Visualizing and Understanding the Relationship between PCA, Auto encoder and K-Means Clustering

Presented By

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Introduction and Outline

Step 1: Relation between PCA Guided K-means and K-means (simulation)

Step 2 : Relation between PCA and Linear Auto encoder (proof + simulation)

Step 1 : Relation between PCA Guided K-means and K-means

Dataset : IMDB Movie data

Data Dimensions : 14332×44 removing strings like url 14332 we get $\times$ 38

Data Pre-processing : Fill NA values, Standardisation

In [1]:

```python
# Loading the Libraries
import numpy as np
import pandas as pd
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import MinMaxScaler
from keras.layers import Input, Dense
from keras import regularizers, Model, optimizers
import seaborn as sns
import keras

from sklearn import datasets
%matplotlib inline
import warnings
warnings.filterwarnings('ignore')
```

```
Using TensorFlow backend.
```

Loading the data

In [ ]:
```
data = pd.read_csv('imdb.csv',error_bad_lines=False);
```

Data Pre-processing

In [3]:

```
data.head()
movie = data
str_list = []
for colname, colvalue in movie.iteritems():
    if type(colvalue[1]) == str:
         str_list.append(colname)
num_list = movie.columns.difference(str_list)
movie_num = movie[num_list]
movie_num.head()
movie_num = movie_num.fillna(value=0, axis=1)
X = movie_num.values
X_std = StandardScaler().fit_transform(X)
movie_num.head()
```

Out[3]:

	Action	Adult	Adventure	Animation	Biography	Comedy	Crime	Documentary	Drama	Family	...	duration	imdbRating	nrOf(
0	0	0	0	0	0	1	0	0	1	1	...	3240.0	8.4	3
1	0	0	1	0	0	1	0	0	0	1	...	5700.0	8.3	3
2	0	0	0	0	0	0	0	0	1	0	...	9180.0	8.4	2
3	1	0	1	0	0	1	0	0	0	0	...	6420.0	8.3	3
4	0	0	0	0	0	1	0	0	1	0	...	5220.0	8.7	3

5 rows × 38 columns

Finding the Eigen Values and Eigen Vectors after Calculating Covariance Matrix

Sort the Eigen Values and Store corresponding Eigen Vectors Using Numpy package

In [4]:

```
# Calculating Eigenvectors and eigenvalues of Covariance matrix
mean_vec = np.mean(X_std, axis=0)
covariance_matrix = np.cov(X_std.T)
eig_vals, eig_vecs = np.linalg.eig(covariance_matrix)
eig_pairs = [ (np.abs(eig_vals[i]),eig_vecs[:,i]) for i in
range(len(eig_vals))]
eig_pairs.sort(key = lambda x: x[0], reverse= True)
print('Top 5 Eigenvalues in descending order:')
for i in eig_pairs[:5]:
    print(i[0])
```

```
Top 5 Eigenvalues in descending order:
3.757417563959593
2.2059055052727463
1.9752793363920373
1.7860731429920065
1.5733880931673736
```

Problem : Number of Principal Components to Choose ?

Solution : Explained Variance measure

Idea : Explained Variance Calculates the information of Variance attributed to each of Principal Components

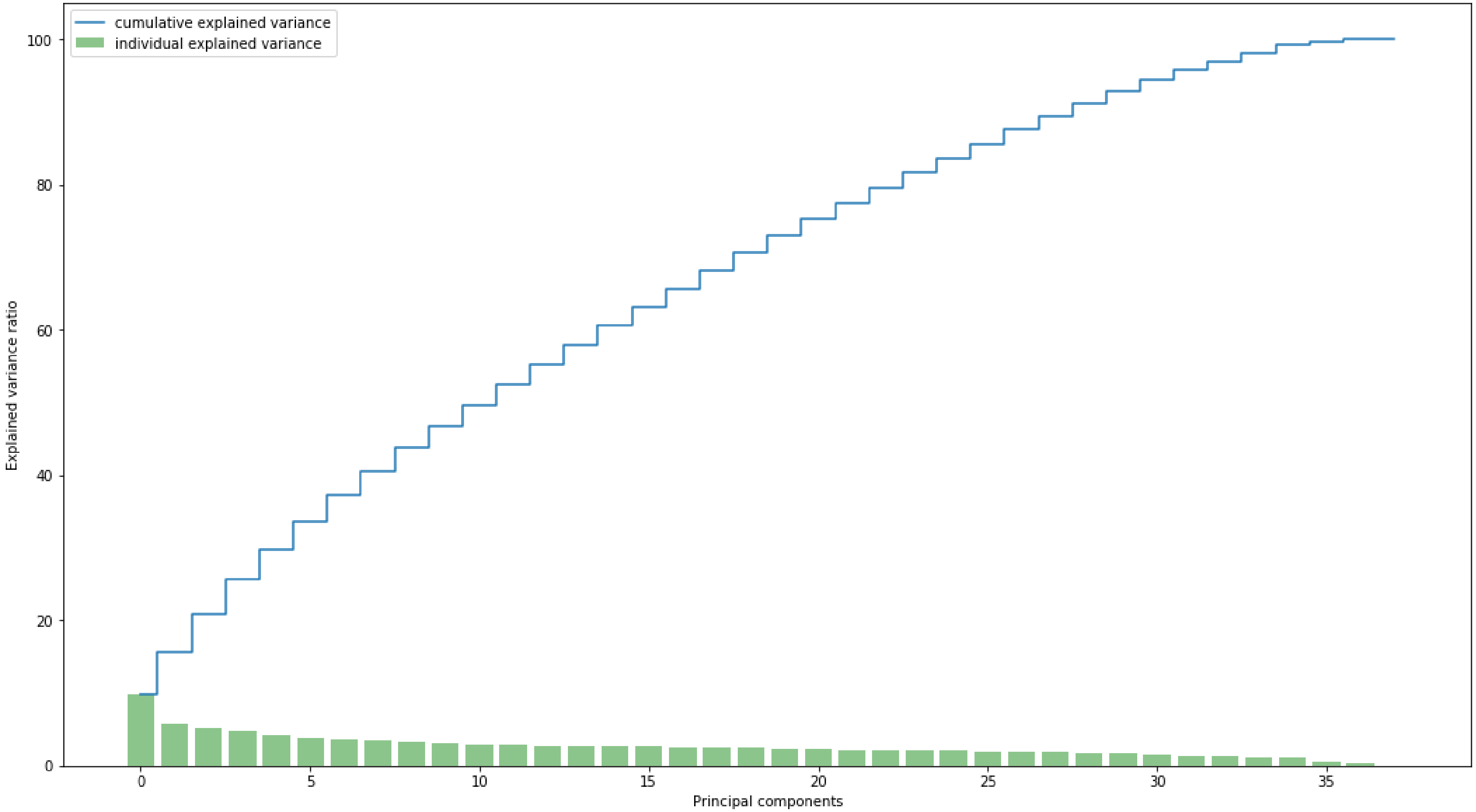
Cummulative Explained variance of k PC's can be Understood as percentage of Variance covered using K PC's

In [5]:

```
tot = sum(eig_vals)
var_exp = [(i/tot)*100 for i in sorted(eig_vals, reverse=True)]
cum_var_exp = np.cumsum(var_exp)
```

In [6]:

```
plt.figure(figsize=(18, 10))
plt.bar(range(38), var_exp, alpha=0.45, align='center', label='individual explai
ned variance', color = 'g')
plt.step(range(38), cum_var_exp, where='mid',label='cumulative explained varianc
e')
plt.ylabel('Explained variance ratio')
plt.xlabel('Principal components')
plt.legend(loc='best')
plt.show()
```



In [7]:

```
print(cum_var_exp[27])
```

```
89.36400271832298
```

Above plot explains 89.3% of Variance can be explained using 27 components.

Running PCA using Principal 27 components

In [8]:

```
pca = PCA(n_components=27)
x_25d = pca.fit_transform(X_std)
x_25d.shape
```

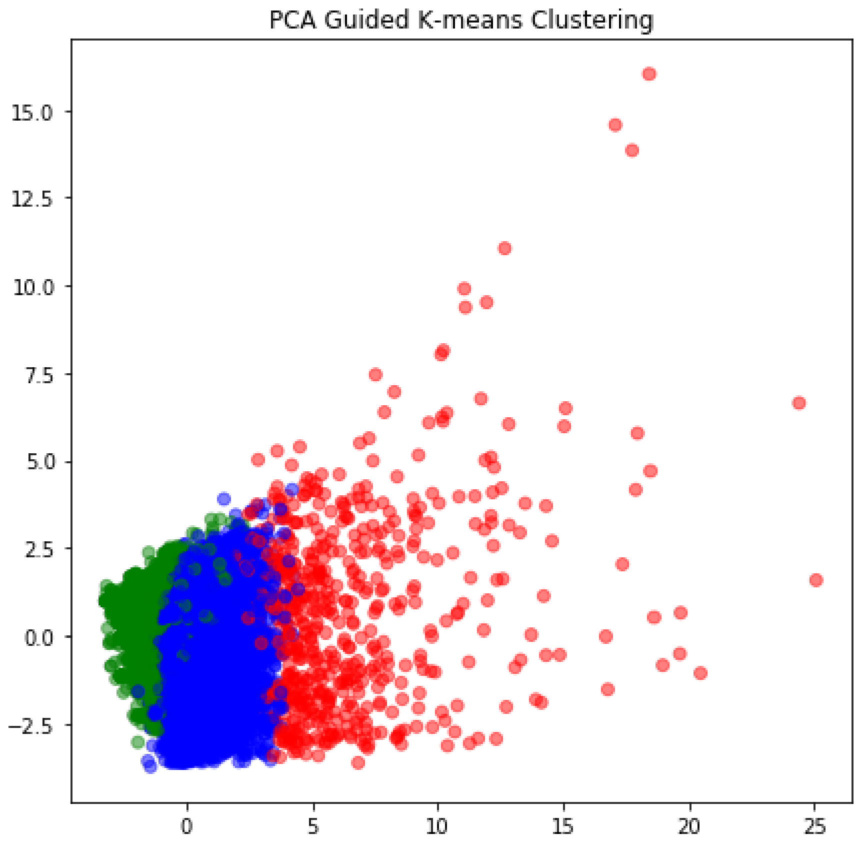
Out[8]:

```
(14332, 27)
```

PCA Guided K-means Clustering Vs K-means Clustering for number of clusters = 3

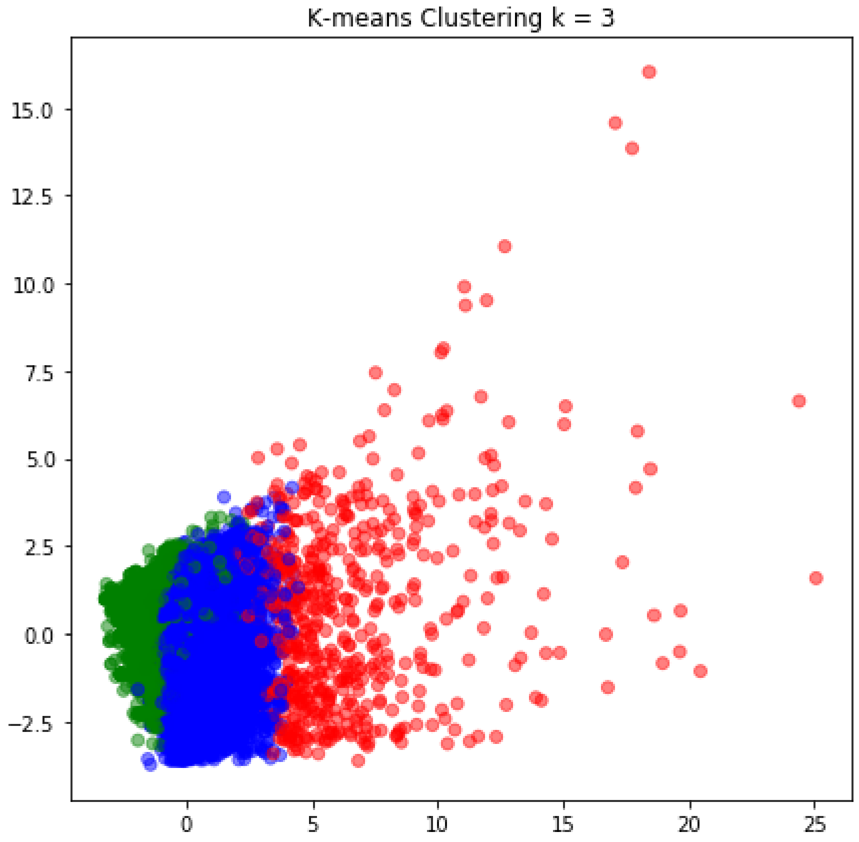
In [9]:

```
kmeans = KMeans(n_clusters=3)
X_clustered = kmeans.fit_predict(x_25d)
LABEL_COLOR_MAP = {0 : 'r',1 : 'g',2 : 'b',3:'y'}
label_color = [LABEL_COLOR_MAP[l] for l in X_clustered]
plt.figure(figsize = (7,7))
plt.scatter(x_25d[:,0],x_25d[:,2], c= label_color, alpha=0.5)
plt.title("PCA Guided K-means Clustering")
plt.show()
```

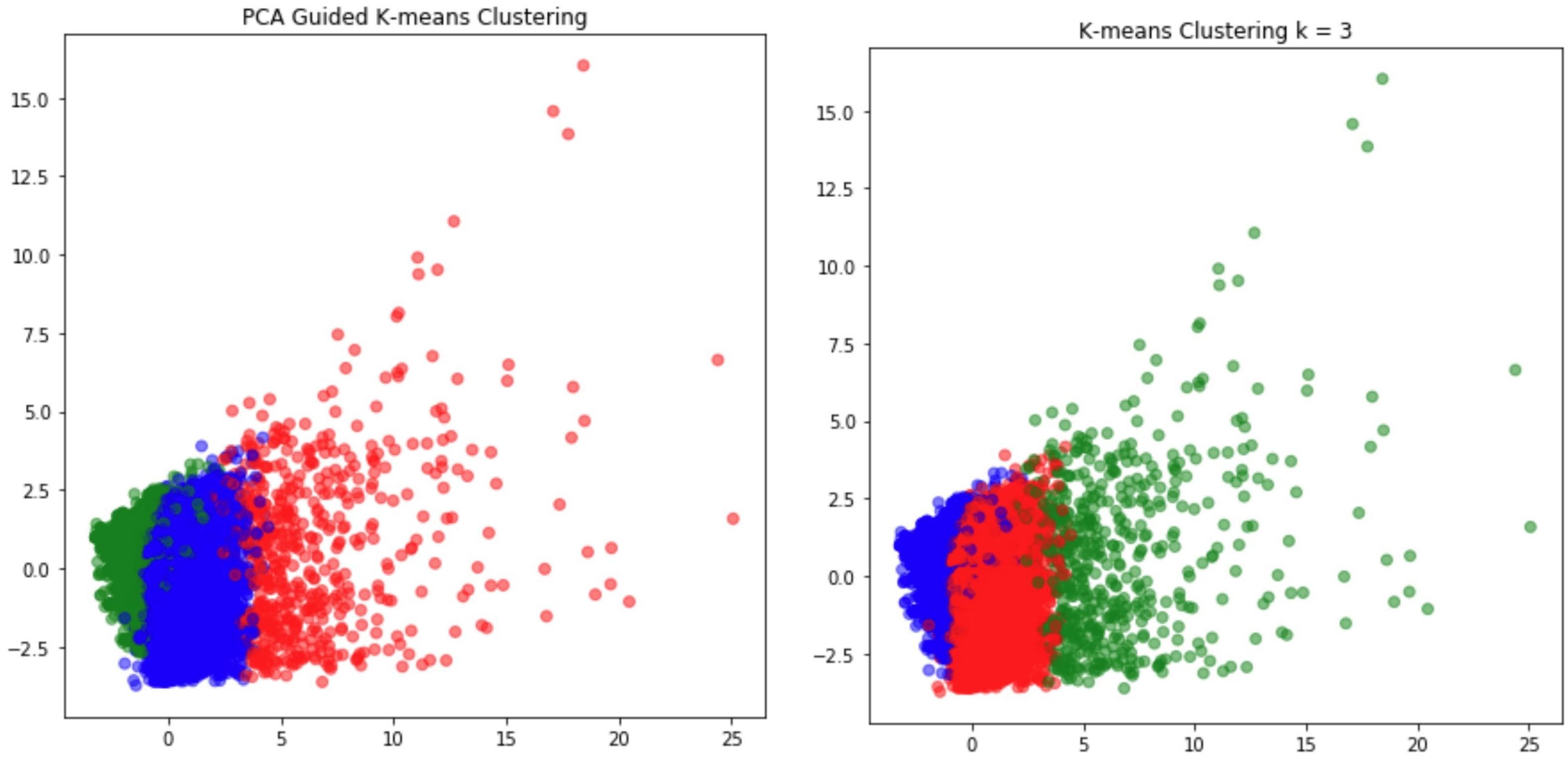


In [10]:

```
kmeans = KMeans(n_clusters=3)
X_clustered = kmeans.fit_predict(X_std)
LABEL_COLOR_MAP = {0 : 'r',1 : 'g',2 : 'b',3:'y'}
label_color = [LABEL_COLOR_MAP[l] for l in X_clustered]
plt.figure(figsize = (7,7))
plt.title("K-means Clustering k = 3")
plt.scatter(x_25d[:,0],x_25d[:,2], c= label_color, alpha=0.5)
plt.show()
```



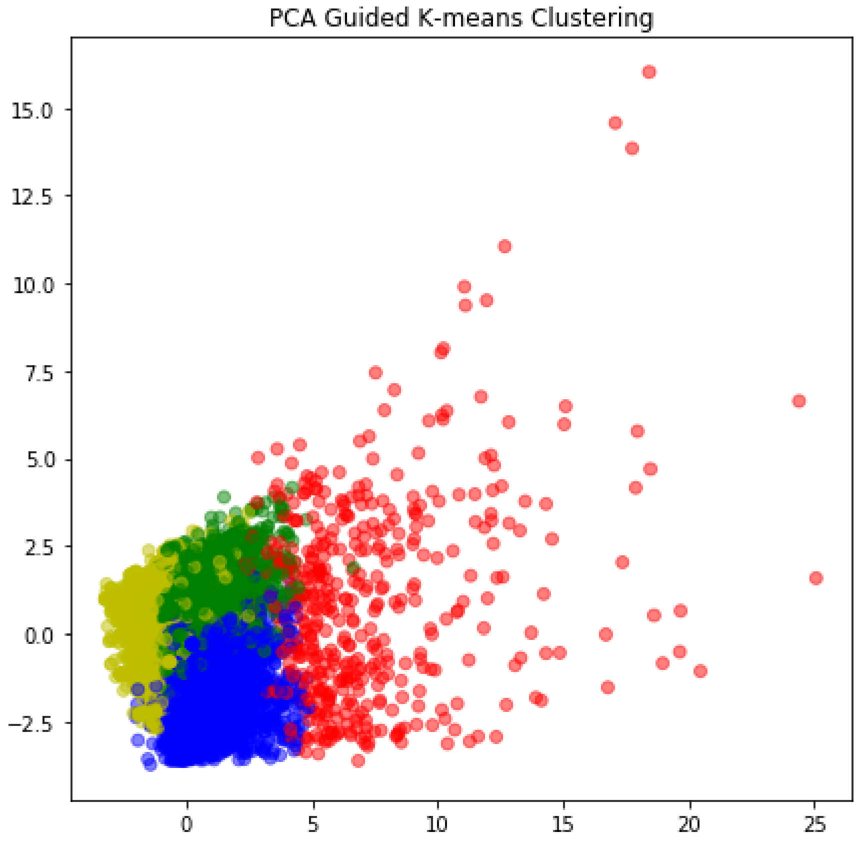
PCA guided K-means Clustering Vs K-means clustering for k =3



PCA Guided K-means Clustering Vs K-means Clustering for number of clusters =4

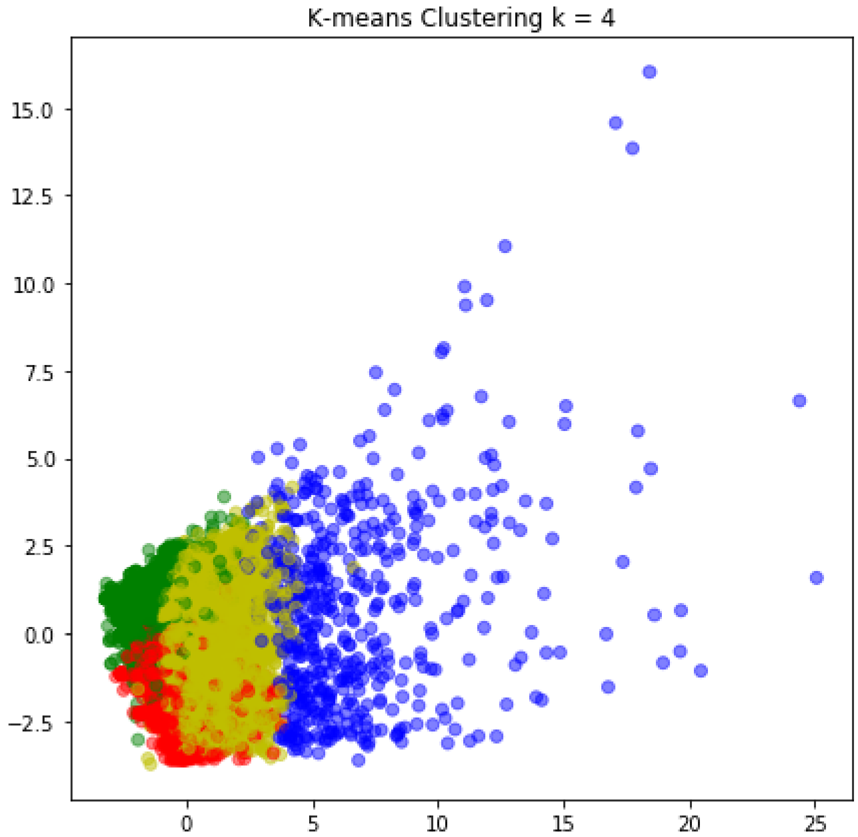
In [11]:

```
kmeans = KMeans(n_clusters=4)
X_clustered = kmeans.fit_predict(x_25d)
LABEL_COLOR_MAP = {0 : 'r',1 : 'g',2 : 'b',3:'y'}
label_color = [LABEL_COLOR_MAP[l] for l in X_clustered]
plt.figure(figsize = (7,7))
plt.scatter(x_25d[:,0],x_25d[:,2], c= label_color, alpha=0.5)
plt.title("PCA Guided K-means Clustering")
plt.show()
```

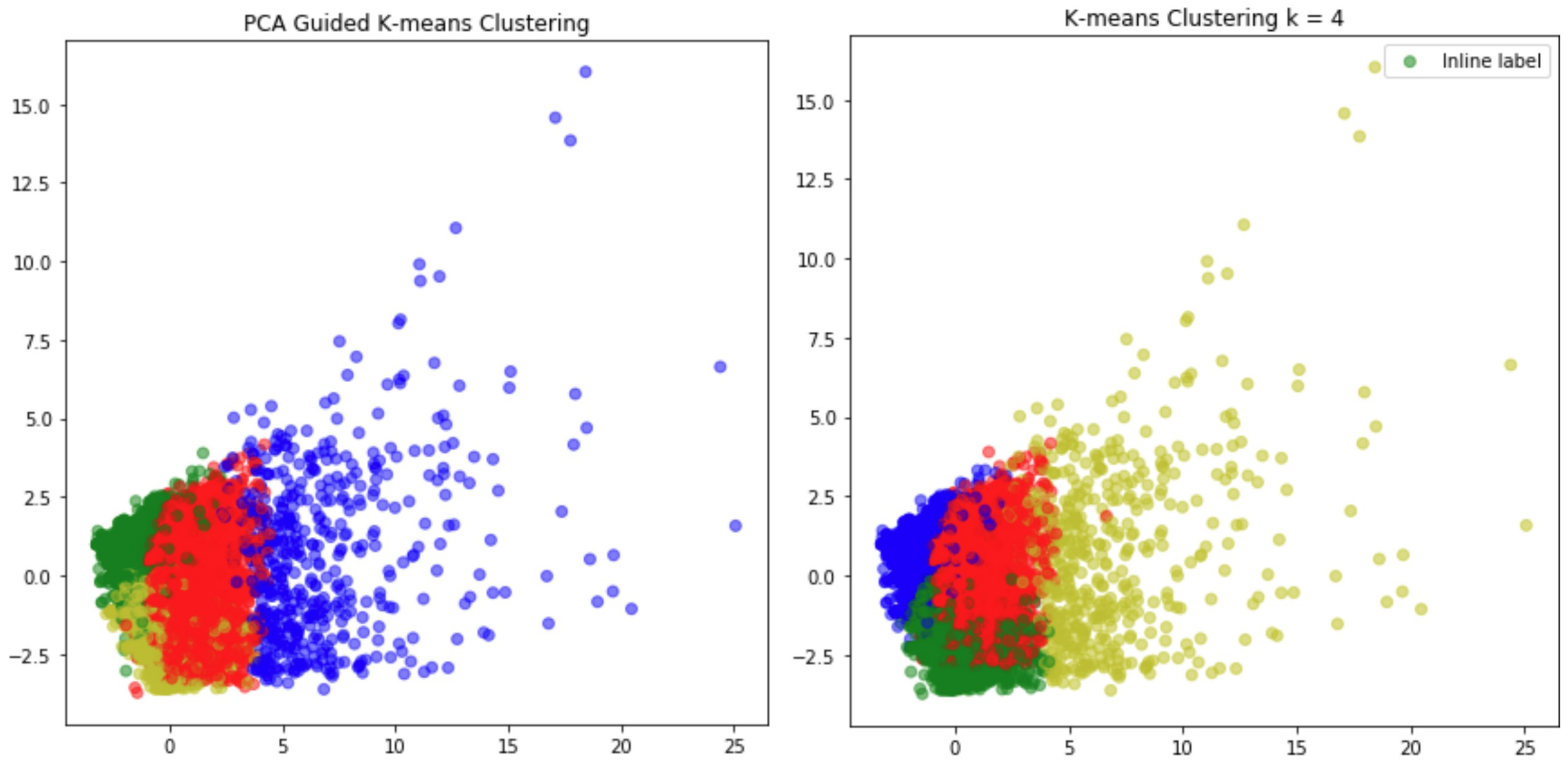


In [12]:

```
kmeans = KMeans(n_clusters=4)
X_clustered = kmeans.fit_predict(X_std)
LABEL_COLOR_MAP = {0 : 'r',1 : 'g',2 : 'b',3:'y'}
label_color = [LABEL_COLOR_MAP[l] for l in X_clustered]
plt.figure(figsize = (7,7))
plt.title("K-means Clustering k = 4")
plt.scatter(x_25d[:,0],x_25d[:,2], c= label_color, alpha=0.5)
plt.show()
```

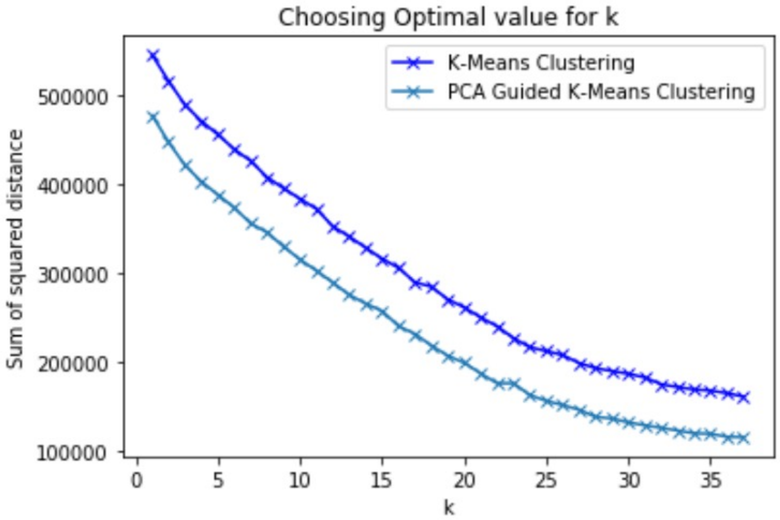


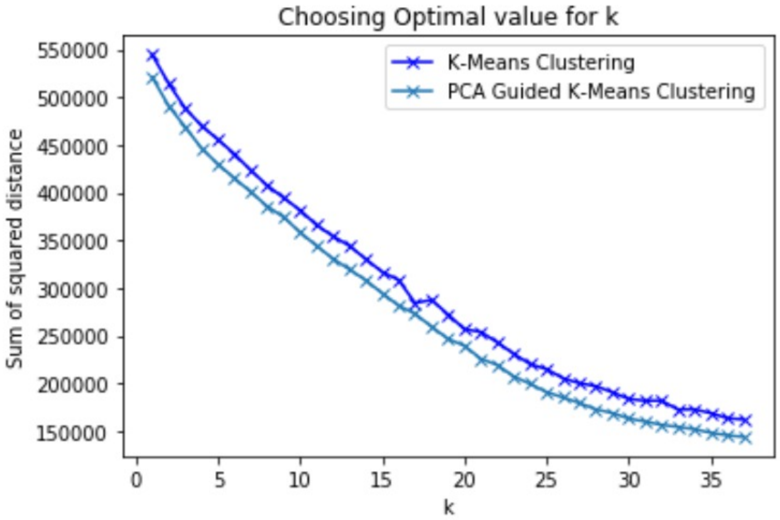
PCA guided K-means clustering Vs K-means clustering for number of clusters = 4



Choosing Optimal Number of Clusters i.e., k

Choosing optimal k PCA guided K-means clustering vs K-means clustering for different principal components





Conclusion of PCA Guided K-means Vs K-Means clustering

PCA guided K-means clustering is very useful if number of dimensions in data are very high.

Advantage : can show approximate results to K-means clustering.

Proof : paper - ”k-means clustering via principal component analysis ”

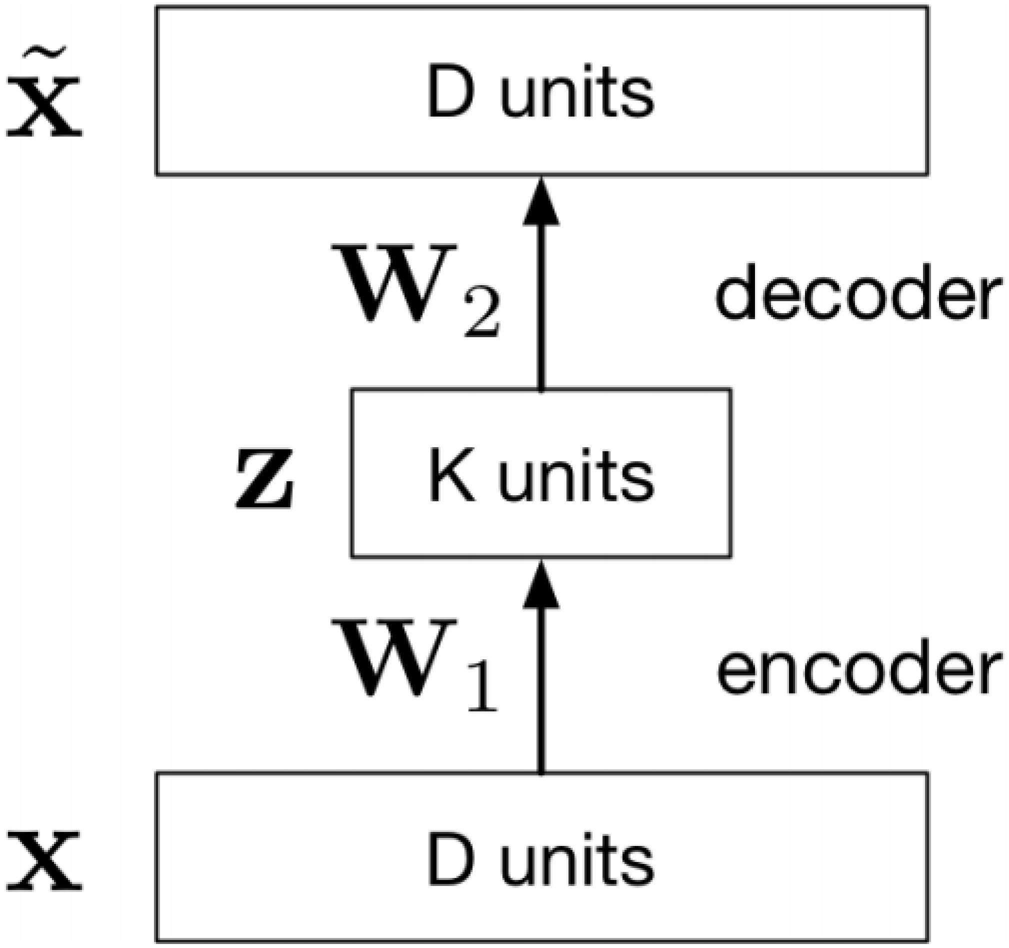
Used data to simulate : IMDB movie data

Step 2 :PCA and Linear Auto encoder

How PCA equivalent to Linear Auto encoder with Squared loss Function ?

In case of PCA, minimum reconstruction error is defined as :

$$\mathcal{L}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|^2$$



$$\mathbf{z} = f(W_1\mathbf{x}); \quad \hat{\mathbf{x}} = g(W_2\mathbf{z})$$

Squared loss error is given by :

$$\min_{\mathbf{W_1},\mathbf{W_2}} \frac{1}{2N} \sum_{n=1}^{N} \left\| \mathbf{x}^{(n)} - \hat{\mathbf{x}}^{(n)} \right\|^2$$

If we Assume functions f and g linear i.e..,

$$\min_{\mathbf{W_1},\mathbf{W_2}} \frac{1}{2N} \sum_{n=1}^{N} \left\| \mathbf{x}^{(n)} - W_2 W_1 \mathbf{x}^{(n)} \right\|^2$$

If we Consider in Auto encoder we have

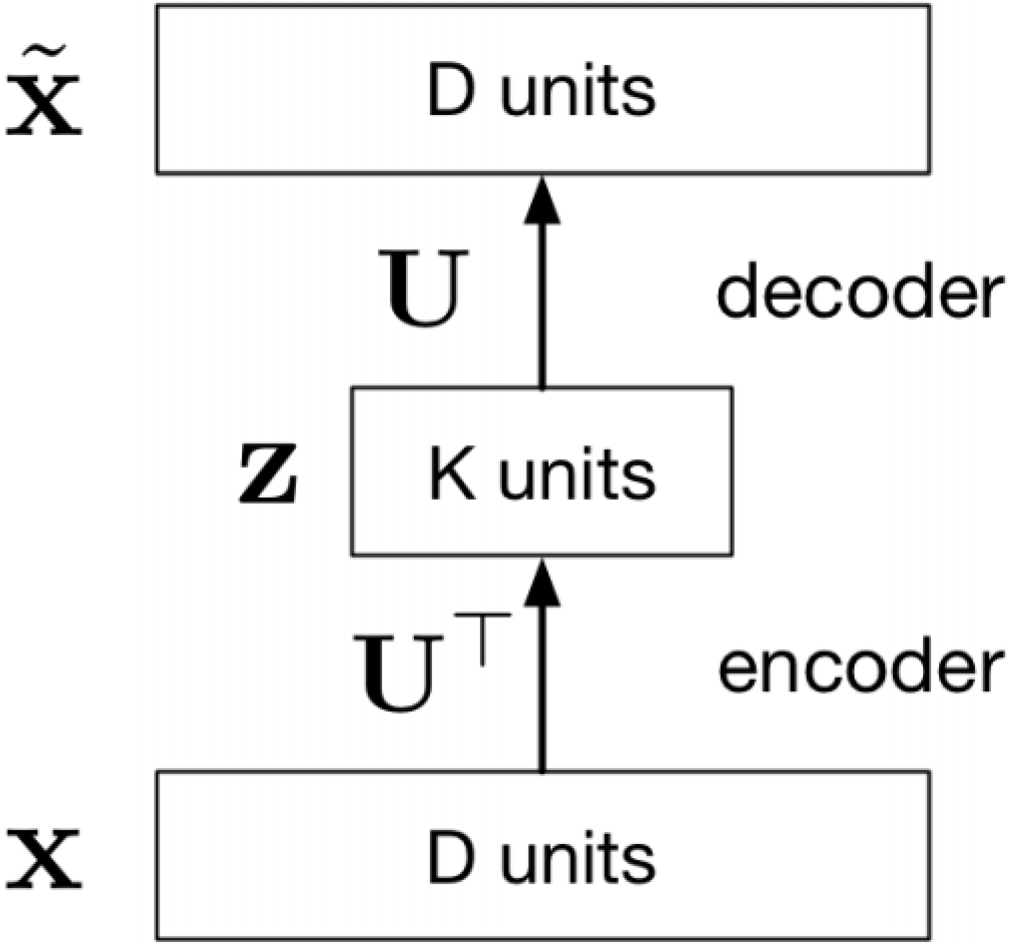
$$\tilde{\mathbf{x}} = \mathbf{W}_2\mathbf{W}_1\mathbf{x}$$

Under the Constraint,

$$\mathbf{W}_2\mathbf{W}_1 = \mathbf{I}$$

The above Optimisation problem of Auto encoder is equivalent to PCA.

Note : Optimal subspace spanned in Auto encoder defined above are equivalent to subspace spanned by Principal Components in PCA



Note : Principal components weights is not equal to Linear Auto encoder weights. But the Subspace spanned by both Principal component weights and Linear auto encoder will be same.

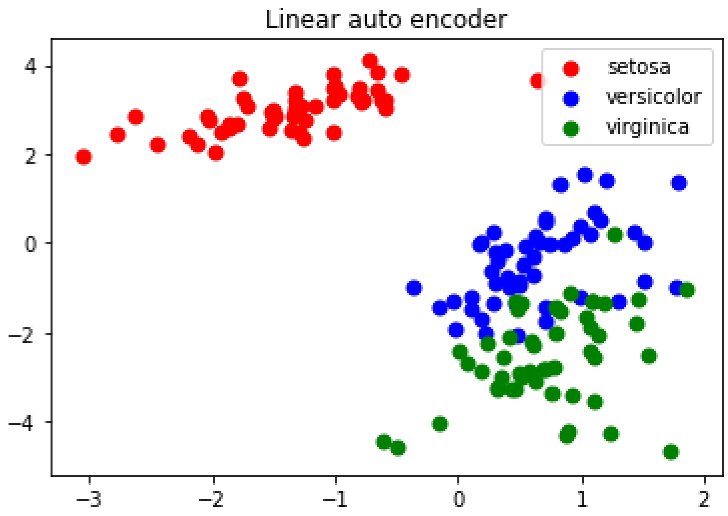
How to recover Principal components from Linear auto Encoder weights ??

Idea : It is shown that first m singular vectors of W_2 are the first m principal components of X.

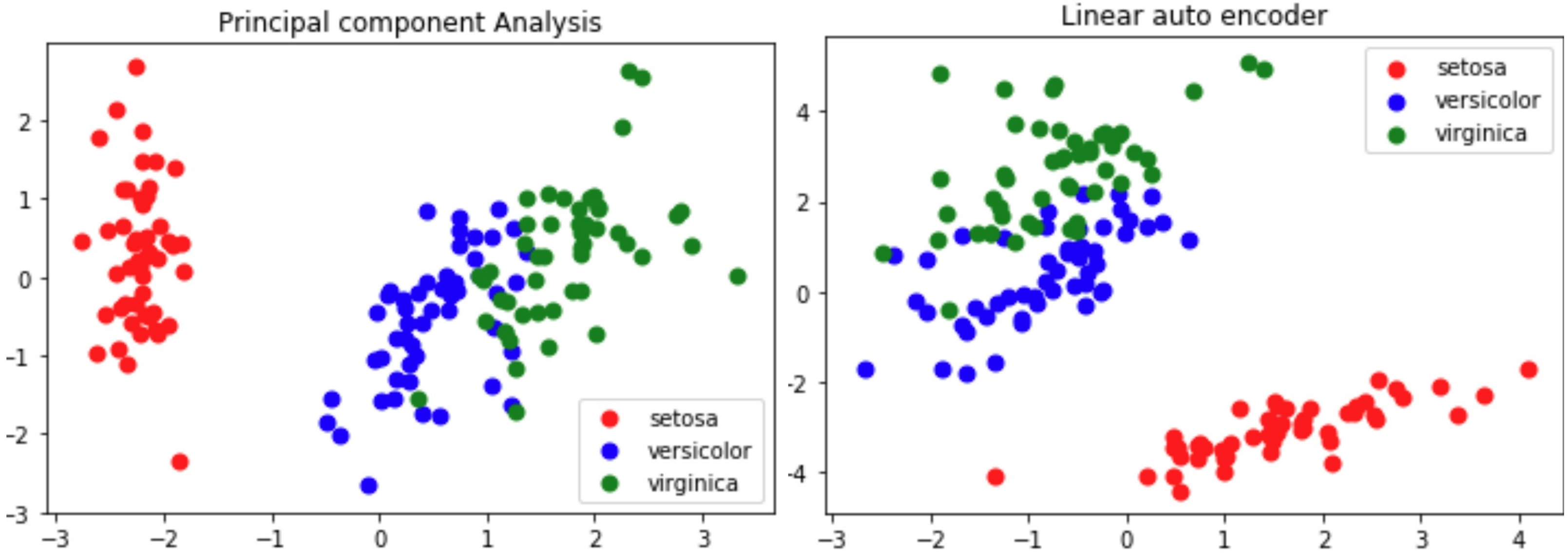
"From Principal Subspaces to Principal Components with Linear Autoencoders"

In [15]:
```
iris = datasets.load_iris()
X = iris.data
y = iris.target
target_names = iris.target_names
scaler = StandardScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)
```

In [19]:
```
encoder = Model(input_img, encoded)
encoded_input = Input(shape=(encoding_dim,))
decoder_layer = autoencoder.layers[-1]
decoder = Model(encoded_input, decoder_layer(encoded_input))
encoded_data = encoder.predict(X_scaled)
X = encoded_data[:,:2]
plt.figure()
colors = ['red', 'blue', 'green']
lw = 2
for color, i, target_name in zip(colors, [0, 1, 2], target_names):
      plt.scatter(X[y == i, 0], X[y == i, 1], color=color, alpha=1., lw=lw,
                  label=target_name)
plt.legend(loc='best', shadow=False, scatterpoints=1)
plt.title("Linear auto encoder")
plt.show()
```



Plot for PCA and Linear auto encoder on IRIS dataset



Conclusion

Studied relation between PCA guided K-means clustering vs K-means clustering.

Studied relation between PCA and auto encoder under constraints.

Future work : How to retrieve principal components from auto encoder weights ?

From Principal Subspaces to Principal Components with Linear Autoencoders

Future work : How well can non linear auto encoder can perform ?

paper : "Reducing the Dimensionality of Data with Neural Networks"