

Sample Code for an Autoencoder for Dr. Goswami

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Introduction and Dataset

In this notebook we will do a test-case with synthetic data comparing classic PCA with an autoencoder to see that the autoencoder is able to take high-dimensional data and extract out the relevant features.

Dataset

Our dataset will be a synthetic dataset in which we will use the sklearn datasets method to create eight “blobs” of data and 30,000 observations. Each blob has a centroid around which the data is clustered in a Gaussian fashion with a standard deviation of 2, i.e. each element of the cluster c , x_c is such that $x_c \sim \mathcal{N}(\text{centroid}_c, c)$. We will have nine features to the data, to which we will add an extra feature, consisting of noise coming from a uniform distribution.

Note on dataset: The author regrets to inform that due to the ongoing shutdowns of internet and communications in Bangladesh that they have had difficulty and delay obtaining actual datasets. This Jupyter notebook therefore serves as a proof of concept that autoencoders can be beneficial and viable in analyzing genomic data via proxy with synthetic data. The author apologizes for this inconvenience.

Introduction and Methodology

Our methodology will be as follows:

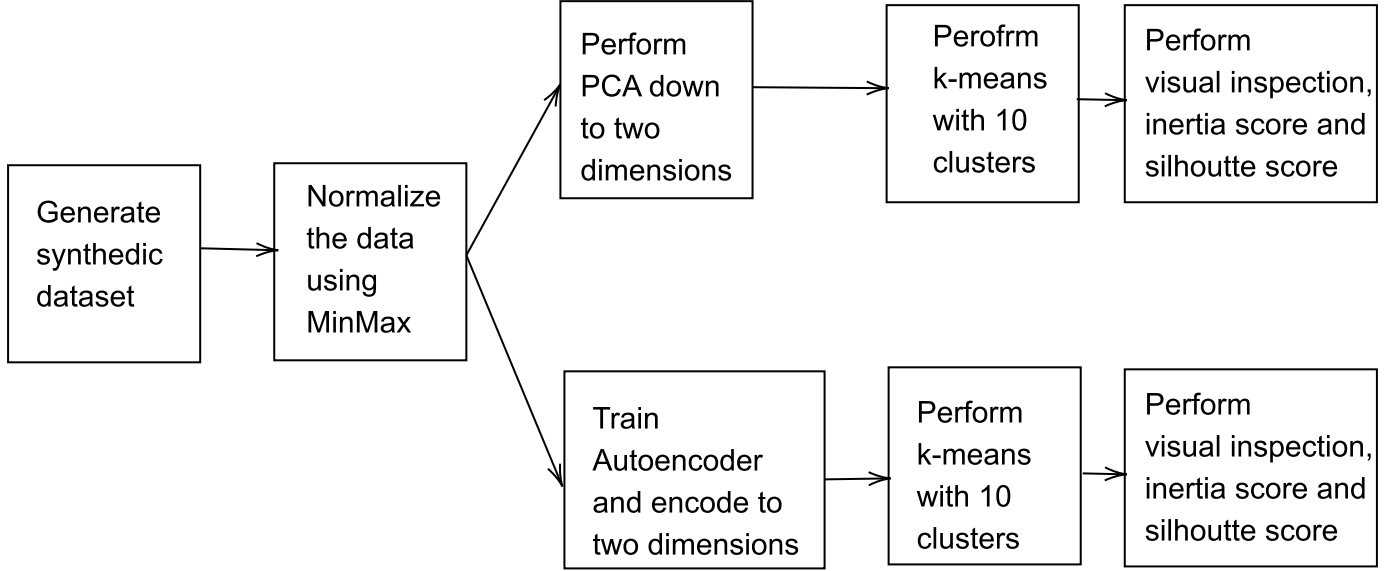


Figure 1: Methodology

In summary, we will take our synthetic dataset and perform normalization using the MinMax Scaler. Upon completion of the PCA transform we will perform a scatterplot and perform a basic visual inspection. Ideally, we would expect to see eight clusters, but even here we will see that PCA will fail dramatically. We will then perform a classic k-means clustering on this reduced space. We will then calculate the relevant scores inertia defined as:

$$\text{Inertia} = \sum_{i=1}^n \sum_{j=1}^k \|x_i - \mu_j\|^2 \cdot \mathbf{1}_{x_i \in C_j}$$

where n is the number of data points, k is the number of clusters μ_j is the centroid of each cluster.

Essentially, the inertial score tells us how “compact” each cluster is. Scores range from $[0, \infty)$. A lower score means a better cluster, although this is not the only metric for measuring clustering effectiveness. One other measure is silhouette score, defined for a single datapoint x_i as:

$$\text{Silhouette}(x_i) = \frac{b(x_i) - a(x_i)}{\max\{a(x_i), b(x_i)\}}$$

Where $a(x_i)$ is the average distance between x_i and all other points in the cluster, mathematically speaking, this is:

$$a(x_i) = \frac{1}{|C_i|-1} \left(\sum_{x_j \in C_k, x_j \neq x_i} \|x_i - x_j\| \right)$$

And where $b(x_i)$ is the minimum average distance between x_i and all other points in other clusters, mathematically speaking, this is:

$$b(x_i) = \min_{C_m \neq C_k} \left(\frac{1}{|C_m|} \sum_{x_j \in C_m} \|x_i - x_j\| \right)$$

The silhouette score method computes the average silhouette score for each point in the dataset. A score closer to one indicates better clustering, zero indicates average clustering and a score closer to -1 indicates poor clustering.

```
#####
#
# The current cell installs packages if not already installed in the hosts
# systems.
# This is supplemented by an extensive requirements.txt file in the folder
#
#####

# import subprocess
# import sys

# def install(package):
#     subprocess.check_call([sys.executable, "-m", "pip", "install", package])

# # List your packages here
# packages = ["numpy", "pandas", "seaborn", "keras", "tensorflow", "matplotlib",
# "scikit-learn"]

# for package in packages:
#     install(package)
```

```
# Import requisite libraries (see cell above)

import numpy as np
np.random.seed(42)
import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
sns.set(style='whitegrid')
```

```
from sklearn.datasets import make_blobs
```

```
# Generate out dataset
```

```
data = make_blobs(  
    n_samples=30000,  
    n_features=9,  
    centers=8,  
    cluster_std=2  
)
```

```
X,y = data
```

```
# Create a random uniform column of noise to be added as a feature
```

```
noise = np.random.uniform(size=len(X))  
noise = pd.Series(noise)
```

```
# Add noise to our dataset. Note that since no one dimension is any  
# special than another dimension it does not matter where we add  
# the noise to
```

```
feat = pd.DataFrame(X)  
feat = pd.concat([feat,noise],axis=1)
```

```
# Rename the columns to be human readable
```

```
feat.columns = [f"X{i+1}" for i in range(len(feat.columns))]
```

```
# Visually inspect our X
```

```
feat
```

	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10
0	-1.136767	7.536911	2.621168	-9.828140	3.865670	1.674786	5.115837	5.617020	-4.750097	0.642509
1	-2.852468	5.484812	0.761357	-5.310830	0.765052	4.604699	0.802374	6.235689	-7.531256	0.601436
2	5.359061	-9.550195	6.925959	5.607171	-9.007517	8.092173	10.609520	0.761276	0.442488	0.143062
3	-1.129229	6.700314	2.486264	-9.299770	3.403568	1.482824	0.175253	7.681944	-5.067821	0.555860
4	0.504382	0.764073	-8.950778	-9.971141	-8.233655	3.444365	2.858322	4.343349	8.237406	0.874118
...
29995	1.694952	-5.769989	1.414679	-6.885614	4.231421	-0.577450	0.401629	8.479906	-9.237994	0.646565
29996	-3.969766	3.027052	10.773146	3.785328	-2.319494	10.762725	7.858389	6.768924	5.738144	0.022102
29997	3.188127	-6.205679	9.776009	5.235112	-5.710168	3.508407	9.290813	3.374623	0.642398	0.683150
29998	-1.153925	1.446702	-5.855630	0.729021	-7.422402	7.574691	8.517585	12.058961	4.634554	0.711099
29999	4.495021	-9.227748	7.160538	9.429177	-3.741316	9.081748	6.549421	-4.734369	0.405850	0.473979

```
# Summary statistics of our dataset for EDA
```

```
feat.describe()
```

	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10
count	30000.000000	30000.000000	30000.000000	30000.000000	30000.000000	30000.000000	30000.000000	30000.000000	30000.000000	30000.000000
mean	-0.114208	1.339915	0.474912	-1.245021	5.033560	3.395521	-0.435639	4.535977	0.787082	0.499431
std	3.454144	6.909265	6.218669	5.188529	4.804423	5.925886	7.488308	5.594253	5.795202	0.289262
min	-10.221948	16.244301	17.057922	15.090140	16.368939	16.264199	17.769535	11.819501	13.793820	0.000086
25%	-2.744997	6.664654	4.094327	-5.957284	7.975855	7.623085	7.214682	0.614334	-4.719394	0.246672
50%	-0.317141	3.240089	1.654777	-0.661242	6.152396	4.735727	1.561951	6.368589	1.306372	0.499086
75%	2.526472	4.944013	4.568410	2.584007	-3.973561	-1.024333	6.959158	8.578064	5.959517	0.750157
max	11.234515	15.793868	16.281236	3.452604	13.693923	16.438185	16.854938	16.083165	15.460923	0.999996

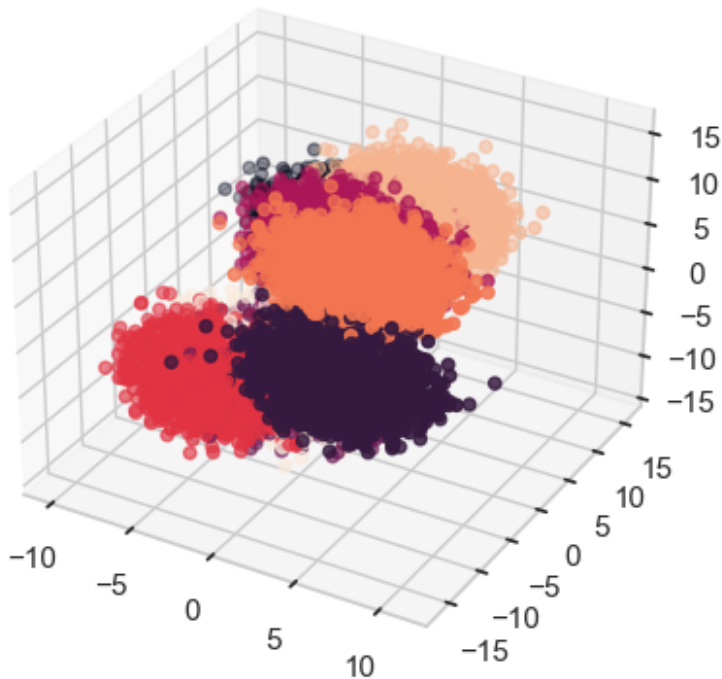
```
# Save our dataset
```

```
feat.to_csv("feat.csv")
```

```
# 3D scatterplot of three arbitrary dimensions
```

```
fig = plt.figure()
```

```
ax = fig.add_subplot(111, projection = '3d')
ax.scatter(feats['X1'],feats['X2'],feats['X9'], c = y)
```



Preprocessing the data

We will use the standard MinMaxScaler from sklearn to scale and preprocess the data

```
# Preprocess our data using MinMaxScaler

from sklearn.preprocessing import MinMaxScaler

scaler = MinMaxScaler()
scaled_data = scaler.fit_transform(feats)
```

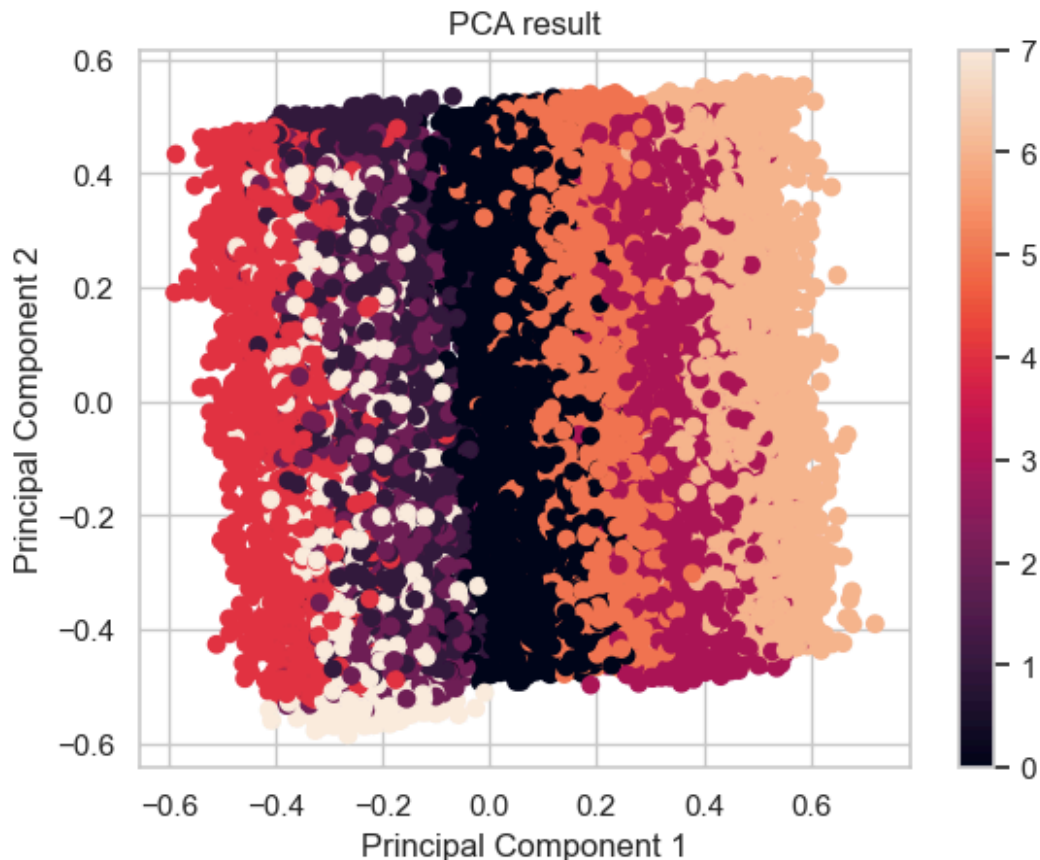
The PCA decomposition

```
from sklearn.decomposition import PCA

pca = PCA(n_components=2)
pca_result = pca.fit_transform(scaled_data)
```

```
# Scatterplot of our reduced dimensions
```

```
plt.scatter(pca_result[:, 0], pca_result[:, 1], c=y)
plt.title('PCA result')
plt.colorbar()
plt.xlabel("Principal Component 1")
plt.ylabel("Principal Component 2")
plt.show()
```



Note that PCA fails dramatically at this dimension reduction task. A priori we know that this dataset has clusters as it was constructed this way but PCA fails to capture the clustering. This is because PCA is a linear transformation and fails to capture any non-linear trends in the data. Note also that the uniform noise dimension results in a projection that is “smeared” yielding no obvious clusters on visual inspection. We will run two separate metrics later on to show how much more effective autoencoders are than regular PCA as a pre-step towards clustering.

Note also that since we have a dimension of uniform noise there exists an eigenvalue and eigenvector in the direction of the uniform noise. Because PCA is again a linear transformation, that direction of the eigenvector induces a horizontal “stripe” pattern as seen in the scatterplot.

K-means done on the encoded data

We now seek to apply classic K-Means on this PCA-result. We will do the same on the

```
from sklearn.cluster import KMeans
```

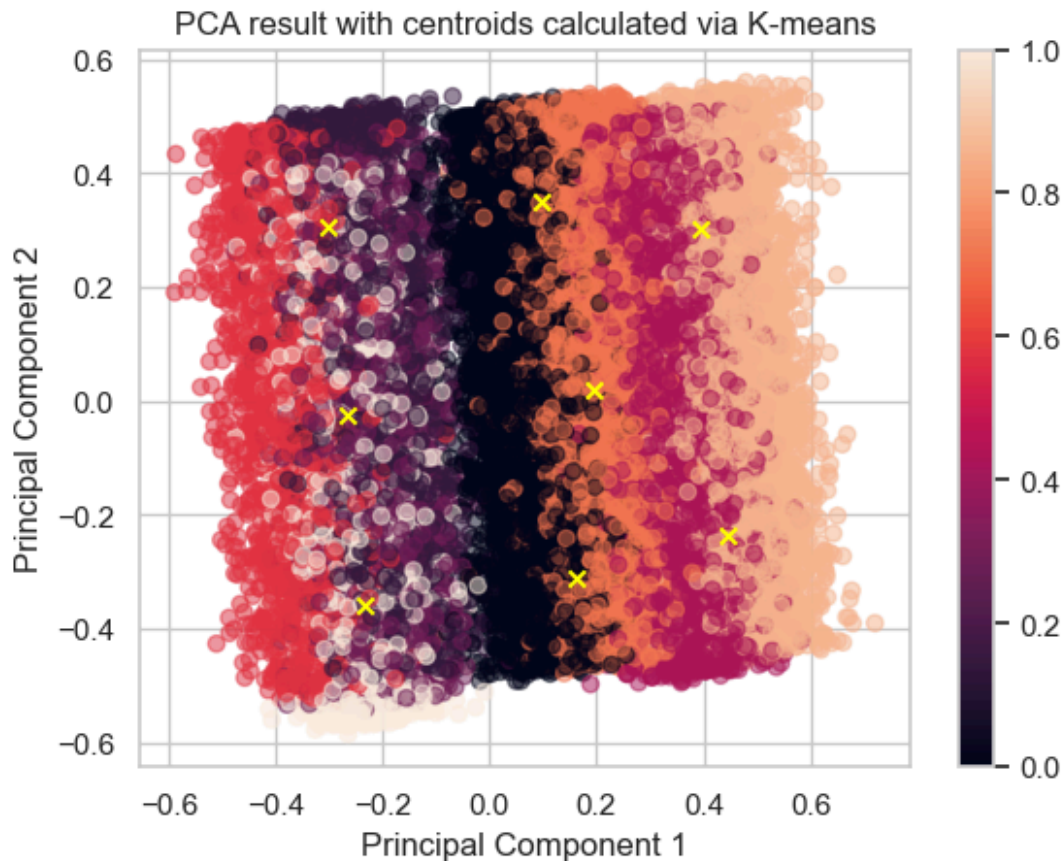
```
kmeans_for_pca = KMeans(n_clusters=8)  
kmeans_for_pca.fit(pca_result)
```

```
KMeans()
```

```
kmeans_for_pca.cluster_centers_
```

```
array([[ 0.39484343,  0.30218081],  
       [-0.26485402, -0.02386432],  
       [ 0.16332751, -0.31207928],  
       [ 0.19432675,  0.01805408],  
       [-0.23347193, -0.36066989],  
       [-0.30190528,  0.30643115],  
       [ 0.09516739,  0.35050887],  
       [ 0.44616033, -0.23692276]])
```

```
plt.scatter(pca_result[:, 0], pca_result[:, 1], c=y, alpha=0.5)  
plt.scatter(kmeans_for_pca.cluster_centers_[0], kmeans_for_pca.cluster_centers_[0, 1], marker='x', c='yellow')  
plt.title('PCA result with centroids calculated via K-means')  
plt.colorbar()  
plt.xlabel("Principal Component 1")  
plt.ylabel("Principal Component 2")  
plt.show()
```

The autoencoder decomposition

We will now create an autoencoder. We will choose a rather deep model, with $10 \rightarrow 5 \rightarrow 2 \rightarrow 5 \rightarrow 10$ layer widths. Our autoencoder will first encode the 10 dimensional data to a 2 dimensional latent space, and then decode it back to 10 dimensions. It will be trained against our dataset until it learns an optimal representation for this dataset into two latent dimensions.

We will then extract out the encoder and visually inspect our 2d latent space. Because neural networks are efficient at learning the underlying structure of unstructured data it's latent space should be noise-free, moreso than the PCA representation. As such, even visually we should see much more clustering than with PCA. Schematically, our autoencoder looks as follows:

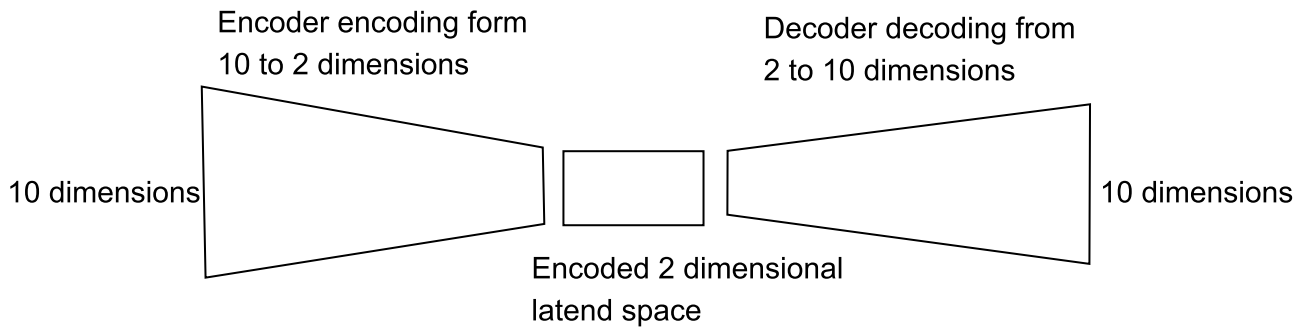


Figure 2: Autoencoder

We will choose the sigmoid function as activation throughout except the last layer of the encoder where we will use the linear activation function. Sigmoid is common in the literature and we will use linear in the last layer so that we may output negative values as well. We will also choose mean squared error loss, with a stochastic gradient descent optimizer and a learning rate of 0.1.

```
# Load requisite libraries
```

```
from tensorflow.keras.models import Model
from tensorflow.keras.layers import Input, Dense
from tensorflow.keras.optimizers import SGD
```

```
# Define the input layer
```

```
input_layer = Input(shape=(scaled_data.shape[1],))
```

```
# Define the encoding layers
```

```
encoded = Dense(8, activation='tanh')(input_layer)
```

```
encoded = Dense(6, activation='tanh')(encoded)
```

```
encoded_output = Dense(2, activation='linear')(encoded)
```

```
# Define the encoder model
```

```
encoder = Model(inputs=input_layer, outputs=encoded_output)
```

```
# Define the decoding layers
```

```
encoded_input = Input(shape=(2,))
```

```
decoded = Dense(6, activation='tanh')(encoded_input)
```

```
decoded = Dense(8, activation='tanh')(decoded)
```

```
decoded_output = Dense(scaled_data.shape[1], activation='linear')(decoded)
```

```
# Define the decoder model
```

```
decoder = Model(inputs=encoded_input, outputs=decoded_output)
```

```
# Define the autoencoder model
autoencoder_input = Input(shape=(scaled_data.shape[1],))
encoded_repr = encoder(autoencoder_input)
reconstructed = decoder(encoded_repr)

autoencoder = Model(inputs=autoencoder_input, outputs=reconstructed)

# Print model summaries
print("Encoder summary:")
encoder.summary()
print("\nDecoder summary:")
decoder.summary()
print("\nAutoencoder summary:")
autoencoder.summary()
```

Encoder summary:

Decoder summary:

Autoencoder summary:

Model: "functional"

Layer (type)	Output Shape	Param #
input_layer (InputLayer)	(None, 10)	0
dense (Dense)	(None, 8)	88
dense_1 (Dense)	(None, 6)	54
dense_2 (Dense)	(None, 2)	14

Total params: 156 (624.00 B)

Trainable params: 156 (624.00 B)

Non-trainable params: 0 (0.00 B)

Model: "functional_1"

Layer (type)	Output Shape	Param #
input_layer_1 (InputLayer)	(None, 2)	0
dense_3 (Dense)	(None, 6)	18
dense_4 (Dense)	(None, 8)	56
dense_5 (Dense)	(None, 10)	90

Total params: 164 (656.00 B)

Trainable params: 164 (656.00 B)

Non-trainable params: 0 (0.00 B)

Model: "functional_2"

Layer (type)	Output Shape	Param #
input_layer_2 (InputLayer)	(None, 10)	0
functional (Functional)	(None, 2)	156
functional_1 (Functional)	(None, 10)	164

Total params: 320 (1.25 KB)

Trainable params: 320 (1.25 KB)

Non-trainable params: 0 (0.00 B)

```
autoencoder.compile(loss='mse',  
                    optimizer=SGD(learning_rate=0.01))
```

```
autoencoder.fit(scaled_data,  
                scaled_data,  
                batch_size = 64,  
                shuffle = True,  
                epochs = 50)
```

```
Epoch 1/50  
469/469 _____ 0s 257us/step - loss: 0.1673  
Epoch 2/50  
469/469 _____ 0s 231us/step - loss: 0.0451  
Epoch 3/50  
469/469 _____ 0s 221us/step - loss: 0.0410  
Epoch 4/50  
469/469 _____ 0s 219us/step - loss: 0.0397  
Epoch 5/50  
469/469 _____ 0s 224us/step - loss: 0.0383  
Epoch 6/50  
469/469 _____ 0s 219us/step - loss: 0.0373  
Epoch 7/50  
469/469 _____ 0s 220us/step - loss: 0.0364  
Epoch 8/50  
469/469 _____ 0s 220us/step - loss: 0.0353  
Epoch 9/50  
469/469 _____ 0s 218us/step - loss: 0.0347  
Epoch 10/50  
469/469 _____ 0s 217us/step - loss: 0.0340  
Epoch 11/50  
469/469 _____ 0s 216us/step - loss: 0.0333  
Epoch 12/50  
469/469 _____ 0s 217us/step - loss: 0.0328  
Epoch 13/50  
469/469 _____ 0s 216us/step - loss: 0.0319  
Epoch 14/50  
469/469 _____ 0s 219us/step - loss: 0.0313  
Epoch 15/50  
469/469 _____ 0s 217us/step - loss: 0.0310  
Epoch 16/50  
469/469 _____ 0s 216us/step - loss: 0.0304  
Epoch 17/50  
469/469 _____ 0s 214us/step - loss: 0.0298  
Epoch 18/50  
469/469 _____ 0s 213us/step - loss: 0.0295
```

```

Epoch 19/50
469/469 _____ 0s 220us/step - loss: 0.0290
Epoch 20/50
469/469 _____ 0s 214us/step - loss: 0.0287
Epoch 21/50
469/469 _____ 0s 218us/step - loss: 0.0284
Epoch 22/50
469/469 _____ 0s 216us/step - loss: 0.0281
Epoch 23/50
469/469 _____ 0s 218us/step - loss: 0.0280
Epoch 24/50
469/469 _____ 0s 233us/step - loss: 0.0276
Epoch 25/50
469/469 _____ 0s 233us/step - loss: 0.0276
Epoch 26/50
469/469 _____ 0s 216us/step - loss: 0.0275
Epoch 27/50
469/469 _____ 0s 212us/step - loss: 0.0273
Epoch 28/50
469/469 _____ 0s 217us/step - loss: 0.0272
Epoch 29/50
469/469 _____ 0s 214us/step - loss: 0.0271
Epoch 30/50
469/469 _____ 0s 213us/step - loss: 0.0271
Epoch 31/50
469/469 _____ 0s 219us/step - loss: 0.0270
Epoch 32/50
469/469 _____ 0s 214us/step - loss: 0.0269
Epoch 33/50
469/469 _____ 0s 218us/step - loss: 0.0268
Epoch 34/50
469/469 _____ 0s 217us/step - loss: 0.0269
Epoch 35/50
469/469 _____ 0s 211us/step - loss: 0.0268
Epoch 36/50
469/469 _____ 0s 212us/step - loss: 0.0267
Epoch 37/50
469/469 _____ 0s 211us/step - loss: 0.0265
Epoch 38/50
469/469 _____ 0s 218us/step - loss: 0.0266
Epoch 39/50
469/469 _____ 0s 216us/step - loss: 0.0265
Epoch 40/50
469/469 _____ 0s 354us/step - loss: 0.0266
Epoch 41/50
469/469 _____ 0s 317us/step - loss: 0.0264
Epoch 42/50
469/469 _____ 0s 231us/step - loss: 0.0265

```

```

Epoch 43/50
469/469 _____ 0s 218us/step - loss: 0.0263
Epoch 44/50
469/469 _____ 0s 214us/step - loss: 0.0262
Epoch 45/50
469/469 _____ 0s 214us/step - loss: 0.0263
Epoch 46/50
469/469 _____ 0s 217us/step - loss: 0.0264
Epoch 47/50
469/469 _____ 0s 214us/step - loss: 0.0261
Epoch 48/50
469/469 _____ 0s 216us/step - loss: 0.0260
Epoch 49/50
469/469 _____ 0s 212us/step - loss: 0.0260
Epoch 50/50
469/469 _____ 0s 217us/step - loss: 0.0260

```

```
<keras.src.callbacks.history.History at 0x30876a9f0>
```

Note that the reconstruction loss here is 0.0389. This is somewhat higher than for PCA although this can be reduced further with more training epochs. The author chose 50 epochs arbitrarily and with consideration for their own access to compute facilities.

```

# Encode our data down to two dimensions using our
# trained autoencoder

```

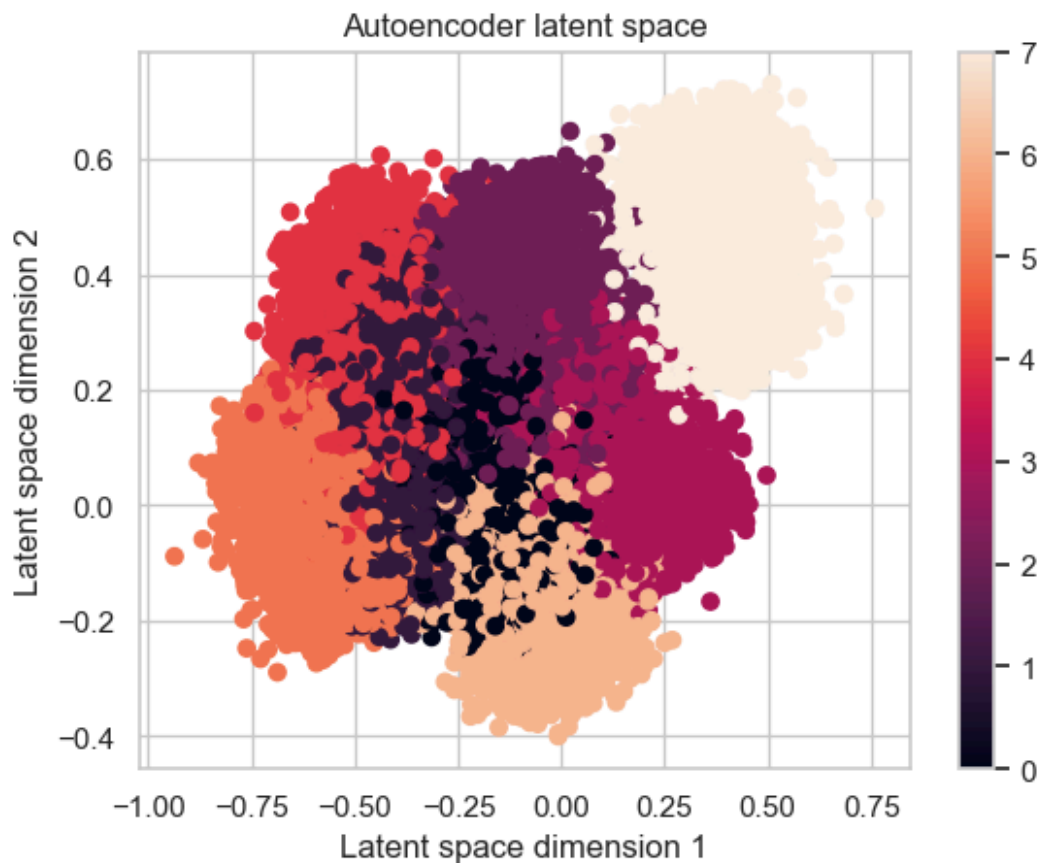
```
encoded_2dim = encoder.predict(scaled_data)
```

```
938/938 _____ 0s 468us/step
```

```

plt.scatter(encoded_2dim[:,0],encoded_2dim[:,1], c = y)
plt.title('Autoencoder latent space')
plt.colorbar()
plt.xlabel("Latent space dimension 1")
plt.ylabel("Latent space dimension 2")
plt.show()

```



Visually we see that our autoencoder has performed much better than the PCA. We see eight clusters very clearly. Not only that the clusters are much more compact than with PCA, and seem well separated. We will quantify this in the next section.

Analysis of results

```
# Train our k-means on the encoded 2 dimensional data
```

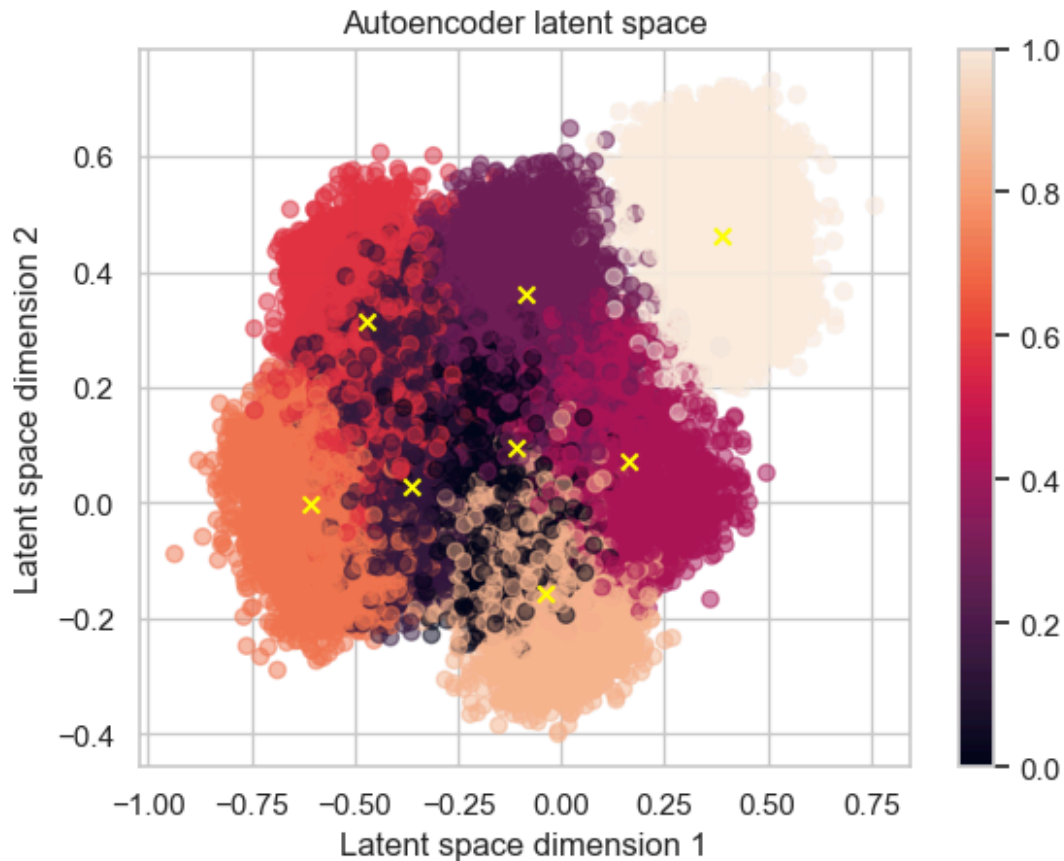
```
kmeans_for_autoencoder = KMeans(n_clusters=8)
kmeans_for_autoencoder.fit(encoded_2dim)
```

```
KMeans()
```

```
plt.scatter(encoded_2dim[:, 0], encoded_2dim[:, 1], c=y, alpha=0.5)
plt.scatter(kmeans_for_autoencoder.cluster_centers[:,
0], kmeans_for_autoencoder.cluster_centers[:, 1], marker='x', c='yellow')
plt.title('Autoencoder latent space')
plt.colorbar()
plt.xlabel("Latent space dimension 1")
```



```
plt.ylabel("Latent space dimension 2")
plt.show()
```



```
# Calculating our inertia for the two k-means
```

```
print("Inertia for k-means after PCA: ", kmeans_for_pca.inertia_)
print("Inertia for k-means after autoencoder: ",
      kmeans_for_autoencoder.inertia_)
```

```
Inertia for k-means after PCA: 544.260274517304
Inertia for k-means after autoencoder: 485.44720458984375
```

```
from sklearn.metrics import silhouette_score

print("Silhouette score for PCA",
      silhouette_score(scaled_data, kmeans_for_pca.labels_))
```

```
print("Silhoutte score for autoencoder",
silhouette_score(scaled_data, kmeans_for_autoencoder.labels_))
```

```
Silhoutte score for PCA 0.11800770665560721
Silhoutte score for autoencoder 0.16393338402522128
```

```
from sklearn.metrics import mean_squared_error

X_reconstructed_from_pca = pca.inverse_transform(pca_result)
X_reconstructed_from_autoencoder = decoder(encoded_2dim)
mean_squared_error(scaled_data, X_reconstructed_from_pca)
```

```
0.02361820017793444
```

Saving our models

Finally we will save our model for future use

```
autoencoder.save("autoencoder.keras")
encoder.save("encoder.keras")
decoder.save("decoder.keras")
```

```
import pickle

with open('pca_model.pkl', 'wb') as file:
    pickle.dump(pca, file)
```

Summary of results

We give here a table summarizing the results:

Attribute	PCA	Autoencoder
Reconstruction loss	0.021	0.039 reconstruction loss can be reduced with more training epochs
Visual	No visual separation between clusters	Clear visual separation between clusters
Inertia lower is better	~ 544 clusters are fall less compact	~ 485 clusters are more compact
Silhoutte Score closer to 1 is better	~ 0.11 substantial overlap between clusters	~ 0.16 far less overlap between clusters

These results indicate that autoencoders may be far better and effective methods of pretraining than standard PCA when it comes to clustering algorithms such as k-means. Indeed autoencoders are able to capture non-linearities in data and suss out complex relationships between data that classical methods such as PCA may not be able to.

This makes autoencoders excellent candidates for dimensionality reduction and analysis for genomic data where high dimensional and intricate relationships exist between features. The field is promising, yet untapped.