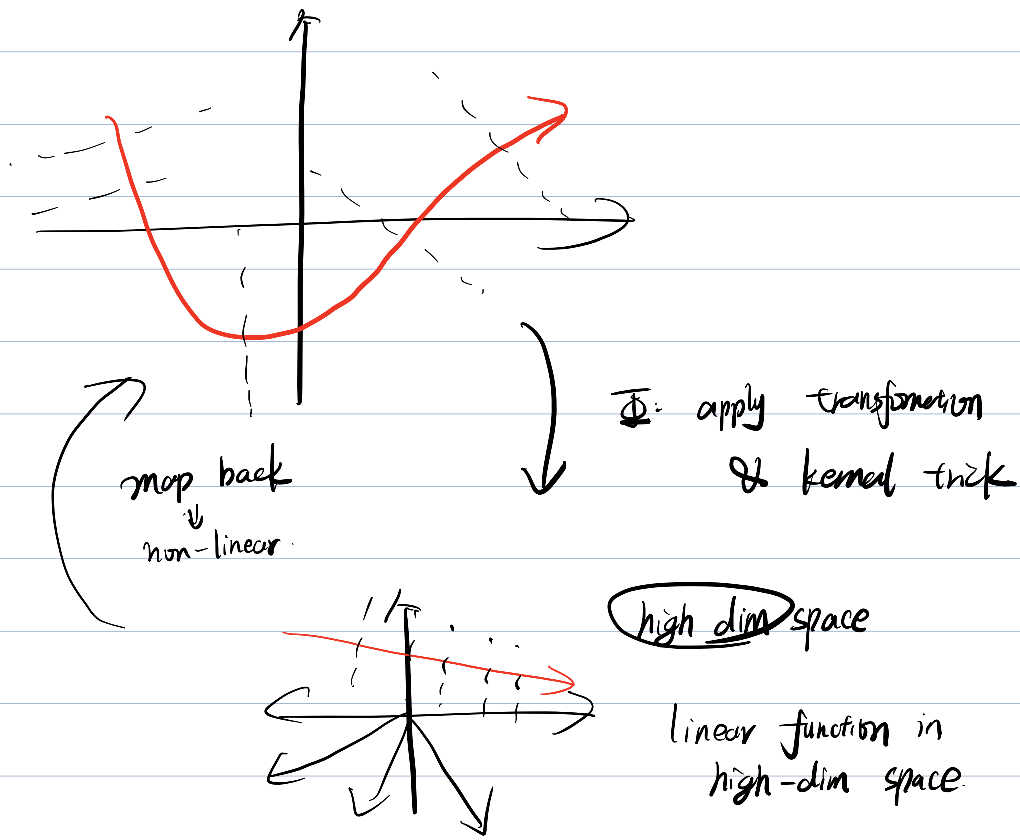
Non linear dim reduction



Kernel PCA

Data $\{x_1, \dots, x_n\}$

- Apply feature transformation

$$x_i \to \phi(x_i)$$

$$[x_1, \dots, x_n] = X \to \Phi = [\phi(x_1), \dots, \phi(x_n)]$$

Assume xformed (transformed) data is centered $\sum_i \phi(x_i) = 0$

- Cov in high-dim space

$$C = \frac{1}{n} \sum_i \phi(x_i)\,\phi(x_i)^T$$ (note: zero mean)

- Find (λ_j, v_j) eigenvalue/ eigenvectors.

$$C v_j = \lambda_j v_j$$

$$\frac{1}{N}\sum_{m=1}^{N} \phi(x_m) \underbrace{\phi(x_m)^T \cdot v_j}_{\substack{\alpha_{mj} \\ \text{scaler}}} = \lambda_j v_j$$

Hence v_j has the form $v_j = \sum_{i}^{N} \alpha_{ij} \phi(x_i) = \Phi \alpha_j$

where $\alpha_j = \begin{bmatrix} \alpha_{1j} \\ \vdots \\ \alpha_{Nj} \end{bmatrix}$

i.e. eigenvectors are combination of $\phi(x_i)$

Substitute for $v_j = \Phi \alpha_j$

$$\frac{1}{N}\sum_{m} \phi(x_m)\phi(x_m)^T \Phi \alpha_j = \lambda_j \underbrace{\Phi \alpha_j}_{\text{span}(\phi(x_1), \dots, \phi(x_n))}$$

eigenvectors are linear combo of $\phi(x_i)$

An equivalent set of equations is to project into the Coordinates of span of Φ & solve there.

$\Rightarrow$ premultiply by Φ^T

$$\Rightarrow \frac{1}{N} \underbrace{\Phi^T \Phi}_{K} \underbrace{\Phi^T \Phi}_{K} \alpha_j = \lambda_j \underbrace{\Phi^T \Phi}_{K} \alpha_j$$

$$\Rightarrow KK\alpha_j = N\lambda_j K\alpha_j$$

① if K is invertible

then $K\alpha_j = N\lambda_j \alpha_j$

② K not invertible

the only differene is there are eigenvectors w/ $\lambda_j = 0$, but these are not principle Components because $\lambda = 0$ solve ① anyway.

Verify: suppose (α_j, λ_j) are ... of K

s.t. $K\alpha_j = N\lambda_j \alpha_j$, $\lambda_j \neq 0$, $\alpha_j^T \alpha_j = 1$

original:

$K \cdot K\alpha_j = N\lambda_j K\alpha_j$

$\Rightarrow \quad N^2\lambda_j^2 \alpha_j = N^2\lambda_j^2\alpha_j$

Kernal centering

$$\tilde{\phi}(x_i) = \phi(x_i) - \underbrace{\frac{1}{N}\sum_k^N \phi(x_k)}_{\text{mean in function space}}$$

$$= \phi(x_i) - \frac{1}{N}\Phi \mathbf{1} \leftarrow \begin{bmatrix} 1 \\ \vdots \end{bmatrix}$$

Centered data

$$\tilde{\Phi} = \Phi - [\tfrac{1}{N}\Phi\mathbf{1}]\mathbf{1}^T = \Phi - \tfrac{1}{N}\Phi\mathbf{1}\mathbf{1}^T = \Phi(I - \tfrac{1}{N}\mathbf{1}\mathbf{1}^T)$$

centered kernal

$$\tilde{K} = \tilde{\Phi}^T\tilde{\Phi} = (I - \tfrac{1}{N}\mathbf{1}\mathbf{1}^T)^T \underbrace{\Phi^T\Phi}_{K} (I - \tfrac{1}{N}\mathbf{1}\mathbf{1}^T)$$

$$= (I - \tfrac{1}{N}\mathbf{1}\mathbf{1}^T) K (I - \tfrac{1}{N}\mathbf{1}\mathbf{1}^T)$$

test kernel

$$\tilde{k}(x_*, x_j) = k(x_*, x_j) - \frac{1}{N}k_*^T\mathbf{1} - \frac{1}{N}k_j^T\mathbf{1} + \frac{1}{N^2}\mathbf{1}^T K \mathbf{1}$$

j^{th} row of K

Summary. KPCA

1) Calculate the kernal matrix $K = [k(x_i, x_j)]_{ij}$
2) Center the kernal $(I - \frac{1}{N}\mathbf{1}\mathbf{1}^T) K (I - \frac{1}{N}\mathbf{1}\mathbf{1}^T)$
3) Find the top D eigenvectors: $\tilde{K}a_j = \lambda_j a_j$, $j = 1 \ldots D$
4) Scale: $\alpha_j \leftarrow \frac{1}{\sqrt{\lambda_j}}\alpha_j$

b) project data X_* : $z_{*,j} = \tilde{K}_*^T \alpha_j$

$$= \sum_i^N \alpha_{ij} K(x_*, x_i)$$

The original PCA needs d-dim eigenvectors

kenal problem needs N-dim eigenvectors

(even if you do not want care about linearility

$\underbrace{d}_{\substack{10000 \\ \text{features}}} \to \underbrace{N}_{\substack{200 \\ \text{datapoints}}}$ $\Rightarrow$ tractable.

Pre-image problem

Given PCA coeff z, we can reconstruct $\hat{x}$, eg. denoising x

$$\hat{x} = \sum_i u_j z_j$$

What about K-PCA