$K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$

PCA → input space

KPCA → PCA on feature space

is not linear in input space.

PCA:

$Cov = \frac{1}{N}\sum_{i=1}^{N} (x_i - m)(x_i - m)^T$

$m = \frac{1}{N}\sum_{i=1}^{N} x_i$

$X = [x_1 \; x_2 \cdots x_N]$

$m = X @ \text{ones}(N,1)/N$

$[m \; m \cdots m] = m @ \text{ones}(1,N)$

$X_c = X - X @ \text{ones}(N,1) @ \text{ones}(1,N)/N$

$X_c = X @ [I_N - \text{ones}(N,N)/N]$

$Cov = X_c @ X_c^T$

$Cov = X @ [I_N - \text{ones}(N,N)/N] @ [I_N - \text{ones}(N,N)/N]^T @ X^T$

$Cov = X_c X_c^T$ $d \times d$

$B = X_c^T X_c$ $N \times N$

$\begin{cases} Cov = U D U^T = X_c X_c^T \\ B = V Z V^T = X_c^T X_c \end{cases}$

u is eigen vector of Cov

$Cov\, u = \lambda u \Rightarrow X_c X_c^T u = \lambda u$

v is eigen vector of B

$B v = z v \Rightarrow X_c^T X_c v = z v$

$\Rightarrow \underline{X_c X_c^T}(X_c v) = z(X_c v)$

$X_c v$ is an eigen vector of $\underline{Cov}$

z is an eigen value of Cov

$u = X_c v$

KPCA:

$Cov = \frac{1}{N}\sum_{i=1}^{N} (\varphi(x_i) - m)(\varphi(x_i) - m)^T$

$m = \frac{1}{N}\sum_{i=1}^{N} \varphi(x_i)$

$Cov = \frac{1}{N}\sum_{i=1}^{N} [\varphi(x_i)\varphi(x_i)^T - m\,\varphi(x_i)^T - \varphi(x_i)\,m^T + m m^T]$

$\varphi(x)^T \varphi(y)$

$\begin{bmatrix} \cancel{\phi(x_1)} \\ \cancel{\phi(x_2)} \\ \vdots \\ \phi(x_N) \end{bmatrix} @ \begin{bmatrix} \phi(x_1) & \phi(x_2) & \cdots & \phi(x_N) \end{bmatrix}$

$K(x_i, x_j)$

$B = X_c^T @ X_c$ $N \times N$

$\boxed{\begin{aligned} B^\phi &= [I_N - \text{ones}(N,N)/N]^T @ \underline{X^{\phi T} @ X^\phi} @ [I_N - \text{ones}(N,N)/N] \\ B^\phi &= [I_N - \text{ones}(N,N)/N] @ G @ [I_N - \text{ones}(N,N)/N] \end{aligned}}$

B eigenvectors v with eigenvalues λ

$\hat{v} \leftarrow v/\sqrt{\lambda}$

? $u = X_c^\phi \hat{v}$

$\|u\|^2 = 1 \Rightarrow u^T u = \hat{v}^T X_c^{\phi T} X_c^\phi \hat{v}$

$\Rightarrow u^T u = \frac{v^T}{\sqrt{\lambda}} \lambda \frac{v}{\sqrt{\lambda}} = \frac{\lambda}{\lambda} = 1$

$x^* \longrightarrow u$

$(\phi(x^*) - m^\phi)^T @ u$

$\underline{\phi(x^*)^T @ X_c^\phi @ \hat{v}} - m^{\phi T} @ X_c^\phi @ \hat{v}$

$- [\frac{1}{N}\sum_{i=1}^{N} \phi(x_i)]^T @ X_c^\phi @ \hat{v}$

$\boxed{\text{proj}(\phi(x^*), u) = \phi(x^*)^T @ X_c^\phi @ \hat{v} - \frac{1}{N}\left[\sum_{i=1}^{N} \phi(x_i)^T @ X_c^\phi\right] @ \hat{v}}$