Hierarchical Heterogeneous Analysis of High-Dimensional Data

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1 Model

- $X = (X_1, ..., X_n)^T \in \mathbb{R}^{n\times p}$, type I features (main G) for all observations, where $X_i \in \mathbb{R}^p$;
- $Z = (Z_1, ..., Z_n)^T \in \mathbb{R}^{n\times q}$, type II features (main E) for all observations, where $Z_i \in \mathbb{R}^q$;
- $y = (y_1, ..., y_n)^T \in \mathbb{R}^n$, the response vector.

1.1 Basic Model

简化后的异质性模型为：

$$y_i = X_i^T \beta_i' + Z_i^T \alpha_i' + \epsilon_i \tag{1.1}$$

其中 $\epsilon_i \sim (iid) N(0, \sigma^2)$

假设所有观测大组可根据基因（X）进行划分，大组中根据环境/图片特征变量（Z）进行进一步的划分。假设有 K 个亚组，则相同亚组中的样有相同参数。

1.2 Object Function

基于高斯混合分布，重参数化后最小化目标函数为（负对数似然+惩罚）：

$$\begin{aligned}
\mathcal{L}(\beta, \alpha, \pi | X, y) &= -\frac{1}{n}\sum_{i=1}^{n} \log p_Y(y) + \mathrm{pen}(\beta', \alpha') \\
&= -\frac{1}{n}\sum_{i=1}^{n} \log \big(\sum_{k=1}^{K} \pi_k f_k(y_i | X_i, Z_i)\big) + \mathrm{pen}(\beta', \alpha') \\
&= -\frac{1}{n}\sum_{i=1}^{n} \log \left\{ \sum_{k=1}^{K} \pi_k \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}\left(y_i - X_i^T\beta_k' - Z_i^T\alpha_k'\right)^2\right)\right\} + \mathrm{pen}(\beta', \alpha') \\
&= -\frac{1}{n}\sum_{i=1}^{n} \log \left\{ \sum_{k=1}^{K} \pi_k \frac{\rho_k}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2\right)\right\} + \mathrm{pen}(\beta, \alpha)
\end{aligned} \tag{1.2}$$

其中重参数化为 $\beta_k = \beta_k'/\sigma_k, \rho_k = 1/\sigma_k$，惩罚函数为

$$
\begin{aligned}
\operatorname{pen}(\beta, \alpha)= & \sum_{k=1}^K \sum_{j=1}^p \operatorname{pen}\left(\left|\beta_{kj}\right|, \lambda_1\right)+\sum_{k=1}^K \sum_{s=1}^q \operatorname{pen}\left(\left|\alpha_{ks}\right|, \lambda_1\right) \\
& +\sum_{k<k^{\prime}} \operatorname{pen}\left(\sqrt{\left\|\beta_k-\beta_{k^{\prime}}\right\|_2^2+\left\|\alpha_k-\alpha_{k^{\prime}}\right\|_2^2}, \lambda_2\right) \\
& +\sum_{k<k^{\prime}} \operatorname{pen}\left(\left\|\beta_k-\beta_{k^{\prime}}\right\|_2, \lambda_3\right)
\end{aligned} \tag{1.3}
$$

第一项惩罚保证基因相关系数的稀疏性；第二，第三项惩罚共同作用以致模型呈现层级结构（Hierarchy）.

1.3 Penalty Function

MCP 惩罚函数

$$
pen_{(\lambda,a)}(\beta)=\begin{cases}\lambda|\beta|-\dfrac{\beta^2}{2a}, & |\beta|\leq a\lambda \\ \dfrac{a}{2}\lambda^2, & |\beta|> a\lambda\end{cases} \tag{1.4}
$$

MCP 惩罚函数对参数求偏导得

$$
pen'_{(\lambda,a)}(\beta)=\begin{cases}\operatorname{sgn}(\beta)\left(\lambda-\frac{|\beta|}{a}\right) & |\beta|\leq a\lambda \\ 0 & \text{otherwise}\end{cases} \tag{1.5}
$$

超参数 a 常取为大于 1 的数。

2 Computation

2.1 Transformation

采用 EM 算法。E 步更新 π，M 步更新参数 β, α。引入变量 C_i 用于指示每个样本属于哪个类别，有后验概率如 2.1 所示

$$
q_{C_i}(c_i)=\frac{\pi_{c_i} f_{c_i}(y_i|X_i, Z_i)}{\sum_{k=1}^K \pi_k f_k(y_i|X_i, Z_i)} \tag{2.1}
$$

目标函数 1.2 中对数似然部分可以放缩如下

$$
\begin{aligned}
\log p_Y(y) &= log\sum_{k=1}^{K} p_{Y,C}(y,c) \\
&= logE_{q_C}\left(\frac{p_{Y,C}(y,c)}{q_C(c)}\right) \\
&\geq E_{q_C}\left(\frac{p_{Y,C}(y,c)}{q_C(c)}\right) \\
&= E_{q_C}\left(logp_{Y,C}(y,c)\right) - E_{q_C}\left(logq_C(c)\right)
\end{aligned} \tag{2.2}
$$

综上，目标函数可以放缩（根据 Gaussian mixture models and the EM algorithm）为

$$
\begin{aligned}
\mathcal{L}(\beta,\alpha,\pi|X,y) &= -\sum_{i=1}^{n}\log p_Y(y) + \mathrm{pen}(\beta,\alpha) \\
&\leq -E_{q_C}\left(logp_{Y,C}(y,c)\right) + E_{q_C}\left(logq_C(c)\right) + \mathrm{pen}(\beta,\alpha)
\end{aligned} \tag{2.3}
$$

在 M 步更新参数 β,α 式 2.3 中 $E_{q_C}(logq_C(c))$ 与参数无关。而 $E_{q_C}\left(logp_{Y,C}(y,c)\right)$ 可以进一步变形

$$
\begin{aligned}
E_{q_C}logp_{Y,C}(y,c) &= E_{q_C}log\left(p_C(c)p_{Y|C}(y)\right) \\
&= E_{q_C}log\left(\prod_{i=1}^{n} p_{C_i}(c_i)p_{Y_i|C_i}(y_i)\right) \\
&= E_{q_C}log\left(\prod_{i=1}^{n}\prod_{k=1}^{K}\pi_{c_i}f_{Y_i|C_i}(y_i)\right)^{I(C_i=k)} \\
&= E_{q_C}\sum_{i=1}^{n}\sum_{k=1}^{K} I(C_i=k)\left(log\pi_{c_i} + logf_{Y_i|C_i}(y_i)\right) \\
&= \sum_{i=1}^{n}\sum_{k=1}^{K} E_{q_C}I(C_i=k)\left(log\pi_{c_i} + logf_{Y_i|C_i}(y_i)\right) \\
&= \sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(log\pi_{c_i} + logf_{Y_i|C_i}(y_i)\right) \\
&= \sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(log\pi_{c_i} + log\rho_k - \frac{1}{2}log2\pi - \frac{1}{2}(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k)^2\right) \\
&= \sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(C - \frac{1}{2}(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k)^2\right)
\end{aligned} \tag{2.4}
$$

其中 C 为与更新参数无关的常数项。此时最小化目标为原目标函数的上界，表达式为

$$
\begin{aligned}
\mathcal{L}(\beta,\alpha|\pi,X,y) =& -\frac{1}{n}\sum_{i=1}^{n}\log p_Y(y)+\mathrm{pen}(\beta,\alpha) \\
\leq& -\frac{1}{n}E_{q_C}\left(logp_{Y,C}(y,c)\right)+\mathrm{pen}(\beta,\alpha) \\
=& -\frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K}q_{C_i}(k)\left(C-\frac{1}{2}(y_i\rho_k-X_i^T\beta_k-Z_i^T\alpha_k)^2\right) \\
&+\sum_{k=1}^{K}\mathrm{pen}\left(\|\beta_k\|_2,\lambda_1\right)+\sum_{k=1}^{K}\mathrm{pen}\left(\|\alpha_k\|_2,\lambda_1\right) \\
&+\sum_{k<k'}\mathrm{pen}\left(\sqrt{\|\beta_k-\beta_{k'}\|_2^2+\|\alpha_k-\alpha_{k'}\|_2^2},\lambda_2\right) \\
&+\sum_{k<k'}\mathrm{pen}\left(\|\beta_k-\beta_{k'}\|_2,\lambda_3\right)
\end{aligned}
\tag{2.5}
$$

2.2 MCP

β, z 均为 p 维向量，现假设目标函数有

$$
\mathcal{L}(x;\lambda)=\frac{\rho}{2}\|x-z\|_2^2+\mathrm{pen}(\|x\|_2;\lambda) \tag{2.6}
$$

则 x 对应解为

$$
x=\begin{cases}\frac{S\left(z,\frac{\lambda}{\rho}\right)}{1-\frac{1}{a\rho}} & \text{if } |z|\leq a\lambda \\ z & \text{if } |z|> a\lambda\end{cases} \tag{2.7}
$$

其中 $S(.,.)$ 为 soft thresholding operator，定义如下

$$
S(x,t)=\mathrm{sign}(x)(|x|-t)_+=x\left(1-\frac{t}{|x|}\right)_+ \tag{2.8}
$$

故 x 解也可写为

$$
x=\begin{cases}\frac{z\left(1-\frac{\lambda}{|z|\rho}\right)_+}{1-\frac{1}{a\rho}} & \text{if } |z|\leq a\lambda \\ z & \text{if } |z|> a\lambda\end{cases} \tag{2.9}
$$

3 Model Preparation

3.1 Version 1 - P for β ADMM

为了尝试推导以及检验代码正确性，先尝试构建较为简单的模型进行实验。考虑以下目标函数

$$
\begin{aligned}
\mathcal{L}^{(1)}(\beta,\alpha) &= -\frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(C-\frac{1}{2}(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k)^2\right) + \sum_{k=1}^{K}\sum_{j=1}^{p}\mathrm{pen}\left(|\beta_{kj}|,\lambda_1\right) \\
&= \frac{1}{2n}\sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 + \sum_{k=1}^{K}\sum_{j=1}^{p}\mathrm{pen}\left(|\beta_{kj}|,\lambda_1\right) + C
\end{aligned}
\tag{3.1}
$$

C 表示与更新参数无关的项，后面均省略。对于类别 k 目标函数为

$$
\mathcal{L}_k^{(1)}(\beta_k,\alpha_k) = \frac{1}{2n}\sum_{i=1}^{n} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 + \sum_{j=1}^{p}\mathrm{pen}\left(|\beta_{kj}|,\lambda_1\right) \tag{3.2}
$$

对应增广拉格朗日函数为

$$
\begin{aligned}
\mathcal{L}_{k,\rho}^{(1)}(\beta_k,\alpha_k,\tau) = \frac{1}{2n}\sum_{i=1}^{n} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 + \sum_{j=1}^{p}\mathrm{pen}\left(|\beta_{kj}|,\lambda_1\right) \\
+ \sum_{j=1}^{p}\mathrm{pen}\left(|\theta_{kj}|,\lambda_1\right) + \tau^T(\beta_k-\theta_k) + \frac{\rho}{2}\|\beta_k-\theta_k\|_2^2
\end{aligned}
\tag{3.3}
$$

τ 为对应的拉格朗日乘子（向量），$\rho > 0$ 为拉格朗日参数。给定 $(\beta_k^{(t)}, \alpha_k^{(t)}, \tau^{(t)})$ 则第 $t+1$ 步更新写为

$$
\beta_k^{(t+1)} \in \underset{\beta\in R^p}{arg\,min}\ \mathcal{L}_{k,\rho}^{(1)}\left(\beta,\theta^{(t)},\tau^{(t)}\right) \tag{3.4}
$$

$$
\theta_k^{(t+1)} \in \underset{\theta\in R^p}{arg\,min}\ \mathcal{L}_{k,\rho}^{(1)}\left(\beta^{(t+1)},\theta,\tau^{(t)}\right) \tag{3.5}
$$

$$
\tau^{(t+1)} = \tau^{(t)} + \rho\left(\beta^{(t+1)} - \theta^{(t+1)}\right) \tag{3.6}
$$

Update β_k 式 3.3 中与 β_k 相关的项为

$$
\begin{aligned}
\mathcal{L}_{k,\rho}^{(1)}(\beta_k) = \frac{1}{2n}\sum_{i=1}^{n} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 + \sum_{j=1}^{p}\mathrm{pen}\left(|\beta_{kj}|,\lambda_1\right) \\
+ \tau^T(\beta_k-\theta_k) + \frac{\rho}{2}\|\beta_k-\theta_k\|_2^2
\end{aligned}
\tag{3.7}
$$

对 β_k 求偏导，得

$$\beta_k = \left(n^{-1}X^T W_k X + \rho I_p\right)^{-1}\left(n^{-1}X^T W_k' y^{\beta_k} + \rho\theta_k - \tau\right) \tag{3.8}$$

其中 $y^{(\beta_k)} = y\rho_k - Z\alpha_k$，$W_k = \rho_k diag(q_{C_1}(k), ..., q_{C_n}(k))$，$I_p$ 为 p 维单位矩阵。

Update θ_k　式 3.3 中与 θ_k 相关的项为

$$\begin{aligned}\mathcal{L}^{(1)}_{k,\rho}(\beta_k) &= \sum_{j=1}^{p} \mathrm{pen}\left(\theta_{kj}, \lambda_1\right) + \tau^T(\beta_k - \theta_k) + \frac{\rho}{2}\|\beta_k - \theta_k\|_2^2 \\ &= \frac{\rho}{2}\|\theta_k - z_k\|_2^2 + \sum_{j=1}^{p} \mathrm{pen}\left(\theta_{kj}, \lambda_1\right)\end{aligned} \tag{3.9}$$

其中 $z_k = \beta_k + \frac{\tau}{\rho}$.

故 $\theta_k = (\theta_{k1}, ..., \theta_{kp})$ 的解为

$$\theta_{kj} = \begin{cases} \frac{S\left(z_{kj}, \frac{\lambda}{\rho}\right)}{1-\frac{1}{a\rho}} & \text{if } |z_{kj}| \le a\lambda \\ z_{kj} & \text{if } |z_{kj}| > a\lambda \end{cases} \tag{3.10}$$

Update ρ_k　惩罚项不涉及 ρ_k，更新 ρ_k 只需要考虑拟合项。式 3.3 中未完全表示出 ρ_k 相关的项，原待最小化的目标函数中与 ρ_k 有关的项应为 3.11.（注意此处 ρ 表示拉格朗日参数，$rho_k = 1/\sigma_k$ 为高斯分布中的参数）

$$\mathcal{L}^{(1)}_{k,\rho}(\rho_k) = -\frac{1}{n}\sum_{i=1}^{n} q_{C_i}(k)\left(log\rho_k - \frac{1}{2}(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k)^2\right) \tag{3.11}$$

对 ρ_k 求导得

$$\frac{\partial\mathcal{L}^{(1)}_{k,\rho}(\rho_k)}{\partial\rho_k} = -\frac{1}{n}\sum_{i=1}^{n} q_{C_i}(k)\left(1/\rho_k - (y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k)y_i\right) \tag{3.12}$$

$\frac{\partial\mathcal{L}^{(1)}_{k,\rho}(\rho_k)}{\partial\rho_k} = 0$ 时，有下式成立。

$$\begin{aligned}&\sum_{i=1}^{n} q_{C_i}(k)\left(-\rho_k^2 y_i^2 + \rho_k(X_i^T\beta_k + Z_i^T\alpha_k)y_i + 1\right) = 0 \\ &-y^T W_k y\rho_k^2 + (X\beta_k + Z\alpha_k)^T W_k y\rho_k + I_n^T W_k I_n = 0\end{aligned} \tag{3.13}$$

这是一个一元二次方程求根问题，因为 ρ_k 应为正值，取两个根中的正值，解为

$$\rho_k = \frac{-B - \sqrt{B^2 - 4AC}}{2A} \tag{3.14}$$

其中 $A = -y^T W_k y,\ B = (X\beta_k + Z\alpha_k)^T W_k y,\ C = 1_n^T W_k 1_n$.

若给定每个样本类别，等价于再各个类别内部使用 ADMM 方法进行迭代求解系数；若未知样本类别，使用 EM 算法进行估计，算法流程见 1

Algorithm 1: Version 1 with sparse penalty for β (ADMM)

Input ：数据 y, X，超参数 $n, p, K, a, \lambda, \rho$

Output: $\beta_k, k = 1, ..., K$ 的估计值

初始化 $q_{C_i}(k) = \frac{1}{K} + \mathrm{N}(0, 0.5^2), k = 1, ..., K, i = 1, ..., n$ 标准化;

repeat

  for $k\ in\ 1 : K$ **do**

    $W_k = diag(q_{C_1}(k), ..., q_{C_n}(k))$;

    更新 $\beta_k^{(iter)} = \left(n^{-1} X^T W_k X + \rho I_p\right)^{-1} \left(n^{-1} X^T W_k' y^{\beta_k} + \rho\theta_k - \tau\right)$;

    更新 $\theta_k^{(iter)} = \begin{cases} \frac{S\left(z_k, \frac{\lambda}{\rho}\right)}{1 - \frac{1}{a\rho}} & \text{if } \|z_k\|_2 \leq a\lambda \\ z & \text{if } \|z_k\|_2 > a\lambda \end{cases}$;

    更新 $\tau^{(iter)} = \tau^{(iter-1)} + \rho(\beta_k^{(iter)} - \theta_k^{(iter)})$.

    更新 $\rho_k^{(iter)} = \frac{-B - \sqrt{B^2 - 4AC}}{2A}$.

      where $A = -y^T W_k y; B = (X\beta_k + Z\alpha_k)^T W_k y; C = 1_n^T W_k 1_n$.

  end for

  计算基于 $\beta_k^{(iter)}$ 得到的后验概率 q_C

    $q_{C_i}^{(iter)}(k) = \frac{\pi_k^{(iter)} f_k(y_i; \beta_k^{(iter)} / \rho_k^{(iter)})}{\sum_{k'=1}^K \pi_{k'}^{(iter)} f_{k'}(y_i; \beta_{k'}^{(iter)} / \rho_k^{(iter)})}, k = 1, ..., K$

  更新 $\pi_k^{(iter)} = \frac{1}{n} \sum_{i=1}^n q_{C_i}^{(iter)}(k)$

until 收敛（$\frac{\|\beta^{(iter)} - \beta^{(iter-1)}\|}{\|\beta^{(iter)}\|}$小于临界值）;

实验结果大体如表 14 所示。

3.2 Version 2 - P for β

依旧对目标函数

$$\mathcal{L}^{(2)}(\beta, \alpha) = \frac{1}{2n} \sum_{i=1}^n \sum_{k=1}^K q_{C_i}(k) \left(y_i \rho_k - X_i^T \beta_k - Z_i^T \alpha_k\right)^2 + \sum_{k=1}^K \sum_{j=1}^p \mathrm{pen}\left(|\beta_{kj}|, \lambda_1\right) \tag{3.15}$$

p	非零个数	epsilon	flexmix	自己迭代
8	3	0	收敛到真值	收敛到真值
8	3	$N(0, 0.5^2)$	收敛到接近真值	收敛到接近真值
40	3	0	全0估计	距离真值有差异，详情见表
40	3	$N(0, 0.5^2)$	全0估计	收敛到接近真值

不同于上一节，现在直接对于 β_{kj} 求偏导进行求解，而不用 ADMM 算法框架进行问题的转化。目标函数中与第 k 类中的参数相关的部分写为 $\mathcal{L}_k^{(2)}$，见 3.16，其中 $y'_{ik} = \rho_k y_i - X_{i(-j)}^T \beta_{k(-j)} - Z_i^T \alpha_k$，$y'_k = (y'_{1k}, ..., y'_{nk})^T \in \mathbb{R}^{n\times 1}$, $X_{i(-j)}$ 表示 X_i 中除第 j 列外的其他特征，$X_{(-j)} = (X_{1(-j)}, ..., X_{n(-j)})^T \in \mathbb{R}^{n\times(p-1)}$，$\tilde{X}_j = (X_{1j}, ..., X_{nj})^T \in \mathbb{R}^{n\times 1}$，$W_k = diag(q_{C_1}(k), ..., q_{C_n}(k)) \in \mathbb{R}^{n\times n}$

$$\begin{aligned}
\mathcal{L}_k^{(2)}(\beta_k, \alpha_k) &= \frac{1}{2n}\sum_{i=1}^n q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 + \sum_{j=1}^p \operatorname{pen}\left(|\beta_{kj}|, \lambda_1\right) \\
&= \frac{1}{2n}\sum_{i=1}^n q_{C_i}(k)\left(y'_{ik} - X_{ij}\beta_{kj}\right)^2 + \sum_{j=1}^p \operatorname{pen}\left(|\beta_{kj}|, \lambda_1\right) \\
&= \frac{1}{2n}\sum_{i=1}^n q_{C_i}(k)\left(y'^2_{ik} - 2X_{ij}y'_i\beta_{kj} + X_{ij}^2\beta_{kj}^2\right) + \sum_{j=1}^p \operatorname{pen}\left(|\beta_{kj}|, \lambda_1\right) \\
&= \frac{1}{2n}\left(\tilde{X}_j^T W_k \tilde{X}_j \beta_{kj}^2 - 2\tilde{X}_j^T W_k y'_k \beta_{kj} + y'^T_k W_k y'_k\right) + \sum_{j=1}^p \operatorname{pen}\left(|\beta_{kj}|, \lambda_1\right) \\
&= \frac{\tilde{X}_j^T W_k \tilde{X}_j}{2n}\left(\beta_{kj} - \frac{\tilde{X}_j^T W_k y'_k}{\tilde{X}_j^T W_k \tilde{X}_j}\right)^2 + \operatorname{pen}\left(|\beta_{kj}|, \lambda_1\right) + C
\end{aligned} \tag{3.16}$$

其中 C 与 β_{kj} 无关，记 $u_{kj} = \tilde{X}_j^T W_k y'_k$，$l_{kj} = \tilde{X}_j^T W_k \tilde{X}_j$，使得上式最小的 β_{kj} 可表示为

$$\beta_{kj} = \begin{cases} \frac{S\left(\frac{u_{kj}}{l_{kj}}, \frac{n\lambda}{l_{kj}}\right)}{1 - \frac{n}{a l_{kj}}} = \frac{S\left(u_{kj}, n\lambda\right)}{l_{kj} - \frac{n}{a}} & \text{if } |\frac{u_{kj}}{l_{kj}}| \le a\lambda \\ \frac{u_{kj}}{l_{kj}} & \text{if } |\frac{u_{kj}}{l_{kj}}| > a\lambda \end{cases} \tag{3.17}$$

算法流程如 2

实验中，若 n=400, p=8 β_k 中非零项长度为 3（实验中设置 $\alpha_k = 0$，上面所有推导可忽略包含 α 项，同时包含 β, α 且不全为 0 的模型在第三部分实验），模型可以稳定收敛到

Algorithm 2: Version 2 with sparse penalty for β

Input ：数据 y, X，超参数 $n, p, K, a, \lambda, \rho$

Output: $\beta_k, k = 1, ..., K$ 的估计值

初始化 $q_{C_i}(k) = \frac{1}{K} + \mathrm{N}(0, 0.5^2), k = 1, ..., K, i = 1, ..., n$ 标准化，或用 flexmix 包结果初始化;

repeat

  for $k\ in\ 1 : K$ **do**

    $W_k = diag(q_{C_1}(k), ..., q_{C_n}(k))$;

    for $j\ in\ 1 : p$ **do**

      $u_{kj} = (\rho_k y - X_{(-j)}\beta_{k(-j)} - Z\alpha_k)^T W_k \tilde{X}_j$

      $l_{kj} = \tilde{X}_j^T W_k \tilde{X}_j$

      更新 $\beta_{kj}^{(iter)} = \begin{cases} \frac{u_{kj}}{l_{kj}} & \frac{u_{kj}}{l_{kj}} > a\lambda \\ \frac{S(\frac{u_{kj}}{l_{kj}}, n\lambda)}{1-\frac{n}{a}}, & \frac{u_{kj}}{L_{kj}} \leqslant a\lambda \end{cases}$

    end for

    更新 $\rho_k^{(iter)} = \frac{-B-\sqrt{B^2-4AC}}{2A}$.

      where $A = -y^T W_k y; B = (X\beta_k + Z\alpha_k)^T W_k y; C = 1_n^T W_k 1_n$.

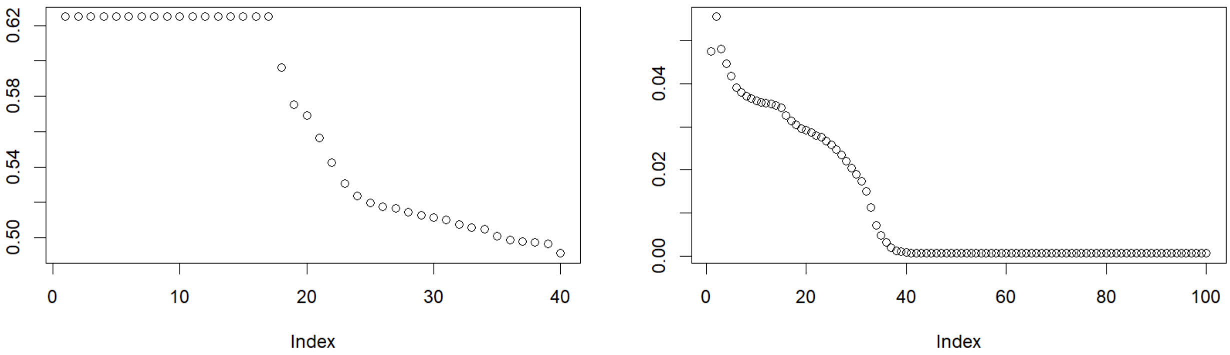
  end for

  计算基于 $\beta_k^{(iter)}$ 得到的后验概率 q_C

    $q_{C_i}^{(iter)}(k) = \frac{\pi_k^{(iter)} f_k(y_i; \beta_k^{(iter)}/\rho_k^{(iter)})}{\sum_{k'=1}^K \pi_{k'}^{(iter)} f_{k'}(y_i; \beta_{k'}^{(iter)}/\rho_k^{(iter)})}, k = 1, ..., K$

  更新 $\pi_k^{(iter)} = \frac{1}{n}\sum_{i=1}^n q_{C_i}^{(iter)}(k)$

until 收敛（$\frac{\|\beta^{(iter)}-\beta^{(iter-1)}\|}{\|\beta^{(iter)}\|}$小于临界值）；



(a) 全 0 初值　　(b) flexmix 初值

图 1: 基于两种初值的参数收敛曲线（仅有 β,α 稀疏惩罚）

真值，当增加误差项或者当 p 增大时，会出现 3,-3 项估计准确而 1,-1 被压为零，或调整参数后出现部分零项估计非零，整个向量偏离真值的情况。在困难情况下使用 flexmix 包作为储值可以收敛。

3.3 Version 3 - P for both β,α

此时目标函数表示为

$$\begin{aligned}\mathcal{L}^{(3)}(\beta,\alpha)=&\frac{1}{2n}\sum_{i=1}^{n}\sum_{k=1}^{K}q_{C_i}(k)\left(y_i\rho_k-X_i^T\beta_k-Z_i^T\alpha_k\right)^2\\&+\sum_{k=1}^{K}\sum_{j=1}^{p}\text{pen}\left(|\beta_{kj}|,\lambda_1\right)+\sum_{k=1}^{K}\sum_{s=1}^{q}\text{pen}\left(|\alpha_{ks}|,\lambda_1\right)\end{aligned}\tag{3.18}$$

当 β_k,α_k 不全为 0 向量时，同时更新 β_k, α_k 的计算流程与上面两种情况相似，只需要注意当更新 β_{kj} 时，对应 $y_i'=\rho_k y_i-X_{i(-j)^T}\beta_{k(-j)}-Z_i^T\alpha_k$，$j=1,2,...,p$；而更新 α_{ks} 时，对应 $y_i'=\rho_k y_i-Z_{i(-s)^T}\alpha_{k(-s)}-X_i^T\beta_k$，$s=1,2,...,q$；

在 p,q 较大时更新难度增大，图 1 对比了 $p=q=20$ 时全 0 初值及基于 flexmix 包结果继续迭代的参数距离真值距离随迭代次数变化曲线。

已经验证，该框架下 $\alpha=0$ 时结果与 Version 2 完全相同。

3.4 Version 4 - P for all

该部分在 Version 3（仅有 β,α 的稀疏惩罚）基础上加上类别压缩惩罚函数，目标函数

补全为最终的

$$
\begin{aligned}
\mathcal{L}^{(4)}(\beta,\alpha) =& \frac{1}{2n}\sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 \\
&+ \sum_{k=1}^{K}\sum_{j=1}^{p}\operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right) + \sum_{k=1}^{K}\sum_{s=1}^{q}\operatorname{pen}\left(|\alpha_{ks}|,\lambda_1\right) \\
&+ \sum_{k<k'}\operatorname{pen}\left(\sqrt{\|\beta_k-\beta_{k'}\|_2^2+\|\alpha_k-\alpha_{k'}\|_2^2},\lambda_2\right) \\
&+ \sum_{k<k'}\operatorname{pen}\left(\|\beta_k-\beta_{k'}\|_2,\lambda_3\right)
\end{aligned}
\tag{3.19}
$$

对应的增广拉格朗日函数为

$$
\begin{aligned}
\mathcal{L}^{(4)}(\beta,\alpha,u,v,\xi,\zeta) =& \frac{1}{2n}\sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 \\
&+ \sum_{k=1}^{K}\sum_{j=1}^{p}\operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right) + \sum_{k=1}^{K}\sum_{s=1}^{q}\operatorname{pen}\left(|\alpha_{ks}|,\lambda_1\right) \\
&+ \sum_{k<k'}\operatorname{pen}\left(\sqrt{\|v_{kk'}\|_2^2+\|w_{kk'}\|_2^2},\lambda_2\right) \\
&+ \sum_{k<k'}\operatorname{pen}\left(\|v_{kk'}\|_2,\lambda_3\right) \\
&+ \sum_{k<k'}\xi_{kk'}^T(\beta_k-\beta_k'-v_{kk'}) + \frac{\tau}{2}\sum_{k<k'}\|\beta_k-\beta_k'-v_{kk'}\|_2^2 \\
&+ \sum_{k<k'}\zeta_{kk'}^T(\alpha_k-\alpha_k'-w_{kk'}) + \frac{\tau}{2}\sum_{k<k'}\|\alpha_k-\alpha_k'-w_{kk'}\|_2^2
\end{aligned}
\tag{3.20}
$$

记 $H_1=\varepsilon\otimes I_p\in\mathbb{R}^{\frac{K(K-1)}{2}p\times Kp}, H_2=\varepsilon\otimes I_q\in\mathbb{R}^{\frac{K(K-1)}{2}q\times Kq}, \varepsilon=\{(e_k-e_{k'}),k<k'\}^T$. $e_k\in\mathbb{R}^{K\times1}$ 为独热向量，除了第 k 个元素为 1 外，其他元素都为 0；I_p,I_q 分别表示维度为 $p\times p, q\times q$ 的单位对角阵。

另外，记

$$
u_{kk'}=(v_{kk'}^T,w_{kk'}^T)^T \tag{3.21}
$$

则增广拉格朗日函数可以改写为

$$
\begin{aligned}
\mathcal{L}^{(4)}(\beta,\alpha,u,v,\xi,\zeta)= & \frac{1}{2n}\sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 \\
& +\sum_{k=1}^{K}\sum_{j=1}^{p}\operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right)+\sum_{k=1}^{K}\sum_{s=1}^{q}\operatorname{pen}\left(|\alpha_{ks}|,\lambda_1\right) \\
& +\sum_{k<k'}\operatorname{pen}\left(\|u_{kk'}\|_2,\lambda_2\right)+\sum_{k<k'}\operatorname{pen}\left(\|v_{kk'}\|_2,\lambda_3\right) \\
& +\frac{\tau}{2}\|H_1\beta - v + \frac{1}{\tau}\xi\|_2^2 - \frac{1}{2\tau}\|\xi\|_2^2 \\
& +\frac{\tau}{2}\|H_2\alpha - w + \frac{1}{\tau}\zeta\|_2^2 - \frac{1}{2\tau}\|\zeta\|_2^2
\end{aligned} \tag{3.22}
$$

若使用 scaled-form，分别记 ξ,ζ 为上面表达式的 $1/\xi, 1/\zeta$

$$
\begin{aligned}
\mathcal{L}^{(4)}(\beta,\alpha,u,v,\xi,\zeta)= & \frac{1}{2n}\sum_{i=1}^{n}\sum_{k=1}^{K} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 \\
& +\sum_{k=1}^{K}\sum_{j=1}^{p}\operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right)+\sum_{k=1}^{K}\sum_{s=1}^{q}\operatorname{pen}\left(|\alpha_{ks}|,\lambda_1\right) \\
& +\sum_{k<k'}\operatorname{pen}\left(\|u_{kk'}\|_2,\lambda_2\right)+\sum_{k<k'}\operatorname{pen}\left(\|v_{kk'}\|_2,\lambda_3\right) \\
& +\frac{\tau}{2}\|H_1\beta - v + \xi\|_2^2 - \frac{\tau}{2}\|\xi\|_2^2 \\
& +\frac{\tau}{2}\|H_2\alpha - w + \zeta\|_2^2 - \frac{\tau}{2}\|\zeta\|_2^2
\end{aligned} \tag{3.23}
$$

注意维度 $\beta \in \mathbb{R}^{Kp\times 1}, \alpha \in \mathbb{R}^{Kq\times 1}, u,\xi \in \mathbb{R}^{\frac{K(K-1)p}{2}\times 1}, w,\zeta \in \mathbb{R}^{\frac{K(K-1)q}{2}\times 1}$。

Update β_{kj} 式子 3.22 中与 β_{kj} 相关的项写为

$$
\begin{aligned}
\mathcal{L}^{(4)}(\beta_{kj}) &= \frac{1}{2n}\sum_{i=1}^{n} q_{C_i}(k)\left(y_i\rho_k - X_i^T\beta_k - Z_i^T\alpha_k\right)^2 + \operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right) + \frac{\tau}{2}\|H_1\beta - v + \xi\|_2^2 \\
&= \frac{1}{2n}\left(l_{kj}\beta_{kj}^2 - 2u_{kj}\beta_{kj}\right) + \frac{\tau}{2}\left(l'_{kj}\beta_{kj}^2 - 2u'_{kj}\beta_{kj}\right) + \operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right) + C(\beta_{kj}) \\
&= \frac{1}{2}\left(L_{kj}\beta_{kj}^2 - 2U_{kj}\beta_{kj}\right) + \operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right) + C(\beta_{kj}) \\
&= \frac{L_{kj}}{2}\left(\beta_{kj} - \frac{U_{kj}}{L_{kj}}\right)^2 + \operatorname{pen}\left(|\beta_{kj}|,\lambda_1\right) + C(\beta_{kj})
\end{aligned} \tag{3.24}
$$

其中 $C(\beta_{kj})$ 表示与 β_{kj} 无关的项，记号补充说明如下：

$$
\begin{cases}
l_{kj} = \tilde{X}_j^{\,T} W_k \tilde{X}_j \\
u_{kj} = \tilde{X}_j^{\,T} W_k \left(\rho_k y - X_{(-j)}\beta_{k(-j)} - Z\alpha_k\right) \\
l'_{kj} = (H_1^T H_1)_{kj,kj} \\
u'_{kj} = \left(H_1^T(v-\xi)\right)_{kj} - \beta^T_{(-kj)}(H_1^T H_1)_{kj,(-kj)} \\
L_{kj} = \dfrac{1}{n} l_{kj} + \tau l'_{kj} \\
U_{kj} = \dfrac{1}{n} u_{kj} + \tau u'_{kj}
\end{cases}
\tag{3.25}
$$

$W_k = diag(q_{C_1}(k), ..., q_{C_n}(k))$，解得

$$
\beta_{kj} = \begin{cases}
\frac{S\left(\frac{U_{kj}}{L_{kj}}, \frac{\lambda}{L_{kj}}\right)}{1-\frac{1}{aL_{kj}}} = \frac{S\left(U_{kj},\lambda\right)}{L_{kj}-\frac{1}{a}} & \text{if } |\frac{U_{kj}}{L_{kj}}| \leq a\lambda \\
\frac{U_{kj}}{L_{kj}} & \text{if } |\frac{U_{kj}}{L_{kj}}| > a\lambda
\end{cases}
\tag{3.26}
$$

Update α_{ks}　更新过程完全类似 β_{kj} 的更新。

Update $v_{kk'}, w_{kk'}$　式子 3.22 中与 $v_{kk'}, w_{kk'}$ 相关的项写为

$$
\begin{aligned}
\mathcal{L}^{(4)}(v_{kk'}, w_{kk'}) = & \sum_{k<k'} \text{pen}\left(\|u_{kk'}\|_2, \lambda_2\right) + \sum_{k<k'} \text{pen}\left(\|v_{kk'}\|_2, \lambda_3\right) \\
& + \frac{\tau}{2}\|H_1\beta - v + \xi\|_2^2 + \frac{\tau}{2}\|H_2\alpha - w + \zeta\|_2^2
\end{aligned}
\tag{3.27}
$$

记

$$
\begin{cases}
\overline{v_{kk'}} = \beta_k - \beta_{k'} + \xi_{kk'} \\
\overline{w_{kk'}} = \alpha_k - \alpha_{k'} + \zeta_{kk'}
\end{cases}
\tag{3.28}
$$

$$
\begin{cases}
u_{kk'} = (v_{kk'}^T, w_{kk'}^T)^T \\
\overline{u_{kk'}} = (\overline{v_{kk'}}^T, \overline{w_{kk'}}^T)^T
\end{cases}
\tag{3.29}
$$

更新分为四种情况

1. 若 $\|\overline{u_{kk'}}\|_2 > a\lambda_2$ 且 $\|\overline{v_{kk'}}\|_2 > a\lambda_3$，则 $w_{kk'} = \overline{w_{kk'}}$，$v_{kk'} = \overline{v_{kk'}}$;
2. 若 $\|\overline{u_{kk'}}\|_2 \leq a\lambda_2$ 且 $\dfrac{(1-\lambda_2/(\tau\|\overline{u}_{kk'}\|_2\|))_+}{1-1/(a\tau)}\|\overline{v_{kk'}}\|_2 > a\lambda_3$,
   则 $w_{kk'} = \dfrac{(1-\lambda_2/(\tau\|\overline{u}_{kk'}\|_2\|))_+}{1-1/(a\tau)}\overline{w_{kk'}}$，$v_{kk'} = \dfrac{(1-\lambda_2/(\tau\|\overline{u}_{kk'}\|_2\|))_+}{1-1/(a\tau)}\overline{v_{kk'}}$;

3. 若 $\|\overline{w_{kk'}}\|_2^2 + \left(\frac{(1-\lambda_3/(\tau\|\overline{v}_{kk'}\|_2\|))_+}{1-1/(a\tau)}\right)^2 \|\overline{v_{kk'}}\|_2^2 > (a\lambda_2)^2$ 且 $\|\overline{v_{kk'}}\|_2 \leq a\lambda_3$，
   则 $w_{kk'} = \overline{w_{kk'}}$，$v_{kk'} = \frac{(1-\lambda_3/(\tau\|\overline{v}_{kk'}\|_2\|))_+}{1-1/(a\tau)}\overline{v_{kk'}}$;

4. 否则，$w_{kk'} = \frac{\overline{w_{kk'}}}{1+\frac{pen'(u_{kk'},\lambda_2)}{\tau\|u_{kk'}\|_2}}$，$v_{kk'} = \frac{\overline{v_{kk'}}}{1+\frac{pen'(u_{kk'},\lambda_2)}{\tau\|u_{kk'}\|_2}+\frac{pen'(v_{kk'},\lambda_3)}{\tau\|v_{kk'}\|_2}}$

Update ξ, ζ

$$\begin{cases} \xi^{(t)} = \xi^{(t-1)} + H_1\beta^{(t)} - v^{(t)} \\ \zeta^{(t)} = \zeta^{(t-1)} + H_2\alpha^{(t)} - w^{(t)} \end{cases} \tag{3.30}$$

3.5 Notes

- $\lambda_2 = 0, \lambda_3 > 0$ 只对 β 进行压组操作，和 α 无关。由于两个惩罚共用相同的 a，若 $\lambda_2 > 0$ 则必有 $\lambda_3 > \lambda_2$;
- 不考虑 ρ，最后如果需要的话再加上。不加不会影响全局最优点，只可能影响收敛速度以及准确性;

References

[1] Yueyong Shi, Yuling Jiao, Yongxiu Cao, and Yan Yan Liu. An alternating direction method of multipliers for mcp-penalized regression with high-dimensional data. *Acta Mathematica Sinica, English Series*, 34:1892–1906, 2018.