

# Implementing Principal Component Analysis (PCA) from Scratch (July 2023)

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**ABSTRACT** Principal component analysis (PCA) is a widely used technique for dimensionality reduction and data visualization. It aims to find orthogonal vectors that capture the most variance in the data, and project the data onto a lower dimension to counter the problem created by high number of dimensions in a dataset. This report implements PCA from scratch using Python and NumPy and applies it to three datasets: a randomly generated dummy Dataset, Iris Dataset and Diabetes Prediction Dataset. After the data from the dataset were subjected to PCA and plots were generated to effectively visualize the transformed data. The dataset was subjected to our PCA implementation and the PCA from scikit-learn library and the results were compared. This report demonstrates the effectiveness of custom implementation of PCA and PCA from scikit-learn library for effective dimension reduction.

**INDEX TERMS** Covariance matrix, Dimensionality Reduction, Eigen Values, Eigen Vectors, Principal Component Analysis

## I. INTRODUCTION

As the number of dimensions grows many problems arise in the dataset. The data becomes increasingly sparse meaning the datapoints are spread out very thinly making it hard to find any kind of pattern or relationship in the data and very high computational power is required for the high dimensional dataset. Also, there is a problem of visualizing the data in high dimensions. This problem is known as the curse of dimensionality. In the real world the collected data may have many features. Among these features there may be features whose values are irrelevant to the context of the dataset or are heavily correlated to other features present in the dataset. These features do not provide any valuable information or insights to the context of the dataset but only increase the complexity of the problem. So, it becomes a very important task to remove such irrelevant features and keep only the features which are relevant to the subject.

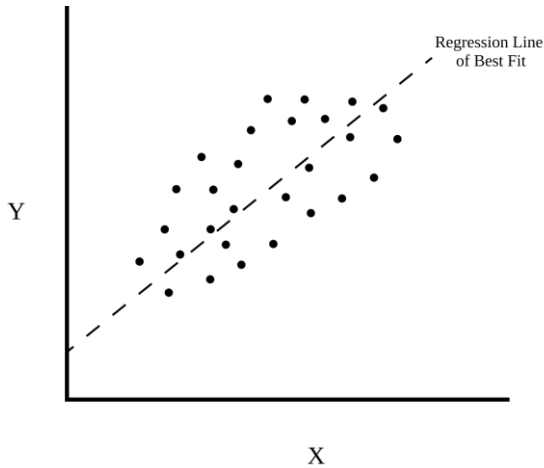
And one of the methods to achieve this task is known as dimensionality reduction.

Principal component analysis (PCA) is a widely used technique for dimensionality reduction and data visualization. It aims to reduce the dimension of the dataset while preserving as much information as possible. It aims to find a set of orthogonal vectors, called principal components, that capture the most variance in the data. The orthogonal vectors are in such order that the first principal component captures the most variance while each subsequent principal component captures the next highest variance in the dataset. The principal components are orthogonal to each other signifying that they are not correlated with each other.

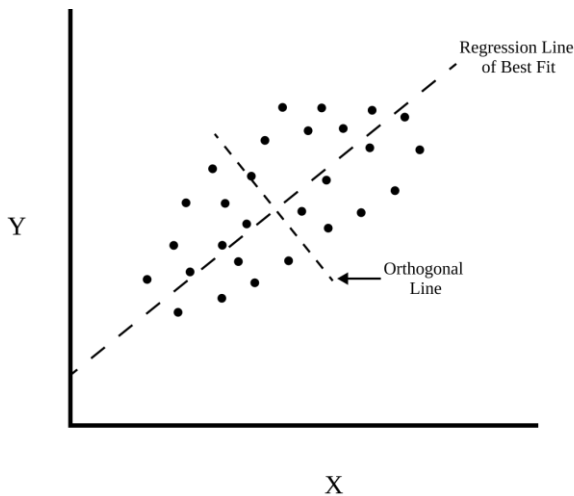
## II. METHODOLOGY

### A. BRIEF THEORY

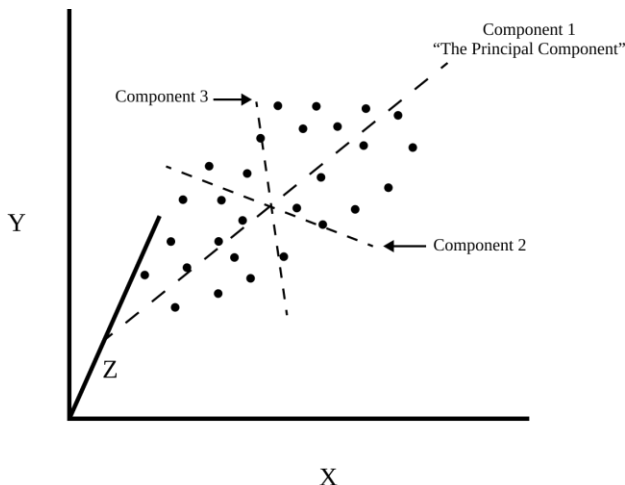
The main concept of PCA is removing any redundant dimensions and keeping the dimensions with the highest variance. PCA selects the principal components that capture all the major variations across the dataset encompassing most of the information present in the dataset.



Suppose we have a dataset with features X and Y then we can fit a regression line onto the dataset. Drawing an orthogonal line to the best fit line we get,



We can see that the data vary mostly along the best fit line. Now, we can project the points onto our new axis and get our new x-axis and y-axis. We can keep drawing lines perpendicular to both lines to get more axis.



This new axis will be our Principal Components. PC1 is generally used to denote the component that captures the most variation, PC2 the next and so on.

### B. WORKING PRINCIPLE

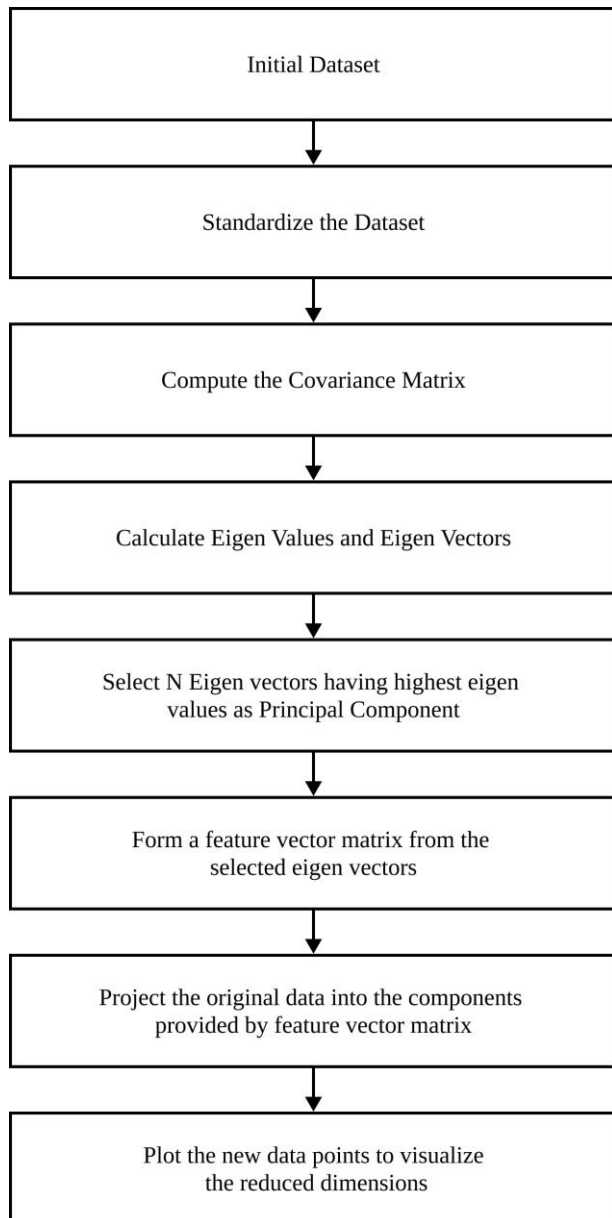
Initially PCA was performed on a random (20 X 2) matrix was generated from a standard normal distribution. Thus, generated matrix had no correlation so PCA could not be applied. Random (2 X 2) matrix was then generated from a uniform distribution. This matrix was then multiplied with the original matrix to generate a new (20 X 2) matrix. Newly generated data was then plotted which resulted in a correlated data point. Standardization was not required as the data from standard normal distribution had 0 mean and multiplying with the (2 X 2) matrix is scaling. Covariance matrix was calculated this, and its value was checked. The required criteria of diagonal element high and off diagonal element nearly 0 was not achieved. Eigenvalues and eigenvectors were extracted from this covariance matrix. Initially both principal components were taken, and a change of basis vector was performed. The variance along Principal Component 1 was very high compared to Principal Component 2 so PC2 was ignored and PC1 was taken. PCA was again using the scikit-learn library and then compared with PCA from scratch. Thus, PCA of random data was completed.

PCA for iris data set firstly involved creating a new data frame and loading the iris data set into the data frame. Features were separated from the class and a matrix of features was created. Calculation of mean and standard deviation showed that the dataset needed to be standardized. Standardization was performed using StandardScaler from scikit-learn. Thus, the dataset had mean 0 and standard deviation of 1. Covariance matrix of the standardized matrix was calculated which did not satisfy our required properties. New basis vectors for the dataset were calculated by eigen decomposition of covariance matrix. Eigenvectors were used to perform changes of basis and projected features were obtained. PCA was again done using decomposition from scikit-learn and compared with PCA from scratch. Thus, PCA of random data was completed.

Diabetes prediction dataset was chosen as our next candidate for PCA. Dataset consisted of 8 features and class. Categorical classes were converted into numerical form. Some of the features were NaN (Not a Number) which was filled with mean value using SimpleImputer. Features was separated from the class and matrix was created. Calculation of mean and standard deviation showed that the dataset needed to be standardized. Standardization was performed. Thus, the dataset had mean 0 and standard deviation of 1. Covariance matrix of the standardized matrix was calculated which did not satisfy our required properties. New basis vectors for the dataset were calculated by eigen decomposition of

covariance matrix. Eigenvectors were used to perform change of basis and projected features was obtained. PCA was again done using scikit-learn library and compared with PCA from scratch. Newly obtained datapoints were the plotted to analyze the result. Thus, PCA of random data was completed.

### C. SYSTEM BLOCK DIAGRAM



#### 1) CREATE A MATRIX OF FEATURE VECTORS

Initially features are selected from which the target is interpreted. These features allow the model to make predictions on new data to assign classes.

#### 2) STANDARDIZE THE DATA

Before starting the PCA process, the feature vectors must be standardized so that they have zero mean and standard deviation of 1. This ensures that all the features have the same scale so that PCA gives equal importance to each feature preventing features with larger scale to disproportionately influence the result. Units are also removed during standardization making interpretation of principal components more meaningful.

#### 3) COVARIANCE MATRIX COMPUTATION

After standardization of features, covariance matrix of the standardized features is calculated. Covariance matrix shows the linear relationship between the features. For PCA decomposition, the diagonal elements of the covariance matrix i.e., Variance of a feature should be maximum, and the non-diagonal elements of the covariance matrix must be minimum. Covariance matrix allows PCA to find the direction of maximum variance. (eqn no 3)

#### 4) CALCULATION OF EIGEN VALUES AND EIGEN VECTORS

The covariance matrix is used of eigen decomposition to get the eigenvalues and eigenvectors. Eigenvalues represent the amount of variance captured by each principal component and eigenvectors represent the direction of each principal component. Each eigenvector is new basis vectors that are used to project the original data into new coordinates.

#### 5) SELECTION OF PRINCIPAL COMPONENT

Eigen values are used to calculate the importance of each principal component. If n number of feature is required, then eigen values are arranged in ascending order and eigenvectors with top n eigenvalue is selected. This ensures that maximum amount of variance is captured thus retaining essential information.

#### 6) FORMATION OF FEATURE MATRIX

Selected eigenvectors are used to form a feature new feature matrix. The feature matrix acts as a new basis for the data, and the new features are orthogonal to each other.

#### 7) PROJECT ORIGINAL DATA INTO THE PRINCIPAL COMPONENTS

Change of basis is performed on the original dataset to project them onto new coordinates. This results in new dataset with reduced number of features. (Change of bias refer to eqn no 4)

#### 8) VISUALIZATION

New data is then plotted to visualize the changes study the result.

## B. MAJOR MATHEMATICAL FORMULAS

### 1) VARIANCE

Variance is used to measure how scattered the data are from a mean value. It is calculated by.

$$Var(x) = \frac{\sum_{i=0}^n (x_i - \bar{x})^2}{n - 1} \quad (1)$$

Where:

$x_i$  = Individual data points

$\bar{x}$  = Mean of all the value

$n$  = Number of data points in the given data.

### 2) COVARIANCE

Covariance is the measure of variance between variables. It describes how variable change to together. Covariance is calculated as

$$Cov(x, y) = \frac{\sum_{i=0}^n (x_i - \bar{x})(y_i - \bar{y})}{n - 1} \quad (2)$$

Where:

$x_i$  = Individual data points of feature x

$\bar{x}$  = Mean of all the value of feature x

$y_i$  = Individual data points of feature y

$\bar{y}$  = Mean of all the value of feature y

$n$  = Number of data points in the given data.

Covariance gives an idea about the trend of the data. Positive covariance indicates that with the increase of x, y also increases whereas negative covariance indicates that with increase in x, y decreases. Zero covariance indicates that there is no relationship between x and y.

### 3) COVARIANCE MATRIX

Covariance Matrix is a square matrix with diagonal elements representing variance and non-diagonal elements representing covariance. Generally, Covariance matrix is represented as

$$\begin{bmatrix} Var(x) & Cov(x, y) \\ Cov(x, y) & Var(y) \end{bmatrix}$$

Where:

$Var(x)$  = Variance of x

$Var(y)$  = Variance of y

$Cov(x, y)$  = Covariance between x and y

Covariance Matrix is calculated as

$$S_x = \frac{1}{n - 1} XX^T \quad (3)$$

Where:

$S_x$  = Square symmetric ( $n \times n$ ) matrix

$X$  =  $n$ -dimensional vector of feature x

### 4) CHANGE OF BASIS

Basis of a vector space is the set of linearly independent vectors that span all the vector space. For e.g. Consider a 2-dimensional space with unit vector  $\hat{i}$  along x axis and  $\hat{j}$  along y axis. These unit vectors can then be scaled so that it can span all the possible points in the 2-dimensional space. In PCA, change on basis plays a vital role to as we map the original data into new one by changing the basis vector. Changing the basis does not change the data only its representation is changed. Changing the basis only projects the data vectors on the basis vectors.

Change of basis is achieved by

$$Y = PX \quad (4)$$

Where:

$Y$  = Data points obtained after linear transformation

$P$  = Basis vectors used for linear transformation

$X$  = Original data points

### 3) EIGEN VALUES AND EIGEN VECTORS

Eigen v

Let  $A$  be an  $n \times n$  matrix, then

An eigen vector is a non-zero vector  $v$  such that

$$Av = \lambda v \quad (5)$$

For some scalar  $\lambda$ .

An eigen value is a scalar  $\lambda$  such that

$$Av = \lambda v \quad (5)$$

Has some non-trivial solution.

If  $Av = \lambda v$  and  $v \neq 0$ , then  $\lambda$  is eigenvalue for  $v$ , and  $v$  is the eigen vector for  $\lambda$ .

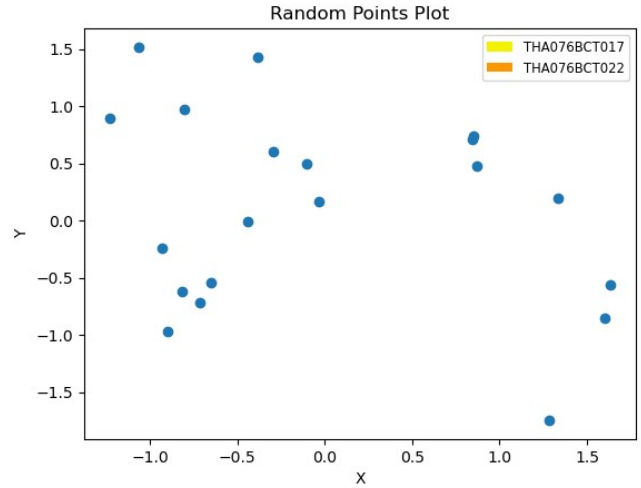
All eigen vectors of a symmetric matrix are perpendicular to each other.

### C. INSTRUMENTATION

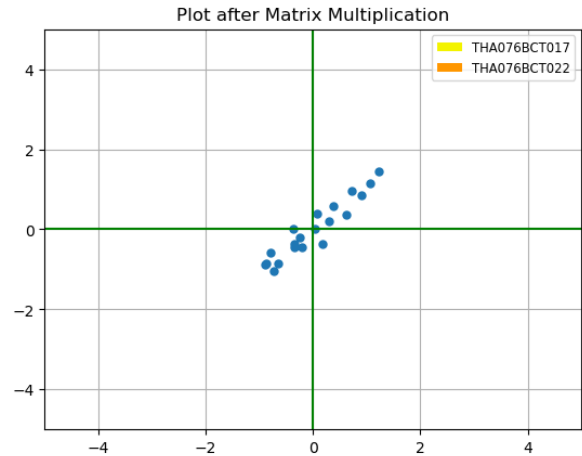
In the implementation of Principal Component Analysis (PCA) using Python, the following libraries and functions were utilized. Numpy, a powerful library for numerical computing, was employed for vector and matrix operations, providing efficient computation capabilities. Pandas, a popular data manipulation library, was used for storing and handling data in the form of dataframes. Scikit-learn, a comprehensive machine learning library, contributed the StandardScaler class for scaling the data, ensuring that all features have similar ranges. The `np.linalg.eig` function from Numpy was utilized to calculate the eigenvalues and eigenvectors, crucial components of PCA. Lastly, the PCA class from scikit-learn was employed to compare the results against the hand-coded implementation, facilitating a convenient and validated approach to PCA analysis.

## III. RESULTS

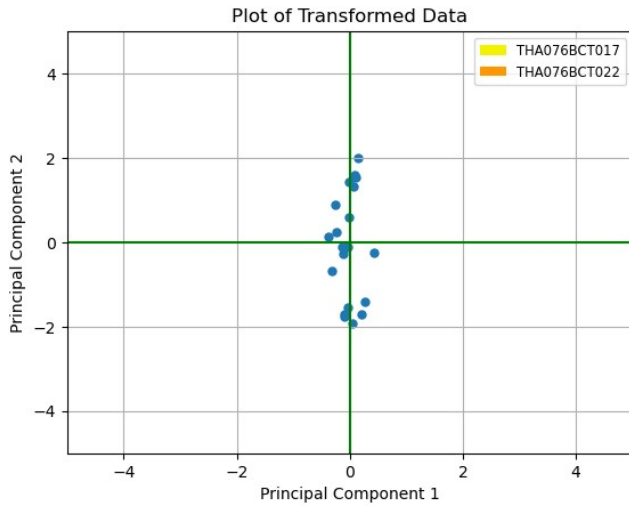
### A. RANDOM DATASET



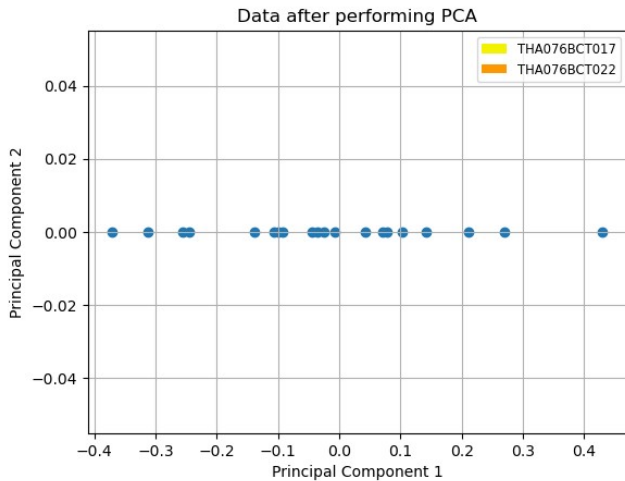
The plot shows the datapoint obtained from standard normal distribution. Since the data is extracted randomly from standard normal distribution, datapoints show no correlation thus PCA cannot be applied. The values generated from a standard normal distribution generates a mean of zero and standard deviation close to 1.



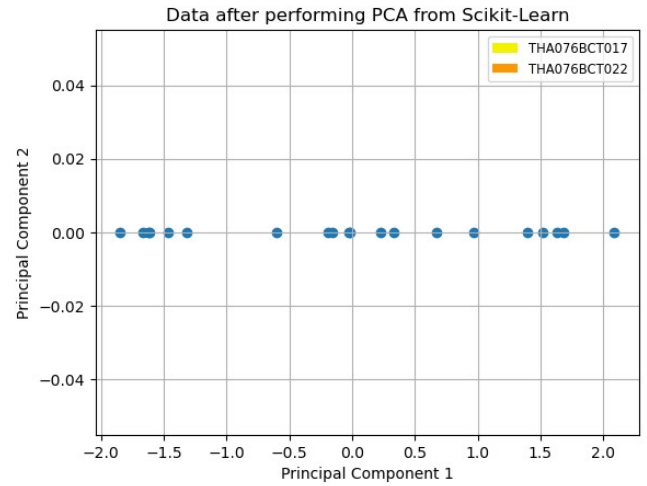
Multiplication with  $(2 \times 2)$  matrix from uniform distribution resulted in the above plot. It is seen that the datapoints are correlated. This is because multiplication with the  $(2 \times 2)$  matrix introduces a linear transformation upon the data. Because the transformation involves a linear combination of the original variables leading to a change in their relationship, as a result the transformed data points become correlated.



The plot was obtained by performing a change of basis vector and data point was projected upon new coordinated system defined by the principal components generated by applying PCA. The Principal Component 1 is as x-axis and Principal Component 2 is at y-axis.



The plot above demonstrated the reduction of the original two-dimensional data into a single dimension using PCA. In this plot the data are varied only in a single dimension x-axis using principal component 1 and the y-axis value which is principal component 2 remains zero.



The above plot was obtained by using the PCA provided by scikit-learn library to reduce the dimension from two-dimensions to a single dimension.

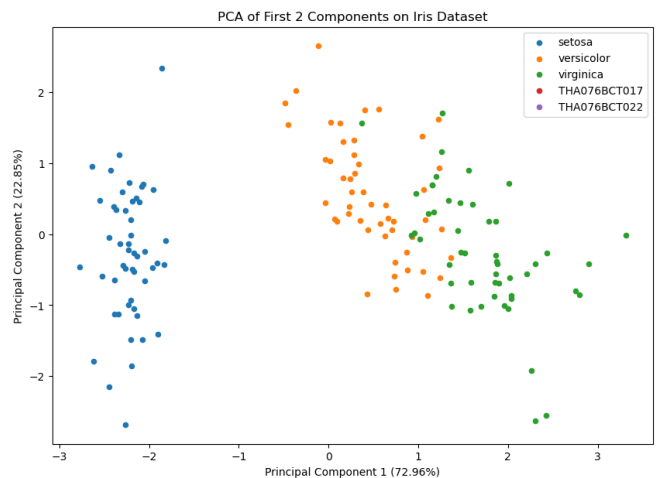
## B. IRIS DATASET

Like the random generated dataset PCA was also applied to the Iris Dataset. The results obtained from applying the PCA on the Iris Dataset are discussed below.

TABLE I  
EXPLAINED VARIANCE FOR IRIS DATASET

Principal Component	Explained Variance	Approx. (in %)
PC1	0.7296	72.96
PC2	0.2285	22.85
PC3	0.03669	3.66
PC4	0.00517	0.51

Table I gives the values of variance captured by every principal component after applying PCA.





The above plot new data points of Iris Dataset after undergoing PCA. This 2-D plot depicts PC1 which covers 72.96% of the variation and PC2 which covers 22.85% of the variation. With only two features of the four, setosa can be seen separated from the other two flowers but there still lies some confusion between versicolor and virginica.

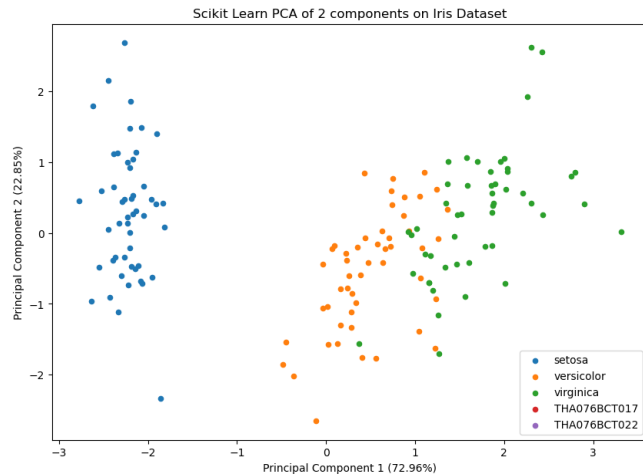


Figure shows the top two PCA accomplished using the decomposition function from scikit-learn. We have observed that the eigenvalues and eigenvectors result in the same value using both methods i.e., applying PCA from scratch and PCA from scikit-learn. The only difference observed was the direction of eigenvectors which was introduced due to a sign difference. This sign difference does not cause any issue for PCA. But for the plot it caused the plot to flip along the y-axis. This occurred due to some difference in mathematical implementation.

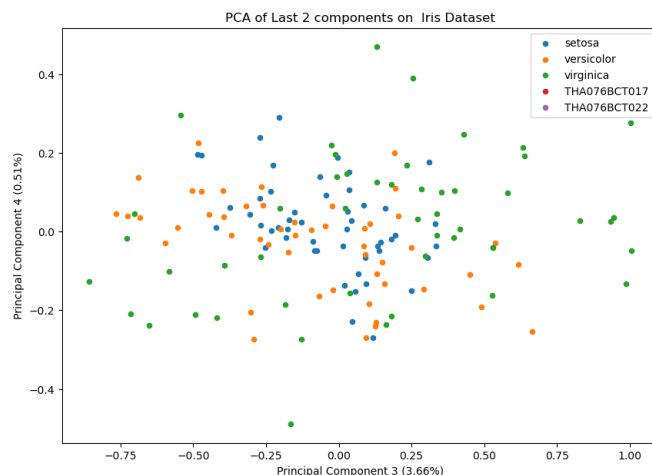


Figure shows the PC3 which captures 3.66% of the variation and PC4 which captures 0.51% of the variation. Separating the flowers was not possible from the available

data points as most of the essential information about the original data was lost because the principal components could not retain most of the information from the dataset.

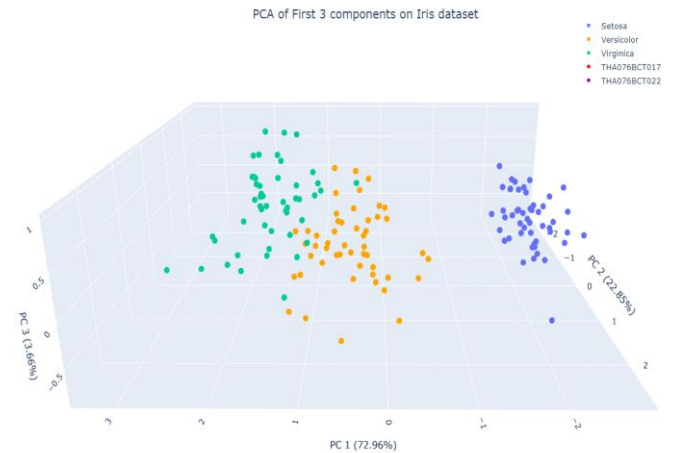


Figure shows 3D plot consisting of PC1, PC2 and PC3. This combination of Principal Component captures the largest amount of variation in the dataset while being easily visualizable. Flowers can be seen to be easily separable as crucial information of the original dataset was retained.

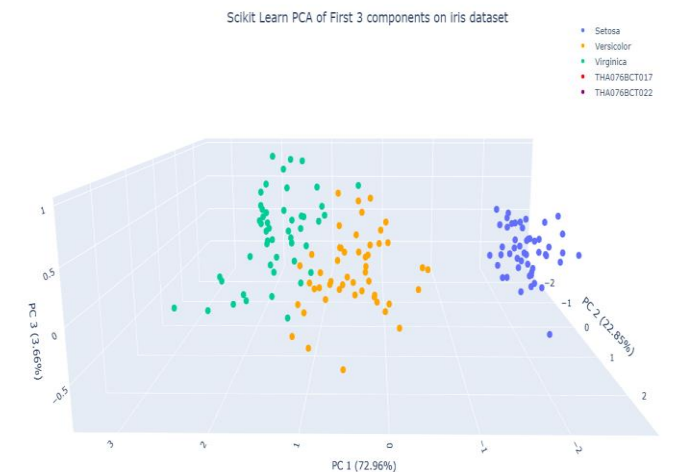


Figure shows top three PC implemented from decomposition using the PCA from scikit-learn library.



Figure shows the 3D plot of PC with least amount of variation captured. As crucial information is lost, separation of the flowers cannot be done.

### C. DIABETES DATASET

Finally, PCA was applied to the Diabetes Detection Dataset. The results obtained from applying the PCA on the Diabetes Detection Dataset are discussed below.

TABLE II  
EXPLAINED VARIANCE FOR DIABETES PREDICTION DATASET

Principal Component	Explained Variance	Approx. (in %)
PC1	0.2150	21.5
PC2	0.1380	13.8
PC3	0.1322	13.22
PC4	0.1196	11.96
PC5	0.1099	10.99
PC6	0.1056	10.56
PC7	0.1041	10.41
PC8	0.0752	7.52

Table II gives the values of variance captured by every principal component after applying PCA on the diabetes detection dataset.

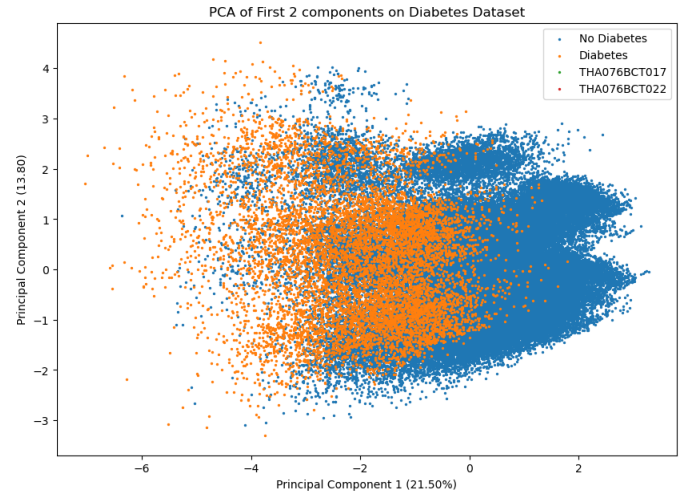


Figure shows the top two principal components for diabetes prediction. Since the original dataset had 8 dimensions so two principal components are not enough to show the difference so not many insights can be gained from this figure.

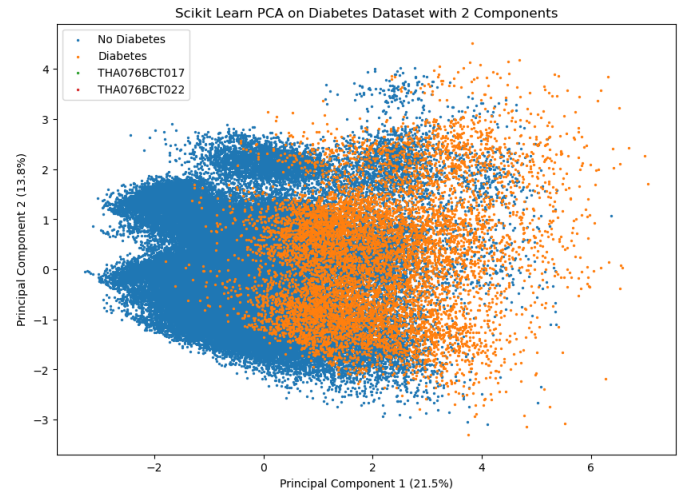
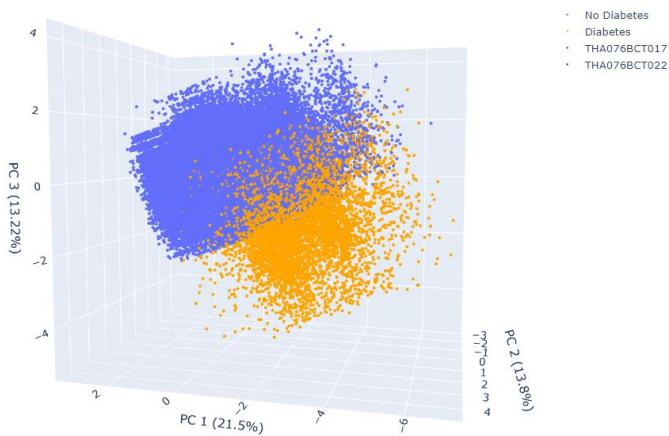


Figure shows top two PC from decomposition from scikit learn. Because of the mathematical implementation of PCA in scikit-learn library and custom one we can see that the plots are flipped on the x-axis.



PCA of First 3 components on Diabetes Dataset



Scikit Learn PCA on Diabetes Dataset with 3 Components

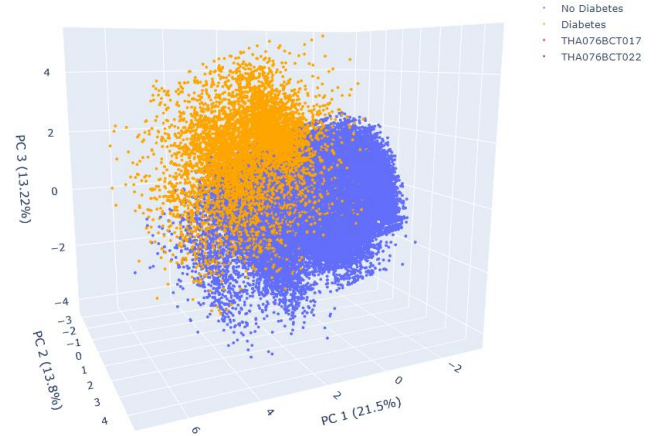


Figure shows 3-d plot of top three PC for diabetes prediction.

Figure shows principal components obtained from scikit-learn that capture the least amount of variance in diabetes prediction dataset.

PCA of last 3 components on Diabetes Dataset

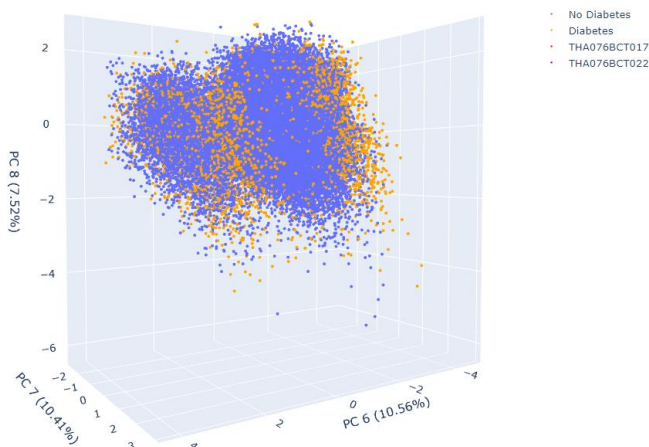


Figure shows principal components that capture the least amount of variance in diabetes prediction dataset.

#### IV. DISCUSSION AND ANALYSIS

Use either SI (MKS) or CGS as primary units. (SI units are strongly encouraged.) English units may be used as secondary units (in parentheses). This applies to papers in data storage. For example, write “15 Gb/cm<sup>2</sup> (100 Gb/in<sup>2</sup>).” An exception is when English units are used as identifiers in trade, such as “3½-in disk drive.” Avoid combining SI and CGS units, such as current in amperes and magnetic field in oersteds. This often leads to confusion because equations do not balance dimensionally. If you must use mixed units, clearly state the units for each quantity in an equation.

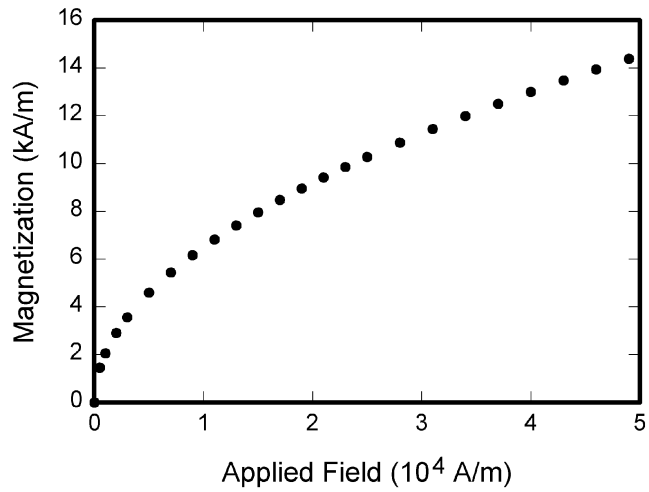
The SI unit for magnetic field strength  $H$  is A/m. However, if you wish to use units of T, either refer to magnetic flux density  $B$  or magnetic field strength symbolized as  $\mu_0 H$ . Use the center dot to separate compound units, e.g., “A·m<sup>2</sup>.”

#### V. CONCLUSION

The word “data” is plural, not singular. The subscript for the permeability of vacuum  $\mu_0$  is zero, not a lowercase letter “o.” The term for residual magnetization is “remanence”; the adjective is “remanent”; do not write “remnance” or “remnant.” Use the word “micrometer” instead of “micron.” A graph within a graph is an “inset,” not an “insert.” The word “alternatively” is preferred to the word “alternately” (unless you really mean something that alternates). Use the word “whereas” instead of “while” (unless you are referring to simultaneous events). Do not use the word “essentially” to mean “approximately” or “effectively.” Do not use the word “issue” as a euphemism for “problem.” When compositions are not specified, separate chemical symbols by en-dashes; for example, “NiMn” indicates the intermetallic compound Ni<sub>0.5</sub>Mn<sub>0.5</sub> whereas “Ni–Mn” indicates an alloy of some composition Ni<sub>x</sub>Mn<sub>1-x</sub>.

Be aware of the different meanings of the homophones “affect” (usually a verb) and “effect” (usually a noun), “complement” and “compliment,” “discreet” and “discrete,”

“principal” (e.g., “principal investigator”) and “principle”



**FIGURE 1.** Magnetization as a function of applied field. Note that “Fig.” is abbreviated. There is a period after the figure number, followed by two spaces. It is good practice to explain the significance of the figure in the caption.

## VI. REFERENCES

#### D. SIZING OF GRAPHICS

Most charts, graphs, and tables are one column wide (3.5 inches / 88 millimeters / 21 picas) or page wide (7.16 inches / 181 millimeters / 43 picas). The maximum depth a graphic can be is 8.5 inches (216 millimeters / 54 picas). When choosing the depth of a graphic, please allow space for a caption. Figures can be sized between column and page widths if the author chooses, however it is recommended that figures are not sized less than column width unless when necessary.

There is currently one publication with column measurements that do not coincide with those listed above. Proceedings of the IEEE has a column measurement of 3.25 inches (82.5 millimeters / 19.5 picas).

The final printed size of author photographs is exactly 1 inch wide by 1.25 inches tall (25.4 millimeters x 31.75 millimeters / 6 picas x 7.5 picas). Author photos printed in editorials measure 1.59 inches wide by 2 inches tall (40 millimeters x 50 millimeters / 9.5 picas x 12 picas).

#### E. RESOLUTION

The proper resolution of your figures will depend on the type of figure it is as defined in the “Types of Figures” section. Author photographs, color, and grayscale figures should be at least 300dpi. Line art, including tables should be a minimum of 600dpi.

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In order to preserve the figures’ integrity across multiple computer platforms, we accept files in the following formats: .EPS/.PDF/.PS. All fonts must be embedded or text converted to outlines in order to achieve the best-quality results.

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The term color space refers to the entire sum of colors that can be represented within the said medium. For our purposes, the three main color spaces are Grayscale, RGB (red/green/blue) and CMYK (cyan/magenta/yellow/black). RGB is generally used with on-screen graphics, whereas CMYK is used for printing purposes.

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When preparing your graphics IEEE suggests that you use of one of the following Open Type fonts: Times New Roman, Helvetica, Arial, Cambria, and Symbol. If you are supplying EPS, PS, or PDF files all fonts must be embedded. Some fonts may only be native to your operating system; without

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A safe option when finalizing your figures is to strip out the fonts before you save the files, creating “outline” type. This converts fonts to artwork what will appear uniformly on any screen.

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##### 1) FIGURE AXIS LABELS

Figure axis labels are often a source of confusion. Use words rather than symbols. As an example, write the quantity “Magnetization,” or “Magnetization  $M$ ,” not just “ $M$ .” Put units in parentheses. Do not label axes only with units. As in Fig. 1, for example, write “Magnetization (A/m)” or “Magnetization ( $A \cdot m^{-1}$ ),” not just “A/m.” Do not label axes with a ratio of quantities and units. For example, write “Temperature (K),” not “Temperature/K.”

Multipliers can be especially confusing. Write “Magnetization (kA/m)” or “Magnetization ( $10^3$  A/m).” Do not write “Magnetization (A/m)  $\times 1000$ ” because the reader would not know whether the top axis label in Fig. 1 meant 16000 A/m or 0.016 A/m. Figure labels should be legible, approximately 8 to 10 point type.

##### 2) SUBFIGURE LABELS IN MULTIPART FIGURES AND TABLES

Multipart figures should be combined and labeled before final submission. Labels should appear centered below each subfigure in 8 point Times New Roman font in the format of (a) (b) (c).

#### J. FILE NAMING

Figures (line artwork or photographs) should be named starting with the first 5 letters of the author’s last name. The next characters in the filename should be the number that represents the sequential location of this image in your article. For example, in author “Anderson’s” paper, the first three figures would be named *ander1.tif*, *ander2.tif*, and *ander3.ps*.

Tables should contain only the body of the table (not the caption) and should be named similarly to figures, except that ‘.t’ is inserted in-between the author’s name and the table number. For example, author Anderson’s first three tables would be named *ander.t1.tif*, *ander.t2.ps*, and *ander.t3.eps*.

Author photographs should be named using the first five characters of the pictured author’s last name. For example, four author photographs for a paper may be named: *oppen.ps*, *moshc.tif*, *chen.eps*, and *duran.pdf*.

If two authors or more have the same last name, their first initial(s) can be substituted for the fifth, fourth, third... letters of their surname until the degree where there is differentiation. For example, two authors Michael and Monica Oppenheimer’s photos would be named *oppmi.tif*, and *oppmo.eps*.

## K. REFERENCING A FIGURE OR TABLE WITHIN YOUR PAPER

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- [4] E. P. Wigner, “Theory of traveling-wave optical laser,” *Phys. Rev.*, vol. 134, pp. A635–A646, Dec. 1965.
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- [7] J. H. Davis and J. R. Cogdell, “Calibration program for the 16-foot antenna,” *Elect. Eng. Res. Lab., Univ. Texas, Austin, TX, USA, Tech. Memo. NGL-006-69-3*, Nov. 15, 1987.

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- [11] *The Founders' Constitution*, Philip B. Kurland and Ralph Lerner, eds., Chicago, IL, USA: Univ. Chicago Press, 1987. [Online]. Available: <http://press-pubs.uchicago.edu/founders/>
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- [15] W. P. Risk, G. S. Kino, and H. J. Shaw, "Fiber-optic frequency shifter using a surface acoustic wave incident at an oblique angle," *Opt. Lett.*, vol. 11, no. 2, pp. 115-117, Feb. 1986.
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- [19] Teralyzer. Lytera UG, Kirchhain, Germany [Online]. Available: [http://www.lytera.de/Terahertz\\_THz\\_Spectroscopy.php?id=home](http://www.lytera.de/Terahertz_THz_Spectroscopy.php?id=home), Accessed on: Jun. 5, 2014

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From 2001 to 2004, he was a Research Assistant with the Princeton Plasma Physics Laboratory. Since 2009, he has been an Assistant Professor with the Mechanical Engineering Department, Texas A&M University, College Station. He is the author of three books, more than 150 articles, and more than 70 inventions. His research interests include high-pressure and high-density nonthermal plasma discharge processes and applications, microscale plasma discharges, discharges in liquids, spectroscopic diagnostics, plasma propulsion, and innovation plasma applications. He is an Associate Editor of the journal *Earth, Moon, Planets*, and holds two patents.

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