- Д-во PCA

Пусть $m \le n$

$$\underset{m\times n}{M} = \underset{m\times m}{U}\,\underset{m\times n}{\Sigma}\,\underset{n\times n}{V^T} = \sum_{i=1}^{r} \sigma_i \underset{m\times 1}{u_i}\,\underset{1\times n}{v_i^T}$$

v_i – столбцы V

v_i^T – строки V^T

$$(U\Sigma)V = \underset{m}{\left[\begin{array}{c|c|c|c} \sigma_1 u_1 & \ldots & \sigma_r u_r & \underset{n-r}{0} \end{array}\right]} \times \underset{n}{\underbrace{\left[\begin{array}{c} v_1^T \\ \hline \vdots \\ \hline v_n^T \end{array}\right]}_{V}} =$$

- PLS

$$\underset{n\times m}{X} = \underset{n\times l}{T}\,\underset{l\times m}{P^T} + \underset{n\times m}{E}$$

$$\underset{n\times p}{Y} = \underset{n\times l}{U}\,\underset{l\times p}{Q^T} + \underset{n\times p}{F}$$

Let's suppose that Y is a vector ($p=1$)

$X^0 = X$

$w^0 = \frac{X^T y}{\|X^T y\|}$

for k in range$(0, l)$:

  $t^k = X^k w^k$

  $t_k = t^{kT} t^k$ - scalar

  $t^k /= t_k$

  $p^k = X^{kT} t^k$

  $q_k = y^T t^k$ - scalar

  if $q_k == 0$:

    $l = k$

    break

  if $k < l-1$:

    $X^{(k+1)} = X^k - t_k t^k p^{kT}$

    $w^{k+1} = X^{(k+1)T} y$

$W = \left[\begin{array}{c|c|c} w^0 & \ldots & w^{l-1} \end{array}\right]$, $P = \ldots$, $q = \ldots$

$B = W(P^T W)^{-1} q$

$B_0 = q_0 - P^{0T} B$

return B, B_0

- Canonical Correlation Analysis

$X = (x_1, \ldots, x_n)^T$, $Y = (y_1, \ldots, y_m)^T$, $\underset{n\times m}{\Sigma_{xy}} = cov(X, Y)$

$$(a', b') = \underset{a\in\mathbb{R}^n,\, b\in\mathbb{R}^m}{\arg\max}\ corr\,(\underbrace{a^T X}, \underbrace{b^T Y})$$

1st pair of canonical variables

Затем ищутся в-ры, максимиз. ту же корреляцию, но с ограничением, что они не должны быть коррел. с 1ой парой канонич. перем.

$$\rho = \frac{a^T \Sigma_{xy} b}{\sqrt{a^T \Sigma_{xx} a}\sqrt{b^T \Sigma_{yy} b}} = \frac{\overbrace{c^T \Sigma_{xx}^{-1/2} \Sigma_{xy} \Sigma_{yy}^{-1/2}}^{\delta^T} d}{\sqrt{c^T c}\,\sqrt{d^T d}}$$

$c := \sqrt{\Sigma_{xx}}\, a$, $d := \sqrt{\Sigma_{yy}}\, b$

По КБШ ЧИСЛ-ЛЬ $\le \sqrt{\delta^T \delta} \cdot \sqrt{d^T d}$

Итого, $\rho \le \frac{\sqrt{\delta^T\delta}}{\sqrt{c^T c}} = \frac{(c^T \Sigma_{xx}^{-1/2} \Sigma_{xy} \Sigma_{yy}^{-1} \Sigma_{yx} \Sigma_{xx}^{-1/2} c)^{1/2}}{(c^T c)^{1/2}}$

max corr $\Leftrightarrow$ $\underline{c \text{ is an eigenvector of } \Sigma_{xx}^{-1/2} \Sigma_{xy} \Sigma_{yy}^{-1} \Sigma_{yx} \Sigma_{xx}^{-1/2}}$

Последующие пары – собств. в-ры, убывающие по величине

Solution: •, d is proportional to $\Sigma_{yy}^{-1/2} \Sigma_{yx} \Sigma_{xx}^{-1/2} c$

<u>ВКЗ</u> a is an eigenvector of $\Sigma_{xx}^{-1} \Sigma_{xy} \Sigma_{yy}^{-1} \Sigma_{yx}$

b is proportional to $\Sigma_{yy}^{-1} \Sigma_{yx} a$

$Nc = \lambda c$

$NMa = \lambda Ma$

$M^{-1}NMa = \lambda a$

Canonical Variables are defined by: $U = c' \Sigma_{xx}^{-1/2} X = a' X$

$V = d' \Sigma_{yy}^{-1/2} Y = b' Y$

PLS Canonical:

$X \in \mathbb{R}^{n\times d}$, $Y \in \mathbb{R}^{n\times t}$, K - number of components

$X_1 := X$, $Y_1 := Y$

for k in $1, \ldots, K$:

a) compute $u_k \in \mathbb{R}^d$, $v_k \in \mathbb{R}^t$ - left and right singular vectors of $\underset{\in d\times t}{C_k} = X_k^T Y_k = U_k \Sigma_k V_k^T$

"weights" $cov(X_k u_k, Y_k v_k)$ is a maximum

$C_k v_k = \sigma_1 u_k$

1ая строка V_k^T 1ый столбец U_k

b) $\xi_k := X_k u_k \in \mathbb{R}^n$, $w_k = Y_k v_k \in \mathbb{R}^n$ "scores"

c) Find $\gamma_k \in \mathbb{R}^d$ such that $\|X_k - \xi_k \gamma_k^T\| \to \min$ $\|$ $\gamma_k^T = (\xi_k^T \xi)^{-1} \xi_k^T X_k$

"loadings"

Find $\delta_k \in \mathbb{R}^d$ such that $\|Y_k - w_k \delta_k^T\| \to \min$

d) $X_{k+1} := X_k - \xi_k \gamma_k^T$

$Y_{k+1} := Y_k - w_k \delta_k^T$

$\xi \to T$

$X = TP^T$ $\Gamma^T \to P^T$

$Y = UQ^T$ $\Omega \to U$

$\Delta^T \to Q^T$

$$X \approx \underbrace{\xi_1 \gamma_1^T + \ldots + \xi_k \gamma_k^T}_{\hat{X}} = \underset{\mathbb{R}^{n\times K}}{\Xi}\,\underset{\mathbb{R}^{K\times d}}{\Gamma^T} = \left[\begin{array}{c|c|c} \xi_1 & \ldots & \xi_k \end{array}\right] \times \left[\begin{array}{c} \gamma_1^T \\ \hline \vdots \\ \hline \gamma_k^T \end{array}\right]$$

$$Y \approx \underbrace{w_1 \delta_1^T + \ldots + w_k \delta_k^T}_{\hat{Y}} = \underset{\mathbb{R}^{n\times k}}{\Omega}\,\underset{\mathbb{R}^{k\times d}}{\Delta^T} = \left[\begin{array}{c|c|c} w_1 & \ldots & w_k \end{array}\right] \times \left[\begin{array}{c} \delta_1^T \\ \hline \vdots \\ \hline \delta_k^T \end{array}\right]$$

What is a P that $\Xi = XP$?

We know that $X = \Xi \Gamma^T$

$\underset{\mathbb{R}^{d\times K}}{P} := U(\Gamma^T U)^{-1}$, where $U = \left[\begin{array}{c|c|c} u_1 & \ldots & u_k \end{array}\right] \in \mathbb{R}^{d\times K}$

$XP = XU(\Gamma^T U)^{-1} = \Xi(\Gamma^T U)(\Gamma^T U)^{-1} = \Xi$

Similarly, $\Omega = Y \cdot V(\Delta^T V)^{-1} \in \mathbb{R}^{t\times K}$

$A(P^T A)^{-1}$

$XA(P^T A)^{-1} =$

$= (TP^T A + EA)(P^T A)^{-1} =$

$\approx T$

$B(Q^T B)^{-1}$.

Centered

$\underset{n\times d}{X}$ $\underset{n\times t}{Y}$

$\frac{1}{n}\underset{d\times t}{X^T Y} = cov(X, Y)$

$\underset{n\times K}{\Xi}$ $\underset{n\times K}{\Omega}$

Откуда брать в-р?

$cov(Xu, Yv)$

Power method.

<u>Assumptions</u>: 1) A has an eigenvalue that is strictly greater than others

2) Let's denote v_1 as an eigenvector of A

Then $\langle v_1, b_0 \rangle \ne 0$

$$b_{k+1} = \frac{A b_k}{\|A b_k\|}$$

<u>The importance of assumptions</u>: $b_k = e^{i\varphi_k} v_1 + r_k$

$$\mu_k = \frac{b_k^T A b_k}{b_k^T b_k} \longrightarrow \lambda_1$$

$c_{k+1} = Ac_k - \langle v_1, c_k \rangle c_k$

$c_{k+1} /= \|c_{k+1}\|$