

Dimensionality Reduction - Vignesh Vishwanath (1947122)

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1 Dimensionality Reduction

The complexity of any classifier or regressor depends on the number of inputs (Both number of samples and features), this determines the time and space complexity of the classifier or regressor. So feature selection (Of which dimensionality reduction is a subset) becomes an important part of the decision making process.

Feature selection, ideally, should not be a separate process and should infact be a part of the decision making algorithm. 1. The complexity of most learning algorithms depend on the number of input samples N , and the dimensions of these samples D . So reducing these implies a direct reduction in time and space complexity of the algorithm. Reducing the dimensions D , also reduces the inference complexity during test times. This also, to a certain extent, helps explain the process of decision making better (Not always). 2. In case of feature extraction. If, for some reason, we decide to exclude feature, we then save the cost of extracting said feature making the pipeline (Of decision making) more efficient. 3. Lower dimensions ensures less chances of overfitting (Usually) and hence a decision making process that is explainable by only a few features is more robust (For smaller datasets) 4. Having lower dimensions help visualization and detecting structure of the data which could prove useful for outlier detection.

2 Multi-Dimensional Scaling

Multi dimensional scaling aims to map the features from an unknown dimensional space to a N dimensional space. Consider N points in the data. The dimensionality of these data points are unknown. Distance d_{ij} , for all points i, j where $i, j = 1, 2, \dots, N$, is given. The distance measure is unknown (Only the values of distance is given). Multi-dimensional scaling projects these data points from the unknown dimensional space to a N dimensional space, such that the euclidean distance between the given points (Say i, j) are as close to the given distances d_{ij} .

Multi-dimensional scaling can be used to reduce dimensions by passing the d dimensional x space as input, the pairwise euclidean distance is calculated to project it to a lower dimensions while preserving the original dimensions.

The pairwise euclidean squared distance between points r and s is given by,

$$d_{rs}^2 = \|\mathbf{x}^r - \mathbf{x}^s\|^2 = \sum_{j=1}^d (x_j^r - x_j^s)^2 = \sum_{j=1}^d (x_j^r)^2 - 2 \sum_{j=1}^d x_j^r x_j^s + \sum_{j=1}^d (x_j^s)^2$$

Now if we define b_{rs} as

$$B = X * X^T$$

or more precisely,

$$b_{rs} = \sum_{j=1}^d x_j^r x_j^s$$

we get d_{rs}^2 as,

$$b_{rr} + b_{ss} - 2b_{rs}$$

Note that this is zero mean. The sum of all data points will be equal to zero. This is a constraint on the data

Using the matrix B, we can get the eigen vectors of B and then the eigen values from those vectors. We choose k dimensions, where, $k < \min(d, N)$

Multi-dimensional scaling does the same thing as PCA, 1. Both have a linear relationship with the original dimension d 2. PCA is calculated on Covariance matrix, whereas MDS is calculated on Correlation matrix. Essentially PCA on correlation matrix is the same as MDS with euclidean distance with unit variance variables. 3. PCA does this more efficiently

The objectives in brief can be written as : 1. As an exploratory technique to identify unrecognized dimensions affecting behavior 2. As a means of obtaining comparative evaluations of objects when the specific bases of comparison are unknown or undefinable

3 Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA)

3.1 Principal component Analysis

In projection methods we try to find the mapping of input space in d dimensions to a new $k(< d)$ dimensions, with minimum loss of information. The projection of x on the direction w is,

$$Z = W^T * X$$

PCA is an unsupervised dimensionality reduction method (Does not require targets). It aims to find the principal component w of x such that w has maximum variance (The difference between different points is maximum). To ensure solution is unique $||w||$ is equal to 1, this also makes the direction important.

Consider,

$$Var(Z) = W^T * X$$

PCA aims to maximize $Var(Z)$ and keep $||W|| = 1$

Additionally the second principal component has to be orthogonal to the previous principal component (Dot product is zero). This ensures the correlation is minimized. In brief: 1. PCA is an unsupervised algorithm(Requires no targets) 2. PCA uses the covariance matrix to find projection

onto the new dimensions. 3. PCA maximizes variance in the data and reduces correlation 4. The eigen values are calculated using eigen vectors and these are arranged in descending order. The first principal component contributes the maximum variance and so on.

3.2 Linear discriminant analysis

Linear discriminant analysis is a supervised technique(Requires targets) for dimensionality reduction, mainly used for classification. Given samples from classes C1 and C2, LDA finds a projection from the original d dimension to $k < \min(d, n)$ dimensions such that the separation between the two classes is maximum. Here n is the number of classes

LDA is also called Fisher's linear discriminant. The objective function is called Fisher's criterion $J(w)$. The Fisher criterion is defined to be the ratio of the between-class variance to the within-class variance.

LDA also finds a projection of the data (Like PCA) but also uses the targets to maximise the distance between classes (Unlike PCA)

The projection is given by,

$$Z = W^T * X$$

While also optimizing the Fisher's Criterion $J(W)$ given by,

$$J(W) = \frac{(m_1 - m_2)^2}{(s_1^2 + s_2^2)}$$

where, m_i is the mean of the class i s_i^2 is the scatter (Within class) of class i

LDA essentially increase the distance between the means of the classes while at the same time decreasing the within class scatter of the class. This is encapsulated by the Fisher's Criterion

In brief: 1. LDA is a dimensionality reduction method that is supervised (Requires targets) 2. LDA is also a classifier of sorts. It aims for maximum separation 3. Uses covariance matrix to find projection. And hence the number of samples has to be big (Otherwise inversion gives a singular value) 4. The resultant features are arranged in descending order of the separation contribution. The first feature separates the the most and so on.

4 Demonstration of Dimensionality Reduction

4.1 Importing necessary libraries

```
[93]: import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.decomposition import PCA
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis as LDA
import tensorflow as tf
from sklearn.model_selection import train_test_split
from mpl_toolkits.mplot3d import Axes3D
```

4.1.1 Get the data from here:

<https://www.kaggle.com/dipayanbiswas/parkinsons-disease-speech-signal-features> The data consists of time series data of speech features of people suffering from parkinsons disease. There are originally 750 features, of which , 300 have been selected. The status of the person is the target variable.

```
[17]: data = pd.read_csv("../Datasets/pd_speech_features.csv")
      data = data.drop(data.columns[300:-1],axis = 1)
      data = data.drop("id",axis = 1)
```

4.2 View data samples

```
[18]: data.head()
```

```
[18]:
```

	gender	PPE	DFA	RPDE	numPulses	numPeriodsPulses	\
0	1	0.85247	0.71826	0.57227	240	239	
1	1	0.76686	0.69481	0.53966	234	233	
2	1	0.85083	0.67604	0.58982	232	231	
3	0	0.41121	0.79672	0.59257	178	177	
4	0	0.32790	0.79782	0.53028	236	235	

	meanPeriodPulses	stdDevPeriodPulses	locPctJitter	locAbsJitter	...	\
0	0.008064		0.000087	0.00218	0.000018	...
1	0.008258		0.000073	0.00195	0.000016	...
2	0.008340		0.000060	0.00176	0.000015	...
3	0.010858		0.000183	0.00419	0.000046	...
4	0.008162		0.002669	0.00535	0.000044	...

	app_LT_entropy_shannon_10_coef	app_LT_entropy_log_1_coef	\
0	-3601122.613	414.6434	
1	-3563560.603	413.5284	
2	-3539902.400	413.0675	
3	-3271399.011	413.6380	
4	-3367165.736	421.1396	

	app_LT_entropy_log_2_coef	app_LT_entropy_log_3_coef	\
0	276.4850	198.5803	
1	275.8597	198.1971	
2	275.5868	198.0149	
3	275.3259	197.2795	
4	279.1703	199.4350	

	app_LT_entropy_log_4_coef	app_LT_entropy_log_5_coef	\
0	153.8978	132.2489	
1	153.6379	132.0522	
2	153.5036	131.9418	

3	152.5940	130.9480
4	153.7788	131.6258

	app_LT_entropy_log_6_coef	app_LT_entropy_log_7_coef \
0	124.1971	127.9812
1	124.0327	127.8282
2	123.9329	127.7329
3	122.8786	126.6411
4	123.3566	127.0837

	app_LT_entropy_log_8_coef	class
0	130.3804	1
1	130.2373	1
2	130.1464	1
3	129.0689	1
4	129.4029	1

[5 rows x 300 columns]

4.3 Checking data dimensions

```
[19]: data.shape
```

```
[19]: (756, 300)
```

4.4 Exploring statistical moments of the data

At first glance it is clear that we need to normalize the data as the mean of different attributes is different. From the features itself we can see that they are on different scales (Exponential, logarithmic) because of the feature extraction.

```
[20]: data.describe()
```

```
[20]:
```

	gender	PPE	DFA	RPDE	numPulses \
count	756.000000	756.000000	756.000000	756.000000	756.000000
mean	0.515873	0.746284	0.700414	0.489058	323.972222
std	0.500079	0.169294	0.069718	0.137442	99.219059
min	0.000000	0.041551	0.543500	0.154300	2.000000
25%	0.000000	0.762833	0.647053	0.386537	251.000000
50%	1.000000	0.809655	0.700525	0.484355	317.000000
75%	1.000000	0.834315	0.754985	0.586515	384.250000
max	1.000000	0.907660	0.852640	0.871230	907.000000

	numPeriodsPulses	meanPeriodPulses	stdDevPeriodPulses	locPctJitter \
count	756.000000	756.000000	756.000000	756.000000
mean	322.678571	0.006360	0.000383	0.002324

std	99.402499	0.001826	0.000728	0.002628
min	1.000000	0.002107	0.000011	0.000210
25%	250.000000	0.005003	0.000049	0.000970
50%	316.000000	0.006048	0.000077	0.001495
75%	383.250000	0.007528	0.000171	0.002520
max	905.000000	0.012966	0.003483	0.027750

	locAbsJitter	...	app_LT_entropy_shannon_10_coef	\
count	7.560000e+02	...	7.560000e+02	
mean	1.673391e-05	...	-4.143375e+06	
std	2.290134e-05	...	4.876751e+05	
min	6.860000e-07	...	-5.882489e+06	
25%	5.260000e-06	...	-4.474741e+06	
50%	9.530000e-06	...	-4.155440e+06	
75%	1.832500e-05	...	-3.802516e+06	
max	2.564800e-04	...	-2.665481e+06	

	app_LT_entropy_log_1_coef	app_LT_entropy_log_2_coef	\
count	756.000000	756.000000	
mean	425.629078	282.711578	
std	22.146419	12.763780	
min	138.297600	115.908600	
25%	419.073075	279.039500	
50%	428.110650	284.092300	
75%	435.746200	288.434200	
max	467.377300	305.941900	

	app_LT_entropy_log_3_coef	app_LT_entropy_log_4_coef	\
count	756.000000	756.000000	
mean	202.511481	156.685856	
std	7.567502	4.475900	
min	106.489700	102.332000	
25%	200.170825	155.049100	
50%	203.374950	157.179700	
75%	206.039200	159.002800	
max	216.634100	166.016500	

	app_LT_entropy_log_5_coef	app_LT_entropy_log_6_coef	\
count	756.000000	756.000000	
mean	134.482587	126.164411	
std	2.819619	2.067284	
min	107.374200	111.134600	
25%	133.138125	124.978700	
50%	134.804800	126.390950	
75%	136.164075	127.547025	
max	141.399600	131.865800	

	app_LT_entropy_log_7_coef	app_LT_entropy_log_8_coef	class
count	756.000000	756.000000	756.000000
mean	129.842591	132.197901	0.746032
std	1.888099	1.632429	0.435568
min	121.331100	126.152000	0.000000
25%	128.718000	131.123125	0.000000
50%	130.046450	132.335200	1.000000
75%	131.134600	133.346950	1.000000
max	135.165000	137.089700	1.000000

[8 rows x 300 columns]

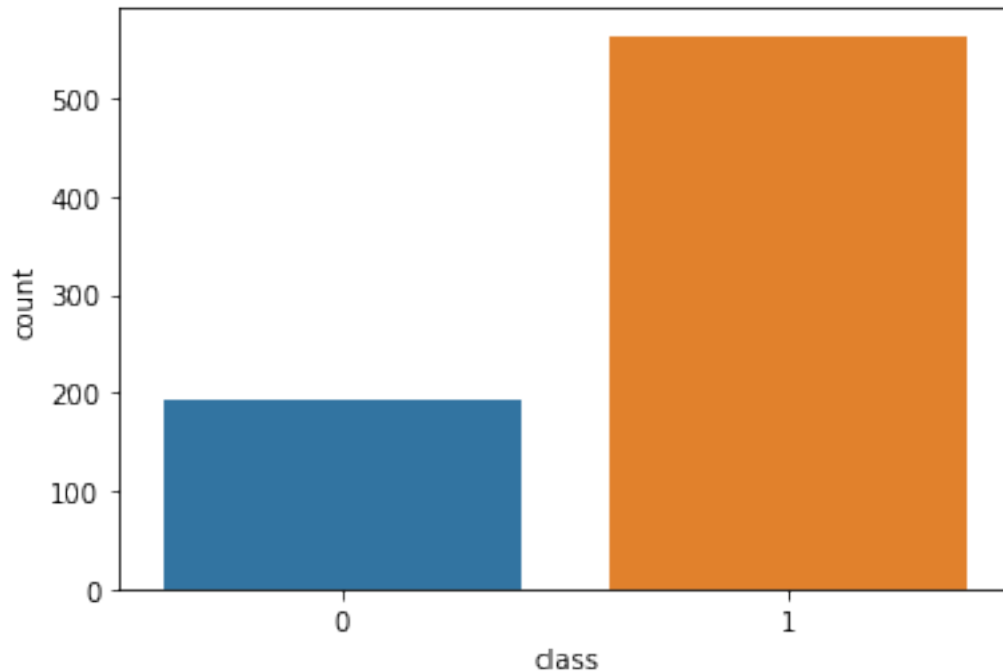
4.5 Exploring the distribution of classes

The class distribution is skewed. From this skewed data we derive the baseline accuracy which is 74%. If the classifier acts like a majority classifier (Outputs a constant value) it will have 74% accuracy. For our model to make a difference we need to exceed this at the least.

```
[22]: target = data["class"]
      data_sec = data[data.columns[:-1]]
```

```
[38]: sns.countplot(target)
      print(target.value_counts())
      print("Baseline", (target.value_counts()[1]/target.shape[0])*100, "%")
```

```
1    564
0    192
Name: class, dtype: int64
Baseline 74.60317460317461 %
```



4.6 Train-Test split

The post distribution is printed later The data is also normalized.

```
[145]: X_train,X_test,Y_train,Y_test = train_test_split(data_sec,target,test_size = 0.2)
```

```
[146]: print(X_train.shape,Y_train.shape)
print(X_test.shape,Y_test.shape)
```

```
(604, 299) (604,)
(152, 299) (152,)
```

```
[147]: X_train = (X_train - X_train.mean())/X_train.std()
X_test = (X_test - X_test.mean())/X_test.std()
```

4.7 Applying PCA on the data

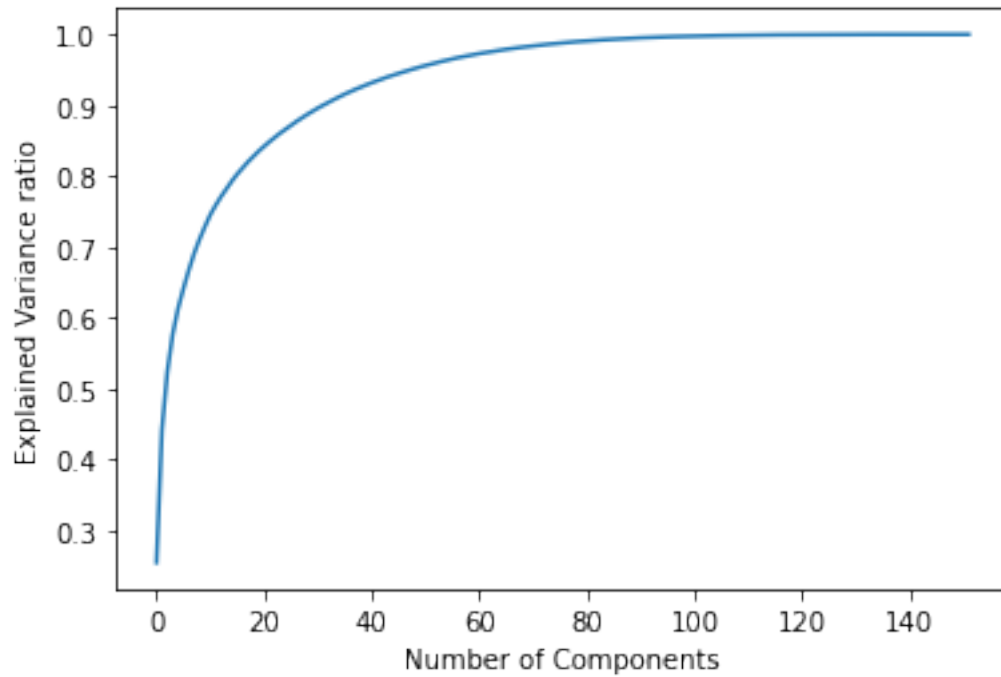
We plot the explained variance ratio vs the number of features to see how many features explain the overall variance. Recall, PCA aims to maximise variance in its principal components

```
[149]: pca = PCA().fit(X_train)
X_pca = pca.fit_transform(X_train)
X_pca_test = pca.fit_transform(X_test)
sums = np.cumsum(pca.explained_variance_ratio_)
plt.plot(np.cumsum(pca.explained_variance_ratio_))
```



```
plt.xlabel("Number of Components")
plt.ylabel("Explained Variance ratio")
```

```
[149]: Text(0, 0.5, 'Explained Variance ratio')
```



```
[72]: sums[80]
```

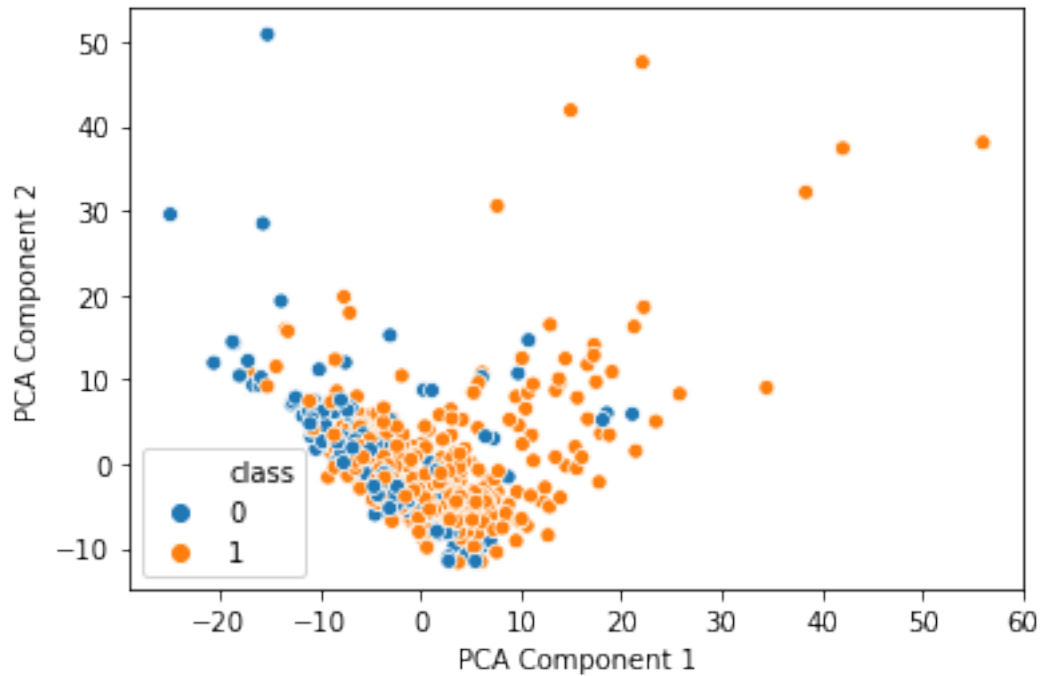
```
[72]: 0.9657289439379847
```

4.8 Visualization of PCA components.

The original data with 300 features cannot be visualized but using PCA, most of the variance can be visualized.

```
[91]: sns.scatterplot(X_pca[:,0],X_pca[:,1],hue = Y_train)
plt.xlabel("PCA Component 1")
plt.ylabel("PCA Component 2")
```

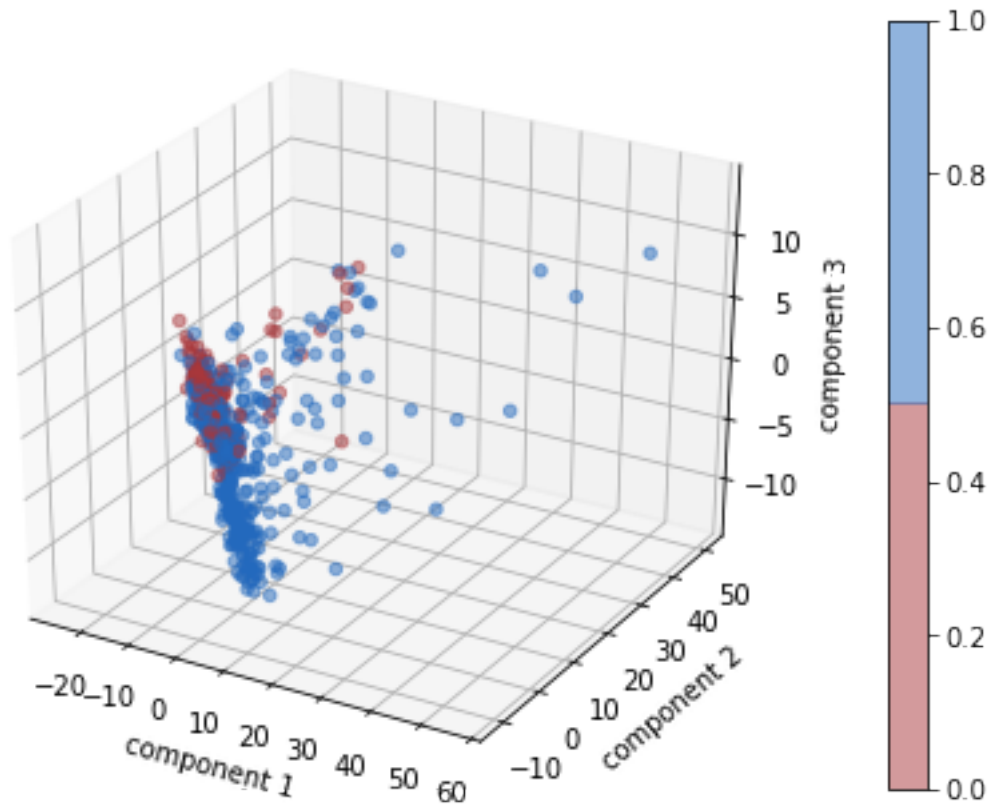
```
[91]: Text(0, 0.5, 'PCA Component 2')
```



4.8.1 3-Dimensional visualization

As we see from both visualizations, the variance is maximized, the separation is not so good. PCA is unsupervised and is not even trying to separate.

```
[102]: ax = Axes3D(plt.figure())
p = ax.scatter(X_pca[:, 0], X_pca[:, 1], X_pca[:, 2],
               c=Y_train, alpha=0.5,
               cmap=plt.cm.get_cmap('vlag_r', 2))
plt.xlabel('component 1')
plt.ylabel('component 2')
ax.set_zlabel('component 3')
plt.colorbar(p);
```



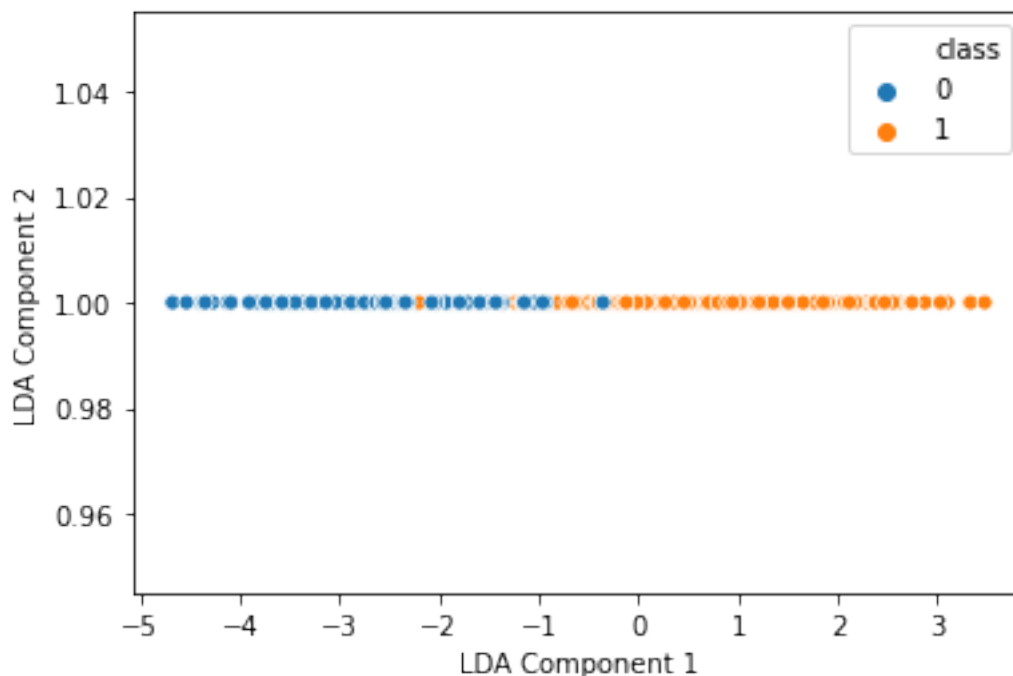
4.9 Applying LDA on the dataset

LDA features have to be less than $\min(\text{number of samples}, \text{number of classes})$. Because number of classes is 2, we obtain only one LDA feature. But this feature maximizes the separation. As we can see from the below plot. It is mostly separated using one dimension.

```
[198]: lda = LDA().fit_transform(X_train,Y_train)
      lda_test = LDA().fit_transform(X_test,Y_test)
```

```
[113]: sns.scatterplot(lda[:,0],1,hue = Y_train)
      plt.xlabel("LDA Component 1")
      plt.ylabel("LDA Component 2")
```

```
[113]: Text(0, 0.5, 'LDA Component 2')
```



```
[110]: lda.shape
```

```
[110]: (604, 1)
```

4.10 Training Neural Net on original data features

We get about 76.31% on the test set. Which is above baseline.

```
[141]: model_orig = tf.keras.models.Sequential([tf.keras.layers.Input(299,1),
                                                tf.keras.layers.Dense(units = 256,activation = tf.nn.relu),
                                                tf.keras.layers.Dense(units = 1,activation = tf.nn.sigmoid)])
model_orig.compile(optimizer = "adam",loss = "binary_crossentropy",metrics = ["accuracy"])
model_orig.build()
model_orig.summary()
model_orig.fit(X_train,Y_train.values,epochs = 10)
```

Model: "sequential_7"

Layer (type)	Output Shape	Param #
dense_13 (Dense)	(1, 256)	76800

```

dense_14 (Dense)                (1, 1)                257
=====
Total params: 77,057
Trainable params: 77,057
Non-trainable params: 0
-----
Epoch 1/10
604/604 [=====] - 1s 2ms/sample - loss: 0.5901 - acc: 0.7715
Epoch 2/10
604/604 [=====] - 1s 2ms/sample - loss: 0.2866 - acc: 0.8775
Epoch 3/10
604/604 [=====] - 1s 2ms/sample - loss: 0.2381 - acc: 0.9023
Epoch 4/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1904 - acc: 0.9338
Epoch 5/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1586 - acc: 0.9487
Epoch 6/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1180 - acc: 0.9619
Epoch 7/10
604/604 [=====] - 1s 2ms/sample - loss: 0.0598 - acc: 0.9834
Epoch 8/10
604/604 [=====] - 1s 2ms/sample - loss: 0.0591 - acc: 0.9884
Epoch 9/10
604/604 [=====] - 1s 2ms/sample - loss: 0.0573 - acc: 0.9818
Epoch 10/10
604/604 [=====] - 1s 2ms/sample - loss: 0.0600 - acc: 0.9818

```

```
[141]: <tensorflow.python.keras.callbacks.History at 0x1febb541888>
```

```
[144]: print(model_orig.evaluate(X_train,Y_train.values)[1]*100)
       print(model_orig.evaluate(X_test,Y_test.values)[1]*100)
```

```

604/604 [=====] - 1s 882us/sample - loss: 0.7026 - acc: 0.9255
92.54966974258423
152/152 [=====] - 0s 886us/sample - loss: 1.3734 - acc: 0.7632
76.31579041481018

```

4.11 Training Neural net on PCA features

We have taken the maximum amount of features, 150. We get about 76.9% test accuracy, which is pretty good. Although a good amount of hyperparameter tuning was required

```
[224]: feat = 150
model_pca = tf.keras.models.Sequential([tf.keras.layers.Input(feat,1),
                                         tf.keras.layers.Dense(units = 1024,activation = tf.nn.relu,kernel_regularizer = tf.keras.regularizers.l2(0.7)),
                                         tf.keras.layers.Dense(units = 1,activation = tf.nn.sigmoid)])
model_pca.compile(optimizer = "adam",loss = "binary_crossentropy",metrics = ["accuracy"])
model_pca.build()
model_pca.summary()
model_pca.fit(X_pca[:, :feat],Y_train.values,epochs = 20)
```

Model: "sequential_42"

Layer (type)	Output Shape	Param #
dense_83 (Dense)	(1, 1024)	154624
dense_84 (Dense)	(1, 1)	1025

Total params: 155,649

Trainable params: 155,649

Non-trainable params: 0

Epoch 1/20

604/604 [=====] - 2s 3ms/sample - loss: 7.3186 - acc: 0.7666

Epoch 2/20

604/604 [=====] - 1s 2ms/sample - loss: 0.7312 - acc: 0.7748

Epoch 3/20

604/604 [=====] - 1s 2ms/sample - loss: 0.7333 - acc: 0.7781

Epoch 4/20

604/604 [=====] - 1s 2ms/sample - loss: 0.7175 - acc: 0.7765

Epoch 5/20

604/604 [=====] - 1s 2ms/sample - loss: 0.6736 - acc: 0.7914

Epoch 6/20

604/604 [=====] - 1s 2ms/sample - loss: 0.6500 - acc: 0.7781

```

Epoch 7/20
604/604 [=====] - 1s 2ms/sample - loss: 0.6322 - acc:
0.7864
Epoch 8/20
604/604 [=====] - 1s 2ms/sample - loss: 0.6201 - acc:
0.7964
Epoch 9/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5922 - acc:
0.8013
Epoch 10/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5757 - acc:
0.7930
Epoch 11/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5883 - acc:
0.7831
Epoch 12/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5669 - acc:
0.7864
Epoch 13/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5607 - acc:
0.7997
Epoch 14/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5600 - acc:
0.8013
Epoch 15/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5571 - acc:
0.7930
Epoch 16/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5412 - acc:
0.8063
Epoch 17/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5478 - acc:
0.8030
Epoch 18/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5466 - acc:
0.8046
Epoch 19/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5422 - acc:
0.7914
Epoch 20/20
604/604 [=====] - 1s 2ms/sample - loss: 0.5381 - acc:
0.7980

```

```
[224]: <tensorflow.python.keras.callbacks.History at 0x1ffa97f2488>
```

```
[225]: print(model_pca.evaluate(X_pca[:, :feat], Y_train.values)[1]*100)
print(model_pca.evaluate(X_pca_test[:, :feat], Y_test.values)[1]*100)
```

```

604/604 [=====] - 1s 2ms/sample - loss: 0.4896 - acc:
0.8477
84.76821184158325
152/152 [=====] - 0s 1ms/sample - loss: 0.7737 - acc:
0.7697
76.97368264198303

```

4.12 Training a Neural net on LDA feature space

Recall, LDA aims to maximize separation and this means that the job of the classifier is made easier (Most times) We get a 100% test accuracy. Which is the best among all of the models.

```

[199]: feat = 1
model_lda = tf.keras.models.Sequential([tf.keras.layers.Input(feat,1),
                                         tf.keras.layers.Dense(units = 256,
                                         activation = tf.nn.relu,kernel_regularizer = tf.keras.regularizers.l2(0.01)),
                                         tf.keras.layers.Dense(units = 1,
                                         activation = tf.nn.sigmoid)])
model_lda.compile(optimizer = "adam",loss = "binary_crossentropy",metrics = ["accuracy"])
model_lda.build()
model_lda.summary()
model_lda.fit(lda[:, :feat],Y_train.values,epochs = 10)

```

Model: "sequential_30"

Layer (type)	Output Shape	Param #
dense_59 (Dense)	(1, 256)	512
dense_60 (Dense)	(1, 1)	257

Total params: 769

Trainable params: 769

Non-trainable params: 0

Epoch 1/10

```

604/604 [=====] - 2s 3ms/sample - loss: 0.2425 - acc:
0.9139

```

Epoch 2/10

```

604/604 [=====] - 1s 2ms/sample - loss: 0.1736 - acc:
0.9255

```

Epoch 3/10

```

604/604 [=====] - 1s 2ms/sample - loss: 0.1689 - acc:
0.9288

```

Epoch 4/10

```

604/604 [=====] - 1s 2ms/sample - loss: 0.1655 - acc:

```



```

0.9321
Epoch 5/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1660 - acc:
0.9305
Epoch 6/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1658 - acc:
0.9338
Epoch 7/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1645 - acc:
0.9321
Epoch 8/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1648 - acc:
0.9288
Epoch 9/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1650 - acc:
0.9288
Epoch 10/10
604/604 [=====] - 1s 2ms/sample - loss: 0.1671 - acc:
0.9272

```

```
[199]: <tensorflow.python.keras.callbacks.History at 0x1ff9ef33188>
```

```
[201]: print(model_lda.evaluate(lda[:, :feat], Y_train.values)[1]*100)
print(model_lda.evaluate(lda_test[:, :feat], Y_test.values)[1]*100)
```

```

604/604 [=====] - 1s 1ms/sample - loss: 0.1579 - acc:
0.9272
92.71523356437683
152/152 [=====] - 0s 1ms/sample - loss: 0.0142 - acc:
1.0000
100.0

```

To see more information about hoe PCA and LDA affects data, visit my other notebook [here](#)

End of Notebook