What is PCA?

PCA is a statistical technique to extract patterns in a dataset. Yes, it is. You maybe know it as dimensionality reduction method, yes it is; but it is actually more than that. PCA simply converts your dataset to identify hidden relationships, similarities or differences, then you can make dimension reduction, data compression or feature extraction over the output of it. However, PCA is the best known and used to reduce the dimensions of dataset.

Why do we need to reduce the dimensions in dataset? Isn't that loosing information? Yes, we loose information when we discard some of the dimensions in our data. However, in some cases our data can have lots of features or variables to apply a machine learning technique to do classification or clustering. Think about user dataset of AmazonVideo, Youtube or Netflix, they can be in million-dimension where each video content is a variable or feature, and multiply it with the number of users they have when you need to extract similarities between users or videos and produce recommendations.

Simply, the more dimensions data has, the harder to process it. Therefore, dimensionality reduction techniques like *PCA, LDA* are applied to extract new powerful features from data and these new features or components are used instead of original features. Although some of data is taken out, selected best components should be enough to process.

First try to understand some terms -

Variance : It is a measure of the variability or it simply measures how spread the data set is. Mathematically, it is the average squared deviation from the mean score. We use the following formula to compute variance *var(x).*

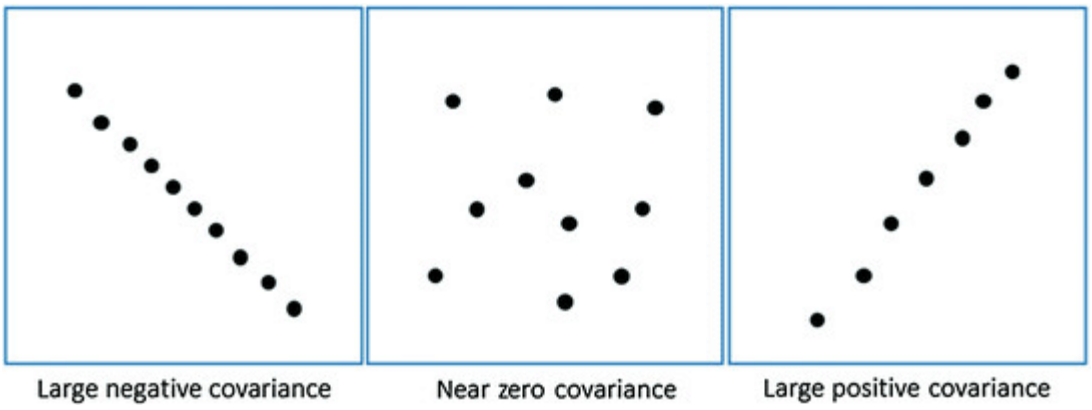
$$var(x) = \frac{\sum (x_i - \bar{x})^2}{N} \qquad cov(x,y) = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{N}$$

Covariance : It is a measure of the extent to which corresponding elements from two sets of ordered data move in the same direction. Formula is shown above denoted by *cov(x,y)* as the covariance of *x* and *y*.

Here, *xi* is the value of x in *ith* dimension.

x bar and *y bar* denote the corresponding mean values.

One way to observe the covariance is how interrelated two data sets are.



Positive covariance means X and Y are positively related i.e. as X increases Y also increases. Negative covariance depicts the exact opposite relation. However, zero covariance means X and Y are not related.

Now lets think about the requirement of data analysis.

Since we try to find the patterns among the data sets so we want the data to be spread out across each dimension. Also, we want the dimensions to be independent. Such that if data has high covariance when represented in some *n* number of dimensions then we replace those dimensions with *linear combination* of those n dimensions. Now that data will only be dependent on linear combination of those related n dimensions. *(related = have high covariance)*

So, what does Principal Component Analysis (PCA) do?

PCA finds a new set of dimensions (or a set of basis of views) such that all the dimensions are orthogonal (and hence linearly independent) and ranked according to the variance of data along them. It means more important principle
axis occurs first. (more important = more variance/more spread out data)

How does PCA work -

1. Calculate the covariance matrix *X* of data points.
2. Calculate eigen vectors and corresponding eigen values.
3. Sort the eigen vectors according to their eigen values in decreasing order.
4. Choose first k eigen vectors and that will be the new k dimensions.
5. Transform the original n dimensional data points into k dimensions.

We have the knowledge of variance and covariance; Let's look into what a ***Covariance matrix*** is.

$$\begin{bmatrix} V_a & C_{a,b} & C_{a,c} & C_{a,d} & C_{a,e} \\ C_{a,b} & V_b & C_{b,c} & C_{b,d} & C_{b,e} \\ C_{a,c} & C_{b,c} & V_c & C_{c,d} & C_{c,e} \\ C_{a,d} & C_{b,d} & C_{c,d} & V_d & C_{d,e} \\ C_{a,e} & C_{b,e} & C_{c,e} & C_{d,e} & V_e \end{bmatrix}$$

A covariance matrix of some data set in 4 dimensions a,b,c,d.

Va : variance along dimension a

Ca,b : Covariance along dimension a and b

If we have a matrix X of m*n dimension such that it holds n data points of m dimensions, then covariance matrix can be calculated as

$$C_x = \frac{1}{n-1}(X - \bar{X})(X - \bar{X})^T \qquad\qquad X^T = Transpose\ of\ X$$

It is important to note that the covariance matrix contains -

* variance of dimensions as the main diagonal elements.
* covariance of dimensions as the off-diagonal elements.

Also, covariance matrix is symmetric. (observe from the image above)

As, we discussed earlier we want the data to be spread out i.e. it should have high variance along dimensions. Also we want to remove correlated dimensions i.e. covariance among the dimensions should be zero (they should be linearly independent). Therefore, our covariance matrix should have -

* large numbers as the main diagonal elements.
* zero values as the off diagonal elements.

We call it a *diagonal matrix*.

So, we have to transform the original data points such that their covariance is a diagonal matrix. The process of transforming a matrix to diagonal matrix is called *diagonalization*.

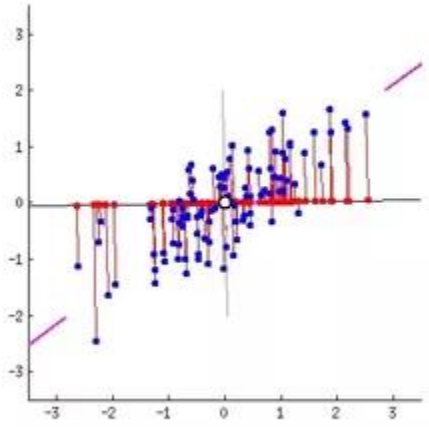
Always normalize your data before doing PCA because if we use data(features here) of different scales, we get misleading components. We can also simply use correlation matrix instead of using covariance matrix if features are of different scales. For the simplicity assume we have already normalized data.

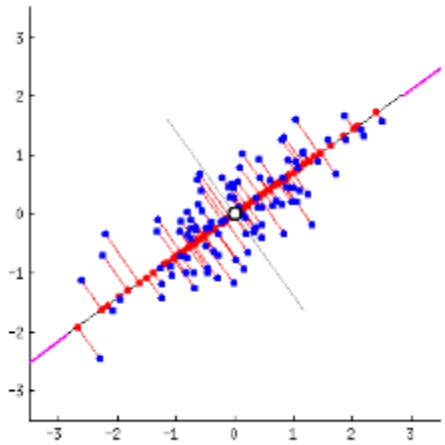
This defines the goal of PCA -

1. Find linearly independent dimensions (or basis of views) which can losslessly represent the data points.

2. Those newly found dimensions should allow us to predict/reconstruct the original dimensions. The reconstruction/projection error should be minimized.

Lets try to understand what I mean by projection error. Suppose we have to transform a 2 dimensional representation of data points to a one dimensional representation. So we will basically try to find a straight line and project data points on them. (A straight line is one dimensional). There are many possibilities to select the straight line. Lets see two such possibilities -





Say magenta line will be our new dimension.

If you see the red lines (connecting the projection of blue points on magenta line) i.e. the perpendicular distance of each data point from the straight line is the projection error. Sum of the error of all data points will be the total projection error.

Our new data points will be the projections (red points) of those original blue data points. As we can see we have transformed 2-dimensional data points to one dimensional data points by projection them on 1 dimensional space i.e. a straight line. That magenta straight line is called *principal axis.* Since we are projecting to a single dimension, we have only one principal axis.

Clearly, second choice of straight line is better because -

* The projection error is less than that in the first case.
* Newly projected red points are more widely spread out than the first case. i.e. more variance.

The above mentioned two points are related i.e. if we minimize the reconstruction error, the variance will increase. How?

Proof

Steps we have performed so far -

* We have calculated the covariance matrix of original data set matrix **X.**

Now we want to transform the original data points such that the covariance matrix of transformed data points is a diagonal matrix. How to do that?

$C_x = covariance\ matrix\ of\ original\ data\ set\ X$
$C_y = covariance\ matrix\ of\ transformed\ data\ set\ Y$
$such\ that,$
$Y = PX$
$For\ simplicity,\ we\ discard\ the\ mean\ term\ and\ assume\ the$
$data\ to\ be\ centered.\ i.e.\ X = (X - \bar{X})$
$So,\ C_x = \frac{1}{n}XX^T$
$C_y = \frac{1}{n}YY^T$
$= \frac{1}{n}(PX)(PX)^T$
$= \frac{1}{n}PXX^TP^T$
$= P(\frac{1}{n}XX^T)P^T$
$= PC_xP^T$

Here's the trick- If we find the matrix of eigen vectors of Cx and use that as P (P is used for transforming X to Y, see the image above) , then Cy (covariance of transformed points) will be a diagonal matrix. Hence Y will be the set of new/transformed data points.
Now, if we want to transform points to k dimensions then we will select first k eigen vectors of the matrix Cx (sorted decreasingly according to eigen values) and form a matrix with them and use them as P.

So, if we have m dimensional original n data points then

*X : m*n*

*P : k*m*

*Y = PX : (k*m)(m*n) = (k*n)*

Hence, our new transformed matrix has n data points having k dimensions.

But why does this trick work?

Proof: First lets look at some theorems -

- Theorem-1:

  The inverse of an orthogonal matrix is its transpose, why?

Let A be an $m * n$ orthogonal
matrix where a_i is
the ith column vector.
The ijth element of $A^T A$ is

$$(\mathrm{A}^T A)_{ij} = a_i^T a_j =$$
$$\begin{cases} 1 \ \ if \ i = j \\ 0 \ \ otherwise \end{cases}$$
Therefore, because $\mathrm{A}^T A = I$,
it follows that $A^{-1} = A^T$.

- Theorem-2 :

Let A be a real symmetric matrix and $\lambda_1, \lambda_2, ..., \lambda_k$ be distinct eigenvalues of A.
Let $u_i \in R^n$ be nonzero such that, $1 \leq i \leq k$.
Then $\{u_1, u_2, .., u_k\}$ forms an orthonormal set.

Proof :

For $i \neq j$, $1 \leq i, j \leq k$, since $A^T = A$, we have
$\lambda_i \langle u_i, u_j \rangle = \langle \lambda_i u_i, u_j \rangle$
$= \langle Au_i, u_j \rangle = \langle u_i, A^T u_j \rangle = \langle u_i, Au_j \rangle$
$= \lambda_j \langle u_i, u_j \rangle$
Since, $i \neq j$ we have $\lambda_i \neq \lambda_j$ and hence $\langle u_i, u_j \rangle = 0$

- Theorem-3 :

Let A be $n * n$ real symmetric matrix such that
all its eigenvales are distinct. Then, there
exists an orthogonal matrix P such that,
$P^{-1} AP = D$
where D is a diagonal matrix with
diagonal entries being the eigenvalues of A.

Proof :

$$Let\ A\ has\ eigenvalues\ \lambda_1, \lambda_2, ..., \lambda_n\ with\ u_i \in R^n$$
$$such\ that\ |u_i| = 1\ and\ Au_i = \lambda_i u_i, 1 \leq i \leq n.$$
$$By\ corollary,\ the\ matrix$$
$$P = [u_1, u_2, .., u_n]$$
$$is\ invertible\ and\ P^{-1}AP = D,\ is\ diagonal\ with\ diagonal\ entries.$$
$$Further,\ by\ theorem - 2,\ (u_1, u_2, .., u_n)\ is\ an\ orthogonal\ set.\ Hence\ P$$
$$is\ in\ fact\ an\ orthogonal\ matrix.$$

Having these theorems, we can say that

A symmetric matrix is diagonalized by a matrix of its orthonormal eigenvectors. Orthonormal vectors are just normalized orthogonal

vectors. (what normalization is? google ;))

$$C_y = PC_xP^T$$
$$= P(E^TDE)P^T$$
$$= P(P^TDP)P^T$$
$$= (PP^T)D(PP^T)$$
$$= (PP^{-1})D(PP^{-1})$$
$$C_Y = D$$

It is evident that the choice of P diagonalizes Cy. This was the goal for PCA. We can summarize the results of PCA in the matrices P and Cy.

- The principal components of X are the eigenvectors of Cx.
- The ith diagonal value of Cy is the variance of X along pi

Conclusion -

$$[new\ data]_{k*n} = [top\ k\ eigenvectors]_{k*m}[original\ data]_{m*n}$$

Note: PCA is an analysis approach. You can do PCA using SVD, or you can do PCA doing the eigen-decomposition (like we did here), or you can do PCA using many other methods. SVD is just another numerical method. So, don't confuse the terms PCA and SVD. However, there are some performance factors of sometimes choosing SVD over eigen-decomposition or the other way around.