Adjust covariance matrix D

2019-12-15

Given the parameters of the linear mixed effect models, i.e. $\beta_1, \beta_2, \Gamma_1, \Gamma_2, D_1, D_2$ and q, the dimension of the D_1 and D_2, the individual purity and the dataset purity can be expressed as:

$$g(\alpha) = g(w) = A_0 + A_1 x'\alpha + \frac{A_2}{2}\alpha' x x' \alpha \tag{1}$$

$$G(\alpha) = A_0 + A_1 \mu_x' \alpha + \frac{A_2}{2}\Big[\alpha' \Sigma_x \alpha + \alpha' \mu_x \mu_x' \alpha\Big] \tag{2}$$

where

$$A_0 = -q + \frac{1}{2}tr(D_2^{-1}D_1) + \frac{1}{2}tr(D_1^{-1}D_2) + \frac{1}{2}(\beta_1 - \beta_2)'(D_1^{-1} + D_2^{-1})(\beta_1 - \beta_2)$$

$$A_1 = (\beta_1 - \beta_2)'(D_1^{-1} + D_2^{-1})(\Gamma_1 - \Gamma_2)$$
$$A_2 = (\Gamma_1 - \Gamma_2)'(D_1^{-1} + D_2^{-1})(\Gamma_1 - \Gamma_2)$$

However, the D matrix is not stable enough. The inverse of D can return a quite large value, i.e. D is singular, we may modify D as $D^* = D + I$.

Since

$$(A + B)^{-1} = (I + A^{-1}B)^{-1}A$$

$$\begin{aligned} D^{-1} =& \Big((D + I) - I\Big)^{-1} \\ &= (I - (D + I)^{-1}I)^{-1}(D + I) \\ &= (I - (D + I)^{-1})^{-1}(D + I) \\ &= (I - D^{*-1})^{-1}D^* \end{aligned}$$

What is their relationship? the purity and purity*?

Ridge regression

Recall the **Linear mixed effect model**

$$Y = X\beta + Z\alpha + \epsilon$$

where Y is the observed vector with $n \times 1$, X is fixed effect design matrix with $n \times p$, β is $p \times 1$, and Z is $n \times q$, the design matrix with random effect. α is $q \times 1$. $Var(\alpha) = G, Var(\epsilon) = R$

Y is from a multivariate normal distribution, with mean equas to $X\beta$, covariance matrix $var(Y) = V = ZGZ'$.

Therefore, the joint distribution of α and Y is

$$\begin{bmatrix} \alpha \\ Y \end{bmatrix} \sim N\Big[\begin{bmatrix} 0 \\ X\beta \end{bmatrix}, \begin{bmatrix} G & GZ' \\ ZG & V \end{bmatrix}\Big]$$

The pdf is

$$f(y,\alpha) = f(y|\alpha)f(\alpha) = \frac{1}{(2\pi)^{(n+q)/2}|R|^{1/2}|G|^{1/2}} \exp\{-\frac{1}{2}[y-X\beta-Z\alpha]'R^{-1}[y-X\beta-Z\alpha]+\alpha'G^{-1}\alpha\}$$

We may then calculate the log likelihood. The derviations of the equation

$$-\frac{1}{2}[y-X\beta-Z\alpha]'R^{-1}[y-X\beta-Z\alpha]+\alpha'G^{-1}\alpha$$

with respect to β and α return:

$$\begin{bmatrix} X'R^{-1}X & X'R^{-1}Z \\ Z'R^{-1}X & Z'R^{-1}Z+G^{-1} \end{bmatrix}\begin{bmatrix} \hat{\beta} \\ \hat{\alpha} \end{bmatrix} = \begin{bmatrix} X'R^{-1}Y \\ Z'R^{-1}Y \end{bmatrix}$$

The solution of $\hat{\beta}$ and $\hat{\alpha}$ are

$$\hat{\beta} = (X'V^{-1}X)^{-1}X'V^{-1}Y$$
$$\hat{\alpha} = GZ'V^{-1}(Y - X\hat{\beta})$$

Previous papers consider the ridge regression with LME, since the matrix of X can be singular, i.e. $X'R^{-1}X$. Therefore, a penalty is added

$$\begin{bmatrix} X'R^{-1}X+kI & X'R^{-1}Z \\ Z'R^{-1}X & Z'R^{-1}Z+G^{-1} \end{bmatrix}\begin{bmatrix} \hat{\beta} \\ \hat{\alpha} \end{bmatrix} = \begin{bmatrix} X'R^{-1}Y \\ Z'R^{-1}Y \end{bmatrix}$$

Few people dealed with singular G matrix. Since the dimension of X and Z are not necessary to be equal, therefore the random effect can be modified to the appropriate dimension.

Following the above idea, can we add a penalty as

$$\begin{bmatrix} X'R^{-1}X & X'R^{-1}Z \\ Z'R^{-1}X & Z'R^{-1}Z+(G+kI)^{-1} \end{bmatrix}\begin{bmatrix} \hat{\beta} \\ \hat{\alpha} \end{bmatrix} = \begin{bmatrix} X'R^{-1}Y \\ Z'R^{-1}Y \end{bmatrix}$$

Then

$$\hat{\alpha} = (Z'R^{-1}Z + (G+kI)^{-1})^{-1}Z'R^{-1}(Y - X\hat{\beta})$$
$$\hat{\beta} = (X'R^{-1}X)^{-1}X'R^{-1}(Y - Z\hat{\alpha})$$

substituting α into β hat