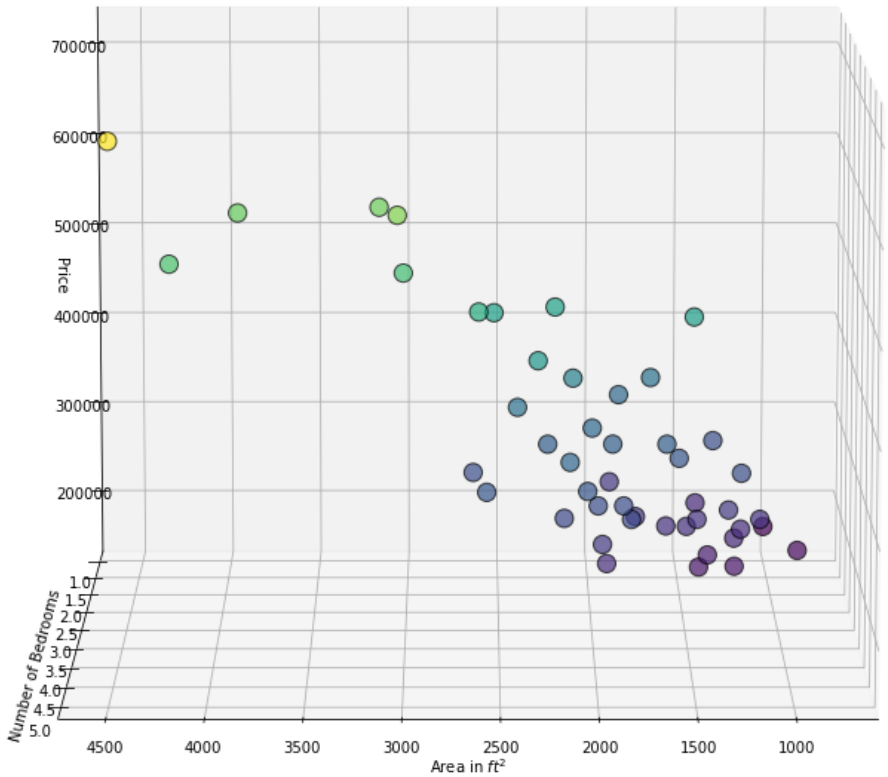
```
[[2104    3]
 [1600    3]
 [2400    3]
 [1416    2]
 [3000    4]]
[[399900]
 [329900]
 [369000]
```

```
[232000]
[539900]]
```

Now we will plot every data points onto a 3D plot for better visualization.

In [ ]:

```
fig = plt.figure(figsize=(15, 15))
ax = fig.add_subplot(111, projection='3d')
ax.view_init(elev=10., azim=90)

ax.set_xlabel('Area in ' + r'$ft^2$')
ax.set_ylabel('Number of Bedrooms')
ax.set_zlabel('Price')

sc = ax.scatter(X[:,0], X[:, 1], y, edgecolor='k', s=150, alpha=.7, c=y)
```



As we can see from X , the range of **first** column **(Area)** is very large while the range of the **second** column **(Number of Bedrooms)** are small. This could cause the Gradient Descent algorithm to be inefficient. Therefore we need to normalize our data using **mean normalization**.

Normalizing data

We can use either **Max - Min Normalization** or **Mean Normalization** . However, I will use

the second one for easier implementation. To use it we have to calculate the mean μ and the standard deviation σ of each column (each feature).

We can write a `for` loop for this but it is not efficient, in the `numpy` library we have `numpy.mean()` to calculate the mean element of an array. By specifying `numpy.mean(X, 0)`, we are calculating the mean μ_i of each column of the array X. The output of this is a row vector containing the mean of each column. (0 specify the zeroth axis meaning the row axis, 1 specify the first axis meaning the column axis). Similarly, we have to calculate the standard deviation σ of X by calling `numpy.std(X, 0)`

In [ ]:
```
def mean_normalization(X) :
    """Normalize the range of each feature in X by using Mean Normalization
    mu = np.mean(X, 0)
    sigma = np.mean(X, 0)

    return (X - mu) / sigma, mu, sigma
```

In [ ]:
```
X, mu, sigma = mean_normalization(X)
print(X[:5])
```

```
[[ 0.05164199 -0.05369128]
 [-0.20027225 -0.05369128]
 [ 0.19959163 -0.05369128]
 [-0.29224094 -0.36912752]
 [ 0.49948954  0.26174497]]
```

Choose the hypothesis

Our goal is to find our hypothesis $f_\theta(x)$, which is a plane, fit the most points.

$$f_\theta(x) = \theta^T X = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

Vectorizating the variables

Vectorization is a powerful tool to make our code more readable and shorter. This uses linear algebra to squeeze variables into matrices to make computation easier.

First we will initialize θ as a column vector containing all θ_i.

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \dots \\ \theta_{n-1} \end{bmatrix}$$

Then we will initialized X as an $m \times n$ matrix.

$$X = \begin{bmatrix} [x^{(0)}]^T \\ [x^{(1)}]^T \\ \dots \\ [x^{(m-1)}]^T \end{bmatrix}$$

With $[x^{(i)}]^T = [x_0^{(i)}, x_1^{(i)}, \ldots, x_{n-1}^{(i)}]$
And because $x_0 = 1$ so X will be:

$$X = \begin{bmatrix} 1 & x_1^{(0)} & x_2^{(0)} & \ldots & x_{n-1}^{(0)} \\ 1 & x_1^{(1)} & x_2^{(1)} & \ldots & x_{n-1}^{(1)} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & x_1^{(m-1)} & x_2^{(m-1)} & \ldots & x_{n-1}^{(m-1)} \end{bmatrix}$$

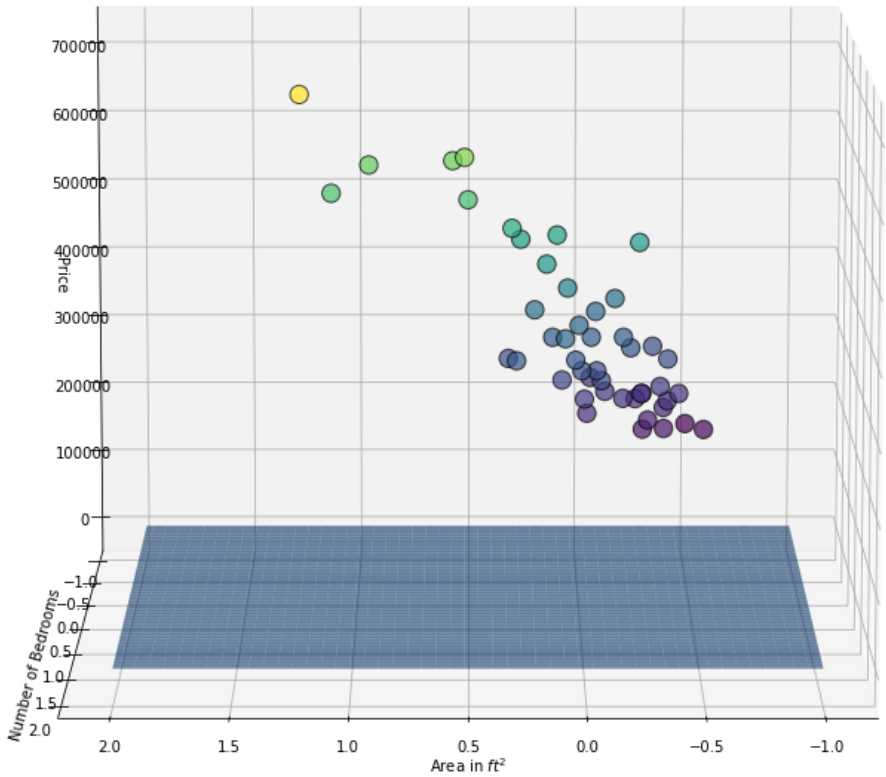
So let's add the bias term to the X (add a column of ones corresponding to θ_0).

In [ ]:
```
X = np.hstack((np.ones((m, 1)), X))
theta = np.zeros((3, 1))

print(X[:5])
print(theta)
```

```
[[ 1.          0.05164199 -0.05369128]
 [ 1.         -0.20027225 -0.05369128]
 [ 1.          0.19959163 -0.05369128]
 [ 1.         -0.29224094 -0.36912752]
 [ 1.          0.49948954  0.26174497]]
[[0.]
 [0.]
 [0.]]
```

With the given θ we can plot on to 3D plot for a better visualization.

In [ ]:
```
fig.clear()

fig = plt.figure(figsize=(15, 15))
ax = fig.add_subplot(111, projection='3d')
ax.view_init(elev=10., azim=90)

ax.set_xlabel('Area in ' + r'$ft^2$')
ax.set_ylabel('Number of Bedrooms')
ax.set_zlabel('Price')

sc = ax.scatter(X[:,1], X[:, 2], y, edgecolor='k', s=150, alpha=.7, c=y)

x_plane, y_plane = np.meshgrid(np.linspace(-1, 2, 100), np.linspace(-1, 2,

z = theta[0] + 0 * x_plane + 0 * y_plane

surf = ax.plot_surface(x_plane, y_plane, z, cmap=plt.cm.RdBu_r, alpha=0.6)
```



Calculate cost function

Cost function $J(\theta)$ can be calculated with the X and θ matrices.

$$J(\theta) = sum((\theta^T X - y)^2)$$

In [ ]:
```
def calculate_cost(theta, x_matrix, y_matrix) :
    return np.sum(np.square(np.dot(x_matrix, theta) - y_matrix)) / (2 * len
```

In [ ]:
```
J = calculate_cost(theta, X, y)
print("Calculate the current cost:", J)
```

```
Calculate the current cost: 65591548106.45744
```

Optimizing our Model

Gradient Descent

As mentioned in the previous section, when updating θ_i , we have to do it simultaneously. The vectorized formula is:

$$\theta = \theta - \alpha \frac{\partial}{\partial \theta} J(\theta)$$

With:

$$\frac{\partial}{\partial \theta} J(\theta) = \frac{X^T . (X . \theta - y)}{m}$$

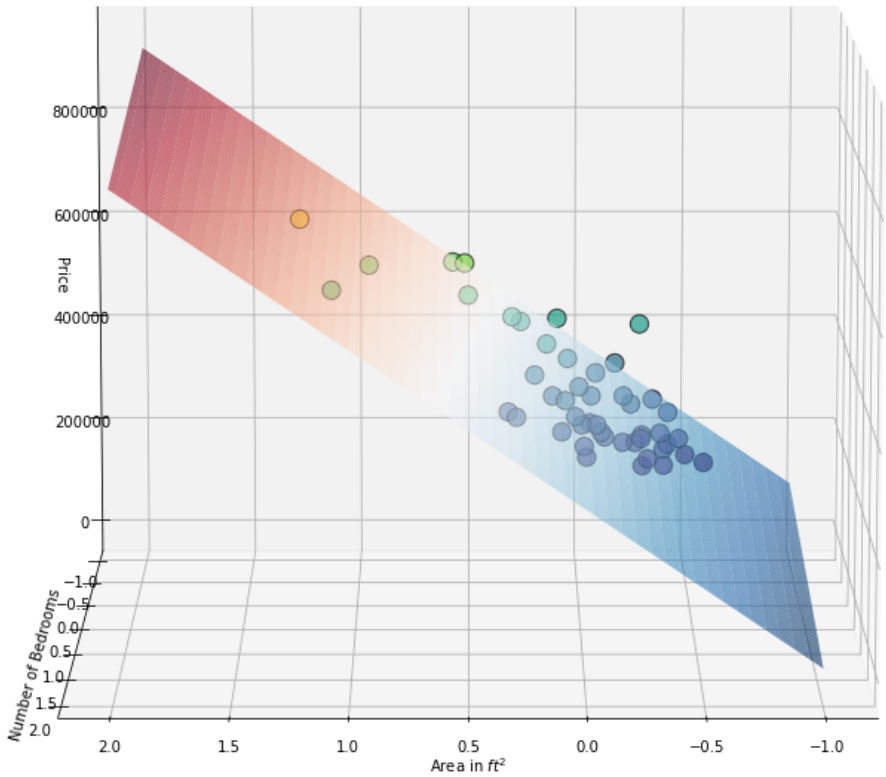
In [ ]:

```
def gradient_descent(theta, x_matrix, y_matrix, learning_rate=1.5, max_itera
    J_history = calculate_cost(theta, x_matrix, y_matrix)

    i = 0

    while i < max_iterations:
        theta = theta - learning_rate / m * (np.dot(x_matrix.T, (np.dot(x_ma

        J_history = np.hstack((J_history, calculate_cost(theta, x_matrix, y_

        i += 1

        if J_history[-1] - J_history[-2] > 1e7 :
            raise ValueError("Learning rate is too high")

    return theta, J_history
```

In [ ]:

```
theta, j_arr = gradient_descent(theta, X, y)

print(theta)

fig.clear()

fig = plt.figure(figsize=(15, 15))
ax = fig.add_subplot(111, projection='3d')
ax.view_init(elev=10., azim=90)

ax.set_xlabel('Area in ' + r'$ft^2$')
ax.set_ylabel('Number of Bedrooms')
ax.set_zlabel('Price')

sc = ax.scatter(X[:,1], X[:, 2], y, edgecolor='k', s=150, alpha=.7, c=y)

x_plane, y_plane = np.meshgrid(np.linspace(-1, 2, 100), np.linspace(-1, 2, 1

z = theta[0] + theta[1] * x_plane + theta[2] * y_plane

surf = ax.plot_surface(x_plane, y_plane, z, cmap=plt.cm.RdBu_r, alpha=0.6)
```

```
[[340412.65957447]
 [278516.12977075]
 [-27701.37973908]]
```

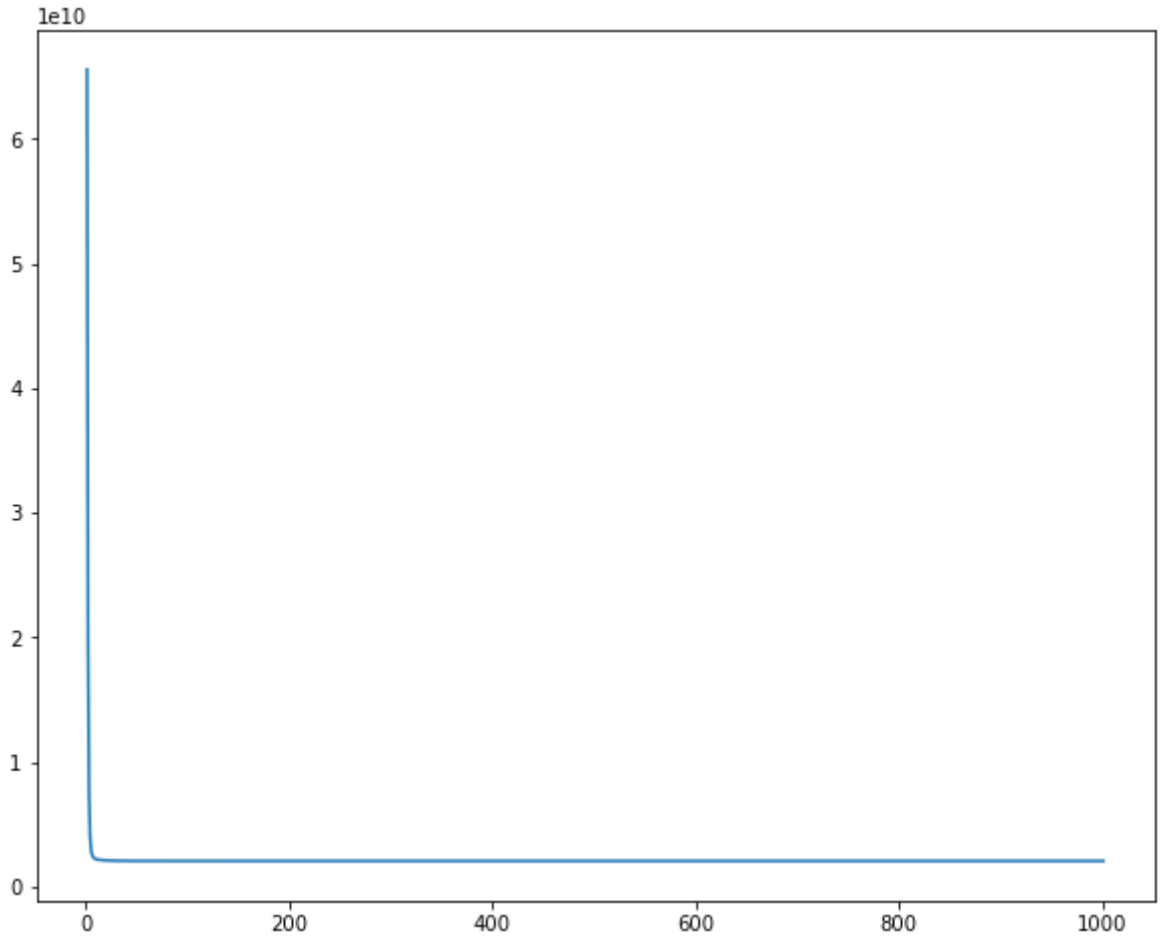


Gradient Descent Performance

In [ ]:

```
plt.plot(range(1, len(j_arr) + 1), j_arr)
print(j_arr[-1])
```

```
2043280050.6028287
```



The plot here shows that our algorithm quickly reaches the optimal θ so we conclude that our learning rate α is sufficient.

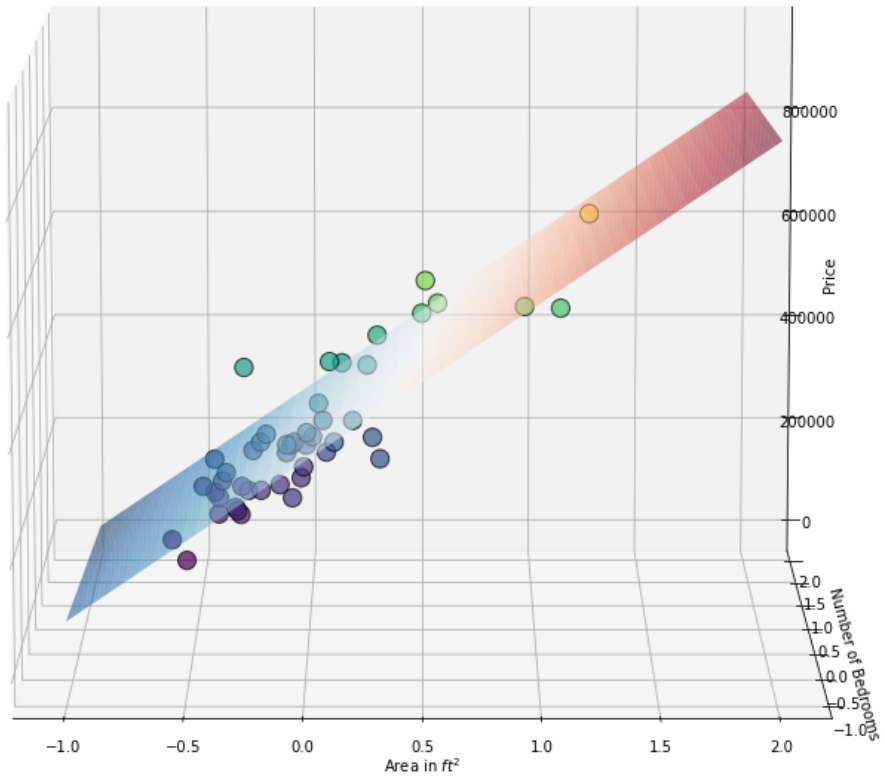
Normal Equation

Since the number of features are small, we can use **Normal Equation** for faster computation.

In [ ]:
```
def normal_equation(x_matrix, y_matrix) :
    return np.linalg.multi_dot((np.linalg.inv(np.dot(x_matrix.T, x_matrix))
```

In [ ]:
```
theta = normal_equation(X, y)

print(theta)

fig.clear()

fig = plt.figure(figsize=(15, 15))
ax = fig.add_subplot(111, projection='3d')
ax.view_init(elev=10., azim=-90)

ax.set_xlabel('Area in ' + r'$ft^2$')
ax.set_ylabel('Number of Bedrooms')
ax.set_zlabel('Price')

sc = ax.scatter(X[:,1], X[:, 2], y, edgecolor='k', s=150, alpha=.7, c=y)

x_plane, y_plane = np.meshgrid(np.linspace(-1, 2, 100), np.linspace(-1, 2,

z = theta[0] + theta[1] * x_plane + theta[2] * y_plane

surf = ax.plot_surface(x_plane, y_plane, z, cmap=plt.cm.RdBu_r, alpha=0.6)
```

```
[[340412.65957447]
 [278516.12977075]
 [-27701.37973908]]
```



We can see that both **Normal Equation** and **Gradient Descent** gives the same result. But as discussed above, when the number of features n is low, we should use the **Normal Equation** for the best performance.

Test our model

Since our hypothesis seems to have fitted with our training set, let's start testing it with testing values.

In [ ]:
```
def predict(theta, X, mu, sigma) :
    X = np.subtract(X, mu) / sigma
    X = np.hstack((1, X))
    return np.dot(X, theta)[0]
```

In [ ]:
```
area = float(input('Area'))
num_of_bed = int(input('Number of Bedrooms'))
print("Predicting the house with {} sq-ft and {} bedrooms: ".format(area, nu
```

```
Predicting the house with 2000.0 sq-ft and 4 bedrooms: 333067.0$
```

We should check R^2 to see if this model really is a good fit for this data set. Let's start this by calculating $SSTO$:

$$SSTO = \frac{1}{2m} \sum_{i=1}^{m} (y_i - y_{mean})^2$$

Then use this to calculate R^2 :

$$R^2 = 1 - \frac{J}{SSTO}$$

In [ ]:

```
SSTO = np.sum(np.square(np.mean(y) - y)) / (2 * m)

r_square = 1 - j_arr[-1] / SSTO

print("Total Sum of Square:", SSTO)
print("R-square:", r_square)
```

```
Total Sum of Square: 7651158707.176097
R-square: 0.7329450180289142
```

As we can see, the R^2 is not too high but not too low. Hence, this is the **optimal** result.