Lecture 11 - Non linear dimensionality Reduction

CS5487 Lecture Notes (2020)
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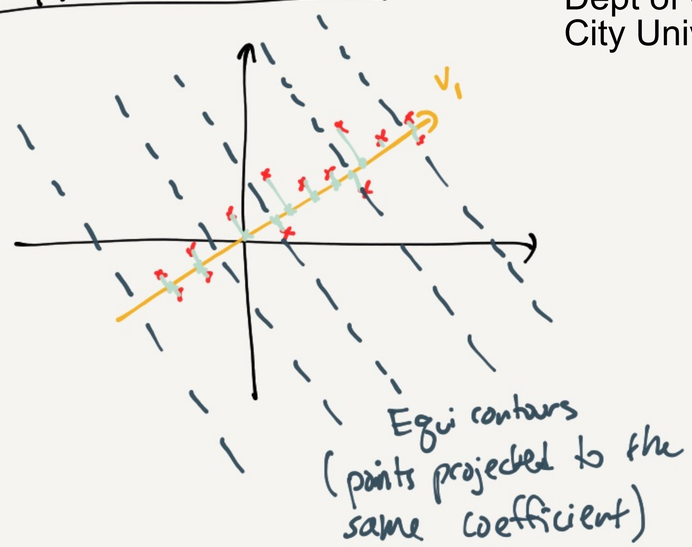
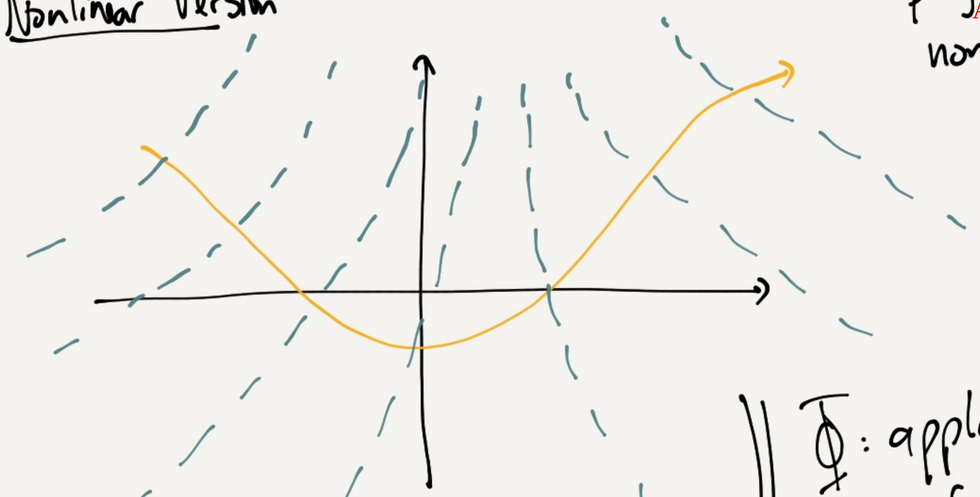
PCA (linear dim reduction)

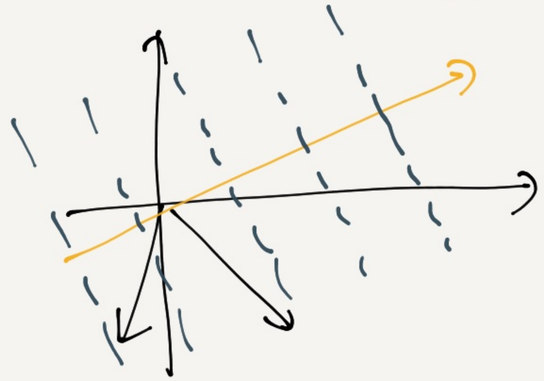


Nonlinear version

project onto nonlinear function.



Φ: apply feature xform



linear xform in high-dim space.

Kernel PCA

- Data: $\{x_1, \dots, x_n\}$
- Apply feature xform to $x_i \rightarrow \phi(x_i)$
  $X \rightarrow \Phi$
- Assume the xformed data is zero-mean (centered)
  i.e. $\sum_i \phi(x_i) = 0$
- Covariance matrix: (assuming zero-mean) $C = \frac{1}{n} \sum_{i=1}^{n} \phi(x_i)\,\phi(x_i)^T$
- Find Eigenvectors/values: (v_j, λ_j) $\quad C v_j = \lambda_j v_j$

$$\frac{1}{n} \sum_{m=1}^{n} \phi(x_m)\,\phi(x_m)^T v_j = \lambda_j v_j$$

($\phi(x_m)^T v_j$: scalar $a_{j,m}$)

$$\lambda_j v_j = \frac{1}{n} \sum_{m=1}^{n} a_{j,m}\, \phi(x_m)$$

Thus v_j has the form:

$$v_j = \sum_i a_{j,i}\, \phi(x_i) \quad \text{for some coefficients } a_{j,i}$$
$$= \Phi a_j, \quad a_j = \begin{bmatrix} a_{j,1} \\ \vdots \\ a_{j,n} \end{bmatrix}$$

Substitute for v_j

$$\Rightarrow \frac{1}{n} \sum_m \phi(x_m)\,\phi(x_m)^T \Phi a_j = \lambda_j \Phi a_j$$

($\sum_m \phi(x_m)\,\phi(x_m)^T = \Phi\Phi^T$)

$$\Rightarrow \frac{1}{n} \Phi\Phi^T \Phi a_j = \lambda_j \Phi a_j$$

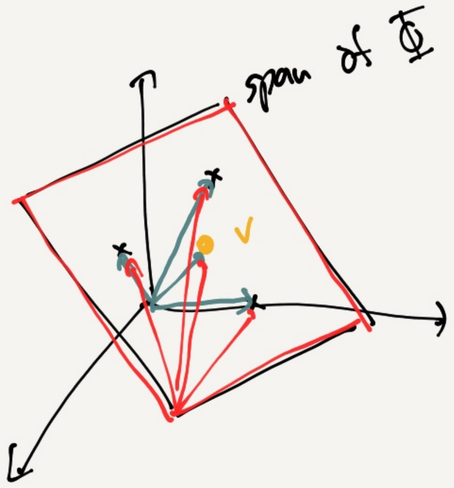
$$\frac{1}{n}\Phi\Phi^T\Phi a_j = \lambda_j \Phi a_j$$

eigenvector is a linear combo of $\phi(x_1) \dots \phi(x_n)$

Pre-multiply by Φ^T:

(equivalent set of equations by projecting onto the span of Φ)

$$\Rightarrow \frac{1}{n}\Phi^T\Phi\Phi^T\Phi a_j = \lambda_j \Phi^T\Phi a_j$$



Apply kernel trick

$$\frac{1}{n}KKa_j = \lambda_j K a_j$$

$$\Rightarrow KKa_j = n\lambda_j K a_j \quad (1)$$

Two possibilities:

1) K is invertible $\Rightarrow$ multiply by K^{-1}

$\Rightarrow$ Solve $Ka_j = n\lambda_j a_j$

2) K is not invertible $\Rightarrow$ the only difference is eigenvectors with $\lambda_j = 0 \Rightarrow$ do not affect the PCA solution.

$\Rightarrow$ Solve $Ka_j = n\lambda_j a_j$

Verification

Suppose (a_j, λ_j) are an eigenpair of K s.t.

✓ $Ka_j = n\lambda_j a_j$, $\lambda_j \neq 0$, $a_j^T a_j = 1$

Then looking at (1):

$$KKa_j = n\lambda_j Ka_j \quad \checkmark$$

($KKa_j = n\lambda_j a_j$, $n\lambda_j Ka_j = n\lambda_j n\lambda_j a_j$)

$$n\lambda_j Ka_j = n^2\lambda_j^2 a_j$$

($n\lambda_j Ka_j = n\lambda_j n\lambda_j a_j$)

$$n^2\lambda_j^2 a_j = n^2\lambda_j^2 a_j \quad \checkmark$$

PC v_j should be normalized

$$v_j^T v_j = 1$$

$$a_j^T \Phi^T \Phi a_j = 1$$

$$a_j^T K a_j = 1$$

($K a_j = n\lambda_j a_j$)

$$n\lambda_j a_j^T a_j = 1$$

$$\Rightarrow a_j \leftarrow \frac{1}{\sqrt{n\lambda_j}} a_j$$

Then $v_j^T v_j = 1$

Kernel Centering - How to center the data in the feature space $\phi(x)$?

Consider x_i, to center $\phi(x_i)$: (1 = vectors of ones)

$$\tilde{\phi}(x_i) = \phi(x_i) - \frac{1}{n}\sum_j \phi(x_j) = \phi(x_i) - \frac{1}{n}\Phi 1$$

Center all data:

$$\tilde{\Phi} = \Phi - \left[\frac{1}{n}\Phi 1\right] 1^T = \Phi\left(I - \frac{1}{n} 1 1^T\right)$$

Centered Kernel:

$$\tilde{K} = \tilde{\Phi}^T \tilde{\Phi} = \left(I - \frac{1}{n} 1 1\right)^T \Phi^T \Phi \left(I - \frac{1}{n} 1 1^T\right)$$

$$\boxed{\tilde{K} = \left(I - \frac{1}{n} 1 1\right)^T K \left(I - \frac{1}{n} 1 1^T\right)}$$

Summary KPCA (kernel PCA)

Given data X:

training:

1) calculate kernel matrix: $K = [k(x_i, x_j)]_{ij}$
2) center kernel: $\tilde{K} = (I - \frac{1}{n} 1 1^T) K (I - \frac{1}{n} 1 1^T)$
3) find the top D eigenvectors of $\tilde{K}$: $\tilde{K} a_j = \lambda_j a_j$
4) scale $a_j \leftarrow \frac{1}{\sqrt{\lambda_j}} a_j$

testing:

5) project x_*: $z_{*j} = \tilde{\phi}(x_*)^T \tilde{\Phi} a_j = \tilde{K}_*^T a_j$

$$\tilde{K}_* = K_* - \frac{1}{n} k_*^T 1 - \frac{1}{n} K 1 + \frac{1}{n^2} 1^T K 1$$

$$K_* = [k(x_*, x_i)]_i$$ ← kernel function btwn new point x_* & data X.

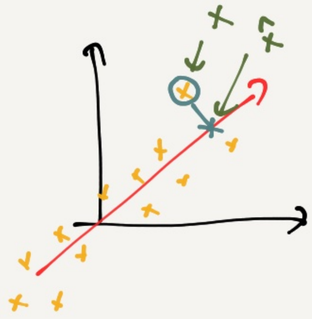
- Same properties of PCA in $\mathcal{H}$
  - the first D PC carry the most variance (in $\mathcal{H}$) minimize the reconstruction error (in $\mathcal{H}$)
  - PC are orthogonal (in $\mathcal{H}$)

Final: the original problem needs a d-dim eigenvector (d = # of features)
⇒ kernelized problem needs a N-dim eigenvector. (N = # of data)

- Kernel version of FLD ⇒ kernel discriminant analysis (10.15)

Pre-image Problem

Given PCA coefficients z, we can reconstruct $\hat{x}$.
(e.g. denoising)



given z,

$$\hat{x} = \sum_j v_j z_j = Vz$$

What about KPCA?

- given a z, what is the high-dim feature?

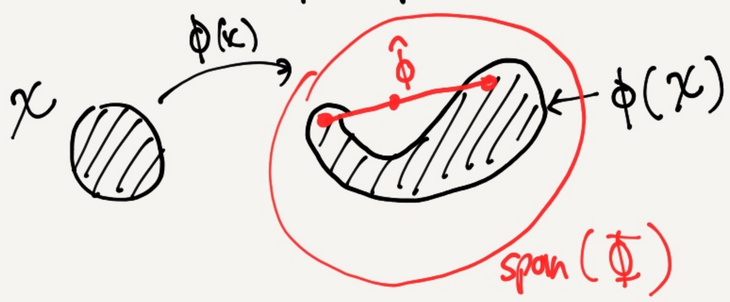
$$\hat{\phi} = \sum_j v_j z_j = \sum_j \Phi a_j z_j = \Phi\left(\sum_j a_j z_j\right)$$

$\hat{\phi}$ ← reconstruction

linear combo of $\phi(x_i)$'s

$\hat{\phi} \in \text{span}(\Phi)$

- But... not all points in $\text{span}(\Phi)$ have a corresponding x in the input space.



Example: let $\phi(x) = \begin{bmatrix} x^2 \\ x \end{bmatrix}$

$x_1 = 1 \Rightarrow \phi(x_1) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$x_2 = 2 \Rightarrow \phi(x_2) = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$

$\hat{\phi} = \phi(x_1) + \phi(x_2) = \begin{bmatrix} 5 \\ 3 \end{bmatrix}$

what is the $\hat{x}$ that gives $\hat{\phi}$?

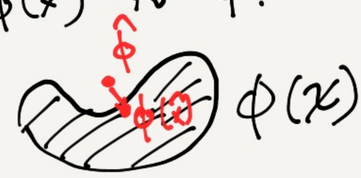
There is no $\phi(\hat{x}) = \hat{\phi}$

Approximate Pre-Image

- Consider the general problem:

$$\hat{\phi} = \Phi\alpha \quad \leftarrow \text{given vector}$$
$$= \sum_i \alpha_i \phi(x_i)$$

- Goal: find $\hat{x}$ that gives the closest $\phi(x)$ to $\hat{\phi}$.
  minimum norm reconstruction.



$$\hat{x} = \underset{x \in \mathcal{X}}{\text{argmin}} \; \| \phi(x) - \hat{\phi} \|^2 \qquad (\hat{\phi} = \Phi\alpha)$$

$$= \underset{x \in \mathcal{X}}{\text{argmin}} \; k(x,x) - 2\sum_i \alpha_i k(x, x_i) + \underbrace{\sum_i \sum_j \alpha_i \alpha_j k(x_i, x_j)}_{\text{constant wrt } x}$$

$$\boxed{\hat{x} = \underset{x \in \mathcal{X}}{\text{argmin}} \; k(x,x) - 2\sum_i \alpha_i k(x, x_i)}$$

Soln 1: (nearest neighbor): select $x \in X$ (dataset)

$$\hat{x} = \underset{j}{\text{argmin}} \; k(x_j, x_j) - 2k_j^T\alpha$$

where k_j = j^{th} column of kernel matrix K

Soln 2: solve the minimization directly w/ optimizer.

Soln 3: Suppose $k(x,x) = 1$, $k(x_i, x_j) \geq 0$ (e.g. Gaussian kernel)
and k is homogeneous, $k(\|x_i - x_j\|)$

$$\hat{x} = \underset{}{\text{argmin}} \; -\sum_i \alpha_i k(x_i, x) = \underset{}{\text{argmax}} \; \sum_i \alpha_i k(x_i, x)$$
$$= \underset{}{\text{argmax}} \; \left(\sum_i \alpha_i k(x_i, x)\right)^2$$

$\Rightarrow$ iterative algorithm:
(like mean-shift w/ weights α_i on each x_i)

$$\hat{x} \leftarrow \frac{\sum_i \alpha_i k'(\|x_i - \hat{x}\|^2)\, x_i}{\sum_i \alpha_i k'(\|x_i - \hat{x}\|^2)}$$