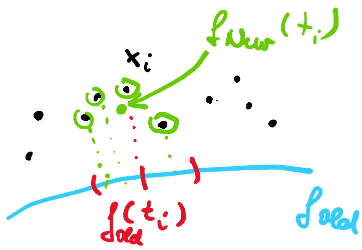
Minule: nPCA

→ 1.) Hl. krivky a plochy → stredom dát
→ projection - expectation algoritmus



• Hl. plochy: analogicky

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2.) Jadrová PCA (Kernel PCA, kPCA)

• priamka / rovina ... nestačí

⇒ (i) nelin. transformácia dát: do "ešte viac"-rozmerného priestoru

(ii) klasické PCA na transf. dátach

(i) transf. $\Phi: \mathbb{R}^k \to \mathbb{R}^p$, $\quad x_i \in \mathbb{R}^k \longmapsto \begin{pmatrix} \Phi_1(x_i) \\ \vdots \\ \Phi_p(x_i) \end{pmatrix} \in \mathbb{R}^p$

$(p >> k)$

(reálne: $p = \infty$)

(ii) S^*: výb. var. matica $\Phi(x_1), \dots, \Phi(x_n)$

$S^* = V \Lambda V^T$: spekt. rozklad

atď.

problém: $\underset{\uparrow \text{ veľká príliš}}{S : p \times p}$

predp.: Φ - centrované: $\sum_{i=1}^{n} \Phi(x_i) = 0_p$

$$\Rightarrow \underset{p \times p}{S^*} = \frac{1}{n} \sum_{i=1}^{n} \Phi(x_i) \cdot \Phi(x_i)^T = \frac{1}{n} \underset{p \times n}{\begin{bmatrix} | & & | \\ \Phi(x_1) & \dots & \Phi(x_n) \\ | & & | \end{bmatrix}} \underbrace{\begin{bmatrix} - \Phi(x_1)^T - \\ \vdots \\ - \Phi(x_n)^T - \end{bmatrix}}_{n \times p}$$

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

$\Phi \in \mathbb{R}^{n \times p}$: matica transf. dát

jadrový trik: $A^T A$ má nenulové kladné vl. hodnoty ako $A A^T$

⇒ vl. hodnoty (a vektory) S^* môžem získať z $\underbrace{\underset{n \times p}{\Phi}\,\underset{p \times n}{\Phi^T}}_{n \times n}$: "iba" $n \times n$

$$K := \Phi \Phi^T = \begin{bmatrix} \Phi(x_1)^T \\ \vdots \\ \Phi(x_n)^T \end{bmatrix} \begin{bmatrix} \Phi(x_1) & \dots & \Phi(x_n) \end{bmatrix} =$$

$$= \begin{bmatrix} \Phi(x_1)^T\Phi(x_1) & \Phi(x_1)^T\Phi(x_2) & \dots & \Phi(x_1)^T\Phi(x_n) \\ \vdots & \vdots & & \vdots \\ \Phi(x_n)^T\Phi(x_1) & \Phi(x_n)^T\Phi(x_2) & \dots & \Phi(x_n)^T\Phi(x_n) \end{bmatrix}_{n\times n}$$

– jadro (kernel)

– mat. skal. súčinov (Gramova matica)

$$K_{ij} = \langle \Phi(x_i), \Phi(x_j) \rangle$$

$\Rightarrow$ stačia skal. súčiny ! : netreba $\Phi(\ )$

$\Rightarrow$ iný pohľad : namiesto $\langle x_i, x_j \rangle = x_i^T x_j$

pracujeme s inými : $\langle \Phi(x_i), \Phi(x_j) \rangle$

Napr. jadrá :

- gaussovské (radial basis function kernel) : $K_{ij} = e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}}$
- laplaceovské : $K_{ij} = e^{-\frac{\|x_i - x_j\|}{\sigma}}$
- sigmoid : $K_{ij} = \tanh(a\langle x_i, x_j\rangle + b)$

  ↳ hyperbolický tangens : $\tanh(z) = \dfrac{e^z - e^{-z}}{e^z + e^{-z}}$

Sklo : gaussovské : $K_{ij} = e^{-\sigma_R \|x_i - x_j\|^2} \Rightarrow \sigma_R = \dfrac{1}{2\sigma^2_{\text{naša}}}$

Tech. detaily : $S^* = V \Lambda V^T \leftarrow$?

$\rightarrow$ vl. h. $\boxed{\lambda_1, \dots, \lambda_r}, 0, \dots, 0$

$\rightarrow$ vl. vekt. $\boxed{v_1, \dots, v_r}, v_{r+1}, \dots, v_p$ – ortonormálne

↳ odteraz iba tieto

↳ špec. : $\|v_j\| = 1$

$r = \text{rank}(S^*)$

$$S^* = \frac{1}{n}\Phi^T\Phi$$

- $\Phi^T\Phi = nS^*$: vl. h. $n\lambda_j =: \tilde{\lambda}_j$ (1)

  : vl. vekt. v_j

- $\Phi\Phi^T =: K$: vl. h. $\tilde{\lambda}_j$ $\Rightarrow K = \underset{n\times r}{B}\ \underset{r\times r}{\tilde{\Lambda}}\ \underset{r\times n}{B^T}$

  : vl. vekt. b_j

  ↳ ortonorm. $\Rightarrow \|b_j\| = 1$

platí : $\tilde{v}_j = \Phi^T b_j$: vl. vektor $\Phi^T\Phi$

↳ overme : $\Phi^T\Phi\,\tilde{v}_j = \Phi^T\Phi\,\Phi^T \dots$

platí: $v_j = \Phi b_j$: vl. vektor $\Phi'\Phi$

↳ overenie: $\Phi^T\Phi \cdot \tilde{v}_j = \underline{\Phi^T} \underbrace{\underbrace{\Phi \Phi^T}_{K} b_j}_{\tilde{\lambda}_j b_j} = \tilde{\lambda}_j \underbrace{\Phi^T b_j}_{v_j} = \tilde{\lambda}_j \tilde{v}_j$ ✓

chceme: $\|v_j\| = 1$

$$\|\tilde{v}_j\|^2 = \|\Phi^T b_j\|^2 = b_j^T \underbrace{\underbrace{\Phi \Phi^T}_{K} b_j}_{\tilde{\lambda}_j b_j} = \tilde{\lambda}_j \underbrace{b_j^T b_j}_{\|b_j\|^2 = 1} = \tilde{\lambda}_j \quad \Rightarrow v_j = \frac{1}{\sqrt{\tilde{\lambda}_j}} \tilde{v}_j = \frac{1}{\sqrt{\tilde{\lambda}_j}} \Phi^T b_j \quad (2)$$

(1) $\Rightarrow$ $\boxed{\Lambda = \frac{1}{n} \tilde{\Lambda}}$ (1^*)

(2) $\Rightarrow$ $\boxed{V} = \left[v_1 \dots v_r \right] = \left[\frac{1}{\tilde{\lambda}_1^{1/2}} \Phi^T b_1, \dots, \frac{1}{\tilde{\lambda}_r^{1/2}} \Phi^T b_r \right] = \boxed{\Phi^T B \tilde{\Lambda}^{-1/2}}$ (2^*)

$\Rightarrow$ stačí spekt. rozklad K, (1^*), (2^*) $\to$ získame spekt. rozklad S^*

<u>skóre</u>: súradnice $\Phi(x_1), \dots, \Phi(x_n)$ vzhľadom na $v_1, \dots, v_r$

$$\Phi(x_i) = V y_i \quad / \cdot V^T \quad \to y_i \in \mathbb{R}^r, \quad i = 1, \dots, n$$

$$V^T \Phi(x_i) = y_i \quad \forall i$$

$$\underbrace{[y_1, \dots, y_n]}_{Y^T} = [V^T\Phi(x_1), \dots, V^T\Phi(x_n)] = V^T \Phi^T$$

$$Y^T = V^T \Phi^T \quad /^T$$

$$\underset{n \times r}{Y} = \Phi V \overset{(2)}{=} \underbrace{\Phi \Phi^T}_{K} B \tilde{\Lambda}^{-1/2} = \underbrace{K B}_{} \tilde{\Lambda}^{-1/2} = B \tilde{\Lambda} \tilde{\Lambda}^{-1/2} = B \tilde{\Lambda}^{1/2}$$

↑ matica skóre

$= B\tilde{\Lambda}$, lebo b_j sú vl. vektory K-čka

$K = B \tilde{\Lambda} B^T \quad / \cdot B_p$

$KB = B\tilde{\Lambda}$

$\Rightarrow$ $\boxed{Y = B \tilde{\Lambda}^{1/2}}$

: aj skóre priamo z K

<u>Pozn.</u>:

- môžeme mať necentrované Φ, potom centrujeme K: $\tilde{K} = (I_n - \frac{1}{n} J_n) K (I_n - \frac{1}{n} J_n)$

  ↑ mat. jednotiek

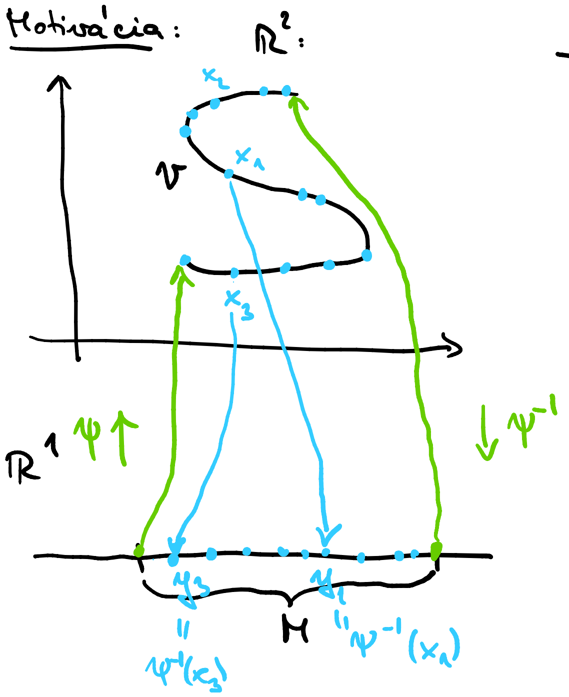
- jadrová PCA: podobná metrickému MS - transformujeme dáta

<u>Pr.</u>:
$$K_{ij} = e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}} = e^{-\frac{D_{ij}^2}{2\sigma^2}}$$

RBF: $K_{ij} = e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}} = e^{-\frac{D_{ij}^2}{2\sigma^2}}$

Isomap (isometric feature mapping - izometrické mapovanie)

Motivácia: $\mathbb{R}^2$:



- vnorenie menejrozmernej štruktúry v $\mathbb{R}^\ell$ (embedding) (krivka v $\mathbb{R}^2$)

varieta (manifold) $\mathcal{V}$: priestor, ktorý sa lokálne podobá na euklidovský, ale môže byť zakrivený

- krivka, kružnica, sféra, ...

$\mathcal{V} \subseteq \mathbb{R}^\ell$, q-rozmerná (krivka $\subseteq \mathbb{R}^2$, 1-rozm.)

$\mathcal{V} = \Psi(M)$ pre $M \subseteq \mathbb{R}^q$

$\Psi: \mathbb{R}^q \to \mathbb{R}^\ell$

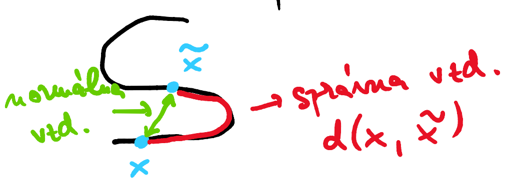
opačné zobr.: $\Psi^{-1}: \mathbb{R}^\ell \to \mathbb{R}^q$

$M = \Psi^{-1}(\mathcal{V})$

- máme $x_1, \dots, x_n \in \mathcal{V} \subseteq \mathbb{R}^\ell$

hľadáme $\underbrace{y_1, \dots, y_n}_{\text{menejrozmerná reprezentácia}} \in M \subseteq \mathbb{R}^q$ a $\mathcal{V}$, kde $y_1 = \Psi^{-1}(x_1)$, ..., $y_n = \Psi^{-1}(x_n)$

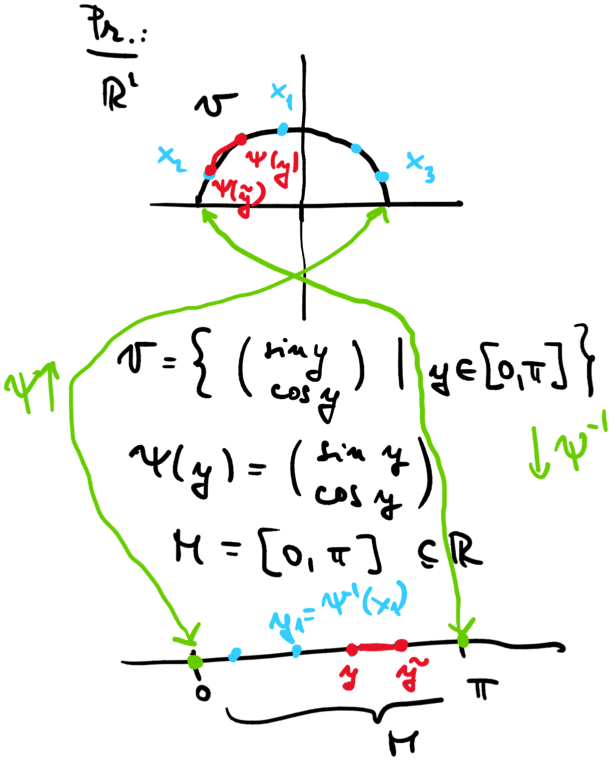
Myšlienka: "správne" vyjadriť vzdialenosti medzi x-kami a potom aplikovať KMŠ



- $d(x, \tilde{x})$ = dĺžka najkratšej krivky vo $\mathcal{V}$, ktorá spája x a $\tilde{x}$

predp.: Ψ je izometrické: $\forall y, \tilde{y} \in M$:

Pr.: $\mathbb{R}^1$



$\mathcal{V} = \left\{ \begin{pmatrix} \sin y \\ \cos y \end{pmatrix} \;\middle|\; y \in [0, \pi] \right\}$

$\Psi(y) = \begin{pmatrix} \sin y \\ \cos y \end{pmatrix}$

$M = [0, \pi] \subseteq \mathbb{R}$

$\Psi^{-1}(x) = \arcsin(x_1)$, $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

$\Psi^{-1}(x) = \arcsin(x_1)$, $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

predp.: Ψ je <u>izometrické</u>: $\forall y, \tilde{y} \in M$:

$$\| y - \tilde{y} \| = \| \Psi(y) - \Psi(\tilde{y}) \|$$

$\Downarrow$

<u>iso</u> map

$$\Psi(y) = \begin{pmatrix} \sin y \\ \cos y \end{pmatrix} \quad \text{pre } [0, \pi]$$

$$\text{nie} \quad \Psi(y) = \begin{pmatrix} \sin(2y) \\ \cos(2y) \end{pmatrix} \quad \text{pre } y \in \underbrace{[0, \pi/2]}_{M}$$