


$$\begin{pmatrix} 1 & 0.999 \\ 0.999 & 1 \end{pmatrix}$$


Boundary Estimation Problem

ML and REML $\hat{\Sigma}$ are close to not being positive definite (degenerate, singular).

- Most variables have zero variances or some variables are a linear combination of others.

p. 140

```
> fit2u.alt <- lme4::lmer(LYMP ~ Phase * Time + (Phase * Time | ID), , REML=F,
  control=lme4::lmerControl(optCtrl=list(maxfun=1e5)))
boundary (singular) fit: see help('isSingular')

> fit2u <- nlme::lme(fixed=LYMP ~ Phase * Time, random=~Phase * Time | ID, data=, method="ML",
  control=nlme::lmeControl(opt="optim", optCtrl=list(maxit=1e5)))
```

In Bayesian statistics, the Wishart distribution is the conjugate prior for the inverse covariance matrix (i.e., the precision matrix $\Omega = \Sigma^{-1}$) of a multivariate normal random vector.

$$\Omega \sim \mathcal{W}(\Psi^{-1}, \nu) \quad \text{Degrees of freedom } \nu > p - 1 \quad \Omega \mid \text{Data} \sim \mathcal{W}((n\mathbf{S} + \Psi)^{-1}, n + \nu)$$

$$\mathbb{E}[\Omega] = \nu \Psi^{-1} \quad \text{Scale matrix } \Psi_{p \times p}^{-1} > 0$$

$$\text{Omega} \sim \text{dwish}(\text{Psi}, \text{nu}) \quad \text{\#JAGS} \quad \text{Omega} \sim \text{wishart}(\text{nu}, \text{InvPsi}); \quad \text{\#Stan}$$

Alternatively, the inverse-Wishart distribution is the conjugate prior for the covariance matrix.

$$\Sigma \sim \mathcal{W}^{-1}(\Psi, \nu) \quad \text{Degrees of freedom } \nu > p - 1 \quad \Sigma \mid \text{Data} \sim \mathcal{W}^{-1}(n\mathbf{S} + \Psi, n + \nu)$$

$$\mathbb{E}[\Sigma] = \frac{\Psi}{\nu - p - 1} \quad \text{for } \nu > p + 1 \quad \text{Scale matrix } \Psi_{p \times p} > 0$$

$$\text{Sigma} \sim \text{inv_wishart}(\text{nu}, \text{Psi}); \quad \text{\#Stan}$$

Remark: If $\Sigma \sim \mathcal{W}\left(\frac{\mathbf{I}_{p \times p}}{2\theta}, \nu\right)$, then $p(\Sigma) \propto \prod_{r=1}^p f_{\Gamma}\left(\lambda_r; \frac{\nu - p + 1}{2}, \theta\right)$. p. 142-143, eq. 6

```
> dgamma(.001, shape=1.5, rate=10^-4) #~0
```

$$(u_{0i}, u_{1i})^{\top} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}_2(\mathbf{0}, \Sigma) \quad \text{and} \quad \Sigma \equiv \begin{pmatrix} \sigma_0^2 & \rho \sigma_0 \sigma_1 \\ \rho \sigma_0 \sigma_1 & \sigma_1^2 \end{pmatrix} \quad \text{for } p = 2 \quad (1)$$

$$\Sigma \sim \mathcal{W}^{-1}((\nu_0 - 3) \cdot \mathbf{S}, \nu_0) \quad \text{Both prior and posterior means are the sample covariance matrix.} \quad (2.1)$$

$$\Sigma \sim \mathcal{W}^{-1}(\mathbf{I}_{2 \times 2}, 2) \quad \text{A multivariate generalization of the inverse-gamma distribution.} \quad (2.2)$$

$$\rho \sim U[-1, 1], \quad \sigma_0^2 \sim \text{Inv-Gamma}(10^{-4}, 10^{-4}), \quad \sigma_1^2 \sim \text{Inv-Gamma}(10^{-4}, 10^{-4}) \quad (2.3)$$

$$\rho \sim U[-1, 1], \quad \sigma_0 \sim U[0, \infty), \quad \sigma_1 \sim U[0, \infty) \quad \text{Unconstrained?} \quad (2.4)$$

$$\rho \sim U[-1, 1], \quad \sigma_0 \sim HC(0, 25), \quad \sigma_1 \sim HC(0, 25) \quad (2.5)$$

$$\Sigma \sim \mathcal{W}(5 \times 10^3 \cdot \mathbf{I}_{2 \times 2}, 4) \quad \text{Let } \theta \text{ be sufficiently small and } \nu = p + 2 \text{ by default.} \quad (2.6)$$

DISCUSSIONS

$$Y_{it} = \left(\underset{\text{fixed intercept}}{\beta_0} + \underset{\text{random intercept}}{u_{0i}} \right) + \left(\underset{\text{fixed slope}}{\beta_1} + \underset{\text{random slope}}{u_{1i}} \right) \cdot t + \epsilon_{it} \quad \text{p. 144}$$

1. What are fixed effects and random effects?
- assumed to be constant for all trials - a subset of the entire population of treatments

2. What is restricted maximum likelihood (REML)?
ML is generally preferred when comparing models with different fixed effects. p. 139

3. Does $|\hat{\Sigma}| > 0$ imply that $\hat{\Sigma} > 0$ and $\hat{\Sigma}^{-1}$ exists? <https://rpubs.com/sherloconan/1015445>

one negative eigenvalue

```
> issue <- matrix(c(1.1295254, 0.4658979, -0.8727553, -0.2521035,
  0.4663502, 1.1937169, -0.9350007, -0.4105077,
  -0.8733574, -0.9346202, 1.1152784, 0.1664068,
  -0.2525762, -0.4106099, 0.1664256, 0.4964147), ncol=4, byrow=T)
```

eigenvalue close to zero

```
> singular <- matrix(c(0.7573508, 0.6297603, -0.78943891, -0.28205123,
  0.6305914, 1.2464388, -1.23028009, -0.53885046,
  -0.7887137, -1.2304128, 1.65066378, 0.08047224,
  -0.2813410, -0.5389635, 0.08109029, 0.78802955), ncol=4, byrow=T)
```

two negative eigenvalues

```
> error <- matrix(c(1.0466132, 1.1008902, -1.3268045, -0.7891338,
  1.1003529, 0.9572582, -1.2419223, -0.7404087,
  -1.3267065, -1.2419124, 1.2020524, 0.7253173,
  -0.7893596, -0.7404482, 0.7249186, 0.7322508), ncol=4, byrow=T)
```

```
> error.sym <- (error + t(error)) / 2
```

```
> CholWishart::dWishart(error.sym, 5, diag(4), log=T) #ERROR
```

R only has a default function `stats::rWishart` to generate random Wishart distributed matrices.

Other packages:

`CholWishart::dWishart` can compute the density of a random Wishart distributed matrix.

`MCMCpack::riwish` can generate a random inverse-Wishart distributed matrix.

`LaplacesDemon::rinvwishart` also generates a random inverse-Wishart distributed matrix.

4. Why Bayes modal (BM) estimation? p. 141, eq. 4
- viewed as maximum penalized likelihood estimation where the prior is a penalty function

5. Constrained data type and variable declaration in Stan

```
parameters {
  cov_matrix[4] Sigma; // 4x4 covariance matrix
}
```