

Appendices to “To Center or Not to Center: That is Not the Question — An Ancillarity-Sufficiency Interweaving Strategy (ASIS) for Boosting MCMC Efficiency”

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A Auxiliary Material for Section 3

A.1 Details of the MCMC Steps in the Poisson Time Series Example

Step 1: This step consists of T substeps, one for each $t = 1, \dots, T$.

For substep t , the target conditional density is

$$p(\xi_t | \xi_{t-1}, \xi_{t+1}, \beta, \rho, \delta, Y) \propto \exp\{-(\xi_t - \mu_t)^2 / (2\sigma_t^2) - d_t e^{X_t \beta + \xi_t}\},$$

where $\mu_t = (Y_t \delta^2 + (\xi_{t-1} + \xi_{t+1})\rho) / (1 + \rho^2)$, $\sigma_t^2 = \delta^2 / (1 + \rho^2)$, if $t \neq 1$ and $t \neq T$, and $\mu_1 = Y_1 \delta^2 + \xi_2 \rho$, $\mu_T = Y_T \delta^2 + \xi_{T-1} \rho$, $\sigma_1^2 = \sigma_T^2 = \delta^2$.

Define $l_t(\xi_t) = \log p(\xi_t | \xi_{t-1}, \xi_{t+1}, \beta, \rho, \delta, Y)$. First, use Newton-Raphson to locate the mode x of l_t and then calculate $l_t''(x)$. Then draw t_5 according to a t distribution with 5 degrees of freedom, and propose $\xi_t^{new} = x + t_5 / \sqrt{-l_t''(x)}$. Draw a uniform random number u between 0 and 1. Accept ξ_t^{new} if

$$u \leq \exp\{l_t(\xi_t^{new}) - l_t(\xi_t^{old}) - h(\xi_t^{new}) + h(\xi_t^{old})\},$$

where $h(\cdot)$ is the log density of t_5 centered at x with scale $1/\sqrt{-l_t''(x)}$.

Step 2_A: The target conditional density is

$$p(\beta | \xi, \rho, \delta, Y) \propto \exp\left\{\sum_t (Y_t X_t \beta - d_t e^{X_t \beta + \xi_t})\right\}.$$

Define $l(\beta) = \log p(\beta | \xi, \rho, \delta, Y)$. First, use Newton-Raphson to locate the mode $\hat{\beta}$ of l , and compute $I = -\partial^2 l(\hat{\beta}) / \partial \beta \partial \beta^\top$. (This amounts to fitting a Poisson GLM and computing

the MLE and the observed Fisher information.) Draw T_5 according to a p-variate t_5 , and propose $\beta^{new} = \hat{\beta} + I^{-1/2}T_5$. Draw $u \sim U(0, 1)$, and accept β^{new} if

$$u \leq \exp\{l(\beta^{new}) - l(\beta^{old}) - H(\beta^{new}) + H(\beta^{old})\},$$

where $H(\cdot)$ is the log density of T_5 centered at $\hat{\beta}$ and with scale $I^{-1/2}$.

Step 2_S: The target conditional density $p(\beta|\eta, \rho, \delta, Y)$ is multivariate normal.

Let $Z^\top = (Z_1^\top, \dots, Z_T^\top)$, where $Z_1 = \sqrt{1 - \rho^2}X_1$ and $Z_t = X_t - \rho X_{t-1}$, $t \geq 2$. Let $\tilde{\eta} = (\sqrt{1 - \rho^2}\eta_1, \eta_2 - \rho\eta_1, \eta_3 - \rho\eta_2, \dots, \eta_T - \rho\eta_{T-1})^\top$. Compute $\hat{\beta} = (Z^\top Z)^{-1}Z^\top \tilde{\eta}$, and then draw $\beta^{new} \sim N_p(\hat{\beta}, (Z^\top Z)^{-1}\delta^2)$. Set $\xi_t^{new} = \eta_t - X_t\beta^{new}$.

Step 3_S: The target conditional density is

$$p(\rho, \delta|\beta, \xi, Y) \propto \delta^{-T} \exp\left\{-\frac{1}{2\delta^2} \left[(1 - \rho^2)\xi_1^2 + \sum_{t=2}^T (\xi_t - \rho\xi_{t-1})^2 \right]\right\}.$$

Compute $\hat{\rho} = \sum_{t=2}^T \xi_t \xi_{t-1} / \sum_{t=2}^{T-1} \xi_t^2$ and $\hat{\delta}^2 = (1 - \hat{\rho}^2)\xi_1^2 + \sum_{t=2}^T (\xi_t - \hat{\rho}\xi_{t-1})^2$. Draw $\delta_{new}^2 = \hat{\delta}^2 / \chi_{T-2}^2$, and $\rho_{new} \sim N(\hat{\rho}, \delta_{new}^2 / \sum_{t=2}^{T-1} \xi_t^2)$, where χ_{T-2}^2 is a χ^2 random variable with $T - 2$ degrees of freedom. Accept δ_{new}^2 and ρ_{new} if $-0.99 \leq \rho_{new} \leq 0.99$.

Step 3_A: The target conditional density is

$$p(\rho, \delta|\beta, \kappa, Y) \propto (1 - \rho^2)^{-1/2} \exp\left\{\sum (\xi_t Y_t - d_t e^{\xi_t + X_t \beta})\right\},$$

where ξ and κ are related by $\kappa_1 = \sqrt{1 - \rho^2}\xi_1/\delta$, and $\kappa_t = (\xi_t - \rho\xi_{t-1})/\delta$, $t \geq 2$. Define $l(\rho, \delta) = \log p(\rho, \delta|\beta, \kappa, Y)$.

Propose a random-walk type move, $(\rho, \delta) \rightarrow (\rho^{new}, \delta^{new})$, by setting $\rho^{new} = \rho + s_1 u_1$ and $\delta^{new} = \delta \exp\{s_2 u_2\}$, where u_1, u_2 are i.i.d Uniform $(-1/2, 1/2)$, and s_1, s_2 are suitable step sizes (which may be tuned adaptively during the burn-in period). Draw a uniform random number u_0 between 0 and 1, and accept $(\rho^{new}, \delta^{new})$ if $-0.99 \leq \rho^{new} \leq 0.99$ and

$$u_0 \leq \exp\{l(\rho^{new}, \delta^{new}) - l(\rho, \delta) + s_2 u_2\}.$$

Repeat the entire procedure several times to achieve a reasonable acceptance rate. Keep ξ updated via (3.7).

Step 3'_A: Same as Step 3_A, except that we fix δ , i.e., we set $s_2 = 0$.

Step 3''_A: Same as Step 3_A, except that we fix ρ , i.e., we set $s_1 = 0$.

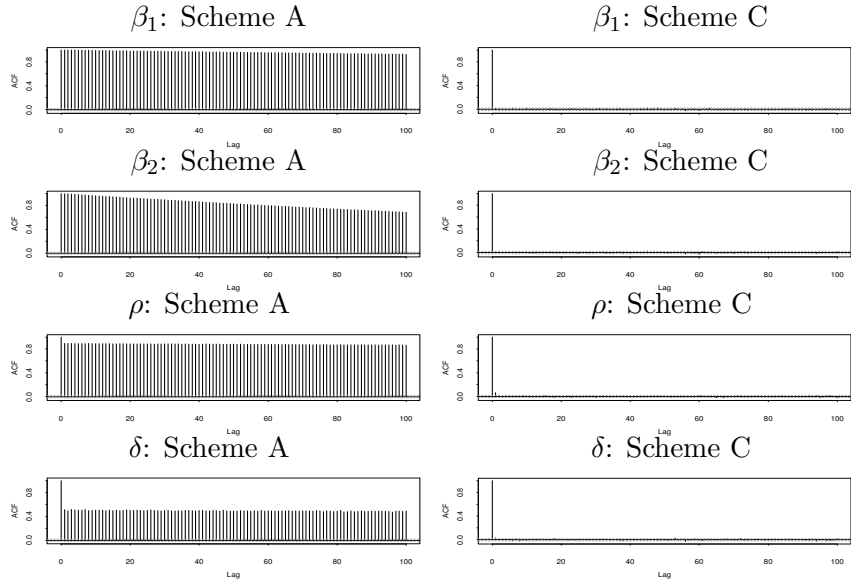


Figure A.1: Comparing Scheme A with Scheme C on DATA1. Autocorrelations of the Monte Carlo draws (excluding the burn-in period) are displayed.

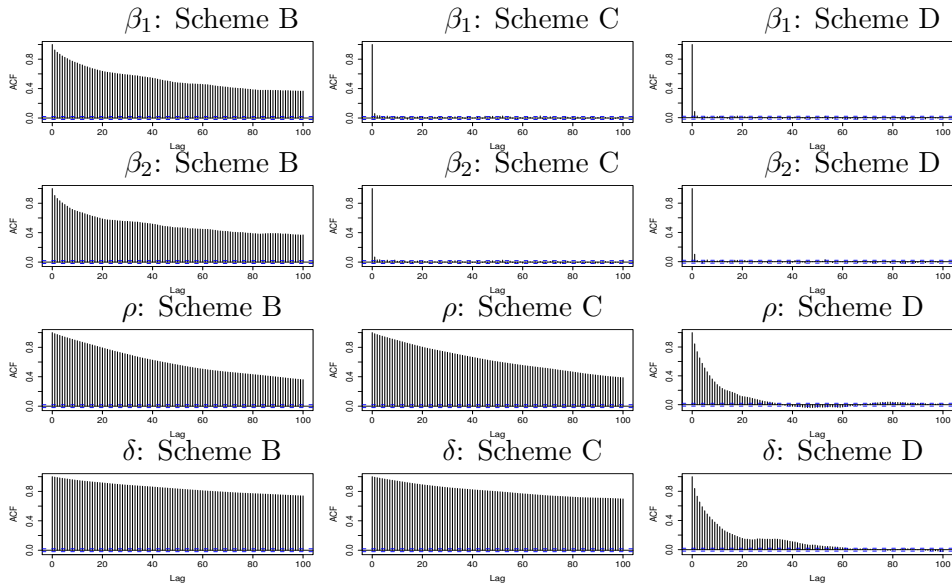


Figure A.2: Autocorrelations under Schemes B, C, and D on DATA2, after the burn-in period.

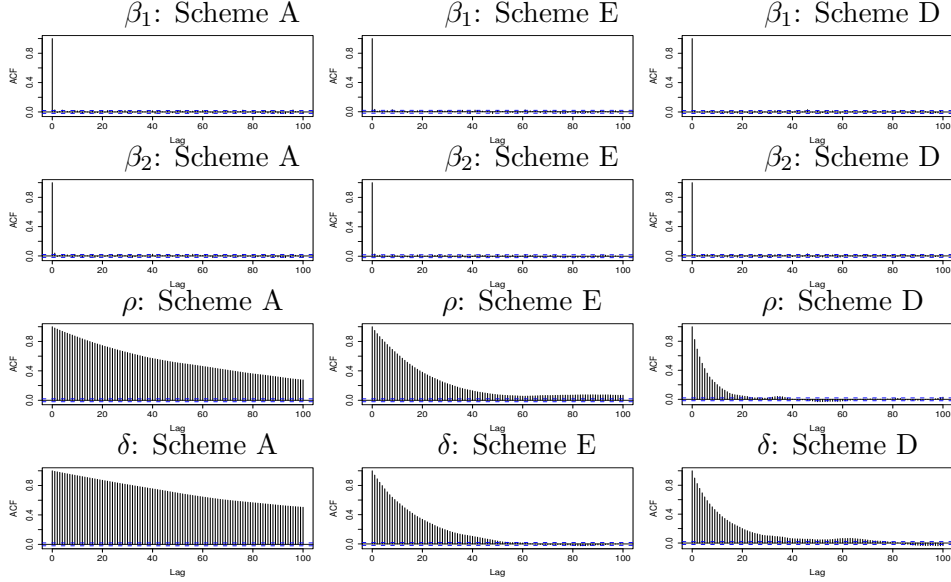


Figure A.3: Autocorrelations under Schemes A, D and E on the Chandra X-ray data, after the burn-in period.

A.2 Autocorrelations Plots of the Monte Carlo Draws (Fig. A.1 – Fig. A.3)

B Auxiliary Material for Section 5

B.1 A Reducible Chain as a Result of Combining Two Transition Kernels (Fig. B.1)

B.2 Proof of Lemma 1

Proof. Let X be \mathcal{A}_1 -measurable and Z be \mathcal{A}_2 -measurable such that $0 < V[X - E(X|\mathcal{M})] < \infty$ and $0 < V[Z - E(Z|\mathcal{M})] < \infty$. Write $X - E(X|\mathcal{M}) = X_0 + X_\perp$ with $X_0 = E(X|\mathcal{N}) - E(X|\mathcal{M})$ and $X_\perp = X - E(X|\mathcal{N})$, and similarly for $Z - E(Z|\mathcal{N})$. Then X_0 and Z_0 are projections onto \mathcal{N} because $\mathcal{M} \subset \mathcal{N}$, and hence they both are \mathcal{N} -measurable, and

$$\begin{aligned} \text{Cov}(X_0, X_\perp) &= \text{Cov}(X_0, Z_\perp) = \text{Cov}(Z_0, Z_\perp) = \text{Cov}(Z_0, X_\perp) = 0, \\ V(X_0 + X_\perp) &= V(X_0) + V(X_\perp), \quad V(Z_0 + Z_\perp) = V(Z_0) + V(Z_\perp). \end{aligned}$$

Consequently,

$$\begin{aligned} \text{Cov}(X_0 + X_\perp, Z_0 + Z_\perp) &= \text{Cov}(X_0, Z_0) + \text{Cov}(X_\perp, Z_\perp) \\ &\leq \sqrt{V(X_0)V(Z_0)} + \mathcal{R}_{\mathcal{N}}(\mathcal{A}_1, \mathcal{A}_2)\sqrt{V(X_\perp)V(Z_\perp)}, \end{aligned} \tag{B.1}$$

by the definition of $\mathcal{R}_{\mathcal{N}}(\mathcal{A}_1, \mathcal{A}_2)$ as in (5.4). It follows that

$$\text{Corr}(X_0 + X_\perp, Z_0 + Z_\perp) \leq R_X R_Z + \mathcal{R}_{\mathcal{N}}(\mathcal{A}_1, \mathcal{A}_2)\sqrt{(1 - R_X^2)(1 - R_Z^2)}, \tag{B.2}$$

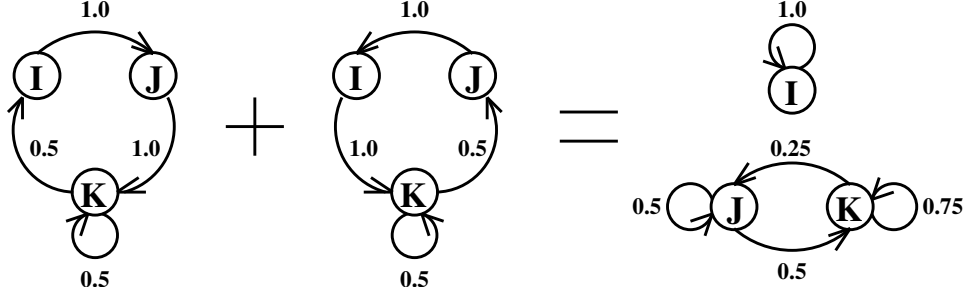


Figure B.1: Alternating two irreducible Markov chains gives a reducible chain. The state space is $\Omega = \{I, J, K\}$, and the target distribution is $\pi = (1/4, 1/4, 1/2)$. Left: transition probability specification (numbers on the arrows) of one chain. Middle: transition probabilities of a second chain with the same stationary distribution. Right: transition probabilities of the combined chain, which becomes reducible even though the original two chains are irreducible.

where (with a bit of abuse of notation)

$$R_X = \sqrt{\frac{V(X_0)}{V(X_0 + X_\perp)}} \quad \text{and} \quad R_Z = \sqrt{\frac{V(Z_0)}{V(Z_0 + Z_\perp)}},$$

where, without lose of generality, we have assumed $V(X_0) > 0$ and $V(Z_0) > 0$. By the simple inequality $\sqrt{(1 - R_X^2)(1 - R_Z^2)} \leq 1 - R_X R_Z$, the right hand side of (B.2) is dominated by

$$\mathcal{R}_{\mathcal{N}}(\mathcal{A}_1, \mathcal{A}_2) + [1 - \mathcal{R}_{\mathcal{N}}(\mathcal{A}_1, \mathcal{A}_2)]R_X R_Z.$$

Noting $X_0 + X_\perp = X - E(X|\mathcal{M})$ and $X_0 = X_{\mathcal{N}} - E(X_{\mathcal{N}}|\mathcal{M})$, where $X_{\mathcal{N}} \equiv E(X|\mathcal{N})$, we have

$$R_X = \frac{\text{Cov}(X_0 + X_\perp, X_0)}{\sqrt{V(X_0 + X_\perp)V(X_0)}} \leq \mathcal{R}_{\mathcal{M}}(\mathcal{A}_1, \mathcal{N}).$$

Similarly $R_Z \leq \mathcal{R}_{\mathcal{M}}(\mathcal{A}_2, \mathcal{N})$. The claim then follows. \square

B.3 Proof of Theorem 1

Proof. With the change of notation $Y_{mis,1} = Y_{mis}$, $Y_{mis,2} = \tilde{Y}_{mis}$, each iteration of GIS as defined in Section 2.3 can be represented by a directed graph, as in (2.13),

$$\theta^{(t)} \longrightarrow Y_{mis,1}^{(t)} \longrightarrow Y_{mis,2}^{(t+1)} \longrightarrow \theta^{(t+1)}.$$

That is, $\theta^{(t)}$ and $Y_{mis,2}^{(t+1)}$ are conditionally independent given $Y_{mis,1}^{(t)}$, etc. Let us focus on the marginal chain $\{\theta^{(t)}\}$ and bound its spectral radius $r_{1\&2}$:

$$r_{1\&2} \leq \mathcal{R}(\theta^{(t)}, \theta^{(t+1)}) \leq \mathcal{R}(\theta^{(t)}, Y_{mis,1}^{(t)}) \mathcal{R}(Y_{mis,1}^{(t)}, Y_{mis,2}^{(t+1)}) \mathcal{R}(Y_{mis,2}^{(t+1)}, \theta^{(t+1)}), \quad (\text{B.3})$$

where we apply (5.6) twice for the last inequality. Under stationarity $\mathcal{R}(\theta^{(t)}, Y_{mis,1}^{(t)})$ is the maximal correlation between θ and $Y_{mis,1}$ in their joint posterior distribution, and likewise for $\mathcal{R}(Y_{mis,2}^{(t+1)}, \theta^{(t+1)})$.

They are related to r_1 and r_2 , the convergence rates of the two ordinary DA schemes via (see Liu *et al.* 1994, 1995)

$$r_1 = \mathcal{R}^2(Y_{mis,1}^{(t)}, \theta^{(t)}), \quad \text{and} \quad r_2 = \mathcal{R}^2(\theta^{(t+1)}, Y_{mis,2}^{(t+1)}).$$

Under stationarity, the distribution of $\{Y_{mis,1}^{(t)}, Y_{mis,2}^{(t+1)}\}$ is simply the joint posterior of $\{Y_{mis,1}, Y_{mis,2}\}$ (with θ integrated out). Hence Theorem 1 follows from (B.3). \square

B.4 Proof of Theorem 2

Proof. We use the same notation as in the proof of Theorem 1. Letting $\mathcal{A} = \sigma(Y_{mis,1}^{(t)}) \cap \sigma(Y_{mis,2}^{(t+1)})$, and applying Lemma 1, we get

$$\begin{aligned} r_{1\&2} &\leq \mathcal{R}(\theta^{(t)}, \theta^{(t+1)}) \\ &\leq \mathcal{R}_{\mathcal{A}}(\theta^{(t)}, \theta^{(t+1)}) + (1 - \mathcal{R}_{\mathcal{A}}(\theta^{(t)}, \theta^{(t+1)}))\mathcal{R}(\theta^{(t)}, \mathcal{A})\mathcal{R}(\mathcal{A}, \theta^{(t+1)}) \\ &= \mathcal{R}^2(\theta, \mathcal{N}) + (1 - \mathcal{R}^2(\theta, \mathcal{N}))\mathcal{R}_{\mathcal{A}}(\theta^{(t)}, \theta^{(t+1)}). \end{aligned}$$

In the last equality, we have used the fact that under stationarity, $\mathcal{R}(\mathcal{A}, \theta^{(t+1)}) = \mathcal{R}(\theta^{(t)}, \mathcal{A}) = \mathcal{R}(\theta, \mathcal{N})$.

Letting $\mathcal{B} = \sigma(Y_{mis,1}^{(t)})$, and applying Lemma 1 again, we get

$$\begin{aligned} \mathcal{R}_{\mathcal{A}}(\theta^{(t)}, \theta^{(t+1)}) &\leq \mathcal{R}_{\mathcal{B}}(\theta^{(t)}, \theta^{(t+1)}) + (1 - \mathcal{R}_{\mathcal{B}}(\theta^{(t)}, \theta^{(t+1)}))\mathcal{R}_{\mathcal{A}}(\theta^{(t)}, \mathcal{B})\mathcal{R}_{\mathcal{A}}(\mathcal{B}, \theta^{(t+1)}) \\ &= \mathcal{R}_{\mathcal{A}}(\theta^{(t)}, Y_{mis,1}^{(t)})\mathcal{R}_{\mathcal{A}}(Y_{mis,1}^{(t)}, \theta^{(t+1)}), \end{aligned}$$

because $\mathcal{R}_{\mathcal{B}}(\theta^{(t)}, \theta^{(t+1)}) = 0$ by conditional independence. Similarly, by taking $\mathcal{B} = \sigma(Y_{mis,2}^{(t+1)})$ and applying Lemma 1, we conclude

$$\mathcal{R}_{\mathcal{A}}(Y_{mis,1}^{(t)}, \theta^{(t+1)}) \leq \mathcal{R}_{\mathcal{A}}(Y_{mis,1}^{(t)}, Y_{mis,2}^{(t+1)})\mathcal{R}_{\mathcal{A}}(Y_{mis,2}^{(t+1)}, \theta^{(t+1)}).$$

Theorem 2 then follows from these three inequalities because, under stationarity, it is easy to show that $\mathcal{R}_{\mathcal{A}}(\theta^{(t)}, Y_{mis,1}^{(t)}) = \mathcal{R}_{\mathcal{N}}(\theta, Y_{mis,1})$, $\mathcal{R}_{\mathcal{A}}(Y_{mis,2}^{(t+1)}, \theta^{(t+1)}) = \mathcal{R}_{\mathcal{N}}(Y_{mis,2}, \theta)$, and $\mathcal{R}_{\mathcal{A}}(Y_{mis,1}^{(t)}, Y_{mis,2}^{(t+1)}) = \mathcal{R}_{\mathcal{N}}(Y_{mis,1}, Y_{mis,2})$. \square

B.5 Proof of Theorem 3

Proof. To prove (5.11), we start by taking $X = \theta^{(t)} = \{\theta_1^{(t)}, \dots, \theta_J^{(t)}\}$, $Z = \theta^{(t+1)} = \{\theta_1^{(t+1)}, \dots, \theta_J^{(t+1)}\}$, and $Y = \theta_1^{(t+1)}$, all with respect to the joint stationary distribution $\{\theta^{(t)}, \theta^{(t+1)}\}$. We then apply the following version of the key inequality (5.8)

$$\mathcal{S}_W(X, Z) \geq \mathcal{S}_Y(X, Z)[\mathcal{S}_W(X, Y) + \mathcal{S}_W(Y, Z) - \mathcal{S}_W(X, Y)\mathcal{S}_W(Y, Z)], \quad (\text{B.4})$$

where W is also a part of $\{\theta^{(t)}, \theta^{(t+1)}\}$ such that $\sigma(W) \subset \sigma(Y)$. Since Y is a part of Z and hence $\mathcal{S}(Y, Z) = 0$, we first take a trivial $W = 0$ in (B.4) to arrive at

$$\mathcal{S}_{CIS} \equiv \mathcal{S}(\theta^{(t)}, \theta^{(t+1)}) \geq \mathcal{S}_{\theta_1^{(t+1)}}(\theta^{(t)}, \theta^{(t+1)})\mathcal{S}(\theta^{(t)}, \theta_1^{(t+1)}). \quad (\text{B.5})$$

Keeping the same X and Z , but now taking $Y = \theta_{\leq 2}^{(t+1)}$ and $W = \theta_1^{(t+1)}$, we apply (B.4) again to obtain

$$\mathcal{S}_{\theta_1^{(t+1)}}(\theta^{(t)}, \theta^{(t+1)}) \geq \mathcal{S}_{\theta_{\leq 2}^{(t+1)}}(\theta^{(t)}, \theta^{(t+1)}) \mathcal{S}_{\theta_1^{(t+1)}}(\theta^{(t)}, \theta_{\leq 2}^{(t+1)}). \quad (\text{B.6})$$

Combining (B.5) and (B.6), we see

$$\mathcal{S}_{CIS} \geq \mathcal{S}_{\theta_{\leq 3}^{(t+1)}}(\theta^{(t)}, \theta^{(t+1)}) \prod_{j=1}^2 \mathcal{S}_{\theta_{\leq j}^{(t+1)}}(\theta^{(t)}, \theta_{\leq j}^{(t+1)}). \quad (\text{B.7})$$

We continue the above argument by taking $Y = \theta_{\leq k}^{(t+1)}$ and $W = \theta_{< k}^{(t+1)}$, and applying (B.4) to $\mathcal{S}_{\theta_{< k}^{(t+1)}}(\theta^{(t)}, \theta^{(t+1)})$ for $k = 3, \dots, J-1$, to reach

$$\mathcal{S}_{CIS} \geq \prod_{j=1}^J \mathcal{S}_{\theta_{\leq j}^{(t+1)}}(\theta^{(t)}, \theta_{\leq j}^{(t+1)}). \quad (\text{B.8})$$

To further factor each term on the right hand side of (B.8), let us first take $X = \theta^{(t)}$, $Z = \theta_{\leq j}^{(t+1)}$, $Y = (\theta_{> j}^{(t)}, \theta_{< j}^{(t+1)})$ and $W = \theta_{< k}^{(t+1)}$, and apply (B.4) again. Note that as long as $j < J$, $\mathcal{S}_{\theta_{< j}^{(t+1)}}(X, Y) = 0$, and hence by (B.4), we have

$$\mathcal{S}_{\theta_{< j}^{(t+1)}}(\theta^{(t)}, \theta_{\leq j}^{(t+1)}) \geq \mathcal{S}_Y(\theta^{(t)}, \theta_{\leq j}^{(t+1)}) \mathcal{S}_{\theta_{< j}^{(t+1)}}(Y, \theta_{\leq j}^{(t+1)}), \quad j = 1, \dots, J-1. \quad (\text{B.9})$$

To deal with the first term on the right-hand side of (B.9), we need the fact that if X_1 and Z_2 are conditionally independent given $\{X_2, X_3, Z_1\}$, then

$$\mathcal{S}_{(Z_1, X_3)}((X_1, X_2, X_3), Z_2) \geq \mathcal{S}_{(Z_1, X_3)}((Z_1, X_2, X_3), Z_2). \quad (\text{B.10})$$

If we let $X_1 = \theta_{< j}^{(t)}$, $X_2 = \theta_j^{(t)}$, $X_3 = \theta_{> j}^{(t)}$, $Z_1 = \theta_{< j}^{(t+1)}$, and $Z_2 = \theta_{\leq j}^{(t+1)}$, then we can apply (B.10) to $\mathcal{S}_Y(\theta^{(t)}, \theta_{\leq j}^{(t+1)})$ because by construction, $\theta_j^{(t+1)}$ and hence $\theta_{\leq j}^{(t+1)}$ is independent of $\theta_{< j}^{(t)}$ when *conditional* on $\theta^{(t+\frac{i-1}{J})}$, the output of the CIS sampler just before the j th component is updated, which is exactly $(\theta_{< j}^{(t+1)}, \theta_j^{(t)}, \theta_{> j}^{(t)}) \equiv \{Z_1, X_2, X_3\}$. Thus

$$\mathcal{S}_Y(\theta^{(t)}, \theta_{\leq j}^{(t+1)}) \geq \mathcal{S}_Y(\theta^{(t+\frac{i-1}{J})}, \theta_{\leq j}^{(t+1)}) \geq \mathcal{S}_j, \quad j = 1, \dots, J-1, \quad (\text{B.11})$$

where \mathcal{S}_j is defined by (5.10). The last inequality in (B.11) is due to the easily verifiable inequality $\mathcal{S}_{\mathcal{M}}(\mathcal{A}_1, \mathcal{A}_2) \geq \mathcal{S}_{\mathcal{M}}(\mathcal{A}_1, \sigma(\mathcal{A}_2 \cup \mathcal{M}))$, and the fact that $\sigma(Y) = \sigma_{j-1} \cap \sigma_j$ and $\sigma(\sigma(\theta_{\leq j}^{(t+1)}) \cup \sigma(Y)) = \sigma_j$.

For $j = J$, (B.10) still applies as long as we take $X_3 = \theta_{> J}^{(t)} = 0$. It then becomes

$$\mathcal{S}_{\theta_{< J}^{(t+1)}}(\theta^{(t)}, \theta_{\leq J}^{(t+1)}) \geq \mathcal{S}_{\theta_{< J}^{(t+1)}}((\theta_{< J}^{(t+1)}, \theta_J^{(t)}, \theta_{\leq J}^{(t+1)}) = \mathcal{S}_J. \quad (\text{B.12})$$

Combining (B.9), (B.11) and (B.12) leads to

$$\mathcal{S}_{CIS} \geq \left(\prod_{j=1}^J \mathcal{S}_j \right) \left[\prod_{j=1}^{J-1} \mathcal{S}_{\theta_{< j}^{(t+1)}}((\theta_{> j}^{(t)}, \theta_{< j}^{(t+1)}), \theta_{\leq j}^{(t+1)}) \right]. \quad (\text{B.13})$$

To show that $\tilde{\mathcal{S}}_G$, the second product on the right hand side of (B.13), is completely determined by π , we note that $(\theta_{<j}^{(t+1)}, \theta_j^{(t+1)}, \theta_{>j}^{(t)})$ is simply $\theta^{(t+\frac{j}{J})}$ in (2.27), which follows π assuming the CIS chain is stationary. We can write $\tilde{\mathcal{S}}_G$ as in (5.12) because $\sigma(\theta_{<j}^{(t+1)}) = \sigma_{j-1} \cap \sigma_J$ and $\sigma(\theta_{>j}^{(t)}, \theta_{<j}^{(t+1)}) = \sigma_{j-1} \cap \sigma_j$, $j = 1, \dots, J$.

To show $\mathcal{S}_G \geq \tilde{\mathcal{S}}_G$, we note that, stochastically, drawing $\theta_j^{(t+1)}$ directly from its full conditional is the same as having $Y_{mis,j}$ and $\tilde{Y}_{mis,j}$ conditionally independent given $\theta_{>j}^{(t)}$ and $\theta_{<j}^{(t+1)}$. Hence $\mathcal{S}_G \geq \tilde{\mathcal{S}}_G$ is a special case of (B.13) with $\mathcal{S}_j = 1$ for all $j = 1, \dots, J$.

To show $\mathcal{S}_G = \tilde{\mathcal{S}}_G$ when $J = 2$, we first note that when $J = 2$, we have $\mathcal{S}_G = 1 - \mathcal{R}(\theta_1, \theta_2)$, where the MCC calculation is with respect to π (see Liu *et al.*, 1994). However, by the definition of $\tilde{\mathcal{S}}_G$, we also have $\mathcal{S}(\theta_1, \theta_2) = 1 - \mathcal{R}(\theta_1, \theta_2)$, and the claim follows. \square

B.6 Proof of Theorem 4

Proof. Because Y_{mis} is sufficient for θ , we can write $p(Y_{obs}|Y_{mis}, \theta)$ as $g(Y_{obs}; Y_{mis})$. Similarly, because \tilde{Y}_{mis} is ancillary, we can write $p(\tilde{Y}_{mis}|\theta)$ as $f(\tilde{Y}_{mis})$. Then the joint posterior density of $(\theta, \tilde{Y}_{mis})$, with respect to the joint product measure of the Haar measure $H(\cdot)$ for θ and Lebesgue measure for \tilde{Y}_{mis} , is

$$\begin{aligned} p(\theta, \tilde{Y}_{mis}|Y_{obs}) &\propto p(Y_{obs}|\tilde{Y}_{mis}, \theta)p(\tilde{Y}_{mis}|\theta)p_0(\theta) \\ &\propto p(Y_{obs}|Y_{mis} = M_\theta^{-1}(\tilde{Y}_{mis}), \theta)p(\tilde{Y}_{mis}|\theta)p_0(\theta) \\ &\propto g(Y_{obs}; M_\theta^{-1}(\tilde{Y}_{mis}))f(\tilde{Y}_{mis})p_0(\theta). \end{aligned} \quad (\text{B.14})$$

Hence the conditional draw at Step 2_A of the interwoven scheme is

$$\theta|(\tilde{Y}_{mis}, Y_{obs}) \sim p_0(\theta)g(Y_{obs}; M_\theta^{-1}(\tilde{Y}_{mis})). \quad (\text{B.15})$$

Noting (B.14) and $Y_{mis} = M_\theta^{-1}(\tilde{Y}_{mis})$, the joint posterior of (θ, Y_{mis}) is

$$p(\theta, Y_{mis}|Y_{obs}) \propto p_0(\theta)f(M_\theta(Y_{mis}))g(Y_{obs}; Y_{mis})J(\theta, Y_{mis}),$$

where $J(\theta, Y_{mis}) = |\det[\partial M(Y_{mis}; \theta)/\partial Y_{mis}]|$. Hence the conditional draw at Step 2_S of the interwoven scheme is

$$\theta|(Y_{mis}, Y_{obs}) \sim p_0(\theta)f(M_\theta(Y_{mis}))J(\theta, Y_{mis}). \quad (\text{B.16})$$

Consider the PX-DA algorithm specified by the Theorem. According to Liu and Wu (1999), when Condition C1 is satisfied we can equivalently implement the optimal PX-DA algorithm (with the uniform prior density on α with respect to the Haar measure) as follows:

(1) Set $\alpha = e$ (identity element of the group). Draw $Y_{mis}|(\theta, Y_{obs})$, which is the same as Step 1 of ASIS. Let $z = Y_{mis}$.

(2) Draw $(\alpha, \theta)|(Y_{mis}^\alpha = z, Y_{obs})$ jointly. This can be accomplished by drawing $\alpha|(z, Y_{obs})$ and then $\theta|(\alpha, z, Y_{obs})$. We first observe that the joint posterior of (α, θ) can be expressed as

$$p(\alpha, \theta|Y_{mis}^\alpha, Y_{obs}) \propto p(Y_{obs}|Y_{mis}^\alpha, \alpha, \theta)p(Y_{mis}^\alpha|\alpha, \theta)p_0(\theta)p(\alpha). \quad (\text{B.17})$$

Since $Y_{mis}^\alpha = M_\alpha(Y_{mis})$, we have

$$\begin{aligned} p(Y_{obs}|Y_{mis}^\alpha, \alpha, \theta) &= p(Y_{obs}|Y_{mis} = M_\alpha^{-1}(Y_{mis}^\alpha), \alpha, \theta) \\ &= g(Y_{obs}; M_\alpha^{-1}(Y_{mis}^\alpha)). \end{aligned} \quad (\text{B.18})$$

But we also have $Y_{mis}^\alpha = M_\alpha(Y_{mis}) = M_\alpha(M_\theta^{-1}(\tilde{Y}_{mis})) = M_{\alpha\theta^{-1}}(\tilde{Y}_{mis})$. Therefore we may obtain $p(Y_{mis}^\alpha|\theta, \alpha)$ via $p(\tilde{Y}_{mis}|\theta) = f(\tilde{Y}_{mis})$. That is,

$$p(Y_{mis}^\alpha|\theta, \alpha) \propto f(M_{\theta\alpha^{-1}}(Y_{mis}^\alpha))J(\theta \cdot \alpha^{-1}, Y_{mis}^\alpha). \quad (\text{B.19})$$

Substituting (B.18–B.19) into (B.17) and noting $p(\alpha) \propto 1$, we have

$$p(\alpha, \theta|z, Y_{obs}) \propto p_0(\theta)f(M_{\theta\alpha^{-1}}(z))g(Y_{obs}; M_{\alpha^{-1}}(z))J(\theta \cdot \alpha^{-1}, z),$$

where z is used as a shorthand for Y_{mis}^α . Now integrate out θ :

$$\begin{aligned} p(\alpha|z, Y_{obs}) &\propto g(Y_{obs}; M_{\alpha^{-1}}(z)) \int p_0(\theta)f(M_{\theta\alpha^{-1}}(z))J(\theta \cdot \alpha^{-1}, z) H(d\theta) \\ (\text{letting } \theta' = \theta \cdot \alpha^{-1}) &\propto g(Y_{obs}; M_{\alpha^{-1}}(z)) \int p_0(\theta' \cdot \alpha)f(M_{\theta'}(z))J(\theta', z) H(d\theta') \\ (\text{by Condition C2}) &\propto g(Y_{obs}; M_{\alpha^{-1}}(z)) \int p_0(\theta')p_0(\alpha)f(M_{\theta'}(z))J(\theta', z) H(d\theta') \\ &\propto g(Y_{obs}; M_{\alpha^{-1}}(z))p_0(\alpha). \end{aligned} \quad (\text{B.20})$$

On the other hand

$$\begin{aligned} p(\theta|\alpha, z, Y_{obs}) &\propto p_0(\theta)f(M_{\theta\alpha^{-1}}(z))J(\theta \cdot \alpha^{-1}, z) \\ &\propto p_0(\theta)f(M_\theta(M_\alpha^{-1}(z)))J(\theta, M_\alpha^{-1}(z)), \end{aligned}$$

which matches equation (B.16), i.e., $p(\theta|Y_{mis}, Y_{obs})$, for $Y_{mis} = M_\alpha^{-1}(z)$.

In summary, when the current iterate is $\theta^{(t)}$, the steps of PX-DA are

Step 1. Same as Step 1 of ASIS.

Step 2a. Let $z = Y_{mis}$, and draw $\alpha|(z, Y_{obs})$ according to (B.20).

Step 2b. Let $z' = M_\alpha^{-1}(z)$, and draw $\theta^{(t+1)} \sim p(\theta|Y_{mis} = z', Y_{obs})$.

Put $\alpha' = \theta^{(t)} \cdot \alpha$. Based on (B.20), Step 2a is equivalent to drawing α' according to

$$\begin{aligned} p(\alpha'|z, Y_{obs}) &\propto g(Y_{obs}; M_{\alpha'^{-1}\theta^{(t)}}(z))p_0([\theta^{(t)}]^{-1} \cdot \alpha') \\ &\propto g(Y_{obs}; M_{\alpha'^{-1}}(w))p_0(\alpha'), \end{aligned} \quad (\text{B.21})$$

where $w = M_{\theta^{(t)}}(z)$. Note this w is the same as \tilde{Y}_{mis} in Step 2_A of ASIS, because $z = Y_{mis}$. Observe that (B.21) matches $p(\theta|\tilde{Y}_{mis} = w, Y_{obs})$ of (B.15) when we equate θ with α' . Therefore if we correspond α' with $\theta^{(t+.5)}$, which is the output of Step 2_A of ASIS, then Step 2a is the same as Step 2_A. Furthermore, with $\alpha' = \theta^{(t+.5)}$, in Step 2b $z' = M_\alpha^{-1}(z) = M_{\alpha'}^{-1}(w) = Y_{mis}$, and we can draw an exact correspondence between Step 2b of PX-DA and Step 2_S of ASIS as well. (Note here the Step 2_A and Step 2_S are in the reversed order, if we match the notation with that for GIS, as defined in Section 2.2; but recall the order does not affect the validity.) \square

C Auxiliary Material for Section 6

The following example illustrates both the relevance and the limitations of Theorem 4. Consider the univariate t model, a well known model for which PX-DA can be applied. We observe $Y_{obs} = (y_1, \dots, y_n)$, where

$$y_i \stackrel{\text{i.i.d.}}{\sim} N(\mu, \sigma^2/q_i), \quad q_i \stackrel{\text{i.i.d.}}{\sim} \chi_\nu^2/\nu.$$

The parameters are $\theta = (\mu, \sigma)$ and the missing data are $q = (q_1, \dots, q_n)^\top$. The degree of freedom ν is assumed known. Assume the standard flat prior on $(\mu, \log(\sigma))$. By introducing a parameter α , this model can be expanded into

$$y_i \stackrel{\text{i.i.d.}}{\sim} N(\mu, \alpha\sigma^2/w_i), \quad w_i \stackrel{\text{i.i.d.}}{\sim} \alpha\chi_\nu^2/\nu,$$

where $w_i = \alpha q_i$. Each iteration of the optimal PX-DA algorithm (see Liu and Wu 1999, and Meng and van Dyk 1999) can be written compactly as

- (1) Draw $q_i \sim \chi_{\nu+1}^2 / [(y_i - \mu)^2/\sigma^2 + \nu]$, independently for $i = 1, \dots, n$;
- (2) Compute $\hat{\mu} = \sum_{i=1}^n q_i y_i / \sum_{i=1}^n q_i$, and then draw

$$\sigma^2 \sim \left[\sum_{i=1}^n q_i (y_i - \hat{\mu})^2 \right] / \chi_{n-1}^2, \quad \mu \sim N \left[\hat{\mu}, \sigma^2 / \sum_{i=1}^n q_i \right];$$

- (3) Redraw $\sigma^2 \sim \sigma^2 \chi_{n\nu}^2 / (\nu \sum_{i=1}^n q_i)$.

These three steps are simply the following conditional draws under the original model:

- (1) $q | (\mu, \sigma, Y_{obs})$;
- (2) $(\mu, \sigma) | (q, Y_{obs})$;
- (3) $\sigma | (\mu, z, Y_{obs})$, where $z = (z_1, \dots, z_n)^\top = (q_1/\sigma^2, \dots, q_n/\sigma^2)^\top$.

In other words, Step 1 draws q , the missing data, given $\theta = (\mu, \sigma)$; Step 2 draws θ given q , which is an AA for θ ; and Step 3 draws σ given z , which is an SA for σ . If we focus on σ , ignoring the part for μ , then the above algorithm is exactly an ASIS sampler for σ ; just as Theorem 4 claims, it coincides with the optimal PX-DA algorithm. However, because z is not an SA for μ , this scheme does not correspond to an ASIS for (μ, σ) as a whole. This suggests that there may be a generalization of Theorem 4 that deals with a form of conditional ASIS. Such results would also shed light on optimality properties of CIS, or reveal an even better formulation.