CS F320 – FOUNDATIONS OF DATA SCIENCE

ASSIGNMENT 2B – PCA Analysis and Determining Optimal Number of Components

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Importing the Libraries

In [1]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import math
import random
```

⏳ Loading the Dataset

In [2]:

```
df = pd.read_csv("Hitters.csv")
df
```

Out[2]:

	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	C
0	293	66	1	30	29	14	1	293	66	1	30	29	
1	315	81	7	24	38	39	14	3449	835	69	321	414	
2	479	130	18	66	72	76	3	1624	457	63	224	266	
3	496	141	20	65	78	37	11	5628	1575	225	828	838	
4	321	87	10	39	42	30	2	396	101	12	48	46	
...	...	...	...	...	...	...	...	...	...	...	...	...	
317	497	127	7	65	48	37	5	2703	806	32	379	311	
318	492	136	5	76	50	94	12	5511	1511	39	897	451	
319	475	126	3	61	43	52	6	1700	433	7	217	93	
320	573	144	9	85	60	78	8	3198	857	97	470	420	
321	631	170	9	77	44	31	11	4908	1457	30	775	357	

322 rows × 20 columns

In [3]:

```
# checking categorical variables
df.select_dtypes(exclude=['number'])
```

Out[3]:

	League	Division	NewLeague
0	A	E	A
1	N	W	N
2	A	W	A
3	N	E	N
4	N	E	N
...	...	...	...
317	N	E	N
318	A	E	A
319	A	W	A
320	A	E	A
321	A	W	A

322 rows × 3 columns

Dropping Categorical Variables

In [4]:

```
# Drop all categorical columns
df = df.select_dtypes(exclude='object')
df
```

Out[4]:

	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	C
0	293	66	1	30	29	14	1	293	66	1	30	29	
1	315	81	7	24	38	39	14	3449	835	69	321	414	
2	479	130	18	66	72	76	3	1624	457	63	224	266	
3	496	141	20	65	78	37	11	5628	1575	225	828	838	
4	321	87	10	39	42	30	2	396	101	12	48	46	
...	...	...	...	...	...	...	...	...	...	...	...	...	
317	497	127	7	65	48	37	5	2703	806	32	379	311	
318	492	136	5	76	50	94	12	5511	1511	39	897	451	
319	475	126	3	61	43	52	6	1700	433	7	217	93	
320	573	144	9	85	60	78	8	3198	857	97	470	420	
321	631	170	9	77	44	31	11	4908	1457	30	775	357	

322 rows × 17 columns

1. Data Understanding and Representation

In [5]:
```
print("Number of records in the given dataset are: ",len(df))
print("Number of features in the given dataset are: ",len(df.columns)-1)
```

```
Number of records in the given dataset are:  322
Number of features in the given dataset are:  16
```

🔬Preprocess and perform exploratory data analysis of the dataset obtained

Replacing NULL values with mean

In [6]:
```
# to check if null values or NAN are present in the dataset
nan_count = df.isna().sum().sum()
null_count = df.isnull().sum().sum()
print("NAN count: ",nan_count)
print("NULL count: ",null_count)
```

```
NAN count:  59
NULL count:  59
```

In [7]:
```
def find_mean(dataset, feature):
    n = len(dataset[feature])
    total_sum = 0
    count_valid_values = 0

    for val in dataset[feature]:
        if isinstance(val, (int, float)) and not np.isnan(val):
            total_sum += val
            count_valid_values += 1

    if count_valid_values == 0:
        return 0

    mean = total_sum / count_valid_values
    return mean
```

In [8]:
```
for feature in df.columns:
    mean = find_mean(df, feature)
    print(feature)
    print(mean)
```

```
AtBat
380.92857142857144
Hits
101.0248447204969
HmRun
10.770186335403727
Runs
50.909937888198755
RBI
48.02795031055901
Walks
38.74223602484472
```

```
Years
7.444099378881988
CAtBat
2648.6832298136646
CHits
717.5714285714286
CHmRun
69.49068322981367
CRuns
358.7950310559006
CRBI
330.11801242236027
CWalks
260.2391304347826
PutOuts
288.9378881987578
Assists
106.91304347826087
Errors
8.040372670807454
Salary
535.9258821292775
```

In [9]:

```
pd.set_option('mode.chained_assignment', None)
```

In [10]:

```
for feature in df.columns:
    mean = find_mean(df,feature)
    df[feature].fillna(mean,inplace=True)
```

In [11]:

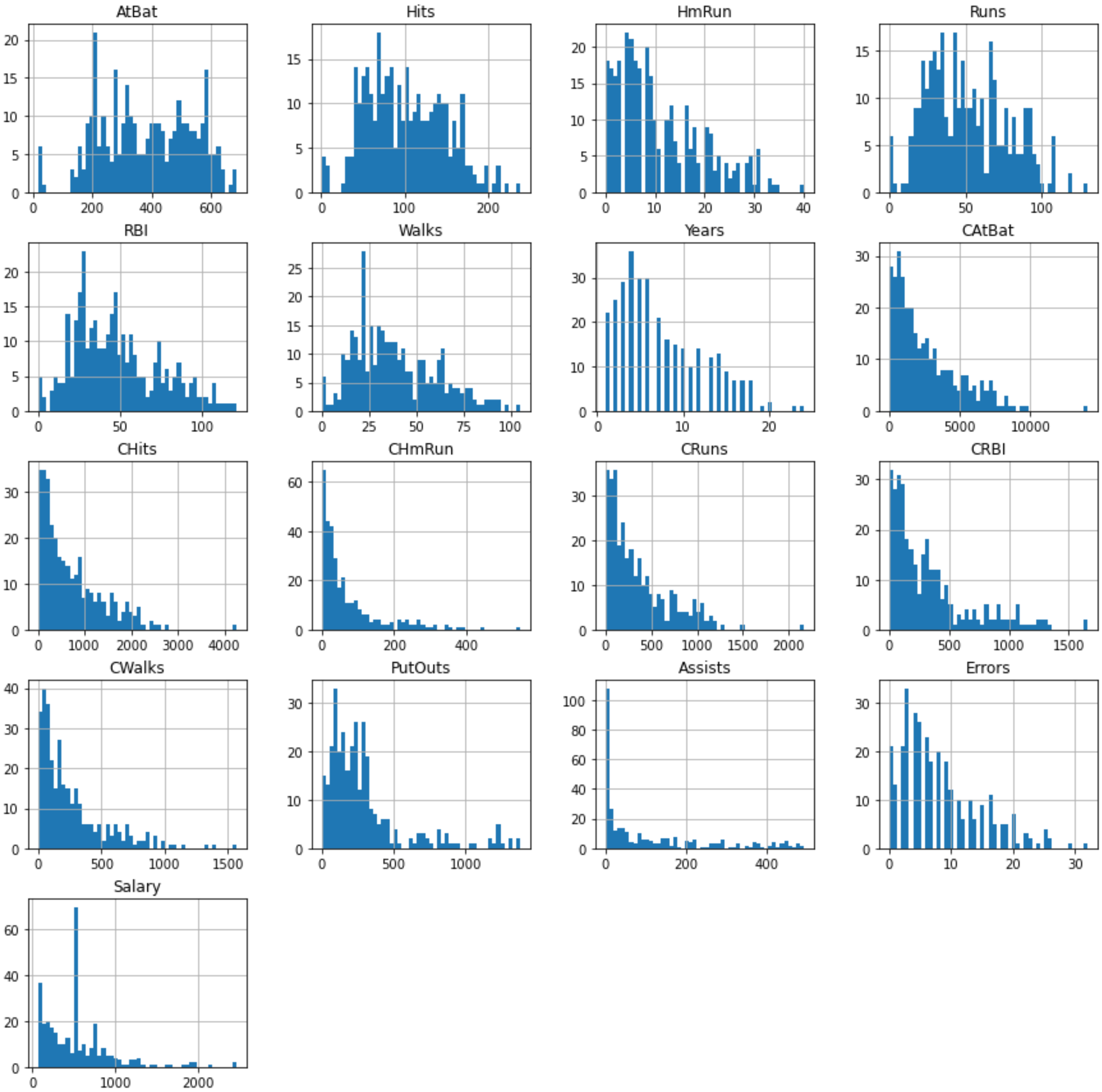
```
nan_count = df.isna().sum().sum()
null_count = df.isnull().sum().sum()
print("NAN count: ",nan_count)
print("NULL count: ",null_count)
```

```
NAN count:  0
NULL count:  0
```

📊 Plotting Histograms

In [12]:

```
df.hist(bins=50,figsize=(15,15))
plt.show()
```



In [13]:

```
# shifting the target attribute to the right most column of the dataset
column_to_shift = 'Salary'
shifted_column = df.pop(column_to_shift)
df[column_to_shift] = shifted_column
```

In [14]:

```
df
```

Out[14]:

	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	C
0	293	66	1	30	29	14	1	293	66	1	30	29	
1	315	81	7	24	38	39	14	3449	835	69	321	414	
2	479	130	18	66	72	76	3	1624	457	63	224	266	
3	496	141	20	65	78	37	11	5628	1575	225	828	838	
4	321	87	10	39	42	30	2	396	101	12	48	46	
...	...	...	...	...	...	...	...	...	...	...	...	...	
317	497	127	7	65	48	37	5	2703	806	32	379	311	
318	492	136	5	76	50	94	12	5511	1511	39	897	451	
319	475	126	3	61	43	52	6	1700	433	7	217	93	

	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	C
320	573	144	9	85	60	78	8	3198	857	97	470	420	
321	631	170	9	77	44	31	11	4908	1457	30	775	357	

322 rows × 17 columns

Feature Scaling

Normalization Method

- Normalization is performed to transform the data to have a mean of 0 and standard deviation of 1
- Normalization is also known as Z-Score Normalization

$$z = \frac{(x-\mu)}{\sigma} \tag{1}$$

In [15]:

```
# function for finding mean of a feature in a given dataset
def find_mean(dataset,feature):
    n = len(dataset[feature])
    sum = 0
    for val in dataset[feature]:
        sum += val
    return sum/n
```

In [16]:

```
# function for finding standard deviation of a feature in a given dataset
def find_standard_deviation(dataset,feature):
    variance, squared_sum = 0,0
    n = len(dataset[feature])
    mean = find_mean(dataset,feature)
    for val in dataset[feature]:
        squared_sum += (val-mean)**2
    variance = squared_sum/n
    return math.sqrt(variance)
```

In [17]:

```
# function for scaling a feature in given dataset
def normalize_feature(dataset,feature):
    mean = find_mean(dataset,feature)
    standard_deviation = find_standard_deviation(dataset,feature)
    normalized_feature = []
    for val in dataset[feature]:
        normalized_feature.append((val-mean)/standard_deviation)
    return normalized_feature
```

In [18]:

```
# function for scaling (standardizing) the whole dataset
def normalize_dataset(dataset):
    df = dataset.drop(columns = 'Salary')
    normalized_df = pd.DataFrame()
    for feature in df.columns:
        normalized_result = normalize_feature(df,feature)
        normalized_df[feature] = normalized_result

# When copying columns from one DataFrame to another, you might get NaN value
```

```
# The issue is caused because the indexes of the DataFrames are different.
# This causes the indexes for each column to be different.
# When pandas tries to align the indexes when assigning columns to the second
# One way to resolve the issue is to homogenize the index values.
# for eg [a,b,c,d] for df1 and indices for df2 are [1,2,3,4]
# that's why use df1.index = df2.index

    normalized_df.index = dataset.index
    normalized_df['Salary'] = dataset['Salary']
    return normalized_df
```

In [19]:

```
# normalizing the complete dataset
df = normalize_dataset(df)
df.head()
```

Out[19]:

	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat
0	-0.574071	-0.755130	-1.123591	-0.804734	-0.728308	-1.145172	-1.310194	-1.015121
1	-0.430437	-0.431732	-0.433579	-1.035649	-0.383827	0.011930	1.332925	0.344876
2	0.640293	0.624699	0.831443	0.580752	0.917547	1.724442	-0.903560	-0.441561
3	0.751283	0.861858	1.061447	0.542266	1.147201	-0.080638	0.722974	1.283860
4	-0.391264	-0.302373	-0.088573	-0.458363	-0.230724	-0.404626	-1.106877	-0.970736

In [20]:

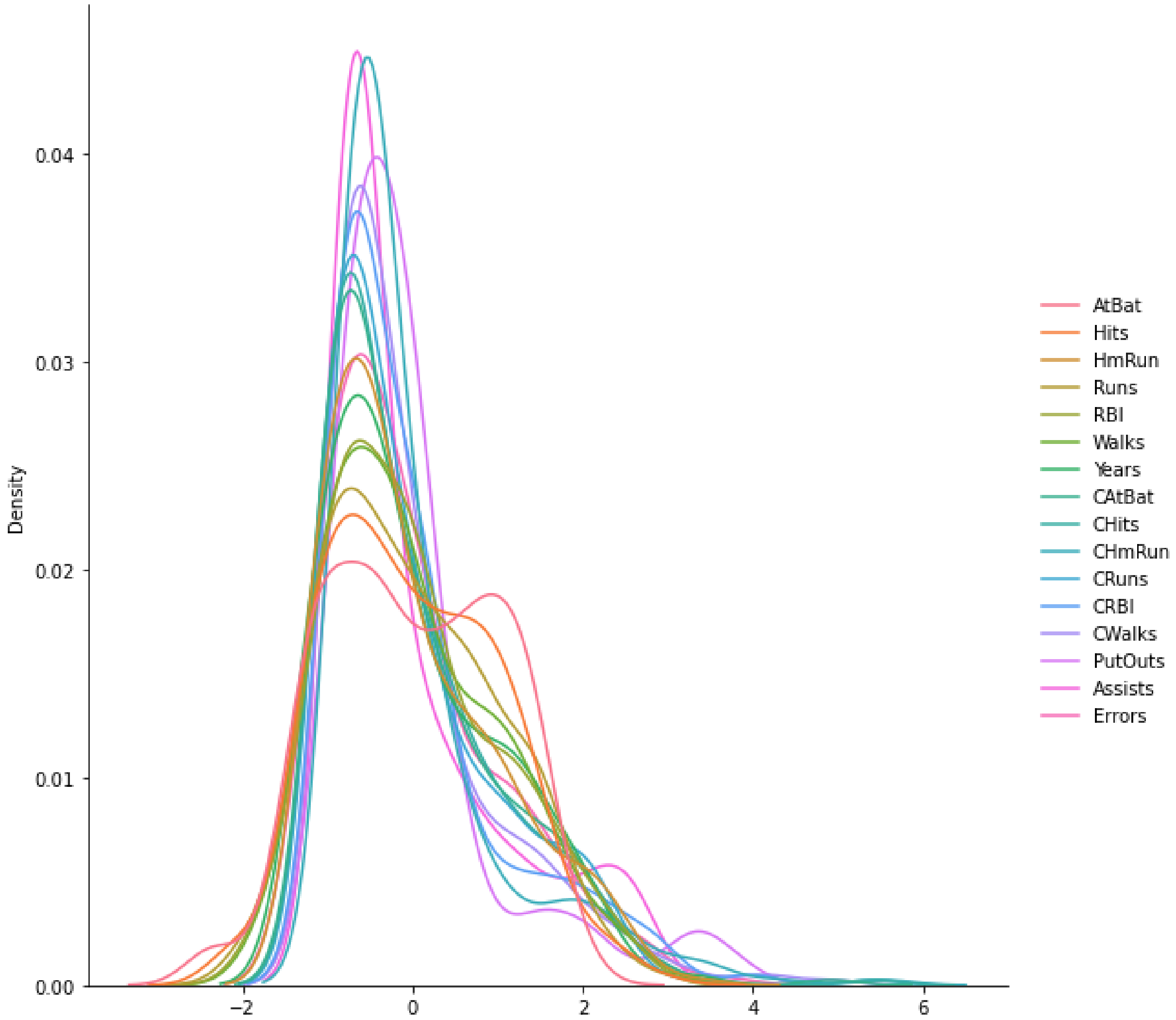
```
# checking mean and variance of each feature after standardizing the dataset
dataset = df.drop(columns = 'Salary')
for feature in dataset:
    print("Mean of",feature,"is",round(find_mean(dataset,feature)))
    print("Standard Deviation of",feature,"is",round(find_standard_deviation(
```

```
Mean of AtBat is 0
Standard Deviation of AtBat is 1
Mean of Hits is 0
Standard Deviation of Hits is 1
Mean of HmRun is 0
Standard Deviation of HmRun is 1
Mean of Runs is 0
Standard Deviation of Runs is 1
Mean of RBI is 0
Standard Deviation of RBI is 1
Mean of Walks is 0
Standard Deviation of Walks is 1
Mean of Years is 0
Standard Deviation of Years is 1
Mean of CAtBat is 0
Standard Deviation of CAtBat is 1
Mean of CHits is 0
Standard Deviation of CHits is 1
Mean of CHmRun is 0
Standard Deviation of CHmRun is 1
Mean of CRuns is 0
Standard Deviation of CRuns is 1
Mean of CRBI is 0
Standard Deviation of CRBI is 1
Mean of CWalks is 0
Standard Deviation of CWalks is 1
Mean of PutOuts is 0
Standard Deviation of PutOuts is 1
Mean of Assists is 0
Standard Deviation of Assists is 1
```

```
Mean of Errors is 0
Standard Deviation of Errors is 1
```

Plot showing distribution of features after Normalization

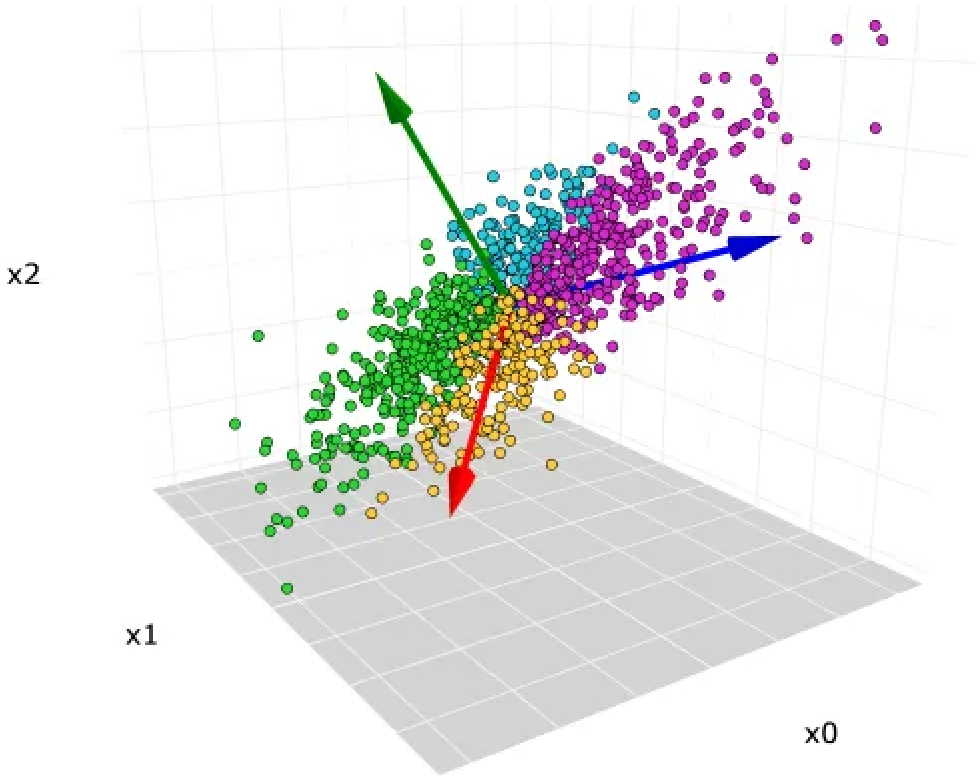
In [21]:
```
# all features following a normal distribution with mean 0 and standard devia
sns.displot(df.drop(columns='Salary'), kind='kde',aspect=1,height=8)
plt.show()
```



Dimensionality Reduction using PCA (Principal Component Analysis)

- It is used to reduce the dimensionality of dataset by transforming a large set into a lower dimensional set that still contains most of the information of the large dataset
- Principal component analysis (PCA) is a technique that transforms a dataset of many features into principal components that "summarize" the variance that underlies the data
- PCA finds a new set of dimensions such that all dimensions are orthogonal and hence linearly independent and ranked according to variance of data along them

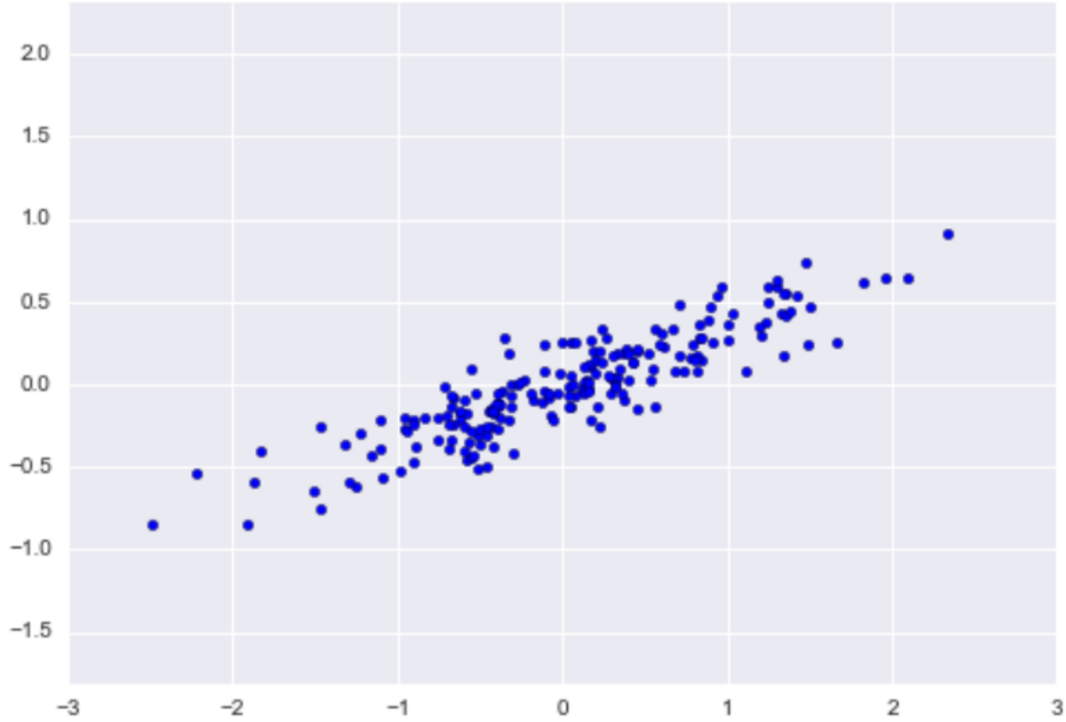
- Eigen vectors point in direction of maximum variance among data, and eigen value gives the importance of that eigen vector



- Let x_1, x_2... x_n be be N training examples, each having D features.
- Mean of N training examples is given by $\bar{x}$, which can be computed as

$$\bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_{n1} + \frac{1}{N}\sum_{n=1}^{N} x_{n2}... + \frac{1}{N}\sum_{n=1}^{N} x_{nd}$$

- Now suppose we have a graph with 2-dimensional points as follows:



- Our motive is to bring down the 2D points to 1D by projecting on a vector. We need to project the points on a 1D vector such that the variance between data points is maximum.

- We need to compute unit vector such that the variance is as maximum as possible.

- We do some mathematical computations as follows:

$$cos\theta = \frac{OA}{OB}$$

$$\bar{u}cdot\bar{x_n} = (||u||)(||x||)cos\theta = (||u||)(OB)cos\theta = (||u||)(OA)$$

- The above equation gives us the below result

$$OA = \frac{\bar{u} \cdot \bar{x_n}}{||u||}$$

- We take projection on unit vector $||u||$ = 1

- Our final result is as follows:

$$OA = \bar{u} \cdot \bar{x_n}$$

- The mean of the projected points is given by

$$\frac{1}{N}\sum_{n=1}^{N} \bar{u} \cdot \bar{x_n} = \bar{u} \cdot \sum_{n=1}^{N} \frac{x_n}{N} = \bar{u} \cdot \bar{x}$$

- Here, $\bar{x}$ is the mean of training points in their dimension

- We then compute variance as

$$Variance = \frac{1}{N}\sum_{n=1}^{N}(\bar{u}\cdot\bar{x_n} - \bar{u}\cdot\bar{x})^2$$

- We then compute $\bar{u}$ which maximizes variance as much as possible such that $||u|| = 1$
- Consider x_n and $\bar{x}$ to be matrices of dx1 size represented as follows

$$\bar{x_n} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_d \end{bmatrix}$$

$$\bar{x} = \begin{bmatrix} \bar{x_1} \\ \bar{x_2} \\ \bar{x_3} \\ \vdots \\ \bar{x_d} \end{bmatrix}$$

- Consider $\bar{u}$ to be a 1xd matrix represented by

$$\bar{u} = [u_1, u_2 \ldots u_d]$$

- We then observe that we need to maximize the following expression

$$max[\frac{1}{N}\sum_{n=1}^{N}(\bar{u}\cdot(\bar{x_n} - \bar{x}))(\bar{u}\cdot(\bar{x_n} - \bar{x})^T]$$

- While trying to maximize the above expression by expanding the same, we get

$$max[\frac{1}{N}\sum_{n=1}^{N}(\bar{u}(x_n - \bar{x})(x_n - \bar{x})^T\bar{u}^T)]$$

- The above expression in turn becomes

$$max[\bar{u}\frac{1}{N}[\sum_{n=1}^{N}(x_n - \bar{x})(x_n - \bar{x})^T]\bar{u}^T]$$

- The above expression simplifies to

$$max[\bar{u}S\bar{u}^T]$$

$$||u|| = 1$$

- Here, S is called covariance matrix
- Principal Component Analysis (PCA) gives linear combination of these features to get matured features
- We then try to convert the above constraint optimization problem to an unconstrained optimization problem, as follows:

$$E(u, \lambda) = max[\bar{u}S\bar{u}^T + \frac{\lambda}{2}(1 - \bar{u}\bar{u}^T)]$$

- Taking derivation with respect to $\bar{u}$ and λ and setting it to 0, we get final answer to be

$$\bar{u}S\bar{u}^T = \lambda$$

- λ is called the eigen value found from the equation

$$|A - \lambda I| = 0$$

- Let u_1, u_2,...u_d be the eigen vectors, and λ_1, λ_2,...λ_d be the eigen values, A is a dxd square matrix, we get

$$A\gamma = \lambda\gamma$$

$$Au_1 = \lambda_1 u_1$$

$$Au_2 = \lambda_2 u_2$$

- Any of d $\bar{u}$ values are feasible solutions, we need to find optimal solution from the following set of equations

$$Su_1 = \lambda_1 u_1$$

$$Su_2 = \lambda_2 u_2$$

$$.$$

$$.$$

$$.$$

$$Su_d = \lambda_d u_d$$

- The above set of equations simplifies to

$$u_1 S u_1^T = \lambda_1$$

$$u_2 S u_2^T = \lambda_2$$

$$.$$

$$.$$

$$.$$

$$u_d S u_d^T = \lambda_d$$

- For instance, if we project all points on eigen vector u_1 then variance comes out to be λ_1

- λ_1, λ_2, ..., λ_d are variances after projecting values/points on eigen vectors u_1, u_2,....,u_d. We need to find that eigen vector which has maximum variance, or simply, maximum λ.

- For instance, consider the first eigen vector to be of the form

$$u_1 = \begin{bmatrix} \bar{u_{11}} \\ \bar{u_{12}} \\ \bar{u_{13}} \\ \vdots \\ \bar{u_{1d}} \end{bmatrix}$$

- Transformed point is

$$u_{11}x_{11} + u_{12}x_{12} + \ldots + u_{1d}x_{1d}$$

- Transformation of a point from multidimensional space (d-dimensional in this case) to a uni-dimensional space is a linear transformation (where multiples are componenents of eigen vectors in PCA)

In [22]:

```
# implementing PCA from scratch

# it will take dataset X and k components needed after PCA
def PCA(X,k):
    k_principal_components = [] # it will store first k eigen vectors
    mean = np.mean(X,axis=0)  # this will find mean for each row
    X = X - mean  # mean centering the data

    # finding the covariance matrix, will give a n*n matrix containing covari
    cov = np.cov(X.T)

    # finding eigenvalues and eigenvectors
    eigenvalues, eigenvectors = np.linalg.eig(cov)

    # transpose eigenvector
    eigenvectors = eigenvectors.T

    # will give indexes according to eigen values, sorted in decreasing order
    idx = np.argsort(eigenvalues)[::-1]
    eigenvalues = eigenvalues[idx]
    eigenvectors = eigenvectors[idx]

    # for finding how much variance does each principal component capture
    explained_variance = eigenvalues / np.sum(eigenvalues)

    # slicing first k eigenvectors
    k_principal_components = eigenvectors[:k]

    # returning the transformed features
    # multiplyinh n*d matrix with d*k matrix to get transformed feature matri
    return np.dot(X,k_principal_components.T), explained_variance, k_principa
```

In [23]:

```
k = 16
# this will return the new dataset
df_pca, explained_variance, k_principal_components = PCA(df.drop(columns="Sal
df_pca = pd.DataFrame(df_pca)
df_pca['Salary'] = df['Salary']
print("Shape of dataset is:", df.shape)
print("Shape of dataset after pca is:",df_pca.shape)
```

```
Shape of dataset is: (322, 17)
Shape of dataset after pca is: (322, 17)
```

In [24]:

```
df_pca
```

Out[24]:

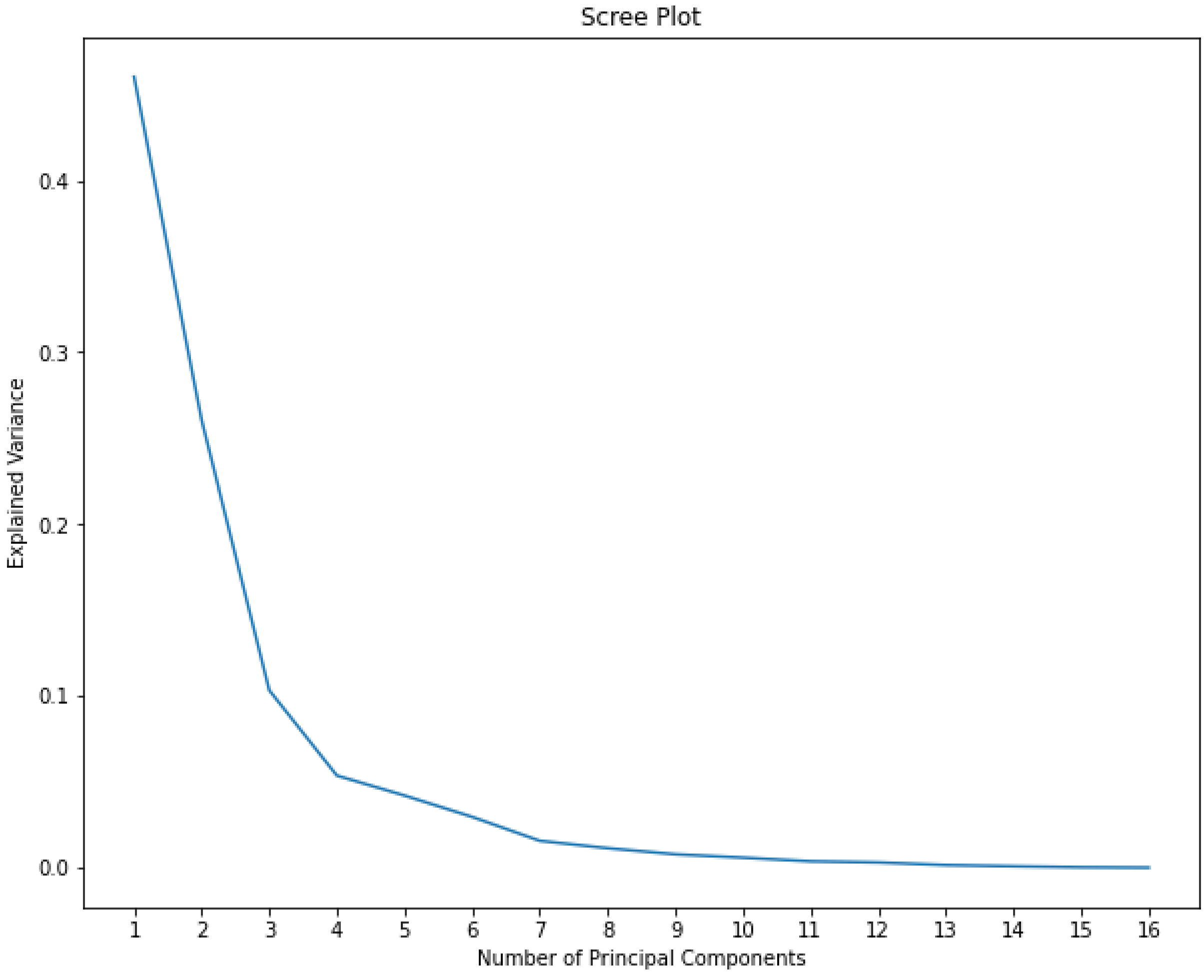
	0	1	2	3	4	5	6	7
0	3.240106	0.253173	0.776066	1.219268	0.727847	-0.049711	1.454681	0.564950
1	-0.245488	-1.302951	0.118040	1.591864	-0.102789	-0.072754	0.321704	-0.575773
2	-0.603883	2.617002	-0.698183	1.752523	-0.267457	-1.094465	0.425861	-0.017763
3	-3.591276	-0.547821	-1.049022	-0.756069	0.780899	0.791621	-0.109723	0.681704
4	2.264528	0.698898	-1.290536	1.718851	-0.145780	0.196242	-0.397752	0.125998
...	...	...	...	...	...	...	...	...
317	0.089503	0.521050	-0.770721	-0.218548	-0.863704	1.056143	0.242847	0.412390
318	-3.339811	0.732713	3.114194	0.207578	-1.935437	-1.441481	0.468249	-0.884348
319	0.951442	0.910086	0.286517	-1.032621	-1.223205	0.212958	0.246514	0.118563
320	-2.091473	2.265826	-0.192745	3.128594	-1.461111	-0.174220	0.175827	0.382475
321	-1.905622	0.311198	-0.356249	-0.135504	-1.236496	2.351643	0.544660	-0.097081

322 rows × 17 columns

Plot showing variance captured by each Principal Component

In [25]:

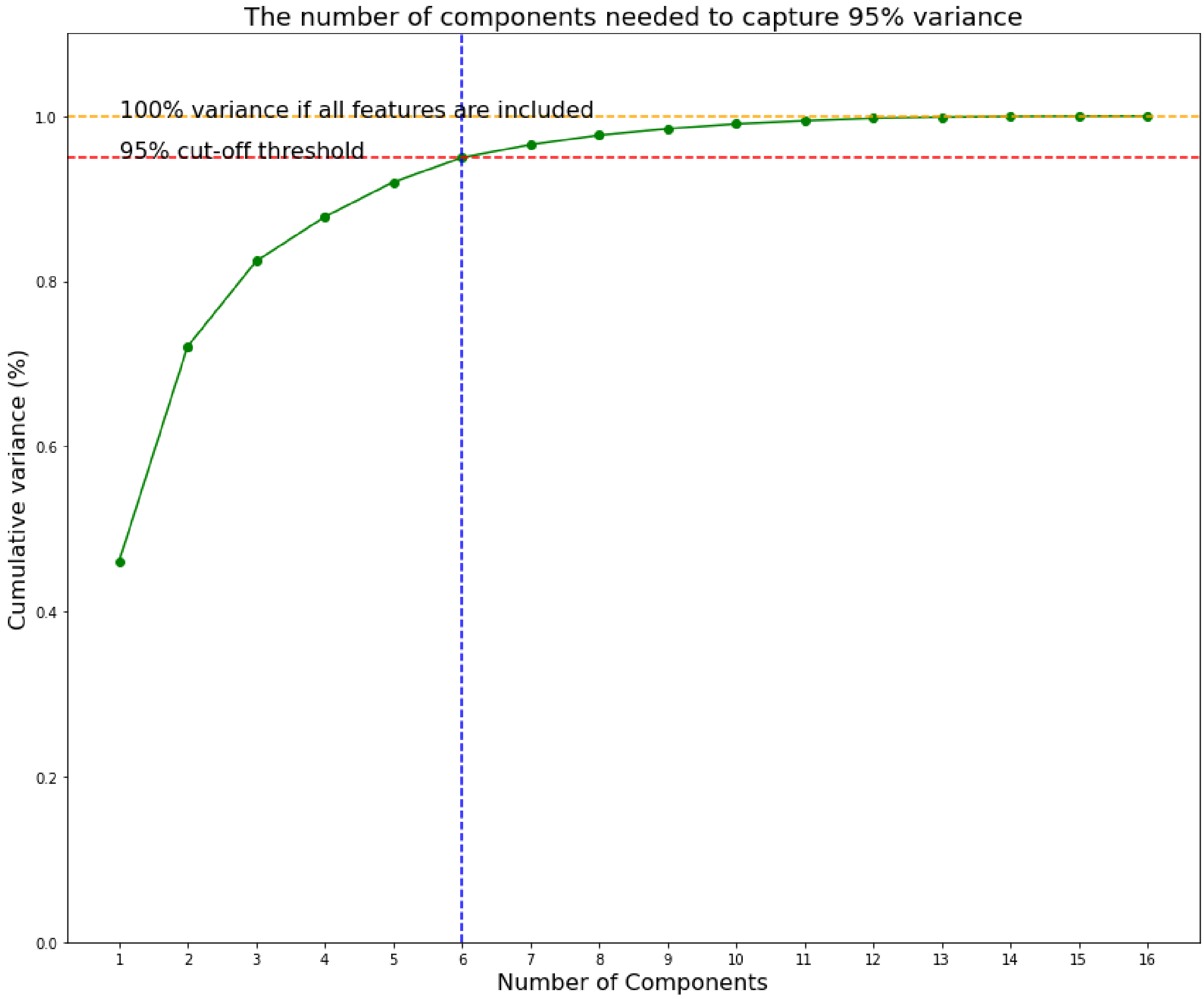
```
num_components = len(explained_variance)
components = np.arange(1, num_components + 1)
plt.figure(figsize=(10, 8))
plt.plot(components, explained_variance)
plt.xlabel('Number of Principal Components')
plt.ylabel('Explained Variance')
plt.title('Scree Plot')
plt.xticks(components)
plt.show()
```



Plot to find out number of Principal Components needed inorder to capture 95% variance in data

In [26]:

```
# finding cumulative variance captured by principal components
y_var = np.cumsum(explained_variance)

plt.figure(figsize=(12,10))
plt.ylim(0.0,1.1)
plt.plot(components, y_var, marker='o', linestyle='-', color='green')

plt.xlabel('Number of Components',fontsize=16)
plt.ylabel('Cumulative variance (%)',fontsize=16)
plt.title('The number of components needed to capture 95% variance',fontsize=
plt.xticks(components)

plt.axhline(y=0.95, color='red', linestyle='--')
plt.axhline(y=1.00, color='orange', linestyle='--')
plt.axvline(x=6.00, color='blue', linestyle='--')
plt.text(1, 0.95, '95% cut-off threshold', color = 'black', fontsize=16)
plt.text(1, 1, '100% variance if all features are included', color = 'black',

plt.tight_layout()
plt.show()
```



- The number of principal components required for efficient prediction might be 6 because we see that the first 6 principal components capture 95% of the complete variance of the data
- We will try a range of components on our regression model to find to determine most efficient number of principal components.

Model Training and MSE/RMSE Calculation

Train-Test Split

In [27]:

```
def split_train_test(data,test_ratio):
    # np.random.seed() is very important as whenever we call the function it
    # it might happen after many calls our model sees all the data and it lea
    # seed function will randomly divide data only once and once the function
    # permuatation of indices whenever called again,hence no overfitting
    np.random.seed(45)
    # it will give random permutation of indices from 0 to len(data)-1
    # now shuffled array will contain random number for eg [0,4,1,99,12,3...]
    shuffled = np.random.permutation(len(data))
    test_set_size = int(len(data)*test_ratio)
    # it will give array of indices from index 0 to test_set_size-1
    test_indices = shuffled[:test_set_size]
    # it will give array of indices from index test_set_size till last
    train_indices = shuffled[test_set_size:]
    # it will return rows from data df corresponding to indices given in trai
```

```
    # so it is returning the train and test data respectively
    return data.iloc[train_indices], data.iloc[test_indices]
```

In [28]:
```
train_set, test_set = split_train_test(df_pca,0.2)
```

In [29]:
```
train_set.shape
```

Out[29]:
```
(258, 17)
```

In [30]:
```
x_train = train_set.drop(columns = 'Salary')
x_test = test_set.drop(columns = 'Salary')
x_train.insert(0,'Ones',1)
x_test.insert(0,'Ones',1)
x_train.columns = range(len(x_train.columns))
x_test.columns = range(len(x_test.columns))
y_train = train_set['Salary']
y_test = test_set['Salary']
```

In [31]:
```
x_train.head()
```

Out[31]:

	0	1	2	3	4	5	6	7	
245	1	-1.043105	-1.497421	-0.202473	1.476653	-0.353427	-0.224182	0.031888	-1.20785
303	1	0.439972	1.821266	1.118801	-0.610235	-1.332483	-0.993179	-0.296966	-0.03879
99	1	0.185414	0.463587	-1.152667	-0.371452	-0.364472	0.432051	0.090698	-0.30147
184	1	-1.598821	1.169536	-0.915390	-0.941744	-0.587221	0.715244	0.196005	0.17748
177	1	-1.915195	1.293846	-2.073940	-1.082417	0.246301	-0.776347	-0.240885	-0.50585

In [32]:
```
x_test.head()
```

Out[32]:

	0	1	2	3	4	5	6	7	
239	1	2.868446	0.118412	1.473357	-0.157607	0.022377	-0.144813	-0.381052	0.13336
301	1	1.107317	2.256892	2.593587	-0.387524	0.104245	0.416844	0.047641	0.6016
292	1	-4.128430	-3.702402	1.555729	0.024108	-0.384057	-0.883853	-0.440187	-0.3175
122	1	0.049561	2.153464	-0.777248	0.054895	-1.821758	0.085294	0.735287	0.20758
279	1	1.815718	1.814290	2.867755	0.267154	-0.556403	-1.313398	0.043599	0.19076

Gradient Descent Algorithm

- We will use this equation to update our linear regression model parameters

$$\theta_j = \theta_j - \alpha \frac{\partial J(\theta)}{\partial \theta_j}, \quad 0 \leq j \leq d \tag{2}$$

$$\frac{\partial J(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} (h_\theta(x) - y^{(i)}) * x_j^{(i)}, \quad h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d \tag{3}$$

- Repeat until convergence

$$\theta_j = \theta_j - \alpha \sum_{i=1}^{n} (h_\theta(x) - y^{(i)}) * x_j^{(i)}, \quad 0 \le j \le d \tag{4}$$

- Such that it minimizes the cost function given by equation

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{n} (h_\theta(x)^{(i)} - y^{(i)})^2 \tag{5}$$

In [33]:

```
def give_train_data(x_train,x_test,k):
    first_k_x_train = x_train.iloc[:,:k+1]
    first_k_x_test = x_test.iloc[:,:k+1]
    return first_k_x_train,first_k_x_test
```

In [34]:

```
def give_weight_vector(k):
    weight_vector = np.zeros(k+1)
    return weight_vector
```

In [35]:

```
# function to find cost value, using the formula for J(theta)
def find_cost(y_actual,y_predicted):
    cost = 0
    for i in range(len(y_actual)):
        cost += (y_predicted[i] - y_actual[i])**2
    return (1/2)*cost
```

In [36]:

```
def print_cost_function(iteration_x_axis_batch,cost_y_axis_batch):
    plt.plot(iteration_x_axis_batch,cost_y_axis_batch)
    plt.xlabel("Iterations")
    plt.ylabel("Cost Value")
    plt.show()
```

In [37]:

```
max_iterations = 10000
```

In [38]:

```
def batch_gradient_descent(x_train,y_train,x_test,k,learning_rate,iteration_x
    prev_cost = 0

    # get x_train and y_train vectors
    x_train_batch, x_test_batch = give_train_data(x_train,x_test,k)

    # get the weight vector with degree weights
    weight_vector = give_weight_vector(k)

    for iteration in range(max_iterations):
        # will give the predicted value, after each iteration using updated w

        y_predicted = np.dot(x_train_batch,weight_vector)
        current_cost = find_cost(y_train,y_predicted)

        # this loop will update all the parameters one by one
        for theta_j in range(len(weight_vector)):

            # defining the xj vector for the column corresponding the weight
            xj_vector = x_train_batch.iloc[:,theta_j]
```

```
            # defining the vector representing the difference between predict
            difference_actual_predicted_vector = (y_predicted-y_train).reshap

            gradient =  np.dot(xj_vector,difference_actual_predicted_vector)
            weight_vector[theta_j] = weight_vector[theta_j] - learning_rate *


        # adding cost to cost array after each iteration
        iteration_x_axis_batch.append(iteration)
        cost_y_axis_batch.append(current_cost)

    return weight_vector
```

In [39]:

```
# function for finding the predicted value
def find_predicted_value(weight_vector,x_train):
    return np.dot(x_train,weight_vector)
```

In [40]:

```
# function for finding mse and sse
def find_mse_rmse(y_actual,y_predicted):
    sse = 0
    for index in range(len(y_actual)):
        sse += (y_actual[index]-y_predicted[index])**2
    mse = sse/len(y_actual)
    rmse = mse**0.5
    return mse,rmse
```

In [41]:

```
# scatter plot for predicted and actual values
def plot_graph_predicted_values(y_actual,y_predicted,length):
    plt.scatter([index for index in range(0,length)],y_predicted)
    plt.scatter([index for index in range(0,length)],y_actual,color='orange')
    plt.legend(['Predicted Values','Actual Values'])
    plt.show()
```

In [42]:

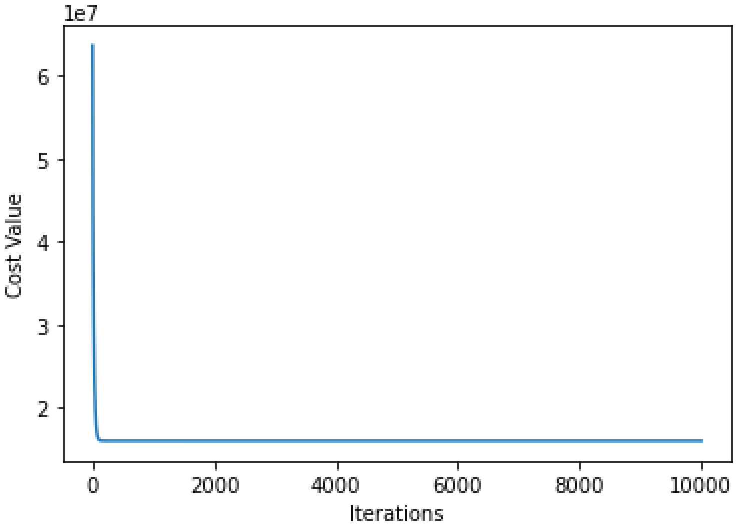
```
def print_score(y_train_actual,x_train,y_test_actual,x_test,weight_vector,ite
    print(f"Cost Function for {k} principal components:\n====================
    print_cost_function(iteration_x_axis_batch,cost_y_axis_batch)

    mse, rmse = find_mse_rmse(y_train_actual,find_predicted_value(weight_vect
    print("Train Result:\n================================================\n"
    print("MSE for this regression model is: ",mse)
    print("RMSE for this regression model is: ",rmse)
    plot_graph_predicted_values(y_train_actual,find_predicted_value(weight_ve

    print("Test Result:\n================================================\n")
    mse, rmse = find_mse_rmse(y_test_actual,find_predicted_value(weight_vecto
    print("MSE for this regression model is: ",mse)
    print("RMSE for this regression model is: ",rmse)
    plot_graph_predicted_values(y_test_actual,find_predicted_value(weight_vec
    return rmse
```

In [43]:

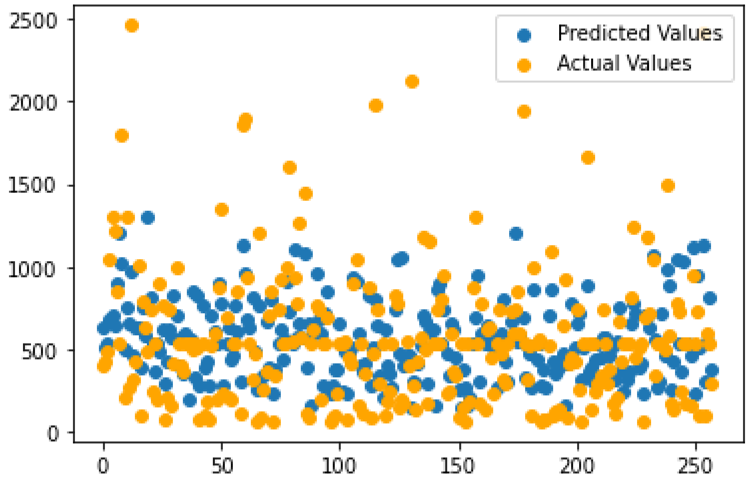
```
# for alpha = 0.0001
learning_rate = 0.0001

y_train = np.array(y_train)
y_test = np.array(y_test)
rmse_arr = []
```

```
# trying for different number of principal components
for k in range(1,17):
    iteration_x_axis_batch = []
    cost_y_axis_batch = []
    weight_vector = batch_gradient_descent(x_train,y_train,x_test,k,learning_
    x_train_k, x_test_k = give_train_data(x_train,x_test,k)
    rmse_arr.append(print_score(y_train,x_train_k,y_test,x_test_k,weight_vect
```

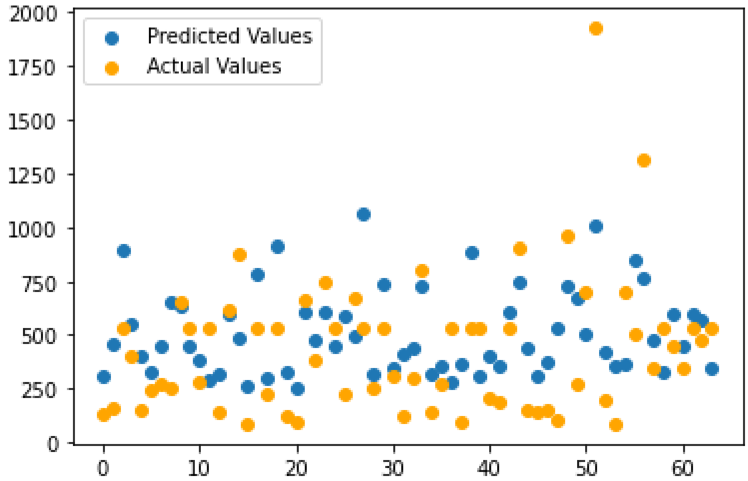
```
Cost Function for 1 principal components:
==================================================
```



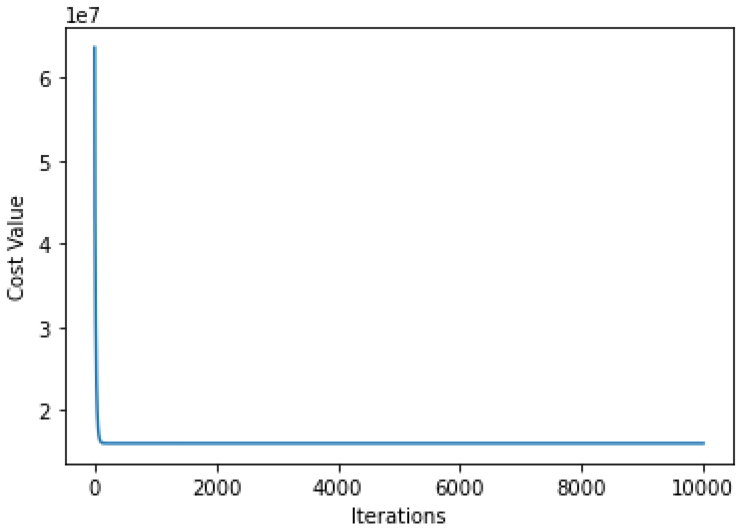

```
Train Result:
==================================================

MSE for this regression model is:  124177.47740796996
RMSE for this regression model is:  352.3882481127456
```



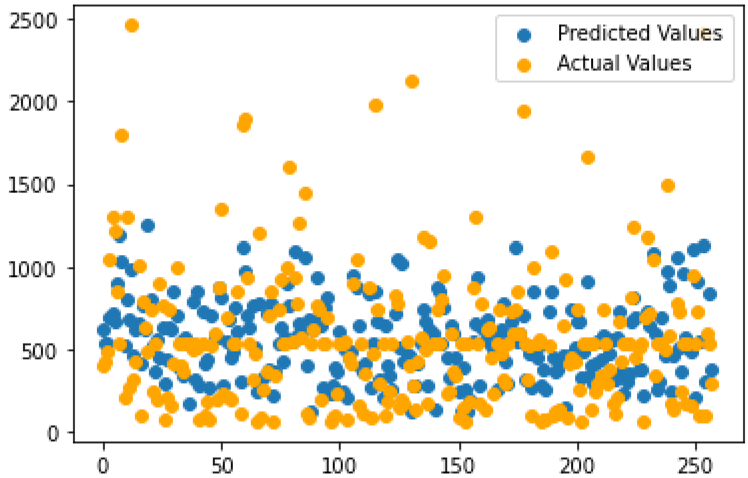

```
Test Result:
==================================================

MSE for this regression model is:  69278.84923246955
RMSE for this regression model is:  263.2087559950648
```



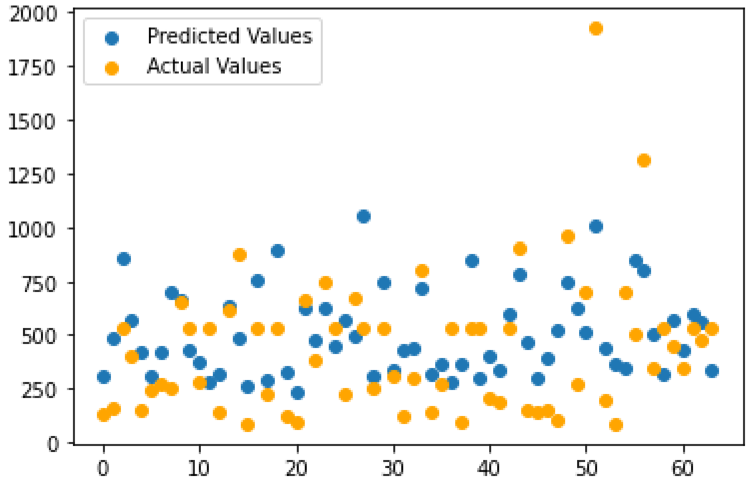

```
Cost Function for 2 principal components:
================================================
```



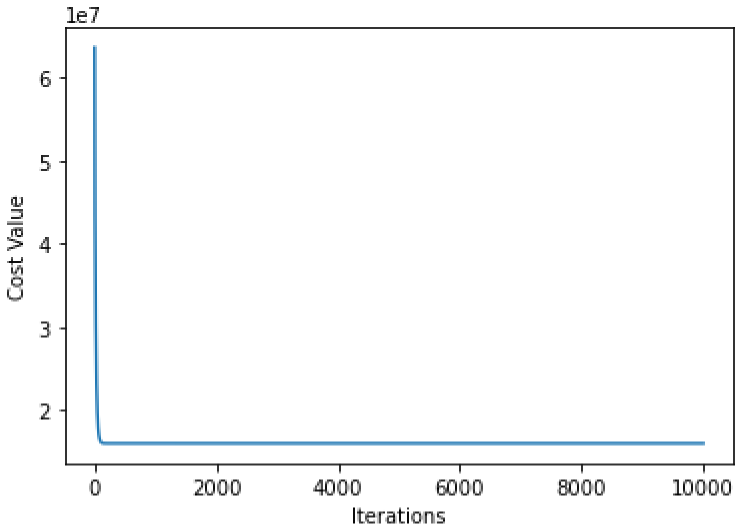

```
Train Result:
================================================

MSE for this regression model is:  123697.4298835931
RMSE for this regression model is:  351.70645413980264
```



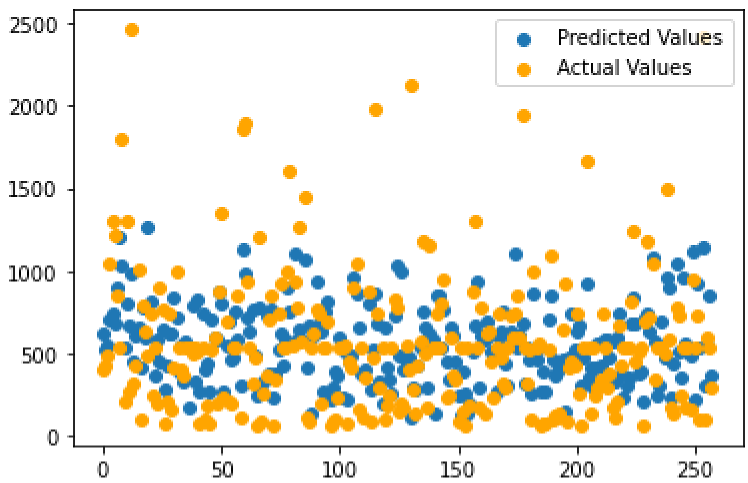

```
Test Result:
================================================

MSE for this regression model is:  67770.56360051801
RMSE for this regression model is:  260.32780028363857
```



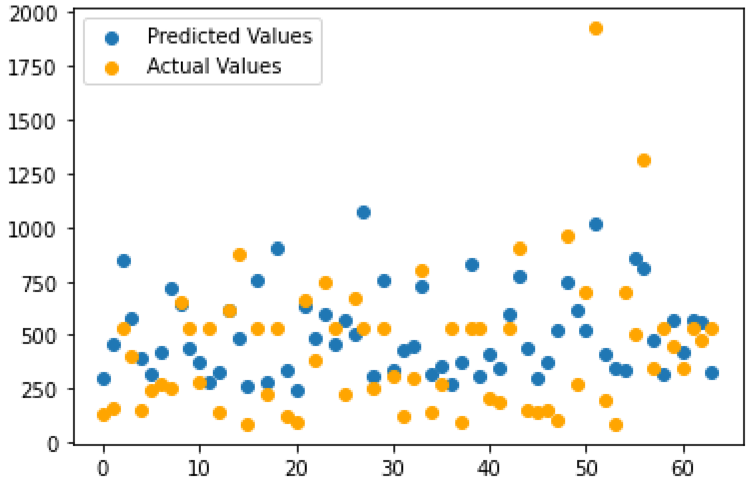

```
Cost Function for 3 principal components:
================================================
```



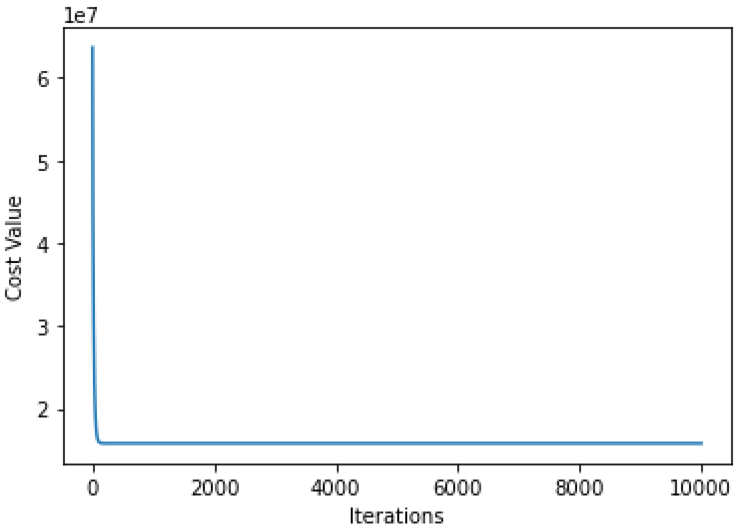

```
Train Result:
================================================

MSE for this regression model is:  123570.97580247452
RMSE for this regression model is:  351.52663597866166
```



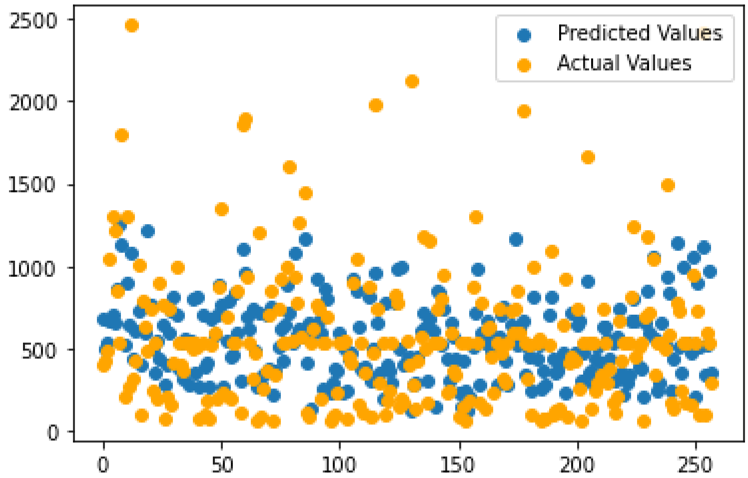

```
Test Result:
================================================

MSE for this regression model is:  66820.58738928533
RMSE for this regression model is:  258.49678409853635
```



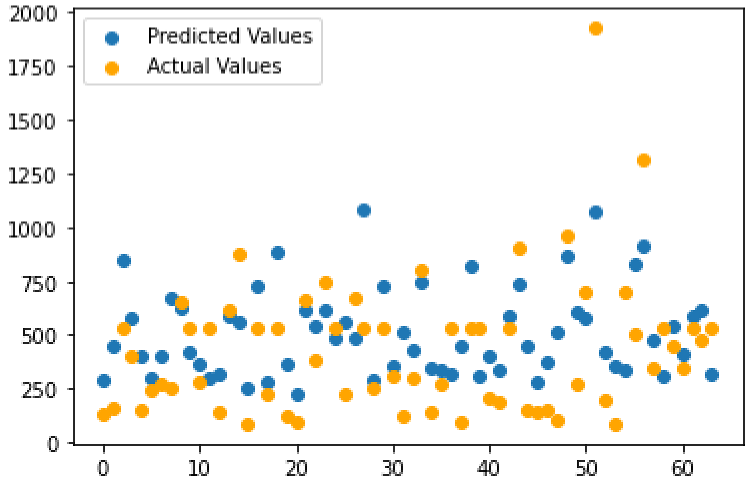

```
Cost Function for 4 principal components:
================================================
```



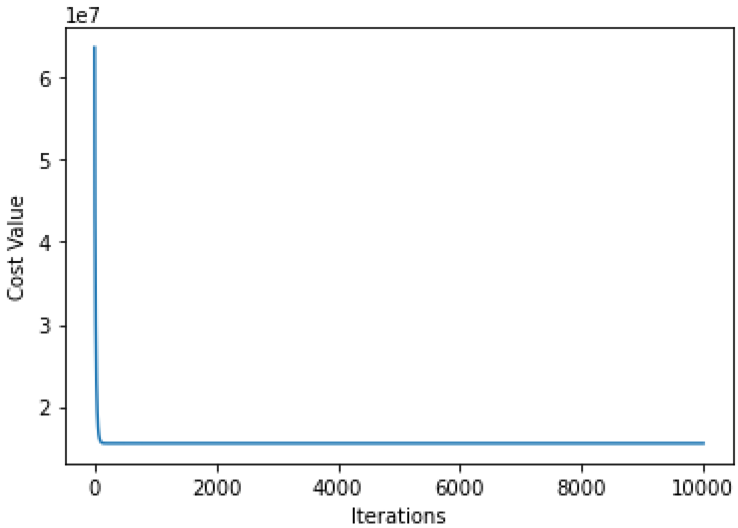

```
Train Result:
================================================

MSE for this regression model is:  122334.69938773432
RMSE for this regression model is:  349.7637765517383
```



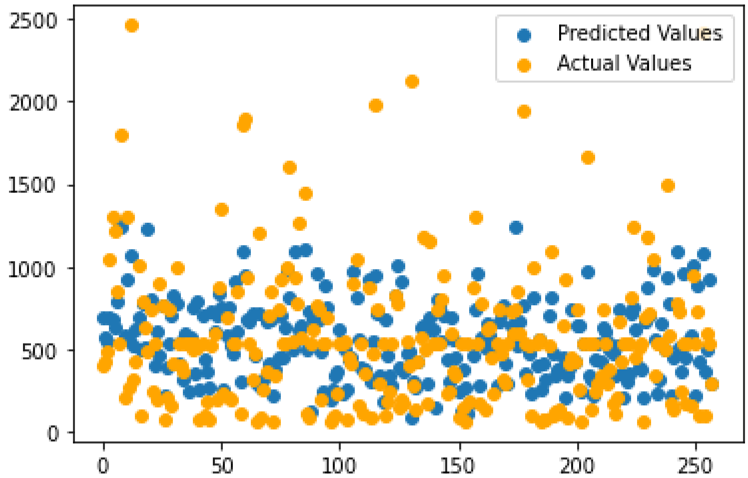

```
Test Result:
================================================

MSE for this regression model is:  62066.5675490257
RMSE for this regression model is:  249.1316269545593
```



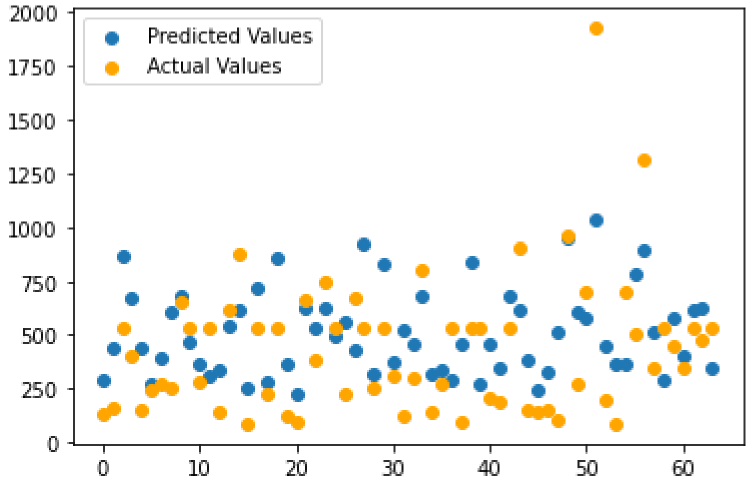

```
Cost Function for 5 principal components:
================================================
```



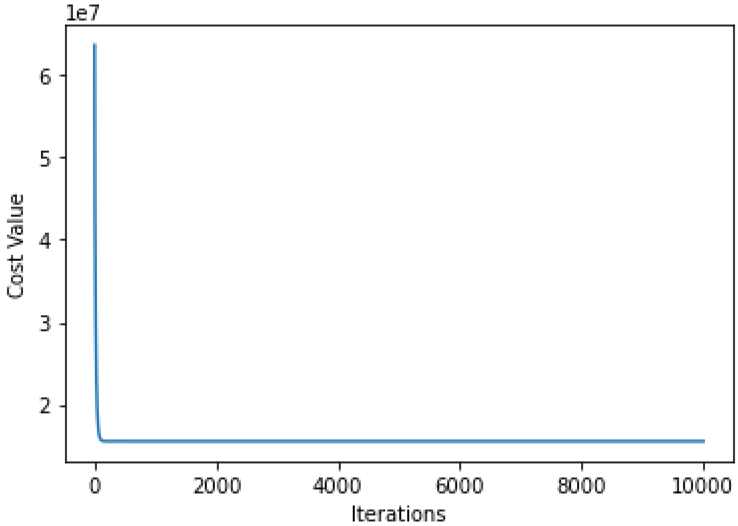

```
Train Result:
================================================

MSE for this regression model is:  120521.4180400181
RMSE for this regression model is:  347.16194785721854
```



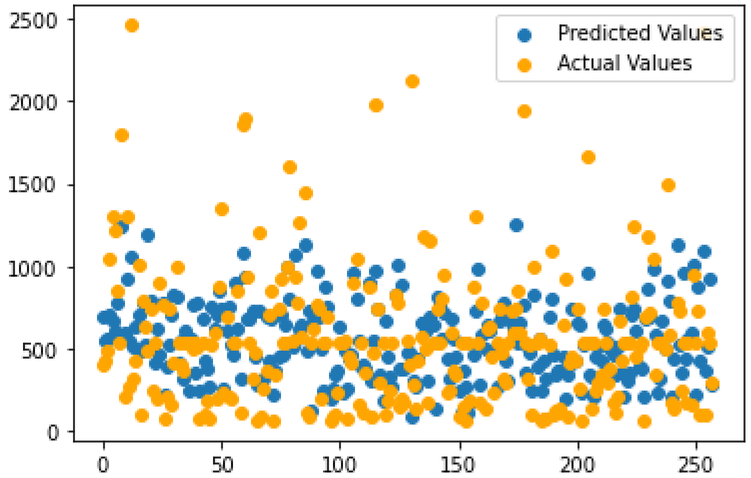

```
Test Result:
================================================

MSE for this regression model is:  63201.32350825243
RMSE for this regression model is:  251.39873410232684
```



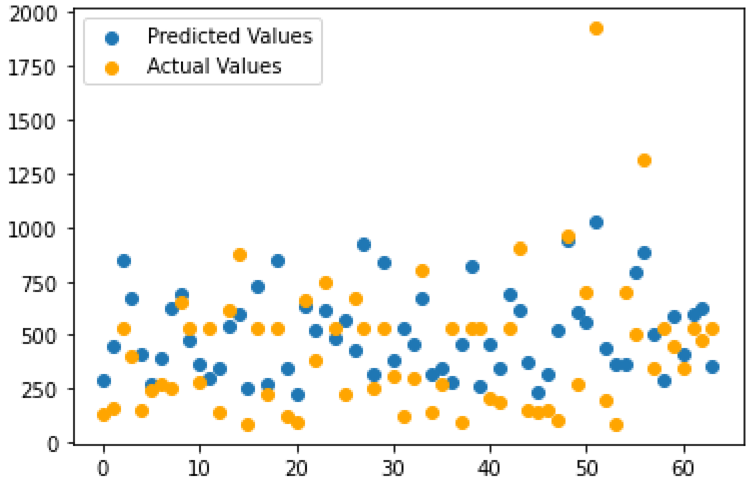

```
Cost Function for 6 principal components:
================================================
```



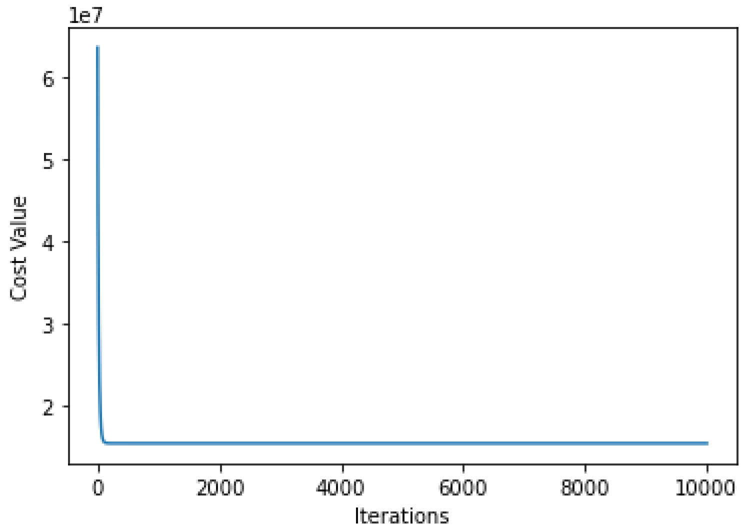

```
Train Result:
================================================

MSE for this regression model is:  120396.31817797363
RMSE for this regression model is:  346.9817260000498
```



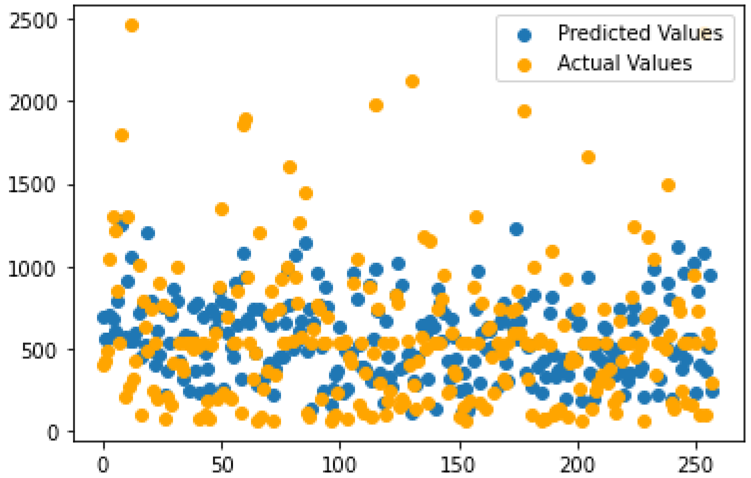

```
Test Result:
================================================

MSE for this regression model is:  63863.26210026061
RMSE for this regression model is:  252.7118163051752
```



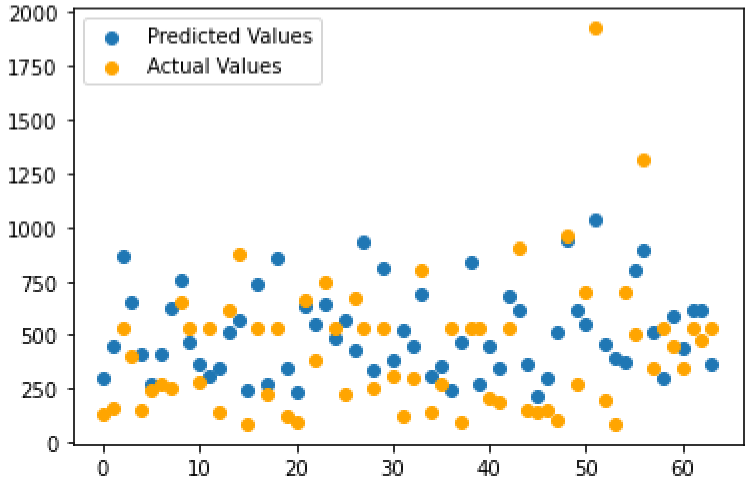

```
Cost Function for 7 principal components:
================================================
```



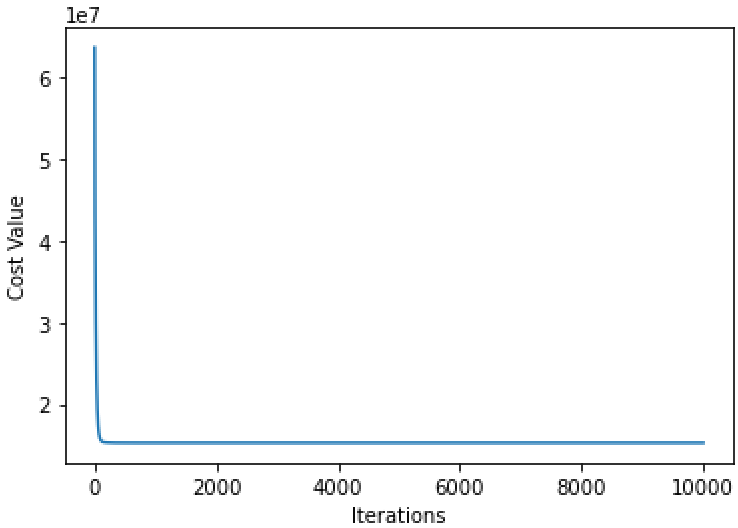

```
Train Result:
================================================

MSE for this regression model is:  120161.94282072148
RMSE for this regression model is:  346.6438270339189
```



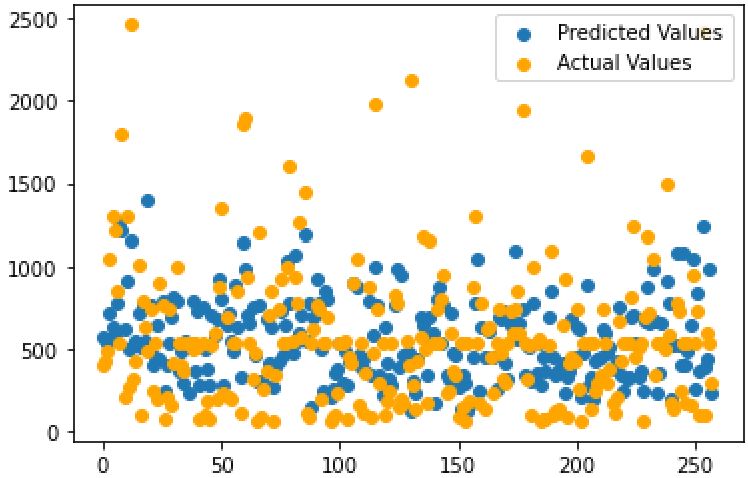

```
Test Result:
================================================

MSE for this regression model is:  64560.02908034867
RMSE for this regression model is:  254.0866566357798
```



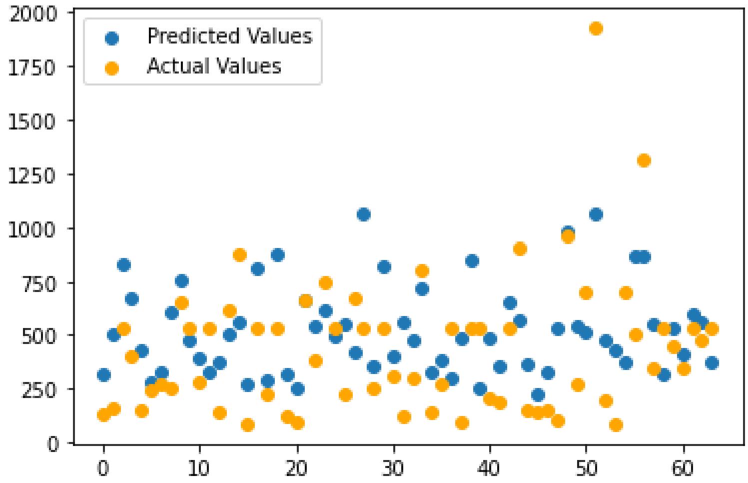

```
Cost Function for 8 principal components:
================================================
```



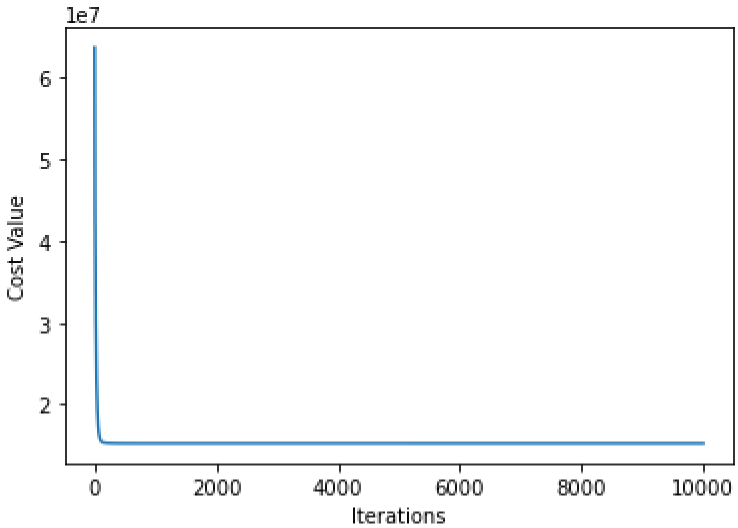

```
Train Result:
================================================

MSE for this regression model is:  118408.7859839223
RMSE for this regression model is:  344.105777318432
```



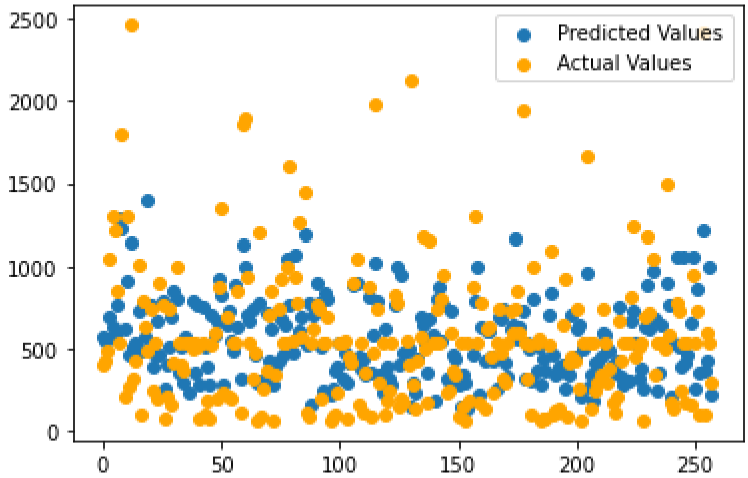

```
Test Result:
================================================

MSE for this regression model is:  69123.42067059061
RMSE for this regression model is:  262.9133330027038
```



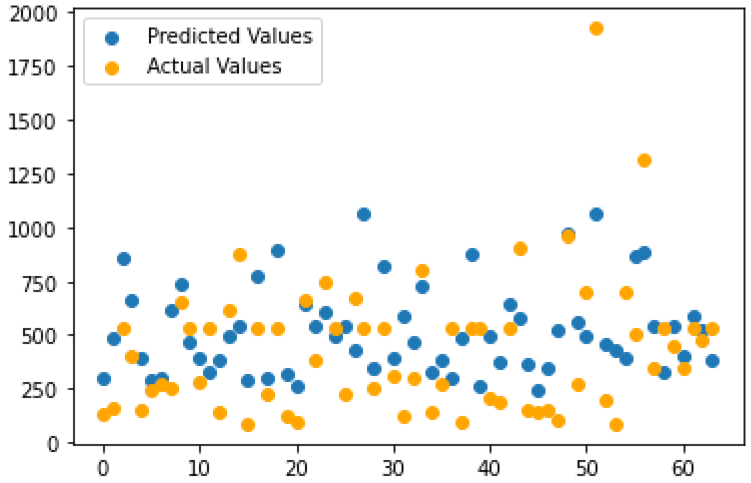

```
Cost Function for 9 principal components:
================================================
```



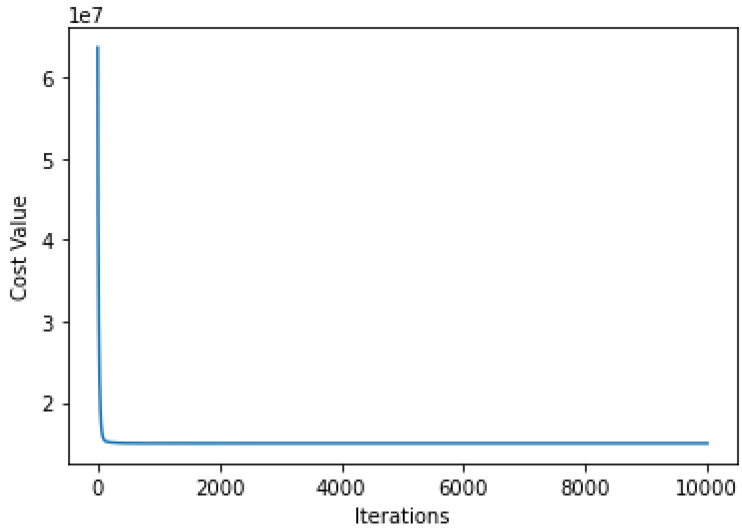

```
Train Result:
================================================

MSE for this regression model is:  118148.52607634694
RMSE for this regression model is:  343.727400822726
```



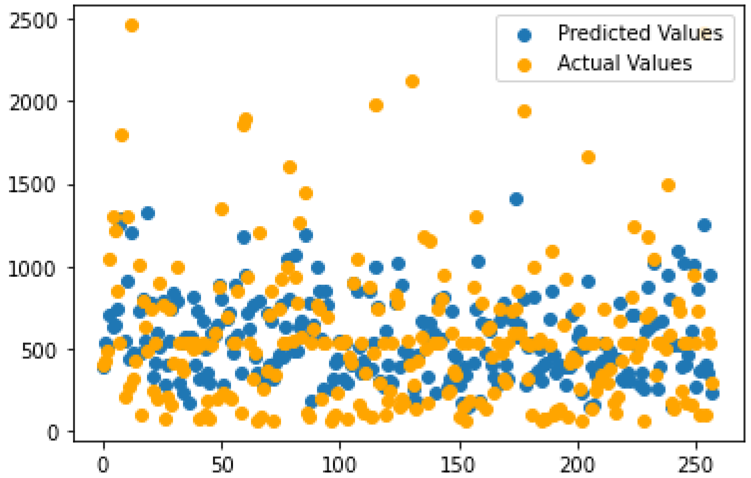

```
Test Result:
================================================

MSE for this regression model is:  69250.44213423833
RMSE for this regression model is:  263.1547874051284
```



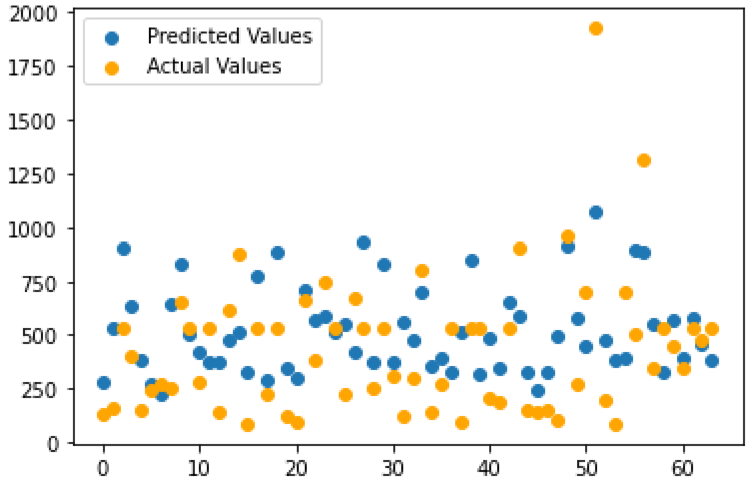

```
Cost Function for 10 principal components:
================================================
```



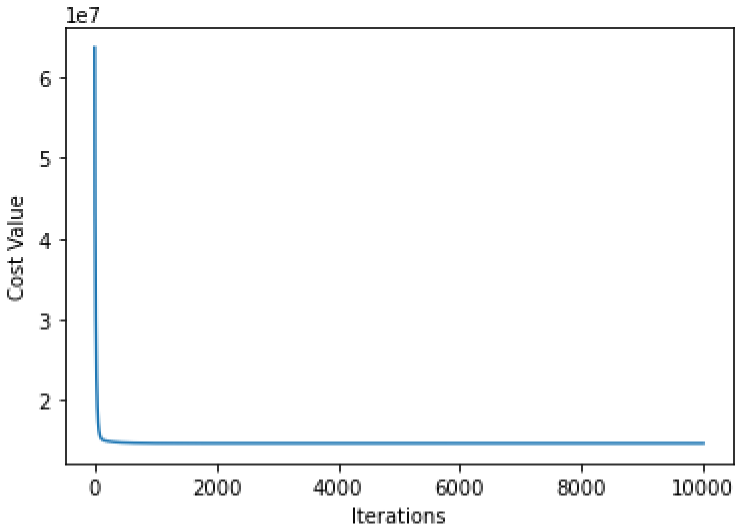

```
Train Result:
================================================

MSE for this regression model is:  116369.78391706859
RMSE for this regression model is:  341.1301568566881
```



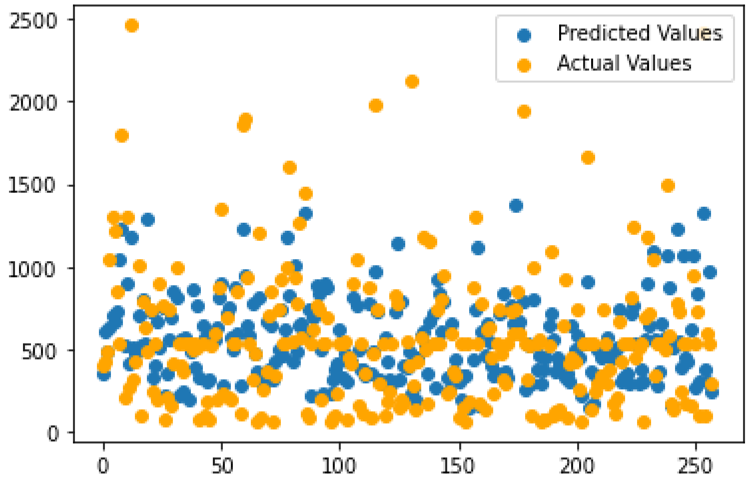

```
Test Result:
================================================

MSE for this regression model is:  68580.68915696764
RMSE for this regression model is:  261.8791499088227
```



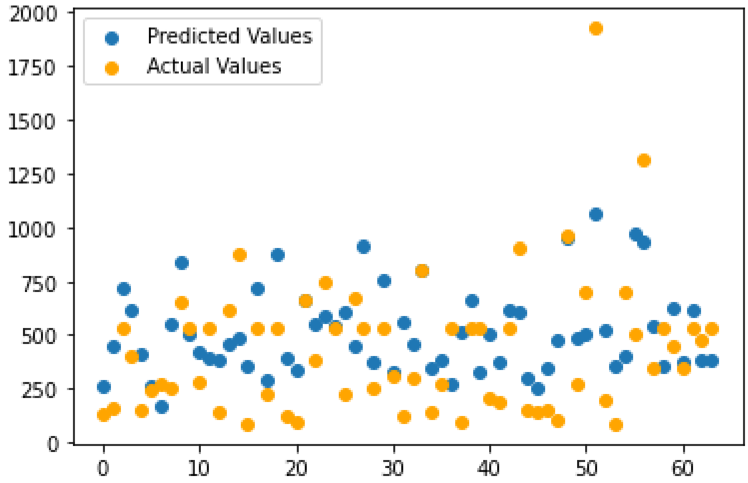

```
Cost Function for 11 principal components:
================================================
```



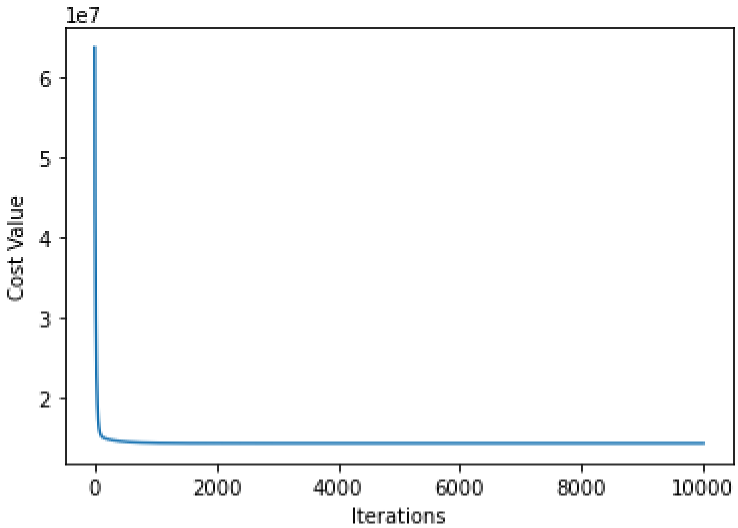

```
Train Result:
================================================

MSE for this regression model is:  113834.33104056367
RMSE for this regression model is:  337.3934365700727
```



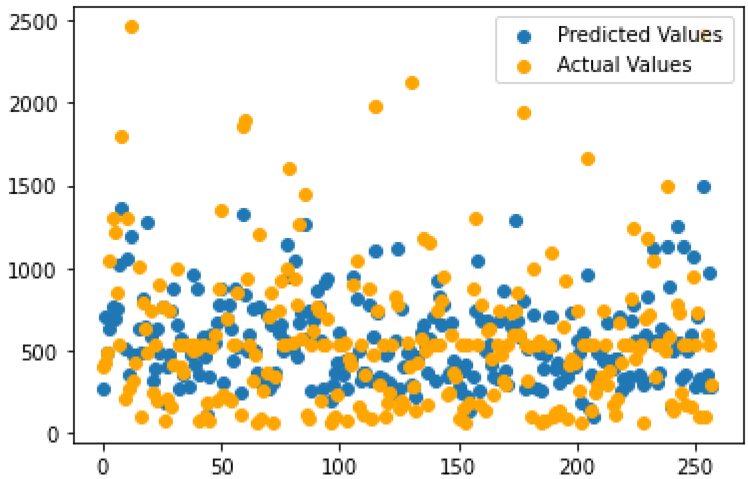

```
Test Result:
================================================

MSE for this regression model is:  63896.603778246
RMSE for this regression model is:  252.77777548322163
```



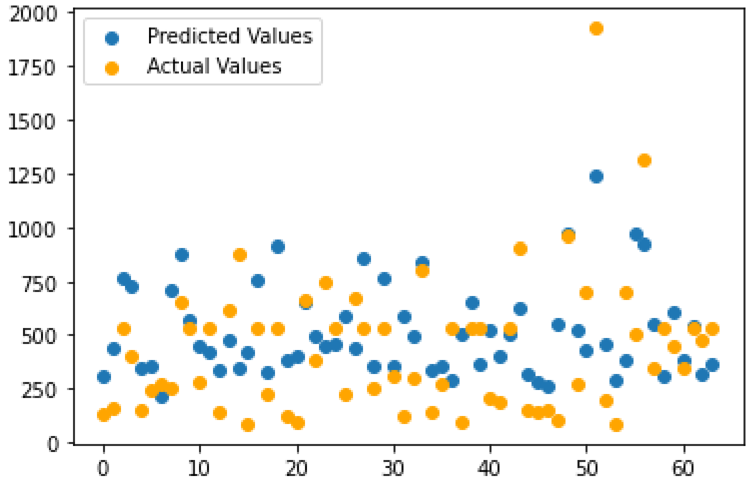

```
Cost Function for 12 principal components:
================================================
```



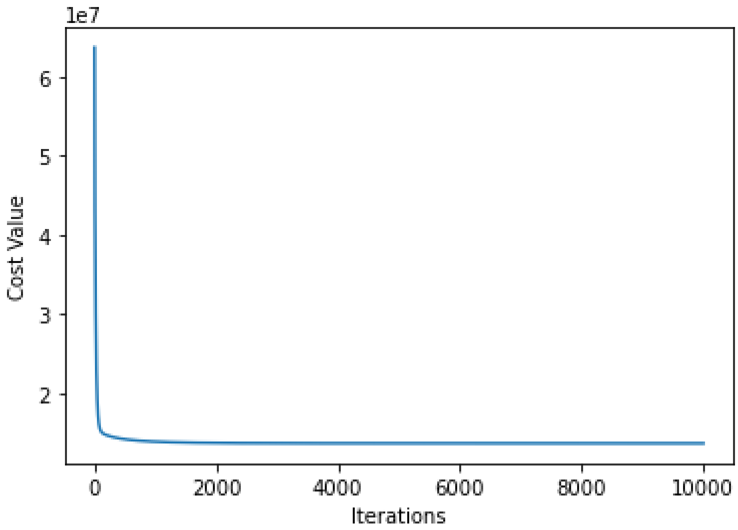

```
Train Result:
================================================

MSE for this regression model is:  110365.84926859835
RMSE for this regression model is:  332.2135597301807
```



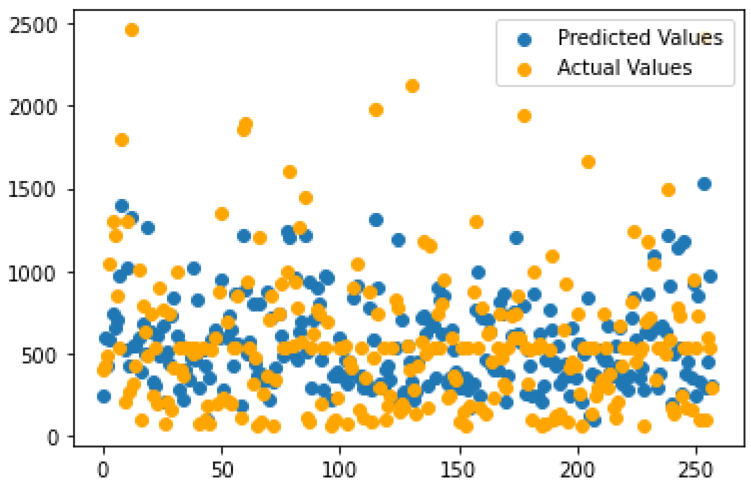

```
Test Result:
================================================

MSE for this regression model is:  67466.74403470497
RMSE for this regression model is:  259.743612115303
```



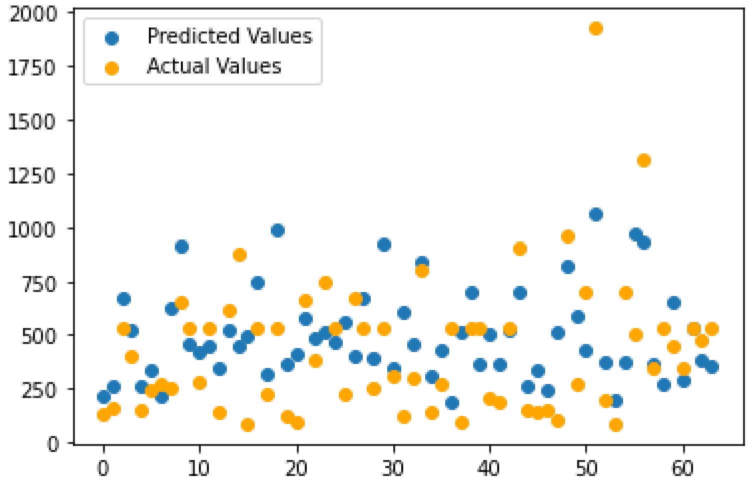

```
Cost Function for 13 principal components:
================================================
```



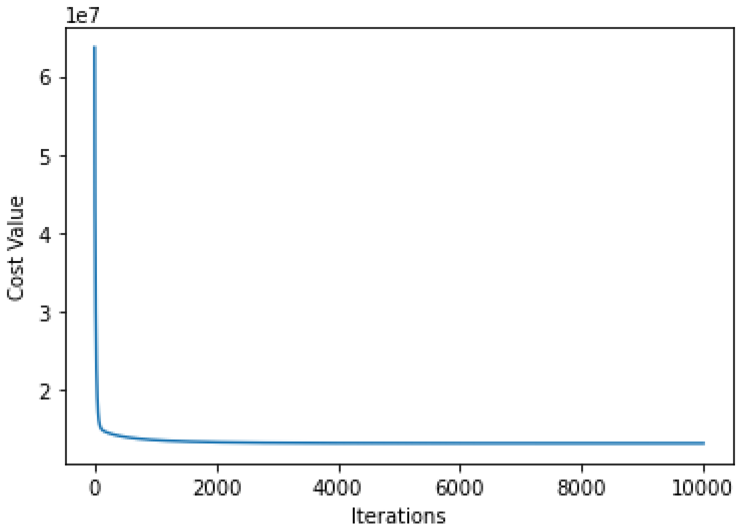

```
Train Result:
================================================

MSE for this regression model is:  105564.36312737507
RMSE for this regression model is:  324.90669911126037
```



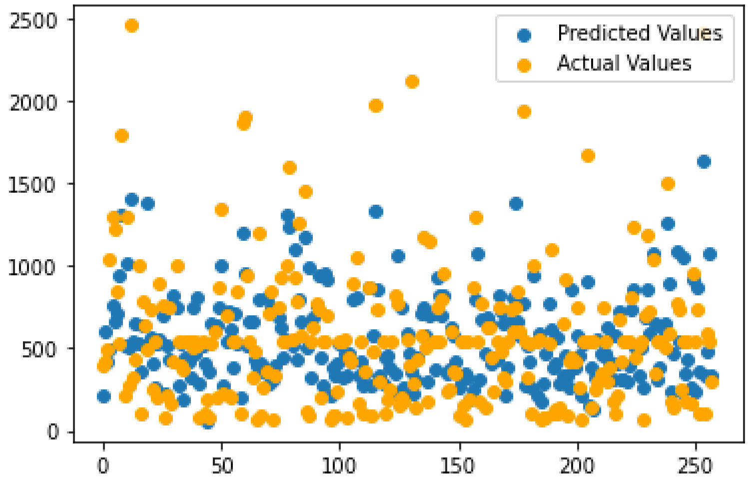

```
Test Result:
================================================

MSE for this regression model is:  66523.98614214815
RMSE for this regression model is:  257.9224421064366
```



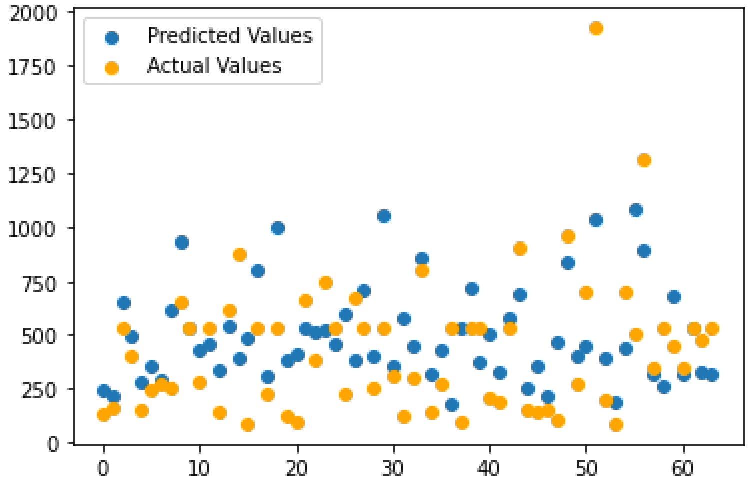

```
Cost Function for 14 principal components:
================================================
```



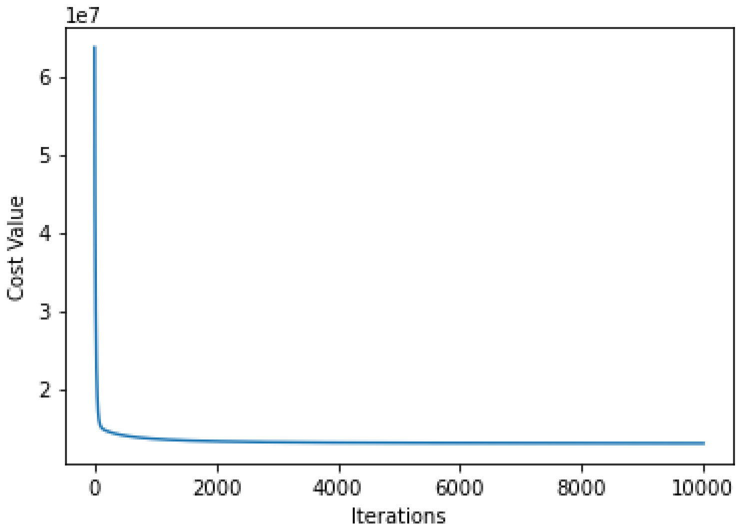

```
Train Result:
================================================

MSE for this regression model is:  102214.10306544695
RMSE for this regression model is:  319.70940409291524
```



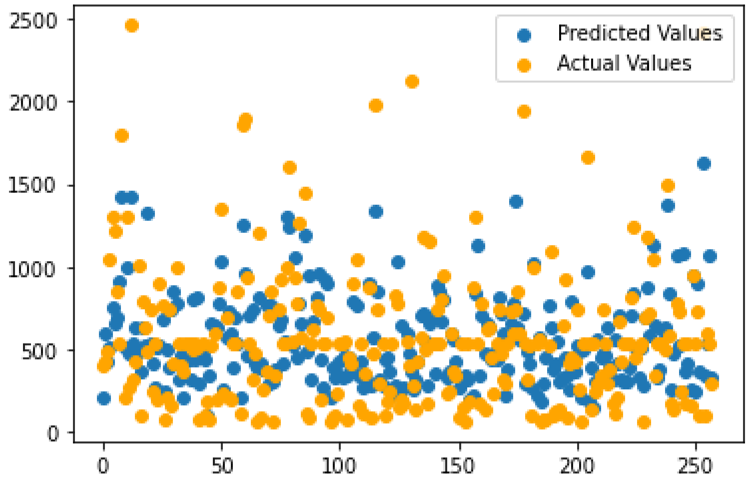

```
Test Result:
================================================

MSE for this regression model is:  71587.0821505513
RMSE for this regression model is:  267.5576239813609
```



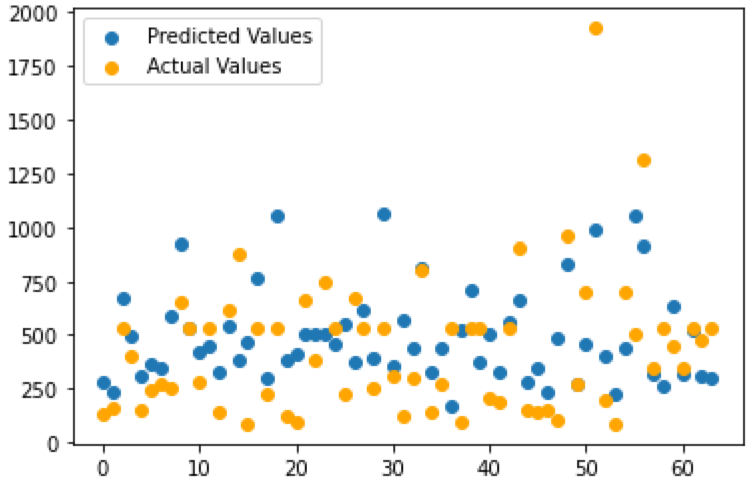

```
Cost Function for 15 principal components:
================================================
```



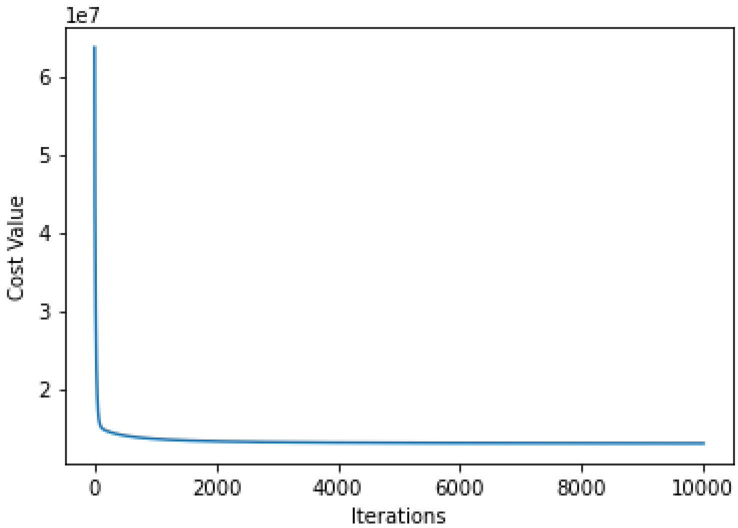

```
Train Result:
================================================

MSE for this regression model is:  100747.2834013865
RMSE for this regression model is:  317.4071256310836
```



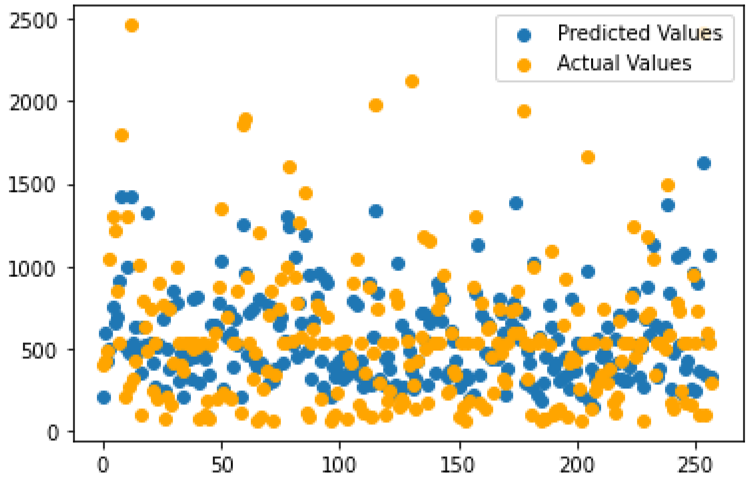

```
Test Result:
================================================

MSE for this regression model is:  72261.0666914737
RMSE for this regression model is:  268.8141861797359
```



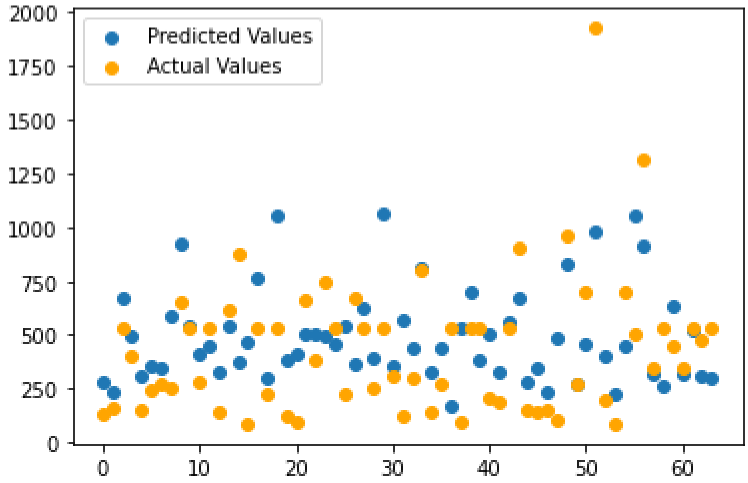

```
Cost Function for 16 principal components:
================================================
```




```
Train Result:
================================================

MSE for this regression model is:  100687.48903965203
RMSE for this regression model is:  317.3129197490263
```



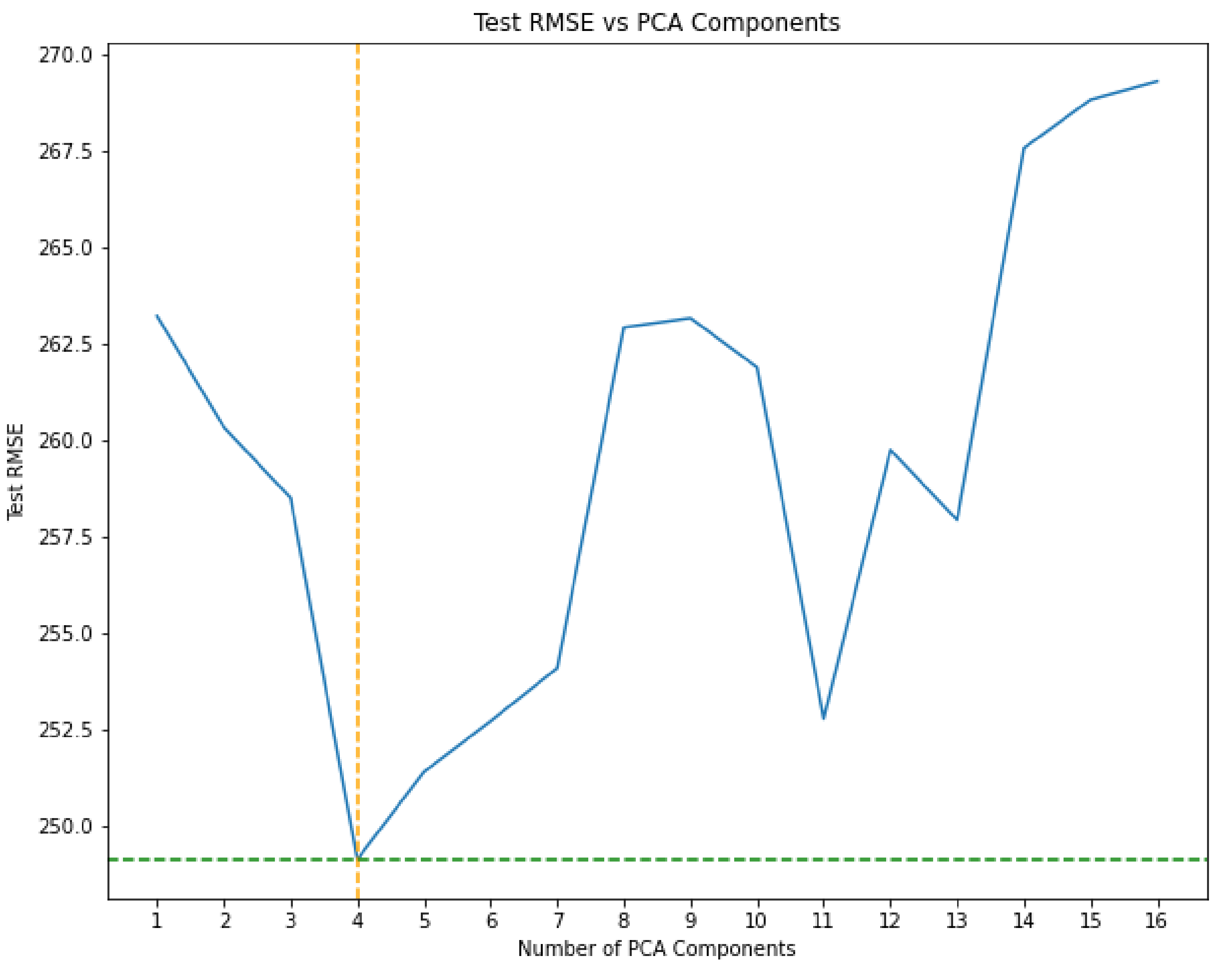

```
Test Result:
================================================

MSE for this regression model is:  72515.0589964796
RMSE for this regression model is:  269.28620275921975
```



Plotting Number of Components vs RMSE

In [44]:

```
# graph showing rmse vs number of pca components
pca_components = [x for x in range(1,17)]
plt.figure(figsize=(10, 8))
plt.plot(pca_components,rmse_arr)
plt.xlabel('Number of PCA Components')
plt.ylabel('Test RMSE')
plt.title('Test RMSE vs PCA Components')
plt.axvline(x=4,color='orange',linestyle='--')
plt.axhline(y=rmse_arr[3],color='green',linestyle='--')
plt.xticks(pca_components)
plt.show()
```



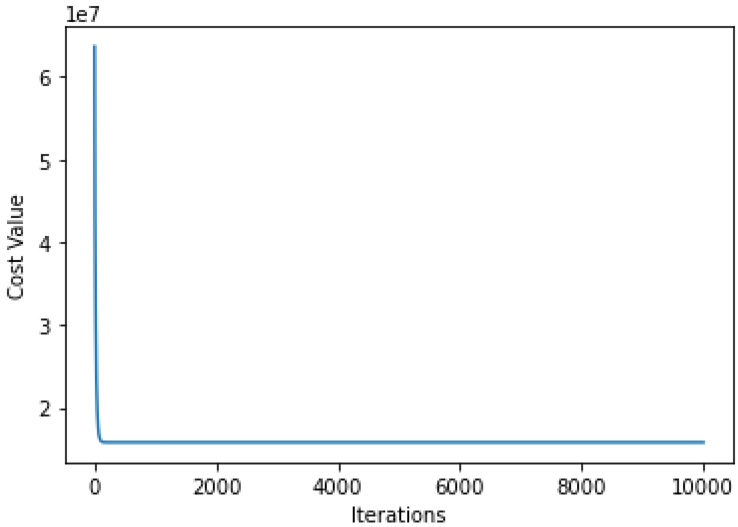
- Initially, as the number of `components increases` , the `RMSE decreases` . This is because a higher number of components capture more variance in the data, allowing the model to predict the underlying patterns better.
- We see that `minimum rmse is captured when we take 4 principal components` . The model captures enough information from the data without overfitting to the noise.
- Beyond 4 number of components, we see that adding more components does not improve the performance. In fact, it `leads to overfitting` , where the model starts `capturing noise` in the data rather than genuine patterns.

Testing the Most Efficient Model

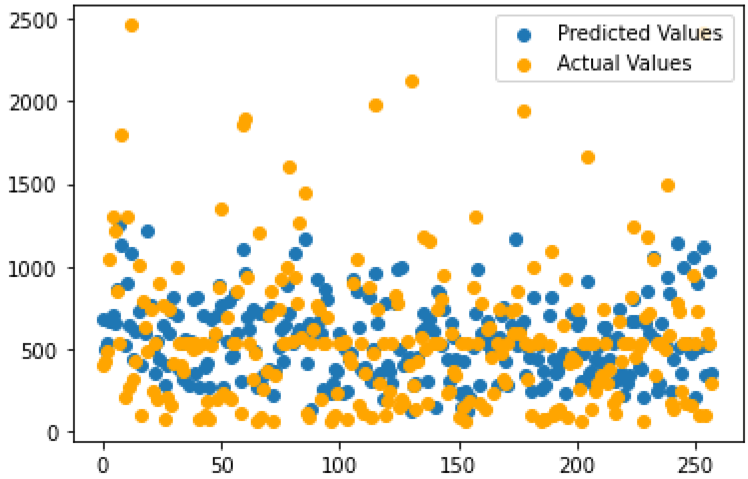
In [45]:
```
# optimal model is one with 4 principal components as per graph
```

In [46]:
```
iteration_x_axis_batch = []
cost_y_axis_batch = []
learning_rate = 0.0001

weight_vector = batch_gradient_descent(x_train,y_train,x_test,4,learning_rate
x_train_k , x_test_k = give_train_data(x_train,x_test,4)
print_score(y_train,x_train_k,y_test,x_test_k,weight_vector,iteration_x_axis_
print()
```

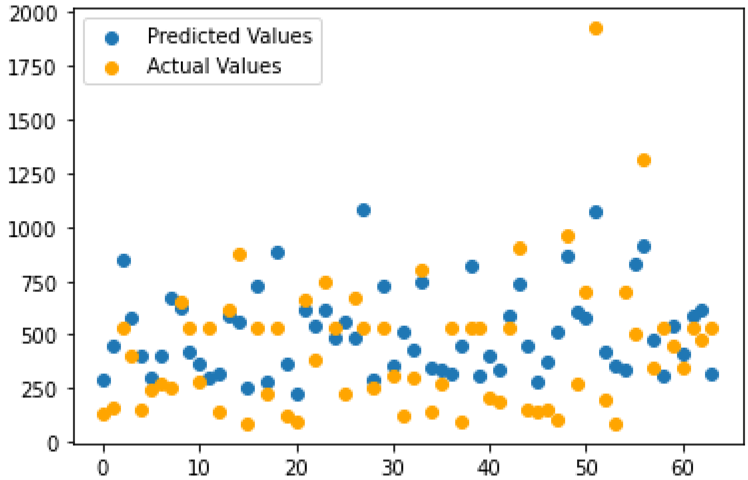
```
Cost Function for 4 principal components:
================================================
```




```
Train Result:
================================================

MSE for this regression model is:  122334.69938773432
RMSE for this regression model is:  349.7637765517383
```




```
Test Result:
================================================

MSE for this regression model is:  62066.5675490257
RMSE for this regression model is:  249.1316269545593
```



In [47]:

```python
y_pred = find_predicted_value(weight_vector,x_test_k)
y_pred
```

Out[47]:

```
array([ 292.09190287,  444.0216452 ,  844.54823872,  579.87082768,
        401.82204258,  298.5314266 ,  403.0507171 ,  668.10867811,
        628.13093754,  422.21433009,  363.55847907,  300.13178713,
        317.8443312 ,  588.79558347,  561.04482364,  248.84498554,
        724.42351648,  277.3756033 ,  888.83650636,  369.28796575,
        223.0068406 ,  618.96757355,  545.69050979,  612.03623706,
        485.98976768,  561.95193564,  487.0417952 , 1077.82394794,
        292.78949674,  727.92596284,  358.9555134 ,  513.57102203,
        431.82978973,  748.1268539 ,  342.57088434,  337.73796565,
        320.67487105,  445.53536206,  824.31655246,  313.31294985,
        401.99808253,  338.63199682,  585.42909667,  734.4708019 ,
        445.25434793,  283.46051658,  376.60885062,  513.26476444,
        871.17425811,  607.48603174,  577.23002525, 1075.34912294,
        418.86287162,  357.32219951,  334.85303463,  828.48092741,
        909.39983168,  473.0545686 ,  307.76323673,  546.23384919,
        414.22476791,  587.62071377,  616.78810425,  319.62583406])
```

In [48]:

```python
# predicted value for a single point
y_pred[:1]
```

Out[48]:

```
array([292.09190287])
```

Conclusion and Analysis

Significance of selecting an appropriate number of components

- PCA reduces the dimensionality of the dataset by transforming it into a new set of uncorrelated variables. This takes care of capturing the required information and not overfitting by capturing the noise of the data.
- A lower number of components simplifies the model and also makes the computation easy.
- It is easier to understand and interpret the contribution of each principal component to the overall prediction.