Penalty on the random effect covariance matrix

2019-01-18

In the EMBARC data, after fitting the LME with random effect for the quadrict term, the covariance matrix D can be almost singular, i.e, with large inverse values. For example, the convariance 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 α and purity vary as the λ value change in the above two approach.

Simulation

Parameter sittings

Outcome data were generated from the model

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

where

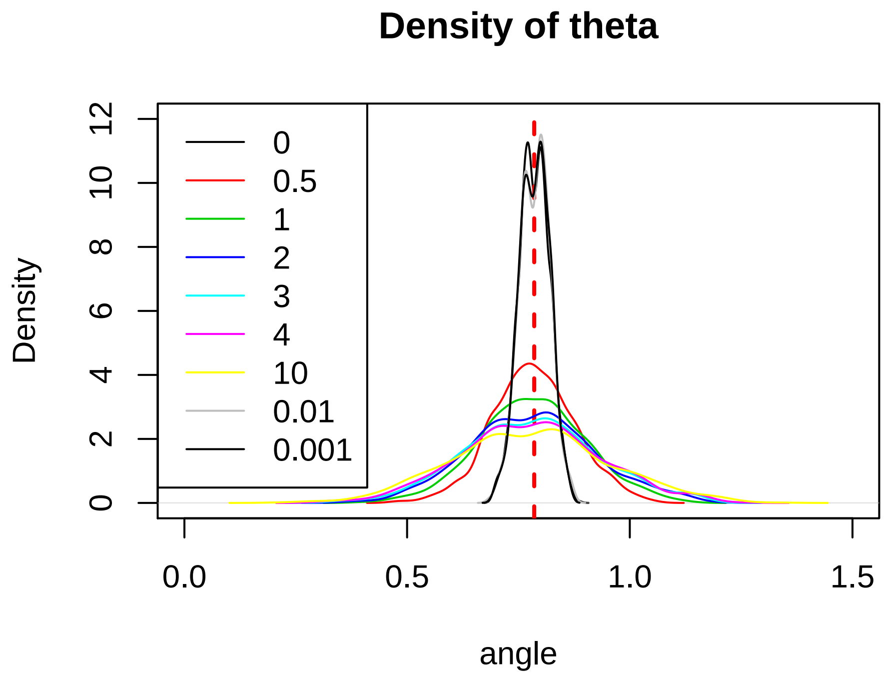
- $\beta_1 = [0, 3.1, 1]', \beta_2 = [0, 3, 0.9]'$
- $\Gamma_1 = [0, 1, 0]', \Gamma_2 = [0, 0, 1]'$, the angle between Γ_1 and Γ_2 was set as $\frac{\pi}{2}$
- D_1 and D_2 are the same as the esimation in the EMBARC dataset
- $X \sim MVN(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix})$
- α can be set as $\alpha = (\cos(\theta), \sin(\theta))$. The true α is set as $(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})$, i.e. $\theta = \frac{\pi}{2}$

Let λ vary within $0, 0.001, 0.01, 0.5, 1, 2, 3, 4, 10$. 1000 iterations were conducted for each λ. The estimated $\hat{\alpha}$ and associated $\hat{\theta}$ and purity were saved.

Results

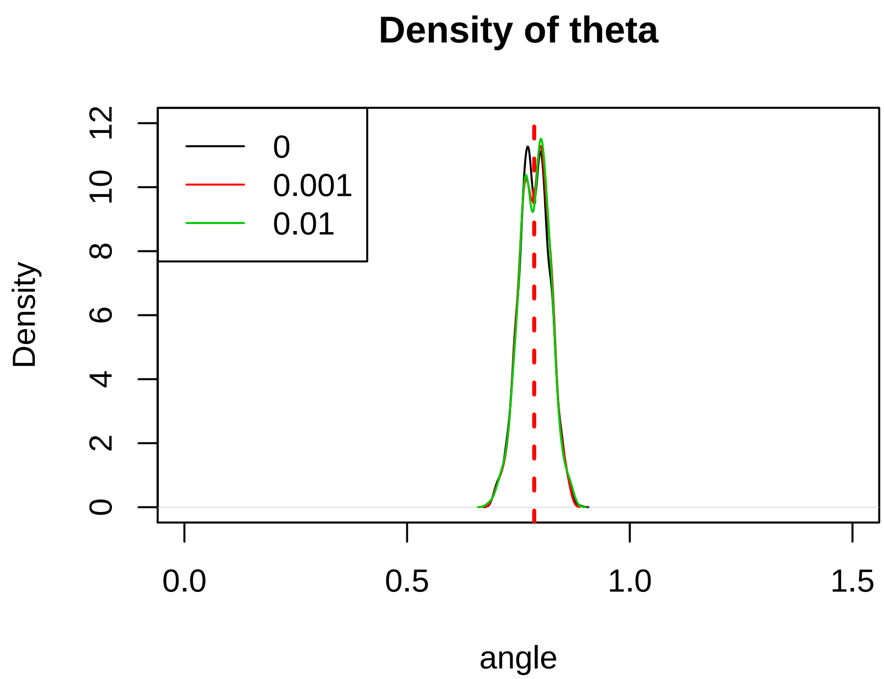
Penalty approach 1, $D^* = D + \lambda I$.

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



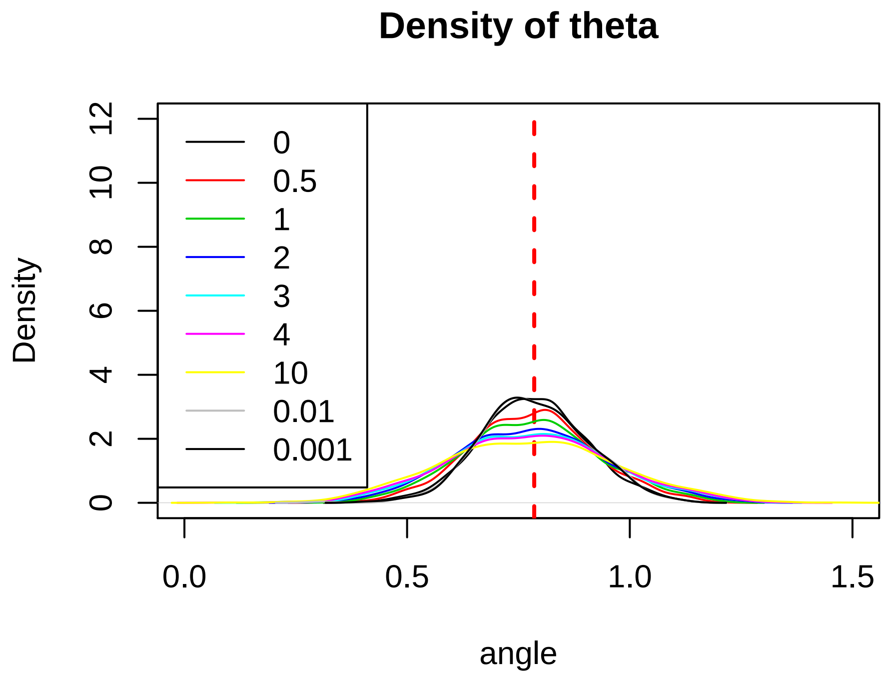
The red vertial line shows the true $\theta = \frac{\pi}{2}$.

Let's look at the scenarios with small $\lambda = 0, 0.001, 0.01$.



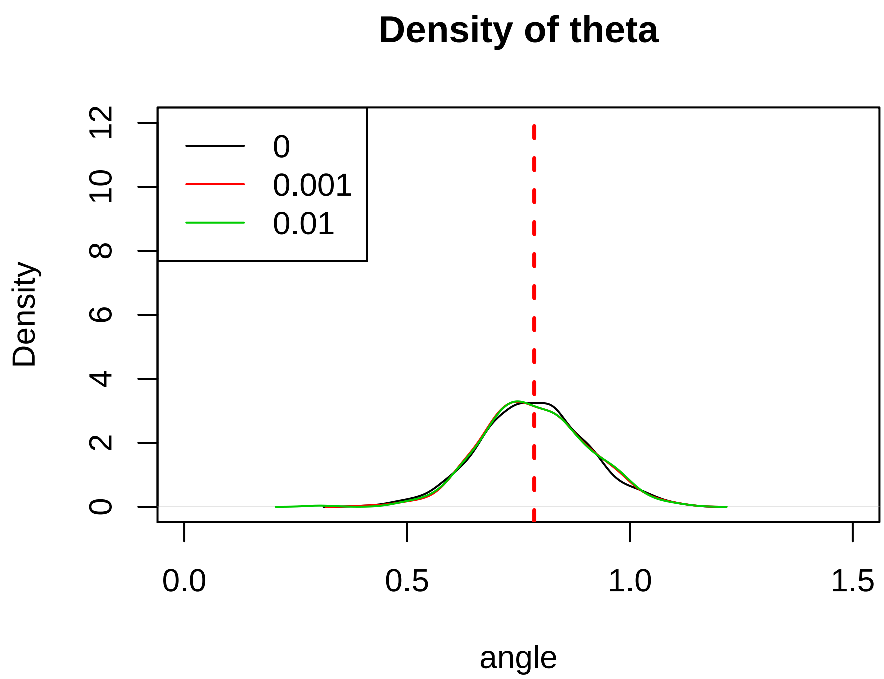
Penalty approach 2, $D^* = D + I^*$.

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

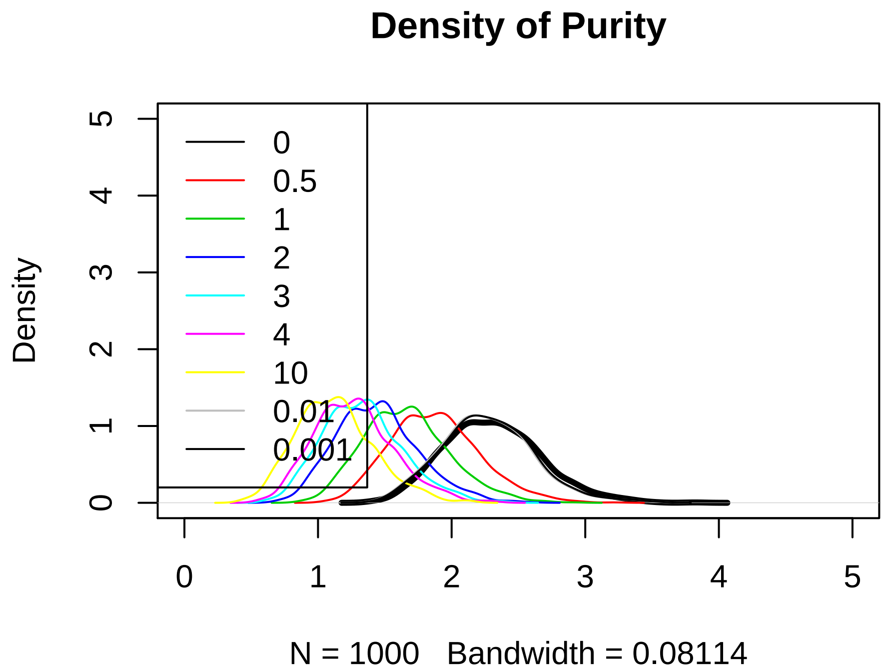


The red vertial line shows the true $\theta = \frac{\pi}{2}$.

Let's look at the scenarios with small $\lambda = 0, 0.001, 0.01$.



The purity plots


Density of Purity
Density
0
0.5
1
2
3
4
10
0.01
0.001
0 1 2 3 4 5
N = 1000 Bandwidth = 0.08114