# **Implementation of Gibbs Sampler**

#### **Full conditional distributions**

Gibbs sampler is the algorithm to sample each unknown variable based on their full conditional distributions. For each iteration of Gibbs sampler, we sample each parameter from their full conditional distributions and iterate through all the parameters. To present the full conditional distribution for all the parameters, we first re-express the model in matrix form.

$$\begin{aligned} \mathbf{y} &= \mathbf{1}\mu + \mathbf{Z}_{\mathbf{g}} \, g + \mathbf{Z}_{\mathbf{h}} \, \mathbf{h} + (\mathbf{Z}_{\mathbf{g}} \, \mathbf{b}) \# (\mathbf{Z}_{\mathbf{h}} \, \mathbf{h}) + \mathbf{\epsilon} \\ \\ &= \mathbf{1}\mu + \mathbf{Z}_{\mathbf{g}} \mathbf{L}_{\mathbf{A}} \boldsymbol{\delta}_{\mathbf{g}} + \mathbf{Z}_{\mathbf{h}} \, \mathbf{L}_{\mathbf{H}} \boldsymbol{\delta}_{\mathbf{h}} + (\mathbf{Z}_{\mathbf{g}} \, \mathbf{L}_{\mathbf{A}} \boldsymbol{\delta}_{\mathbf{b}}) \# [\mathbf{Z}_{\mathbf{h}} \, \mathbf{L}_{\mathbf{H}} \boldsymbol{\delta}_{\mathbf{h}} \, ] + \mathbf{\epsilon} \end{aligned}$$

Where # represents element wise product between two vectors,  $\mathbf{y}$  is a vector of observed phenotypes,  $\mathbf{g}$  is a vector for the main genotype effects,  $\mathbf{Z}_{\mathbf{g}}$  is the incidence matrix that relates each level of  $\mathbf{g}$  to  $\mathbf{y}$ ,  $\mathbf{h}$  is a vector for the main environment effects,  $\mathbf{Z}_{\mathbf{h}}$  is the incidence matrix that related each level of  $\mathbf{h}$  to  $\mathbf{y}$ ,  $\mathbf{b}$  is the regression of the varieties on the main environmental effect. Instead of sampling  $\mathbf{b}$ ,  $\mathbf{g}$ ,  $\mathbf{h}$  directly, we transform them into orthogonal bases as  $\mathbf{\delta}_{\mathbf{g}} = \mathbf{L}_{\mathbf{A}}^{-1}\mathbf{g}$ ,  $\mathbf{\delta}_{\mathbf{b}} = \mathbf{L}_{\mathbf{A}}^{-1}\mathbf{b}$  and  $\mathbf{\delta}_{\mathbf{h}} = \mathbf{L}_{\mathbf{H}}^{-1}\mathbf{h}$  where  $\mathbf{L}_{\mathbf{A}}$  and  $\mathbf{L}_{\mathbf{H}}$  are lower triangular matrix from the Cholesky decomposition of  $\mathbf{A}$  and  $\mathbf{H}$  ( $\mathbf{L}_{\mathbf{A}}\mathbf{L}_{\mathbf{A}'} = \mathbf{A}$ ,  $\mathbf{L}_{\mathbf{H}}\mathbf{L}_{\mathbf{H}'} = \mathbf{H}$ ). The  $\mathbf{\delta}_{\mathbf{g}}$ ,  $\mathbf{\delta}_{\mathbf{b}}$  and  $\mathbf{\delta}_{\mathbf{h}}$  all follow IID Normal distribution:  $\mathbf{\delta}_{\mathbf{g}} \sim \mathbf{N}(\mathbf{0}, \mathbf{I}\sigma_{g}^{2})$ ,  $\mathbf{\delta}_{\mathbf{b}} \sim \mathbf{N}(\mathbf{0}, \mathbf{I}\sigma_{b}^{2})$  and  $\mathbf{\delta}_{\mathbf{h}} \sim \mathbf{N}(\mathbf{0}, \mathbf{I}\sigma_{b}^{2})$ .

### **Observation 1**

For any model  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ , when sampling a location parameter  $\beta_i$  in the model, all other parameters will be treated as known. Let  $\tilde{\mathbf{y}} = \mathbf{y} - \mathbf{X}_{-i} \boldsymbol{\beta}_{-i} = \mathbf{X}_{i} \beta_{i} + \boldsymbol{\epsilon}$ , the

conditional distribution of the new data vector  $\tilde{\mathbf{y}}$  will be  $p(\tilde{\mathbf{y}}|\mathbf{X}_{\mathbf{i}}\beta_i) \sim N(\mathbf{X}_{\mathbf{i}}\beta_i, \mathbf{I}\sigma_{\epsilon}^2)$ . Now let the prior distribution be  $\boldsymbol{\beta} \sim N(\mathbf{0}, \mathbf{I}\sigma_{\beta}^2)$ ,  $\sigma_{\epsilon}^2 \sim \chi^{-2}(\nu_{\epsilon}, S_{\epsilon}^2)$  and  $\sigma_{\beta}^2 \sim \chi^{-2}(\nu_{\beta}, S_{\beta}^2)$ , we will have the following full conditional posterior distribution for  $\beta_i$ ,  $\sigma_{\epsilon}^2$  and  $\sigma_{\beta}^2$  as:

$$p(\beta_i | \text{ELSE}) \sim N(C^{-1}r, C^{-1}), \text{ where } C = \frac{\mathbf{x_i}^T \mathbf{x_i}}{\sigma_{\epsilon}^2} + \frac{1}{\sigma_{\beta}^2} \text{ and } \mathbf{r} = \frac{\mathbf{x_i}^T \tilde{\mathbf{y}}}{\sigma_{\epsilon}^2}$$

$$p(\sigma_{\epsilon}^2 | \text{ELSE}) \sim \chi^{-2} (n + \nu_{\epsilon}, \frac{\nu_{\epsilon} S_{\epsilon}^2 + \epsilon' \epsilon}{n + \nu_{\epsilon}}), \text{ where n is the number of observations}$$

$$p(\sigma_{\beta}^2 | \text{ELSE}) \sim \chi^{-2} (q_{\beta} + \nu_{\beta}, \frac{\nu_{\beta} S_{\beta}^2 + \beta^T \beta}{q_{\beta} + \nu_{\beta}}), \text{ where } q_{\beta} \text{ is the number of levels in } \boldsymbol{\beta}.$$

We can use the rules of Observation 1 to express the full conditional distributions for the unknown parameters. In table 2, we listed the  $\mathbf{X_i}$  and C for each of the location parameters for  $\mu$ ,  $\delta_{h_i}$ ,  $\delta_{b_i}$  and  $\delta_{g_i}$ .

Table 1 The X and C needed to obtain the full conditional distributions for  $\mu$ ,  $\delta_{h_i}$ ,  $\delta_{b_i}$  and  $\delta_{g_i}$  from Observation 1.

Parameters	X <sub>i</sub>	С
μ	1	$rac{11'}{\sigma_{\epsilon}^2}$
$\delta_{h_{m{i}}}$	$Z_h L_{H_i} \# (Z_g b + 1)$	$\frac{\mathbf{X_i}'\mathbf{X_i}}{\sigma_{\epsilon}^2} + \frac{1}{\sigma_h^2}$
$\delta_{b_i}$	$(\mathbf{Z_h}\mathbf{h})\#(\mathbf{Z_g}\mathbf{L_A}_i)$	$\frac{\mathbf{X_i}'\mathbf{X_i}}{\sigma_\epsilon^2} + \frac{1}{\sigma_h^2}$
$\delta_{g_{i}}$	$\mathbf{Z_g}\mathbf{L_A}_i$	$\frac{\mathbf{X_i}'\mathbf{X_i}}{\sigma_{\epsilon}^2} + \frac{1}{\sigma_g^2}$

The full conditional distributions for the variance components will be:

$$p(\sigma_{\epsilon}^{2}|\text{ELSE}) \sim \chi^{-2}(n + \nu_{\epsilon}, \frac{\nu_{\epsilon}S_{\epsilon}^{2} + \epsilon'\epsilon}{n + \nu_{\epsilon}}), \ \sigma_{g}^{2}|\text{ELSE} \sim \chi^{-2}(q_{g} + \nu_{g}, \frac{\nu_{g}S_{g}^{2} + \delta_{g}'\delta_{g}}{q_{g} + \nu_{g}}), \ \sigma_{b}^{2}|\text{ELSE} \sim \chi^{-2}(q_{g} + \nu_{b}, \frac{\nu_{b}S_{b}^{2} + \delta_{b}'\delta_{b}}{q_{g} + \nu_{b}}) \ \text{and} \ \sigma_{h}^{2}|\text{ELSE} \sim \chi^{-2}(q_{h} + \nu_{h}, \frac{\nu_{h}S_{h}^{2} + \delta_{h}'\delta_{h}}{q_{h} + \nu_{h}}), \ \text{where} \ q_{g} \ \text{is the}$$
 number of levels for the varieties, and  $q_{h}$  is the number of levels for the environments.

### **Implementation of Gibbs Sampler**

For each iteration of Gibbs Sampler, we sample each parameter from their full conditional distributions, the detailed implementation is as following:

- 1. Set initial values for all the parameters.
- 2. Set initial values for missing values of y (denote here as  $y_{NA}$ ).
- 3. Sample  $\delta_{h_i}$ , and update  $\epsilon$ . Do this for all i from 1 to  $q_h$ .
- 4. Sample  $\delta_{b_i}$  and update  $\epsilon$ . Sample  $\delta_{g_i}$  and update  $\epsilon$ . Do this for all i from 1 to  $q_g$ .
- 5. Sample  $\sigma_{\epsilon}^2$ ,  $\sigma_h^2$ ,  $\sigma_b^2$ ,  $\sigma_g^2$  from their full conditional distributions.
- 6. Sample  $\mu$  and update  $\epsilon$ .
- 7. Update  $\hat{y}=y-\epsilon$ .
- 8. Sample  $\mathbf{y}_{\mathrm{NA}}$  from N( $\widehat{\mathbf{y}}_{\mathrm{NA}}$  ,  $\mathbf{I}\sigma_{\epsilon}^{2}$ ). Update  $\mathbf{y}_{\mathrm{NA}}$  and  $\epsilon$ .
- 9. Repeat steps 2 through 8 for the number of specified iterations.

## References

Su, G., P. Madsen, M. S. Lund, D. Sorensen, I. R. Korsgaard, and J. Jensen. 2006. Bayesian analysis of the linear reaction norm model with unknown covariates. Journal Of Animal Science. 84:1651-1657.