**Linear Algebra behind Principal Component Analysis**

# Introduction

Let’s start with a basic question – what is algebra?

In our elementary classes, we had performed addition, subtraction, multiplication etc. of numbers and we called them Arithmetic. Basically the operations on numbers or its manipulation is called Arithmetic. And when these operations or manipulations involves abstract symbols (like alphabets, Greek symbols), they are called Algebra.

Use of algebra can be traced back in 1600BC by Babylon and Egyptians and if we think why abstract symbols came into simpler arithmetic must owe to the exorbitant trade and merchandising.

And then came in geometry and Greeks to form the Pythagoras theorem, thus widening Algebra.

Now there are many fields of mathematics with algebra in the name such as Elementary Algebra, Abstract Algebra, and Linear Algebra etc. And here our topic of discussion is Linear Algebra.

# Linear Algebra

Linear Algebra is the study of linear equation or combinations involving an array of numbers or symbols called matrices. In modern mathematics, Linear Algebra is the study of linear equations and vector spaces (nothing but a wider view on matrices).

A Vector space is defined as a set V on which there are 2 operations, one is addition and other is multiplication by scalars such that the following properties hold:

1. x+y = y+x , x,y € V
2. (x+y)+z = x+(y+z) x,y,z€ V
3. There exists an element 0€V, such that x+0 =x, for every x€V
4. For every x€V, there exists -x€V, such that x+(-x)=0
5. λ(x+y) = λx+λy, for all x,y€V and λ is scalar
6. (λ+µ)x = λx+µx for all x€V and scalars µ,λ
7. (λµ)x = λ(µx) for all x€V and scalars µ,λ
8. 1x = x) for all x€V

V is Real vector space, when scalars belong to Real numbers and Complex Vector Space when scalars belong to Complex space.

Using the above properties, we can very well prove that a set of (m×n) matrices is a Vector Space.

# Matrices and algebra on matrices

Matrices and its algebra are a part of a professional’s day to day activity. We use arrays for variety of manipulations such as solving system of linear equations, optimizing and reducing dimensionality using PCA etc.

Most of the times the software solves our requirement without much effort and sometimes we lack a basic understanding of the same. This article is attempted to give a basic understanding of linear algebra behind PCA.

Let’s start with – what is a matrix?

An m×n matrix is an array of m rows and n columns. A 3×2 matrix can be denoted as

A=

## Types of matrices

### Square matrix

A matrix with number of columns equals to number of rows is called a square matrix.

### Zero matrix

A matrix with all elements zero is called a zero matrix. For e.g.

### Identity matrix

A square matrix where all the diagonal elements are one and rest are zero is called an Identity matrix. Identity matrix id denoted by I.

### Diagonal matrix

Diagonal matrix are square matrix or a rectangular matrix with diagonal elements non-zero and rest all the elements are zero. A 3×3 diagonal matrix is given below

### Triangular matrix

An upper or lower triangular matrix is a square matrix with non-zero elements above or below the diagonal respective.

An Upper diagonal matrix is

A lower diagonal matrix is

## Addition of matrices

Matrices can be added only if they are of the same dimension, addition of 2×2 matrix is given as below:

+ =

## Multiplication of matrices

Multiplication of matrix by scalar is also called dot product and is as shown below,

λ =

Matrix multiplication of 2 matrices requires number of columns of the first matrix to be equal to the number of rows of the second.

An m×n matrix multiplied with n×k matrix produces an m×k matrix. Matrix multiplication of a 3×2 and a 2×3 matrix produces a 3×3 matrix as given below:

. =

Product of an Identity matrix I and a matrix A of same dimensions returns the matrix A.

A×I = A = I×A

## Transpose of a matrix

When we swap the rows and columns of a matrix, the resulting matrix is called transpose of A and is denoted by AT.

A =

AT =

If a square matrix A holds a property of AT = A then A is called a **symmetric** matrix. And if the square matrix A holds a property of AT = - A then A is called a **skew symmetric** matrix

A square matrix A is called **orthogonal** if A AT  = AT A = I

## Determinant of a matrix

Any large matrix would be easily interpretable it if can be perceived as a linear combination for its columns, or in other words it can be viewed as a matrix decomposition.

Determinant of matrix is the first step towards matrix decomposition, it’s a function which helps to view an n×n matrix as a linear combination of its columns.

Mathematically, Determinant is defined as a function that maps an n×n matrix to a scalar which satisfies the properties

1. If any 2 rows or columns of a determinant (Det) is interchanged, the determinant changes sign.
2. Determinant of an identity matrix is 1.
3. If each element of a row or column of a determinant is multiplied by a constant k, then its value gets multiplied by k.
4. If the elements of a row or column of a determinant are expressed as the sum of two or more elements, then the determinant can be expressed as the sum of two or more determinants.

Determinant of a 2×2 matrix is given as

Det = a1×b2 + a2×b1

Determinant of a 3×3 matrix can be given as

Det = a1×Det + b1×Det + c1×Det

An n×n Square matrix A is **invertible**, if there exists an n×n matrix B such that, A.B = I = B.A. this matrix B is called inverse of A, denoted by A-1.

To find the inverse of a 2x2 matrix: swap the positions of a1 and b2, put negatives in front of b1 and a2, and divide everything by the determinant (a1b2-a2b1) ≠0.

# Eigenvalues and Eigenvectors

Eigenvalues are eigenvectors are the crux of principal component analysis, helping us understand the dimensionality reduction. Let’s see the definition:

Eigenvalue of an n×n matrix A is a scalar λ, for which there exists a non-zero n×1 matrix such that Ax = λx and the column matrix x is called an eigenvector associated with λ. A scalar is an eigenvalue of A if and only if det(A - λIn ) = 0.

From the above definition, we can see that, an n×n matrix is decomposed into its eigenvalues and eigenvectors without losing important information.

# Principal Component Analysis (Linear) PCA

Principal component analysis reduces the dimensionality of a multivariate data by extracting useful information from the data and forming new variables called principal components (PCs), which explains most variance of the data. This method is particularly useful when the data has high correlation amongst the variables. Principal components are derived from linear combinations of the raw variables in the data. Number of PCs could be less than or equal to the number of the variables in the original data.

Let A be an m×n matrix for which need to reduce the dimensionality using PCA. (Since a multivariate data consists of different scales, it is recommended to standardize the matrix.), we follow the below steps to get to the new principal components for X.

1. Calculate the covariance matrix C=AAT – Covariance matrix of A is an n×n matrix consisting of variances in the variables as diagonal elements of the matrix and covariance between the variables as non-diagonal elements. Since the goal of PCA is to explain the maximum variance of the data, creating a covariance matrix, rightly satisfies the goal.
2. Eigen decomposition on the covariance matrix C – as defined in section IV, this covariance matrix can now be decomposed into it eigenvalues and eigenvector

C=λX,

Where λ consists of eigenvalues and X is an eigenvector matrix. X is an n×n matrix and the columns of X is called principal components or loadings. And the columns of the matrix X comes as ordered by their corresponding eigenvalues.

1. How to reduce the dimension? – From the eigenvector matrix X, we can select the first r number of columns which can explain the maximum variance(r<n). Thus we form a new n×r matrix Y, which has smaller dimension than the original matrix explaining the most variance in the data.
2. Creation of projection matrix P = AY – Projection matrix represents the projection of the original matrix into a smaller dimension. P is an m×r matrix

We can now look into performing PCA using Iris data.