

PCA:

1. Scale the given matrix X with respect to its mean i.e $X - \bar{X}$

2. Find covariance matrix of given matrix X

$$\text{covariance matrix } (\Sigma) = \frac{XX^T}{n-1}$$

3. Find the eigen values of the system

$$\Sigma \alpha_i = \lambda_i \alpha_i$$

where α_i is an eigen vector corresponding to the eigen value λ_i

These α_i are called principal components.

4. The components corresponding to larger eigen values explain most of the variance in the data and are hence considered important whereas the eigen vectors corresponding to lower eigen values can be discarded.

KPCA:

1. Project the data onto a higher dimensional space that makes it linearly separable (similar to SVM). this is done by adding a new dimension which is a function of existing dimensions.

The high dimensional mapping is represented as ϕ .

$$\text{ex: } (x_1, x_2) \rightarrow (x_1, x_2, x_1^2 + x_2^2). \quad \phi: \mathbb{R}^2 \rightarrow \mathbb{R}^3.$$

2. The covariance matrix in the higher dimension is represented as

$$\Sigma = \phi(X)\phi(X)^T.$$

3. This can be easily calculated as dotproduct of feature vectors in the high dimensional space without actually calculating the high dimensional representation.

4. Typically done via kernel method to obtain a matrix as follows.

$$K = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots & k(x_1, x_d) \\ k(x_2, x_1) & k(x_2, x_2) & \dots & k(x_2, x_d) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_d, x_1) & k(x_d, x_2) & \dots & k(x_d, x_d) \end{bmatrix}$$

$k(x_1, x_2)$ is called the kernel function. Typically Gaussian function used.

$$k(x, y) = \exp \left(-\frac{\|x - y\|^2}{2\sigma^2} \right)$$

most used ones are linear, polynomial and sigmoid kernel functions.

1. pick a kernel function $k(x_i, x_j)$.

2. Calculate the kernel matrix K .

3. Center the Kernel matrix.

4. solve the eigen system $\tilde{K} \alpha_i = \lambda_i \alpha_i$.

same as PCA.