

PCA

Basics: vectors have multiple representations in different bases.

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = c_1 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + c_3 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = x_1 \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix} + x_2 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

PCA represents the data as a linear combination of principal components.

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = c_1 [PC_1] + c_2 [PC_2] + \dots + c_n [PC_n]$$

Rewrite the first system:

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} \leftrightarrow v = Bc$$

Projection

The first PC is vector which maximizes the variance of the projection of the data, D , onto that vector.

Def. orthogonal: \mathbf{a} and \mathbf{b} are orthogonal if their inner product is 0.

The projection of \mathbf{a} and \mathbf{b} is thus given by:

$$proj_b(a) = \frac{a^T b}{b^T b} b$$

So for many points (lines, because all points will form a line with the origin) $a_1 \dots a_n$, with their respective projections on \mathbf{b} , $c_1 \dots c_n$, we wish to "minimize their variance". Note that we can write variance as:

$$Var(X) = \frac{1}{n} X^T X$$

Now we can properly state our objective:

$$\max_{\|v\|=1} var(proj_v D)$$

The projection of D on v can be written as:

$$\begin{bmatrix} proj_v d_1 \\ \vdots \\ proj_v d_n \end{bmatrix} = \begin{bmatrix} v^T d_1 \\ \vdots \\ v^T d_n \end{bmatrix} = D^T v$$

And we can rewrite $var(D^T v)$ in a quadratic form, because quadratic forms are easy to maximize analytically.

$$(D^T v)^T (D^T v) = v^T D D^T v$$

To maximize quadratic forms in general, given:

$$x^T A x, A^T = A, \|x\| = 1$$

We use the following theorem about symmetric matrices, stated without proof, if we have a symmetric matrix A , then we can decompose it in terms of 2 matrices E and V , as follows:

$$A^T = A \Rightarrow A = E V E^T, E^T = E^{-1}, V = \begin{bmatrix} v_1 & 0 \\ 0 & v_2 \end{bmatrix}$$

The matrix E is composed of the eigenvectors of A , and V are the eigenvalues.

Since DD^T is necessarily symmetric, we can use that decomposition trick:

$$DD^T = E V E^T$$

Where E is a matrix of the principal components of DD^T .

~Fine~