

# Penalty on the random effect covariance matrix

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In the EMBARC data, after fitting the LME with random effect for the quadric term, the covariance matrix  $D$  can be almost singular, i.e, with large inverse values. For example, the covariance for drug group is,

	tt	I(tt^2)
tt	1.0157249	-0.1040613
I(tt^2)	-0.1040613	0.0149248

The inverse is

	tt	I(tt^2)
tt	3.446265	24.0287
I(tt^2)	24.028696	234.5401

If we add a penalty on the covariance, it may restrict the inverse of the matrix in a reasonable range and therefore decreases the variance of the estimation. However, on the other hand, the bias is induced.

There are two ways to add the penalty, one is

$$D^* = D + \lambda I$$

where  $I$  is the identity matrix, or

$$D^* = D + I^*$$

where  $I^* = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \lambda \end{pmatrix}$

We conduct simulation to see how the estimation of  $\alpha$  and purity vary as the  $\lambda$  value change in the above two approach.

## Simulation

### Parameter settings

Outcome data were generated from the model

$$Y_i \sim N(\beta_i + \Gamma_i(\alpha'X), D_i), i = \{1, 2\}$$

where

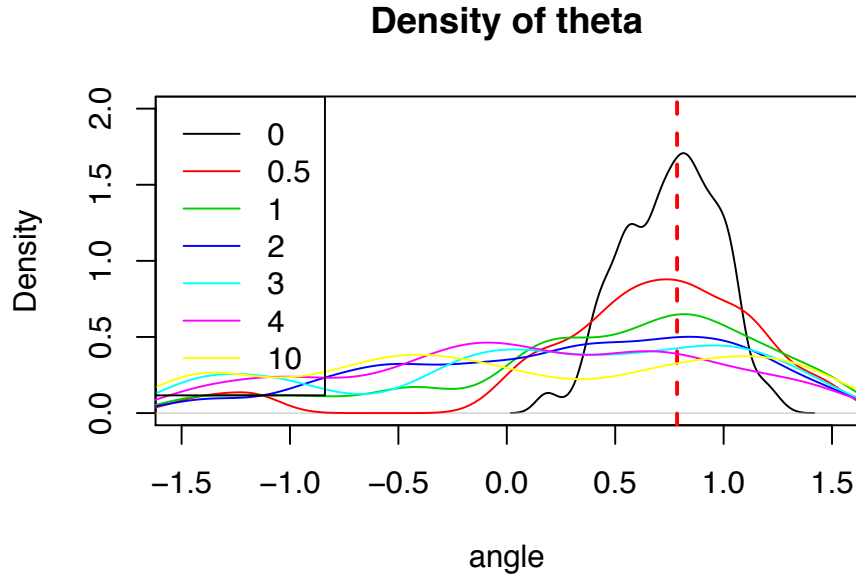
- $\beta_1 = [0, 3.1, 1]'$ ,  $\beta_2 = [0, 3, 0.9]'$
- $\Gamma_1 = [0, 1, 0]'$ ,  $\Gamma_2 = [0, 0, 1]'$ , the angle between  $\Gamma_1$  and  $\Gamma_2$  was set as  $\frac{\pi}{2}$
- $D_1$  and  $D_2$  are the same as the estimation in the EMBARC dataset
- $X \sim MVN\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$
- $\alpha$  can be set as  $\alpha = (\cos(\theta), \sin(\theta))$ . The true  $\alpha$  is set as  $(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})$ , i.e.  $\theta = \frac{\pi}{2}$

Let  $\lambda$  vary within 0, 0.5, 1, 2, 3, 4, 10. 1000 iterations were conducted for each  $\lambda$ . The estimated  $\hat{\alpha}$  and associated  $\hat{\theta}$  and purity were saved.

## Results

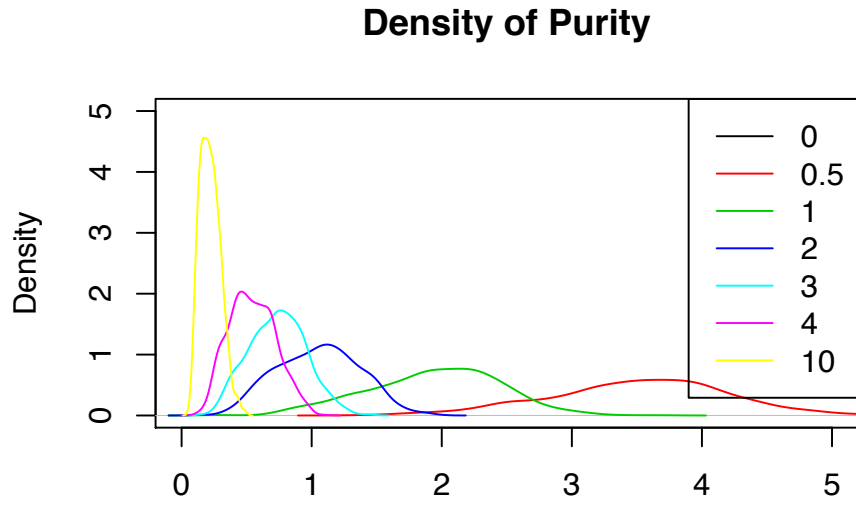
**Penalty approach 1**,  $D^* = D + \lambda I$ .

The following plots draw the histogram of estimated  $\hat{\theta}$  under different  $\lambda$



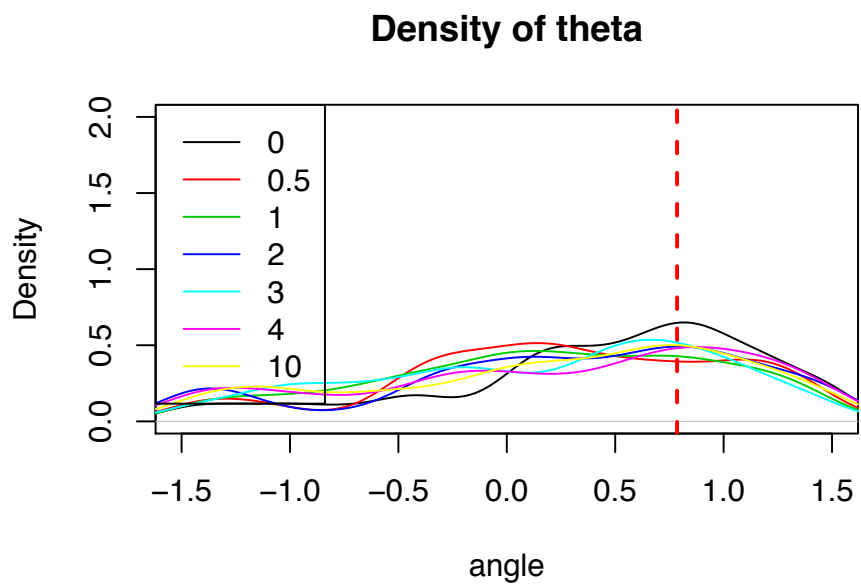
The red vertical line shows the true  $\theta = \frac{\pi}{2}$ .

The purity plots



**Penalty approach 2**,  $D^* = D + I^*$ .

The following plots draw the histogram of estimated  $\hat{\theta}$  under different  $\lambda$



The red vertical line shows the true  $\theta = \frac{\pi}{2}$ .

The purity plots

