正则广义典型相关分析

RGCCA

REGULARIZED GENERALIZED CANONICAL CORRELATION ANALYSIS

正则广义典型相关分析 RGCCA

- 用于解决什么样的问题：

如何关联在同组个体上观测得到的多个变量块。

例：

研究个体生理与心理差异, 需要详细研究有关的变量的集合间的关系. 例如,针对同一个人可以比较其心理测试分数与其身体测量结果. 问题在于, 如何确定这些数据显示出的存在于生理与心理的独立关系的数量和性质, 以及如何从系统中的相关的多样性中提取出这些独立关系的合适特征.

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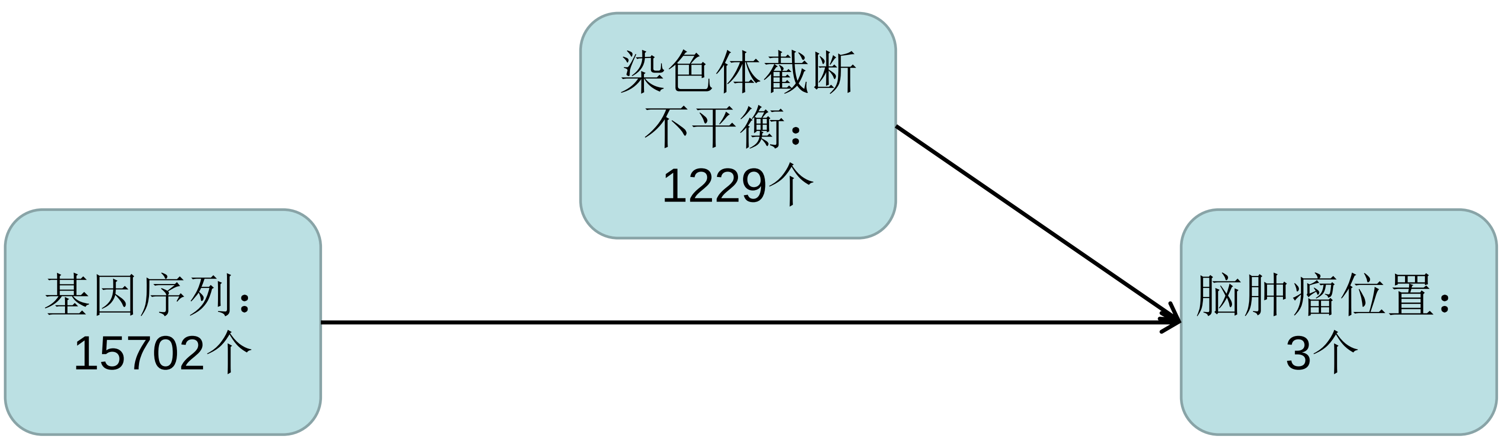
- RGCCA是在同组个体上观测得到的多个变量块的线性关系建模的框架：

考虑块间连接的网络，RGCCA寻找块变量的线性组合使得：

1. 块组件良好的解释自己的块；
2. 假设中相连的块的块组件高度相关。



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依次介绍：

- 总体广义标准相关分析的定义；总体水平上驻定方程组的构造；搜寻总体驻定方程组的解；总体GCCA的PLS算法的构造；收敛性质；

（下一次）

- 块协方差矩阵的收缩估计；样本水平上静态方程的构造；搜寻样本水平上驻定方程组的解；
- SGCCA的定义、算法、收敛性质
- 从CCA到SGCCA的发展历程

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准备工作：

记J为定义在同一总体的p_j维0均值列随机向量$x_j = (x_{j1}, x_{j2}, \dots, x_{jp_j})^T$,以及$p_j$维非随机列向量$\alpha_j = (\alpha_{j1}, \alpha_{j2}, \dots, \alpha_{jp_j})^T$.通过定义矩阵$C = \{c_{jk}\}$来描述随机向量间连接形成的网络: 当$x_j$与$x_k$相连时$c_{jk} = 1$否则为0.

考虑两个线性组件$\eta_j = \sum_h \alpha_{jh} x_{jh} = \alpha_j^T x_j$,$\eta_k = \sum_h \alpha_{kh} x_{kh} = \alpha_k^T x_k$, 两个随机变量$\eta_j$与$\eta_k$的相关系数为:

$$\rho(\alpha_j^T x_j, \alpha_k^T x_k) = \frac{\alpha_j^T \Sigma_{jk} \alpha_k}{(\alpha_j^T \Sigma_{jj} \alpha_j)^{\frac{1}{2}} (\alpha_k^T \Sigma_{kk} \alpha_k)^{\frac{1}{2}}}$$

其中$\Sigma_{jj} = \boldsymbol{E}(x_j^T x_j)$,$\Sigma_{kk} = \boldsymbol{E}(x_k^T x_k)$,$\Sigma_{jk} = \boldsymbol{E}(x_j^T x_k)$且假设$\Sigma_{jj}, \Sigma_{kk}, \Sigma_{jk}$满秩.

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- 定义：总体广义标准相关分析

$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1,j\neq k}^{J} c_{jk}\, g\big(\rho(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k)\big) \tag{2}$$

subject to the constraints $\operatorname{Var}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j) = 1, \quad j = 1, \ldots, J,$

由于记 $\Sigma_{jj} = E(x_j^T x_j), \Sigma_{kk} = E(x_k^T x_k), \Sigma_{jk} = E(x_j^T x_k),$
且假设 x_j 是均值为0的列随机向量，$j = 1, \ldots, J$
故 $Var(a_j^T x_j) = a_j^T \Sigma_{jj} a_j$ ，且

$$\rho(\alpha_j^T x_j, \alpha_k^T x_k) = \frac{Cov(\alpha_j^T x_j, \alpha_k^T x_k)}{\sqrt{Var(\alpha_j^T x_j) Var(\alpha_k^T x_k)}}$$

$$= \alpha_j^T E(x_j^T x_k)\alpha_k$$

$$= \alpha_j^T \Sigma_{jk}\alpha_k$$

$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1,j\neq k} c_{jk}\, g\big(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\big) \tag{3}$$

subject to the constraints $\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J.$

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$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1, j\neq k}^{J} c_{jk}\, g\left(\rho\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right) \quad (2)$$

$$\text{subject to the constraints} \quad \text{Var}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j) = 1, \quad j = 1, \ldots, J,$$

- 定义：总体广义标准相关分析

$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1, j\neq k}^{J} c_{jk}\, g\left(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\right) \quad (3)$$

$$\text{subject to the constraints} \quad \boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J.$$

其中 $g(x) = x$ 或 $g(x) = x^2$ 或 $g(x) = |x|$

Horst scheme

factorial scheme

centroid scheme

最为常见

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$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1, j\neq k}^{J} c_{jk}\, g\big(\rho(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k)\big) \tag{2}$$

subject to the constraints $\mathrm{Var}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j) = 1, \quad j = 1, \ldots, J,$

- 定义：总体广义标准相关分析

$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1, j\neq k}^{J} c_{jk}\, g\big(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\big) \tag{3}$$

subject to the constraints $\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J.$

考虑（3）的拉格朗日函数：

$$F(\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_J, \lambda_1, \ldots, \lambda_J) = \sum_{j,k=1, j\neq k}^{J} c_{jk}\, g\big(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\big) - \varphi \sum_{j=1}^{J} \frac{\lambda_j}{2}\big(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j - 1\big), \tag{4}$$

$\varphi = 1$ → Horst scheme → $g(x) = x$

$\varphi = 2$ → factorial scheme → $g(x) = x^2$

$\varphi = 1$ → centroid scheme → $g(x) = |x|$

假设：$\alpha_j^T \Sigma_{jk} \alpha_k \neq 0$

否则可定义：$c_{jk} = 0$

因此若：$g(x) = |x|$

可将g'视为其导数。

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$$\underset{\alpha_1,\ldots,\alpha_J}{\text{Maximize}} \sum_{j,k=1,j\neq k}^{J} c_{jk}\, g(\rho(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k)) \quad (2)$$

$$\text{subject to the constraints} \quad \text{Var}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j) = 1, \quad j = 1, \ldots, J,$$

- 定义：总体广义标准相关分析

$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1,j\neq k}^{J} c_{jk}\, g\left(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\right) \quad (3)$$

$$\text{subject to the constraints} \quad \boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J.$$

考虑（3）的拉格朗日函数：

$$F(\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_J, \lambda_1, \ldots, \lambda_J) = \sum_{j,k=1,j\neq k}^{J} c_{jk}\, g\left(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\right) - \varphi \sum_{j=1}^{J} \frac{\lambda_j}{2}\left(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j - 1\right), \quad (4)$$

$$\frac{\partial F}{\partial \alpha_j} = \sum_{k=1,k\neq j}^{J} c_{jk}\, g'(\alpha_j^T \Sigma_{jk} \alpha_k) \Sigma_{jk} \alpha_k - \varphi \lambda_j \Sigma_{jj} \alpha_j \quad , \quad j = 1, \ldots, J$$

$$\frac{\partial F}{\partial \lambda_j} = \frac{\varphi}{2}(\alpha_j^T \Sigma_{jj} \alpha_j - 1) \quad , \quad j = 1, \ldots, J$$

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$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1,j\neq k}^{J} c_{jk} g(\rho(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k)) \qquad (2)$$

$$\text{subject to the constraints} \quad \text{Var}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j) = 1, \quad j = 1, \ldots, J,$$

- 定义：总体广义标准相关分析

$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1,j\neq k}^{J} c_{jk} g(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k) \qquad (3)$$

$$\text{subject to the constraints} \quad \boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J.$$

$$\frac{\partial F}{\partial \alpha_j} = \sum_{k=1,k\neq j}^{J} c_{jk} g'(\alpha_j^T \Sigma_{jk} \alpha_k) \Sigma_{jk} \alpha_k - \varphi \lambda_j \Sigma_{jj} \alpha_j \quad , \quad j = 1, \ldots, J$$

$$\frac{\partial F}{\partial \lambda_j} = \frac{\varphi}{2}(\alpha_j^T \Sigma_{jj} \alpha_j - 1) \quad , \quad j = 1, \ldots, J$$

令上式全部为0： $$\frac{1}{\varphi} \boldsymbol{\Sigma}_{jj}^{-1} \sum_{k=1,k\neq j}^{J} c_{jk} g'(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k) \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k = \lambda_j \boldsymbol{\alpha}_j, \quad j = 1, \ldots, J \qquad (5)$$

且： $$\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J. \qquad (6)$$

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$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1,j\neq k}^{J} c_{jk} g(\rho(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k)) \tag{2}$$

$$\text{subject to the constraints} \quad \mathrm{Var}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j) = 1, \quad j = 1, \ldots, J,$$

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$$\underset{\boldsymbol{\alpha}_1,\ldots,\boldsymbol{\alpha}_J}{\text{Maximize}} \sum_{j,k=1,j\neq k}^{J} c_{jk} g\left(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\right) \tag{3}$$

$$\text{subject to the constraints} \quad \boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J.$$

$$\begin{cases} \dfrac{1}{\varphi} \boldsymbol{\Sigma}_{jj}^{-1} \displaystyle\sum_{k=1,k\neq j}^{J} c_{jk} g'\left(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k\right) \boldsymbol{\Sigma}_{jk} \boldsymbol{\alpha}_k = \lambda_j \boldsymbol{\alpha}_j, \quad j = 1, \ldots, J & (5) \\ \boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J. & (6) \end{cases}$$

该方程组没有解析解。

但可以用于构造（3）的一个单调收敛算法（即将介绍）

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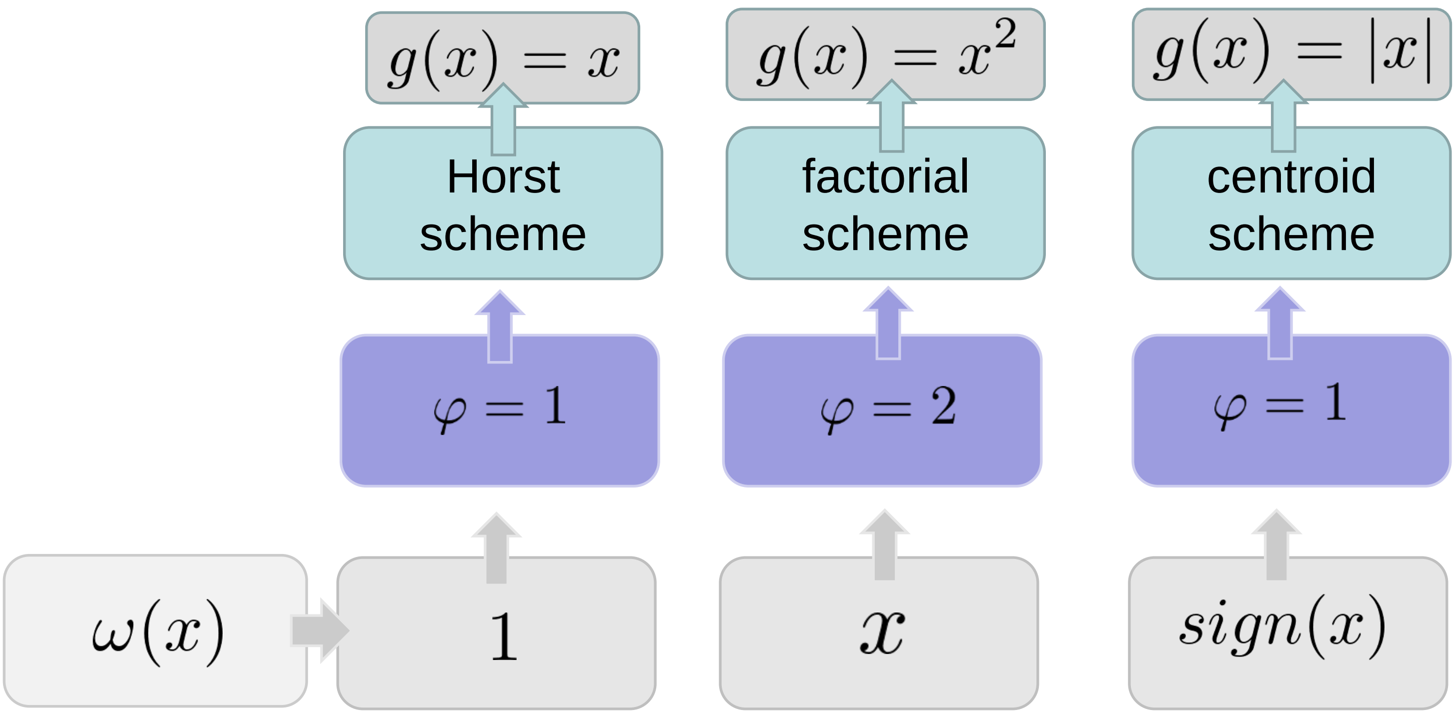
介绍算法前的准备工作：

用 $Cov(\alpha_j^T x_j, \alpha_k^T x_k)$ 而不用 $\alpha_j^T \Sigma_{jk} \alpha_k$ 便于数学处理。

记 $\omega(x) = \frac{1}{\varphi} g'(x)$ (提高下述可读性)



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介绍算法前的准备工作：由于算法借鉴了PLS（偏最小二乘路径模型），下面援引该模型中的部分术语。

外权向量：α_j
(a vector of outer weights)

外部组件：$\eta_j = \alpha_j^T x_j$
(an outer component)

内部组件：
(an inner component)

$$\nu_j = \sum_{k=1, k\neq j}^{J} c_{jk} w\big(\mathrm{Cov}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k)\big)\boldsymbol{\alpha}_k^t \boldsymbol{x}_k. \tag{7}$$

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内部组件：
(an inner component)

$$\nu_j = \sum_{k=1,k\neq j}^{J} c_{jk} w\big(\mathrm{Cov}(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k)\big)\boldsymbol{\alpha}_k^t \boldsymbol{x}_k. \qquad (7)$$

Horst $g(x) = x$ $\quad \nu_j = \sum_{k=1,k\neq j}^{J} c_{jk}\alpha_k^T x_k$

Factorial $g(x) = x^2$ $\quad \nu_j = \sum_{k=1,k\neq j}^{J} c_{jk} Cov(\alpha_j^T x_j, \alpha_k^T x_k)\alpha_k^T x_k$

Centroid $g(x) = |x|$ $\quad \nu_j = \sum_{k=1,k\neq j}^{J} c_{jk} sign(Cov(\alpha_j^T x_j, \alpha_k^T x_k))\alpha_k^T x_k$

下面利用内部组件简化静态方程组(5)

$$\begin{cases} \dfrac{1}{\varphi}\boldsymbol{\Sigma}_{jj}^{-1} \displaystyle\sum_{k=1,k\neq j}^{J} c_{jk} g'\big(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k\big)\boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k = \lambda_j \boldsymbol{\alpha}_j, \quad j = 1, \ldots, J & (5) \\ \boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj}\boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J. & (6) \end{cases}$$

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内部组件：
(an inner component)

$$\nu_j = \sum_{k=1,k\neq j}^{J} c_{jk} w\left(\mathrm{Cov}\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right)\boldsymbol{\alpha}_k^t \boldsymbol{x}_k. \tag{7}$$

下面利用内部组件简化静态方程组(5)
利用下述表达式：

$$\begin{aligned}\mathrm{Cov}(\boldsymbol{x}_j, \nu_j) = E(\boldsymbol{x}_j \nu_j) &= E\left(\boldsymbol{x}_j \sum_{k=1,k\neq j}^{J} c_{jk} w\left(\mathrm{Cov}\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right)\boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right) \\ &= \sum_{k=1,k\neq j}^{J} c_{jk} w\left(\mathrm{Cov}\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right)\boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k \\ &= \frac{1}{\varphi} \sum_{k=1,k\neq j}^{J} c_{jk} g'\left(\mathrm{Cov}\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right)\boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k \end{aligned} \tag{8}$$

以及约束(6)：

$$\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J. \tag{6}$$

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利用下述表达式：

$$\mathrm{Cov}(\boldsymbol{x}_j, \nu_j) = E(\boldsymbol{x}_j \nu_j) = E\left(\boldsymbol{x}_j \sum_{k=1,k\neq j}^{J} c_{jk} w\left(\mathrm{Cov}\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right)\boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)$$

$$= \sum_{k=1,k\neq j}^{J} c_{jk} w\left(\mathrm{Cov}\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right)\boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k$$

$$= \frac{1}{\varphi} \sum_{k=1,k\neq j}^{J} c_{jk} g'\left(\mathrm{Cov}\left(\boldsymbol{\alpha}_j^t \boldsymbol{x}_j, \boldsymbol{\alpha}_k^t \boldsymbol{x}_k\right)\right)\boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k \tag{8}$$

以及约束(6)：

$$\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jj} \boldsymbol{\alpha}_j = 1, \quad j = 1, \ldots, J. \tag{6}$$

$$\frac{1}{\varphi}\boldsymbol{\Sigma}_{jj}^{-1} \sum_{k=1,k\neq j}^{J} c_{jk} g'\left(\boldsymbol{\alpha}_j^t \boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k\right)\boldsymbol{\Sigma}_{jk}\boldsymbol{\alpha}_k = \lambda_j \boldsymbol{\alpha}_j, \quad j = 1, \ldots, J \tag{5}$$

$$\Sigma_{jj}^{-1} Cov(x_j, \nu_j) = \lambda_j \alpha_j, \quad j = 1 \ldots, J \text{且}\ \alpha_j^T \Sigma_{jj} \alpha_j = 1, \quad j = 1, \ldots, J$$

$$\lambda_j^2 = (Cov(x_j, \nu_j))^T \Sigma_{jj}^{-1} Cov(x_j, \nu_j)$$

$$\boldsymbol{\alpha}_j = \left[\mathrm{Cov}(\boldsymbol{x}_j, \nu_j)^t \boldsymbol{\Sigma}_{jj}^{-1} \mathrm{Cov}(\boldsymbol{x}_j, \nu_j)\right]^{-1/2} \boldsymbol{\Sigma}_{jj}^{-1} \mathrm{Cov}(\boldsymbol{x}_j, \nu_j), \quad j = 1, \ldots, J. \tag{9}$$

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算法如右图所示：
该算法的基本特征：
每次替换都是最优的，
且顺序的。
即：在替换 α_{j+1}^{s}
前必有 $\alpha_j^s \rightarrow \alpha_j^{s+1}$

（类似用于求解线性方程组的Guass-Seide迭代算法）
这个顺序的方法诱导出该算法的单调收敛性。

下面的命题具体阐述了该算法的顺序性和最优性。
(optimal &sequantial)

A. Initialisation

A1. Choose J arbitrary vectors $\tilde{\boldsymbol{\alpha}}_1^0, \tilde{\boldsymbol{\alpha}}_2^0, \ldots, \tilde{\boldsymbol{\alpha}}_J^0$. 选取J个随机向量

A2. Compute normalized outer weight vectors $\boldsymbol{\alpha}_1^0, \boldsymbol{\alpha}_2^0, \ldots, \boldsymbol{\alpha}_J^0$ as
计算标准化外权向量

$$\boldsymbol{\alpha}_j^0 = \left[(\tilde{\boldsymbol{\alpha}}_j^0)^t \boldsymbol{\Sigma}_{jj}^{-1} \tilde{\boldsymbol{\alpha}}_j^0\right]^{-1/2} \boldsymbol{\Sigma}_{jj}^{-1} \tilde{\boldsymbol{\alpha}}_j^0.$$

此时有：$(\alpha_j^0)^T \Sigma_{jj} (\alpha_j^0) = 1$

For $s = 0, 1, \ldots$ **(until convergence)**
For $j = 1, 2, \ldots, J$

B. Computing the inner component ν_j^s

Compute the inner component according to the selected scheme:

$$\nu_j^s = \sum_{k<j} c_{jk} w\left[\mathrm{Cov}\left((\boldsymbol{\alpha}_j^s)^t \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^{s+1})^t \boldsymbol{x}_k\right)\right] (\boldsymbol{\alpha}_k^{s+1})^t \boldsymbol{x}_k + \sum_{k>j} c_{jk} w\left[\mathrm{Cov}\left((\boldsymbol{\alpha}_j^s)^t \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^{s})^t \boldsymbol{x}_k\right)\right] (\boldsymbol{\alpha}_k^{s})^t \boldsymbol{x}_k$$

where $w(x) = 1$ for the Horst scheme, x for the factorial scheme and $\mathrm{sign}(x)$ for the centroid scheme.

C. Computing the outer weight vector $\boldsymbol{\alpha}_j^{s+1}$

Compute the outer weight vector

$$\boldsymbol{\alpha}_j^{s+1} = \left[\mathrm{Cov}(\boldsymbol{x}_j, \nu_j^s)^t \boldsymbol{\Sigma}_{jj}^{-1} \mathrm{Cov}(\boldsymbol{x}_j, \nu_j^s)\right]^{-1/2} \boldsymbol{\Sigma}_{jj}^{-1} \mathrm{Cov}(\boldsymbol{x}_j, \nu_j^s).$$

End
End

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命题：记 $\alpha_j^s,\ j=1,\dots,J,\ s=0,1,\dots$ 为一列由总体RGCCA的上述算法生成的外权向量，

$$f(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\dots,\boldsymbol{\alpha}_J)=\sum_{j,k=1,j\neq k}^{J} c_{jk}g\left[\rho\left(\boldsymbol{\alpha}_j^t\boldsymbol{x}_j,\boldsymbol{\alpha}_k^t\boldsymbol{x}_k\right)\right]. \tag{11}$$

则下述不等式成立：

$$\forall s\quad f\left(\boldsymbol{\alpha}_1^s,\boldsymbol{\alpha}_2^s,\dots,\boldsymbol{\alpha}_J^s\right)\le f\left(\boldsymbol{\alpha}_1^{s+1},\boldsymbol{\alpha}_2^{s+1},\dots,\boldsymbol{\alpha}_J^{s+1}\right). \tag{12}$$

证明思路：由下述引理可证得上述命题：

引理：对 $j=1,\dots,J,\ s=0,1,2,\dots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s+1})^Tx_k)] + \sum_{k>j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s})^Tx_k)]$$

则下述性质成立：

$$\forall s\quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$$

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引理：对 $j=1,\ldots,J,\ s=0,1,2,\ldots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s+1})^Tx_k)]+\sum_{k>j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s})^Tx_k)]$$

则下述性质成立：

$$\forall s\quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$$

Step1:利用引理证明命题

$$\forall s\quad f(\boldsymbol{\alpha}_1^s,\boldsymbol{\alpha}_2^s,\ldots,\boldsymbol{\alpha}_J^s)\le f(\boldsymbol{\alpha}_1^{s+1},\boldsymbol{\alpha}_2^{s+1},\ldots,\boldsymbol{\alpha}_J^{s+1}).\tag{12}$$

$$\begin{aligned}\sum_{j=1}^J[f_j^s(\alpha_j^{s+1})-f_j^s(\alpha_j^s)]=&\sum_{j=1}^J\{\sum_{k<j}c_{jk}g[Cov((\alpha_j^{s+1})^Tx_j,(\alpha_k^{s+1})^Tx_k)]\\&+\sum_{k>j}c_{jk}g[Cov((\alpha_j^{s+1})^Tx_j,(\alpha_k^{s})^Tx_k)]\\&-\sum_{k<j}c_{jk}g[Cov((\alpha_j^{s})^Tx_j,(\alpha_k^{s+1})^Tx_k)]\\&-\sum_{k<j}c_{jk}g[Cov((\alpha_j^{s})^Tx_j,(\alpha_k^{s})^Tx_k)]\}\\=&\frac{1}{2}\sum_{j,k=1,\ j\neq k}^J c_{jk}g[Cov((\alpha_j^{s+1})^Tx_j,(\alpha_k^{s+1})^Tx_k)]-\frac{1}{2}\sum_{j,k=1,\ j\neq k}^J c_{jk}g[Cov((\alpha_j^{s})^Tx_j,(\alpha_k^{s})^Tx_k)]\\=&\frac{1}{2}[f(\alpha_1^{s+1},\ldots,\alpha_J^{s+1})-f(\alpha_1^s,\ldots,\alpha_J^s)]\end{aligned}$$

正则广义典型相关分析 RGCCA

Step2:证明引理

引理：对 $j=1,\dots,J,\ s=0,1,2,\dots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s+1})^Tx_k)]+\sum_{k>j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s})^Tx_k)]$$

则下述性质成立： $\forall s\quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$

证明： $f_j^s(\alpha_j^s)$可写成

$$\begin{aligned}
f_j^s(\alpha_j^s)&=\sum_{k<j}c_{jk}g[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s+1})^Tx_k)]+\sum_{k>j}c_{jk}g[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)]\\
&=\sum_{k<j}c_{jk}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s+1})^Tx_k)]Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s+1})^Tx_k)\\
&+\sum_{k>j}c_{jk}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)]Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)\\
&=Cov\{(\alpha_j^s)^Tx_j,\sum_{k<j}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)](\alpha_k^{s+1})^Tx_k+\sum_{k>j}\}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)](\alpha_k^{s})^Tx_k\}\\
&=Cov((\alpha_j^s)^Tx_j,\nu_j^s)\qquad (36)
\end{aligned}$$

利用 ν_j^s和α_j^{s+1} 的定义：

$$\alpha_j^s=[Cov(x_j,\nu_j^s)^T\Sigma_{jj}^{-1}Cov(x_j,\nu_j^s)]^{-\frac{1}{2}}\Sigma_{jj}^{-1}Cov(x_j,\nu_j^s)$$

有下述不等式成立：

$$f_j^s(\alpha_j^s)=Cov((\alpha_j^s)^Tx_j,\nu_j^s)\le Cov((\alpha_j^{s+1})^Tx_j,\nu_j^s)$$

即证

$$(\alpha_j^s)^TCov(x_j,\nu_j^s)\le[(Cov(x_j,\nu_j^s))^T\Sigma_{jj}^{-1}(Cov(x_j,\nu_j^s))]^{-\frac{1}{2}}$$

即证

$$[Cov(x_j,\nu_j^s)]^T(\alpha_j^s)(\alpha_j^s)^T[Cov(x_j,\nu_j^s)]\le[Cov(x_j,\nu_j^s)]^T\Sigma_{jj}^{-1}[Cov(x_j,\nu_j^s)]$$

已知 $(\alpha_j^s)^T\Sigma_{jj}(\alpha_j^s)=1$

A. Initialisation

A1. Choose J arbitrary vectors $\tilde{\boldsymbol\alpha}_1^0,\tilde{\boldsymbol\alpha}_2^0,\dots,\tilde{\boldsymbol\alpha}_J^0$.
A2. Compute normalized outer weight vectors $\boldsymbol\alpha_1^0,\boldsymbol\alpha_2^0,\dots,\boldsymbol\alpha_J^0$ as

$$\boldsymbol\alpha_j^0=[(\tilde{\boldsymbol\alpha}_j^0)'\boldsymbol\Sigma_{jj}^{-1}\tilde{\boldsymbol\alpha}_j^0]^{-1/2}\boldsymbol\Sigma_{jj}^{-1}\tilde{\boldsymbol\alpha}_j^0.$$

For $s=0,1,\dots$ **(until convergence)**
For $j=1,2,\dots,J$

B. Computing the inner component ν_j^s
Compute the inner component according to the selected scheme:

$$\nu_j^s=\sum_{k<j}c_{jk}w[\mathrm{Cov}((\boldsymbol\alpha_j^s)'\boldsymbol x_j,(\boldsymbol\alpha_k^{s+1})'\boldsymbol x_k)](\boldsymbol\alpha_k^{s+1})'\boldsymbol x_k+\sum_{k>j}c_{jk}w[\mathrm{Cov}((\boldsymbol\alpha_j^s)'\boldsymbol x_j,(\boldsymbol\alpha_k^{s})'\boldsymbol x_k)](\boldsymbol\alpha_k^{s})'\boldsymbol x_k$$

where $w(x)=1$ for the Horst scheme, x for the factorial scheme and $\mathrm{sign}(x)$ for the centroid scheme.

C. Computing the outer weight vector $\boldsymbol\alpha_j^{s+1}$
Compute the outer weight vector

$$\boldsymbol\alpha_j^{s+1}=[\mathrm{Cov}(\boldsymbol x_j,\nu_j^s)'\boldsymbol\Sigma_{jj}^{-1}\mathrm{Cov}(\boldsymbol x_j,\nu_j^s)]^{-1/2}\boldsymbol\Sigma_{jj}^{-1}\mathrm{Cov}(\boldsymbol x_j,\nu_j^s).$$

End
End

正则广义典型相关分析
RGCCA

Step2:证明引理

引理：对 $j=1,\dots,J,\ s=0,1,2,\dots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s+1})^Tx_k)]$$
$$+\sum_{k>j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s})^Tx_k)]$$

则下述性质成立： $\forall s\quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$

证明：(续)

有下述不等式成立：

$$f_j^s(\alpha_j^s)=Cov((\alpha_j^s)^Tx_j,\nu_j^s)\le Cov((\alpha_j^{s+1})^Tx_j,\nu_j^s)$$

即证

$$(\alpha_j^s)^TCov(x_j,\nu_j^s)\le[(Cov(x_j,\nu_j^s))^T\Sigma_{jj}^{-1}(Cov(x_j,\nu_j^s))]^{-\frac{1}{2}}$$

即证

$$[Cov(x_j,\nu_j^s)]^T(\alpha_j^s)(\alpha_j^s)^T[Cov(x_j,\nu_j^s)]$$
$$\le[Cov(x_j,\nu_j^s)]^T\Sigma_{jj}^{-1}[Cov(x_j,\nu_j^s)]$$

已知 $(\alpha_j^s)^T\Sigma_{jj}(\alpha_j^s)=1$

下证 $\begin{cases}\text{已知}x^TAx=1,\ A\in S_n^+\\ \text{则}A^{-1}-xx^T\text{半正定}\end{cases}$

由 $A\in S_n^+$，存在正交矩阵 P 使 $A=P^TP$

$x^TAx=1\Rightarrow x^TP^TPx=1$ 而 $y\mapsto Py\quad \mathbb{R}^n\to\mathbb{R}^n$ 是双射

问题转化为 $\begin{cases}\text{已知}x^Tx=1\\ \text{则}\ I-xx^T\ \text{半正定}\end{cases}$

$$\begin{cases}\forall a\in\mathbb{R}^n,\ a^T(A^{-1}-xx^T)a\ge 0\\ \Leftrightarrow\forall b\in\mathbb{R}^n,\ b^TP^T(A^{-1}-xx^T)Pb\ge 0\\ \Leftrightarrow\forall b\in\mathbb{R}^n,\ b^T(I-P^Txx^TP)b\ge 0\\ \text{而}\ x^TAx=1\Leftrightarrow x^TPP^Tx=1\end{cases}$$

A. Initialisation

A1. Choose J arbitrary vectors $\tilde{\boldsymbol{\alpha}}_1^0,\tilde{\boldsymbol{\alpha}}_2^0,\dots,\tilde{\boldsymbol{\alpha}}_J^0$.

A2. Compute normalized outer weight vectors $\boldsymbol{\alpha}_1^0,\boldsymbol{\alpha}_2^0,\dots,\boldsymbol{\alpha}_J^0$ as

$$\boldsymbol{\alpha}_j^0=[(\tilde{\boldsymbol{\alpha}}_j^0)^t\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0.$$

For $s=0,1,\dots$ **(until convergence)**

For $j=1,2,\dots,J$

B. Computing the inner component ν_j^s

Compute the inner component according to the selected scheme:

$$\nu_j^s=\sum_{k<j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k$$
$$+\sum_{k>j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k$$

where $w(x)=1$ for the Horst scheme, x for the factorial scheme and $\mathrm{sign}(x)$ for the centroid scheme.

C. Computing the outer weight vector $\boldsymbol{\alpha}_j^{s+1}$

Compute the outer weight vector

$$\boldsymbol{\alpha}_j^{s+1}=[\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)^t\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s).$$

End

End

令 $B=I-xx^T$ 则 $B^2=(I-xx^T)(I-xx^T)$

$=I-xx^t-xx^T+xx^Txx^T$

$=1-xx^T$

$=B$

即 $B^T=B,\ B^2=B$

则其特征值为0或1,故半正定。

正则广义典型相关分析 RGCCA

Step2:证明引理

引理：对 $j=1,\ldots,J,\ s=0,1,2,\ldots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s+1})^Tx_k)]$$
$$+\sum_{k>j}c_{jk}g[Cov((\alpha_j)^Tx_j,(\alpha_k^{s})^Tx_k)]$$

则下述性质成立： $\forall s \quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$

证明：$f_j^s(\alpha_j^s)$可写成

$$\begin{aligned}
f_j^s(\alpha_j^s)=&\sum_{k<j}c_{jk}g[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s+1})^Tx_k)]+\sum_{k>j}c_{jk}g[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)]\\
=&\sum_{k<j}c_{jk}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s+1})^Tx_k)]Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s+1})^Tx_k)\\
&+\sum_{k>j}c_{jk}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)]Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)\\
=&Cov\{(\alpha_j^s)^Tx_j,\sum_{k<j}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)](\alpha_k^{s+1})^Tx_k+\sum_{k>j}\}\omega[Cov((\alpha_j^s)^Tx_j,(\alpha_k^{s})^Tx_k)](\alpha_k^{s})^Tx_k\}\\
=&Cov((\alpha_j^s)^Tx_j,\nu_j^s) \qquad (36)
\end{aligned}$$

利用 ν_j^s和α_j^{s+1} 的定义：

$$\alpha_j^s=[Cov(x_j,\nu_j^s)^T\Sigma_{jj}^{-1}Cov(x_j,\nu_j^s)]^{-\frac{1}{2}}\Sigma_{jj}^{-1}Cov(x_j,\nu_j^s)$$

有下述不等式成立：

$$f_j^s(\alpha_j^s)=Cov((\alpha_j^s)^Tx_j,\nu_j^s)\le Cov((\alpha_j^{s+1})^Tx_j,\nu_j^s)$$

且有等式：

$$\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,\nu_j^s)=\sum_{k<j}c_{jk}w\big[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)\big]\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)$$
$$+\sum_{k>j}c_{jk}w\big[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k)\big]\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k). \qquad (38)$$

下面对三种不同的g分别进行讨论：

A. Initialisation

A1. Choose J arbitrary vectors $\tilde{\boldsymbol{\alpha}}_1^0,\tilde{\boldsymbol{\alpha}}_2^0,\ldots,\tilde{\boldsymbol{\alpha}}_J^0$.
A2. Compute normalized outer weight vectors $\boldsymbol{\alpha}_1^0,\boldsymbol{\alpha}_2^0,\ldots,\boldsymbol{\alpha}_J^0$ as

$$\boldsymbol{\alpha}_j^0=\big[(\tilde{\boldsymbol{\alpha}}_j^0)'\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0\big]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0.$$

For $s=0,1,\ldots$ **(until convergence)**
For $j=1,2,\ldots,J$

B. Computing the inner component ν_j^s
Compute the inner component according to the selected scheme:

$$\nu_j^s=\sum_{k<j}c_{jk}w\big[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)\big](\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k$$
$$+\sum_{k>j}c_{jk}w\big[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k)\big](\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k$$

where $w(x)=1$ for the Horst scheme, x for the factorial scheme and $\mathrm{sign}(x)$ for the centroid scheme.

C. Computing the outer weight vector $\boldsymbol{\alpha}_j^{s+1}$
Compute the outer weight vector

$$\boldsymbol{\alpha}_j^{s+1}=\big[\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)'\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)\big]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s).$$

End
End

正则广义典型相关分析
RGCCA

Step2:证明引理

$$f_j^s(\alpha_j^s)=Cov((\alpha_j^s)^T x_j,\nu_j^s)\le Cov((\alpha_j^{s+1})^T x_j,\nu_j^s)$$

$$\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,\nu_j^s)=\sum_{k<j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)]\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)$$
$$+\sum_{k>j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^s)'\boldsymbol{x}_k)]\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^s)'\boldsymbol{x}_k). \quad (38)$$

引理：对 $j=1,\dots,J,\ s=0,1,2,\dots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^T x_j,(\alpha_k^{s+1})^T x_k)]+\sum_{k>j}c_{jk}g[Cov((\alpha_j)^T x_j,(\alpha_k^s)^T x_k)]$$

则下述性质成立： $\forall s\quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$

Horst scheme $\quad g(x)=x\ ,\omega(x)=1$

(38)

$$\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,\nu_j^s)=\sum_{k<j}c_{jk}\,\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)$$
$$+\sum_{k>j}c_{jk}\,\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^s)'\boldsymbol{x}_k)=f_j^s(\boldsymbol{\alpha}_j^{s+1}) \quad (39)$$

又已得 $f_j^s(\alpha_j^s)=Cov((\alpha_j^s)^T x_j,\nu_j^s)\le Cov((\alpha_j^{s+1})^T x_j,\nu_j^s)$

故可证得 $\quad f_j^s(\boldsymbol{\alpha}_j^s)\le f_j^s(\boldsymbol{\alpha}_j^{s+1})\quad \square$

A. Initialisation

A1. Choose J arbitrary vectors $\tilde{\boldsymbol{\alpha}}_1^0,\tilde{\boldsymbol{\alpha}}_2^0,\dots,\tilde{\boldsymbol{\alpha}}_J^0$.
A2. Compute normalized outer weight vectors $\boldsymbol{\alpha}_1^0,\boldsymbol{\alpha}_2^0,\dots,\boldsymbol{\alpha}_J^0$ as

$$\boldsymbol{\alpha}_j^0=[(\tilde{\boldsymbol{\alpha}}_j^0)'\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0.$$

For $s=0,1,\dots$ **(until convergence)**
For $j=1,2,\dots,J$

B. Computing the inner component ν_j^s
Compute the inner component according to the selected scheme:

$$\nu_j^s=\sum_{k<j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k+\sum_{k>j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^s)'\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^s)'\boldsymbol{x}_k$$

where $w(x)=1$ for the Horst scheme, x for the factorial scheme and $\mathrm{sign}(x)$ for the centroid scheme.

C. Computing the outer weight vector $\boldsymbol{\alpha}_j^{s+1}$
Compute the outer weight vector

$$\boldsymbol{\alpha}_j^{s+1}=[\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)'\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s).$$

End
End

正则广义典型相关分析 RGCCA

Step2:证明引理

引理：对 $j=1,\dots,J,\ s=0,1,2,\dots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^T x_j,(\alpha_k^{s+1})^T x_k)] + \sum_{k>j}c_{jk}g[Cov((\alpha_j)^T x_j,(\alpha_k^{s})^T x_k)]$$

则下述性质成立： $\forall s \quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$

$$f_j^s(\alpha_j^s)=Cov((\alpha_j^s)^T x_j,\nu_j^s)\le Cov((\alpha_j^{s+1})^T x_j,\nu_j^s)$$

$$\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})^t\boldsymbol{x}_j,\nu_j^s)=\sum_{k<j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k)]\,\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k) + \sum_{k>j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k)]\,\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k). \quad (38)$$

Centroid scheme $g(x)=|x|,\omega(x)=sign(x)$

(38) ⇒

$$f_j^s(\boldsymbol{\alpha}_j^s)=\sum_{k<j}c_{jk}|\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k)|+\sum_{k>j}c_{jk}|\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k)| \quad (40)$$

且 $\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})^t\boldsymbol{x}_j,\nu_j^s)$

$$=\sum_{k<j}c_{jk}\,\mathrm{sign}([\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k)])\,\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k) + \sum_{k>j}c_{jk}\,\mathrm{sign}([\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k)])\,\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k). \quad (41)$$

从而

$$f_j^s(\alpha_j^s)\le Cov((\alpha_j^{s+1})^T x_j,\nu_j^s)\le f_j^s(\alpha_j^{s+1}) \quad \square$$

A. Initialisation

A1. Choose J arbitrary vectors $\tilde{\boldsymbol{\alpha}}_1^0,\tilde{\boldsymbol{\alpha}}_2^0,\dots,\tilde{\boldsymbol{\alpha}}_J^0$.

A2. Compute normalized outer weight vectors $\boldsymbol{\alpha}_1^0,\boldsymbol{\alpha}_2^0,\dots,\boldsymbol{\alpha}_J^0$ as

$$\boldsymbol{\alpha}_j^0=[(\tilde{\boldsymbol{\alpha}}_j^0)^t\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0.$$

For $s=0,1,\dots$ **(until convergence)**

For $j=1,2,\dots,J$

B. Computing the inner component ν_j^s

Compute the inner component according to the selected scheme:

$$\nu_j^s=\sum_{k<j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^{s+1})^t\boldsymbol{x}_k + \sum_{k>j}c_{jk}w[\mathrm{Cov}((\boldsymbol{\alpha}_j^{s})^t\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^{s})^t\boldsymbol{x}_k$$

where $w(x)=1$ for the Horst scheme, x for the factorial scheme and $\mathrm{sign}(x)$ for the centroid scheme.

C. Computing the outer weight vector $\boldsymbol{\alpha}_j^{s+1}$

Compute the outer weight vector

$$\boldsymbol{\alpha}_j^{s+1}=[\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)^t\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s)]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\mathrm{Cov}(\boldsymbol{x}_j,\nu_j^s).$$

End

End

正则广义典型相关分析
RGCCA

Step2:证明引理

引理：对 $j=1,\ldots,J,\ \ s=0,1,2,\ldots$ 定义函数：

$$f_j^s(\alpha_j)=\sum_{k<j}c_{jk}g[Cov((\alpha_j)^T x_j,(\alpha_k^{s+1})^T x_k)]$$
$$+\sum_{k>j}c_{jk}g[Cov((\alpha_j)^T x_j,(\alpha_k^{s})^T x_k)]$$

则下述性质成立： $\forall s \quad f_j^s(\alpha_j^s)\le f_j^s(\alpha_j^{s+1})$

$$f_j^s(\alpha_j^s)=Cov((\alpha_j^s)^T x_j,\nu_j^s)\le Cov((\alpha_j^{s+1})^T x_j,\nu_j^s)$$

$$\operatorname{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,\nu_j^s)=\sum_{k<j}c_{jk}w[\operatorname{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)]\operatorname{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)$$
$$+\sum_{k>j}c_{jk}w[\operatorname{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k)]\operatorname{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k). \quad (38)$$

Factorial scheme $\quad g(x)=x^2,\omega(x)=x$

(38)⇨

$$f_j^s(\boldsymbol{\alpha}_j^s)=\sum_{k<j}c_{jk}\operatorname{Cov}^2((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)+\sum_{k>j}c_{jk}\operatorname{Cov}^2((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k) \quad (43)$$

且

$$\operatorname{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,\nu_j^s)=\sum_{k<j}c_{jk}[\operatorname{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)]\operatorname{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)$$
$$+\sum_{k>j}c_{jk}[\operatorname{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k)]\operatorname{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k). \quad (44)$$

(44)右侧是两个向量得标量积。利用Cautchy-Schwartz不等式和$c_{jk}^2=c_{jk}$

$$\operatorname{Cov}((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,\nu_j^s)$$
$$\le\left[\sum_{k<j}c_{jk}\operatorname{Cov}^2((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)+\sum_{k>j}c_{jk}\operatorname{Cov}^2((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k)\right]^{1/2}$$
$$\times\left[\sum_{k<j}c_{jk}\operatorname{Cov}^2((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)+\sum_{k>j}c_{jk}\operatorname{Cov}^2((\boldsymbol{\alpha}_j^{s+1})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k)\right]^{1/2}. \quad (45)$$

A. *Initialisation*

A1. Choose J arbitrary vectors $\tilde{\boldsymbol{\alpha}}_1^0,\tilde{\boldsymbol{\alpha}}_2^0,\ldots,\tilde{\boldsymbol{\alpha}}_J^0$.
A2. Compute normalized outer weight vectors $\boldsymbol{\alpha}_1^0,\boldsymbol{\alpha}_2^0,\ldots,\boldsymbol{\alpha}_J^0$ as

$$\boldsymbol{\alpha}_j^0=[(\tilde{\boldsymbol{\alpha}}_j^0)'\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\tilde{\boldsymbol{\alpha}}_j^0.$$

For $s=0,1,\ldots$ **(until convergence)**
For $j=1,2,\ldots,J$

B. *Computing the inner component* ν_j^s
Compute the inner component according to the selected scheme:

$$\nu_j^s=\sum_{k<j}c_{jk}w[\operatorname{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^{s+1})'\boldsymbol{x}_k$$
$$+\sum_{k>j}c_{jk}w[\operatorname{Cov}((\boldsymbol{\alpha}_j^{s})'\boldsymbol{x}_j,(\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k)](\boldsymbol{\alpha}_k^{s})'\boldsymbol{x}_k$$

where $w(x)=1$ for the Horst scheme, x for the factorial scheme and $\operatorname{sign}(x)$ for the centroid scheme.

C. *Computing the outer weight vector* $\boldsymbol{\alpha}_j^{s+1}$
Compute the outer weight vector

$$\boldsymbol{\alpha}_j^{s+1}=[\operatorname{Cov}(\boldsymbol{x}_j,\nu_j^s)'\boldsymbol{\Sigma}_{jj}^{-1}\operatorname{Cov}(\boldsymbol{x}_j,\nu_j^s)]^{-1/2}\boldsymbol{\Sigma}_{jj}^{-1}\operatorname{Cov}(\boldsymbol{x}_j,\nu_j^s).$$

End
End

正则广义典型相关分析
RGCCA

Step2:证明引理

$$f_j^s(\alpha_j^s) = Cov((\alpha_j^s)^T x_j, \nu_j^s) \le Cov((\alpha_j^{s+1})^T x_j, \nu_j^s)$$

$$\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})' \boldsymbol{x}_j, \nu_j^s) = \sum_{k<j} c_{jk} w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^{s+1})' \boldsymbol{x}_k)] \mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^{s+1})' \boldsymbol{x}_k)$$

$$+ \sum_{k>j} c_{jk} w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^s)' \boldsymbol{x}_k)] \mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^s)' \boldsymbol{x}_k). \quad (38)$$

引理：对 $j = 1, \ldots, J, \ s = 0, 1, 2, \ldots$ 定义函数：

$$f_j^s(\alpha_j) = \sum_{k<j} c_{jk} g[Cov((\alpha_j)^T x_j, (\alpha_k^{s+1})^T x_k)] + \sum_{k>j} c_{jk} g[Cov((\alpha_j)^T x_j, (\alpha_k^s)^T x_k)]$$

则下述性质成立： $\forall s \quad f_j^s(\alpha_j^s) \le f_j^s(\alpha_j^{s+1})$

Factorial scheme

$$g(x) = x^2, \omega(x) = x$$

$$\mathrm{Cov}((\boldsymbol{\alpha}_j^{s+1})' \boldsymbol{x}_j, \nu_j^s)$$

$$\le \left[\sum_{k<j} c_{jk} \mathrm{Cov}^2((\boldsymbol{\alpha}_j^s)' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^{s+1})' \boldsymbol{x}_k) + \sum_{k>j} c_{jk} \mathrm{Cov}^2((\boldsymbol{\alpha}_j^s)' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^s)' \boldsymbol{x}_k)\right]^{1/2}$$

$$\times \left[\sum_{k<j} c_{jk} \mathrm{Cov}^2((\boldsymbol{\alpha}_j^{s+1})' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^{s+1})' \boldsymbol{x}_k) + \sum_{k>j} c_{jk} \mathrm{Cov}^2((\boldsymbol{\alpha}_j^{s+1})' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^s)' \boldsymbol{x}_k)\right]^{1/2}. \quad (45)$$

从而

$$f_j^s(\boldsymbol{\alpha}_j^s) \le [f_j^s(\boldsymbol{\alpha}_j^s)]^{1/2} [f_j^s(\boldsymbol{\alpha}_j^{s+1})]^{1/2} \quad (46)$$

从而

$$f_j^s(\boldsymbol{\alpha}_j^s) \le f_j^s(\boldsymbol{\alpha}_j^{s+1}).$$

$\square$

至此证明了引理，即证明了定理，从而证明了该算法的最优性和顺序性。

A. *Initialisation*

A1. Choose J arbitrary vectors $\tilde{\boldsymbol{\alpha}}_1^0, \tilde{\boldsymbol{\alpha}}_2^0, \ldots, \tilde{\boldsymbol{\alpha}}_J^0$.

A2. Compute normalized outer weight vectors $\boldsymbol{\alpha}_1^0, \boldsymbol{\alpha}_2^0, \ldots, \boldsymbol{\alpha}_J^0$ as

$$\boldsymbol{\alpha}_j^0 = [(\tilde{\boldsymbol{\alpha}}_j^0)' \boldsymbol{\Sigma}_{jj}^{-1} \tilde{\boldsymbol{\alpha}}_j^0]^{-1/2} \boldsymbol{\Sigma}_{jj}^{-1} \tilde{\boldsymbol{\alpha}}_j^0.$$

For $s = 0, 1, \ldots$ **(until convergence)**

For $j = 1, 2, \ldots, J$

B. *Computing the inner component* ν_j^s

Compute the inner component according to the selected scheme:

$$\nu_j^s = \sum_{k<j} c_{jk} w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^{s+1})' \boldsymbol{x}_k)] (\boldsymbol{\alpha}_k^{s+1})' \boldsymbol{x}_k$$

$$+ \sum_{k>j} c_{jk} w[\mathrm{Cov}((\boldsymbol{\alpha}_j^s)' \boldsymbol{x}_j, (\boldsymbol{\alpha}_k^s)' \boldsymbol{x}_k)] (\boldsymbol{\alpha}_k^s)' \boldsymbol{x}_k$$

where $w(x) = 1$ for the Horst scheme, x for the factorial scheme and $\mathrm{sign}(x)$ for the centroid scheme.

C. *Computing the outer weight vector* $\boldsymbol{\alpha}_j^{s+1}$

Compute the outer weight vector

$$\boldsymbol{\alpha}_j^{s+1} = [\mathrm{Cov}(\boldsymbol{x}_j, \nu_j^s)' \boldsymbol{\Sigma}_{jj}^{-1} \mathrm{Cov}(\boldsymbol{x}_j, \nu_j^s)]^{-1/2} \boldsymbol{\Sigma}_{jj}^{-1} \mathrm{Cov}(\boldsymbol{x}_j, \nu_j^s).$$

End

End

谢谢！