

Independent Metropolis-Hastings Steps for Generalized Linear Models with Latent Gaussian Processes via Global Conditional Laplace Approximations

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Abstract

KEY WORDS:

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1 Introduction

2 Fitting GLMMs with LGPs

We consider a class of generalized linear mixed models (GLMMs; Stroup, 2012) with latent Gaussian processes (LGP). We will conceptualize our class of models using the strategy of Berliner (1996) and Wikle et al. (2003), that is hierarchically with a data model conditional on parameters and a latent process, a process model conditional on parameters, and finally a parameter model. Suppose we observe an m -dimensional vector \mathbf{z}_i for each observational unit i , and let $\mathbf{z}_{1:n} = (\mathbf{z}'_1, \mathbf{z}'_2, \dots, \mathbf{z}'_n)'$ where n is the number of observational units. We assume these observations are conditionally independent given a set of observation-specific location parameters and some common data level parameter ϕ . Let μ_i denote the location parameter for observation i and $\mu_{1:n} = (\mu'_1, \mu'_2, \dots, \mu'_n)'$. Then the data model is $\mathbf{z}_i | \mu, \phi \stackrel{ind}{\sim} [z | \mu_i, \phi]$ where $[z | \mu, \phi]$ is some known parameterized family of densities for the \mathbf{z}_i s indexed by μ and ϕ ; often an exponential family. The location parameters are a known function of a LGP, i.e. $\mu_i = g(\mathbf{y}_i)$ where g is known and $\mathbf{y}_{1:n}$ is a LGP where $\mathbf{y}_{1:n} = (\mathbf{y}'_1, \mathbf{y}'_2, \dots, \mathbf{y}'_n)'$. Then at the process level we model $\mathbf{y}_{1:n}$ as sum of function of fixed effects and random effects, namely $\mathbf{y}_{1:n} = \mathbf{X}_{1:n}\beta + \mathbf{S}_{1:n}\delta$ where $\mathbf{X}_{1:n}$ and $\mathbf{S}_{1:n}$ are known $mn \times p$ and $mn \times r$ matrices respectively, i.e. $\mathbf{X}_{1:n} = (\mathbf{X}'_1, \mathbf{X}'_2, \dots, \mathbf{X}'_n)'$ where \mathbf{X}_i a $m \times p$ matrix and similarly for $\mathbf{S}_{1:n}$. In addition β and δ are unknown p -dimensional and r -dimensional column vectors respectively. Further, we assume $\delta \sim N(\mathbf{0}, \Sigma)$ The process model can be more succinctly written as $\mathbf{y}_{1:n} \sim N(\mathbf{X}_{1:n}\beta, \mathbf{S}_{1:n}\Sigma\mathbf{S}'_{1:n})$ so that $\mathbf{y}_{1:n}$ s mean is structured by $\mathbf{X}_{1:n}$ and its covariance matrix is structured by $\mathbf{S}_{1:n}$. Further, we assume that Σ depends on the unknown parameter ϕ to allow for, e.g., parsimonious representations of Σ . We allow ϕ to enter both the data model and Σ , though in many applications they will depend on distinct components of ϕ . The leaves the unknown parameters (ϕ, β) , which in the parameter model obtain a joint

prior distribution denoted by $[\phi, \beta]$. For notational simplicity, let $\mathbf{D}_n = (\mathbf{z}_{1:n}, \mathbf{X}_{1:n}, \mathbf{S}_{1:n})$ denote all data in the model and $\boldsymbol{\theta} = (\phi, \beta)$ denote all model parameters.

A common MCMC approach in these models is data augmentation (DA; Tanner and Wong, 1987). That is, a two step Gibbs sampler consisting of a draw from $[\boldsymbol{\theta}|\mathbf{y}_{1:n}, \mathbf{D}_n]$ and a draw from $[\mathbf{y}_{1:n}|\boldsymbol{\theta}, \mathbf{D}_n]$ iterated repeatedly. In GLMMs with non-Gaussian data models, $[\mathbf{y}_{1:n}|\boldsymbol{\theta}, \mathbf{D}_n]$ is typically intractable and thus requires a MH step. Often a random walk proposal is used here, but if a good approximation for $[\mathbf{y}_{1:n}|\boldsymbol{\theta}, \mathbf{D}_n]$ is available, then an independent MH (IMH) Gibbs step is attractive. Laplace approximations (LAs) provide a useful approach for constructing a good IMH proposal density for $\mathbf{y}_{1:n}$'s conditional posterior.

3 Laplace Approximations

Let $\boldsymbol{\omega}$ be the model parameter and \mathbf{D}_n the observed data so that $[\boldsymbol{\omega}|\mathbf{D}_n]$ is the posterior distribution, available up to a normalizing constant. Further let $\boldsymbol{\omega}_n^*$ denote the posterior mode of $[\boldsymbol{\omega}|\mathbf{D}_n]$ and let $\mathbf{H}_n(\boldsymbol{\omega}_n^*)$ denote the Hessian matrix of $\log[\boldsymbol{\omega}|\mathbf{D}_n]$ evaluated at $\boldsymbol{\omega}_n^*$. Then under suitable regularity conditions $\boldsymbol{\omega}$'s posterior distribution is asymptotically normal (Schervish, 1997, Sections 7.4.2 and 7.4.3), so for a fixed but large value of n , $\boldsymbol{\omega}|\mathbf{D}_n \stackrel{a}{\sim} N(\boldsymbol{\omega}_n^*, -\mathbf{H}_n^{-1}(\boldsymbol{\omega}_n^*))$ where the notation $\stackrel{a}{\sim}$ means ‘‘approximately distributed as.’’ We do not discuss the precise technical conditions necessary for this result here, but intuitively for the approximation to be good each element of $\boldsymbol{\omega}$ must have enough ‘‘observations’’ for asymptotics to kick in. We put ‘‘observations’’ in scare quotes because often rather than data, it is other elements of $\boldsymbol{\omega}$ are directly informing on another element, e.g. in the GLMM case above $\boldsymbol{\omega} = (\boldsymbol{\theta}, \mathbf{y}_{1:n})$ and $\mathbf{y}_{1:n}$ is directly informing on $\boldsymbol{\theta}$. In that case the asymptotic argument does not apply to $\boldsymbol{\omega}$, but it typically does apply for $\boldsymbol{\theta}$ alone so that if $\mathbf{y}_{1:n}$ assumed to be Gaussian conditional on $\boldsymbol{\theta}$, then a normal approximation may still be reasonable for the posterior of $\boldsymbol{\omega}$. It ‘‘may’’ be reasonable because the non-Gaussian data model implies

that $\mathbf{y}_{1:n}$ is non-Gaussian in its full conditional posterior, but it is still often approximately Gaussian. We call this LA a global LA (GLA) since it approximates the full joint posterior of $\boldsymbol{\omega} = (\boldsymbol{\theta}, \mathbf{y}_{1:n})$.

If the GLA is good, it can be used as a proposal distribution in a single step IMH algorithm to draw from $\boldsymbol{\omega}$'s posterior distribution. Typically a t_{df} proposal is used instead of a normal with df set small enough so that its tails dominate the posterior's, which ensures that the Markov chain is uniformly ergodic (Robert and Casella, 2013, Theorem 7.8). Often $\boldsymbol{\theta}$ contains too many parameters relative to the amount of data available so that $\boldsymbol{\theta}$ is not approximately normal in its marginal posterior, but because of the latent Gaussian assumption $\mathbf{y}_{1:n}$ is still approximately normal in its full conditional posterior. In this context, a conditional LA can be constructed to the density $[\mathbf{y}_{1:n}|\boldsymbol{\theta}, \mathbf{D}_n]$ directly. We call this a *local* conditional LA (LCLA) since the LA approximation is recomputed for each value of $\boldsymbol{\theta}$. Using the LCLA in the context of a Gibbs sampler as the IMH proposal for $\mathbf{y}_{1:n}$ while sampling ***theta*** in one or more hopefully conjugate form Gibbs steps is attractive when the LCLA is good since the acceptance rate of the Metropolis step will be high. However, constructing any of these LAs typically requires numerical optimization since the data model is non-Gaussian. For the GLA this optimization only needs to be performed once, so as long as it is doable it only represents a fixed cost of running the resulting IMH algorithm. However, the IMHwG algorithm that results from the LCLA requires a numerical optimization to be run each MCMC iteration in order to update the conditional posterior mode and approximate covariance matrix. So while IMWwG using the LCLA may have nice MCMC properties, the computational cost can make it significantly less attractive and in some cases even prohibitive.

We propose using a simple method in order to keep the fixed cost associated with the GLA from becoming a variable cost when apply to a conditional distribution: use the conditional distribution implied by the GLA as the IMH proposal. We call this a global *conditional* LA

(GCLA) since it is an approximation to $\mathbf{y}_{1:n}$'s conditional posterior that relies on the GLA. More formally, suppose the GLA is given by the posterior mode $(\boldsymbol{\theta}^*, \mathbf{y}_{1:n}^*)$ with approximate covariance matrix $\boldsymbol{\Omega}^*$ given by

$$\boldsymbol{\Omega}^* = (-\mathbf{H}^*)^{-1} = \begin{bmatrix} \boldsymbol{\Omega}_{\theta}^* & \boldsymbol{\Omega}_{\theta y}^* \\ \boldsymbol{\Omega}_{y\theta}^* & \boldsymbol{\Omega}_y^* \end{bmatrix}.$$

Then the GCLA to $\mathbf{y}_{1:n}$'s conditional posterior is $\mathbf{y}_{1:n}|\boldsymbol{\theta}, \mathbf{D}_n \stackrel{a}{\sim} N(\tilde{\mathbf{y}}_{1:n}, \tilde{\boldsymbol{\Omega}}_y)$, where $\tilde{\boldsymbol{\theta}}_y = \mathbf{y}_{1:n}^* + \boldsymbol{\Omega}_{y\theta}^*(\boldsymbol{\Omega}_{\theta}^*)^{-1}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$ and $\tilde{\boldsymbol{\Omega}}_y = \boldsymbol{\Omega}_y^* - \boldsymbol{\Omega}_{y\theta}^*(\boldsymbol{\Omega}_{\theta}^*)^{-1}\boldsymbol{\Omega}_{\theta y}^*$. The GCLA may be worse than the LCLA since the LCLA directly approximates the target conditional posterior, but the computation savings realized from only having to run the optimization algorithm once are typically significant and make it worthwhile. A problem with using either approximation is that by moving from an IMH algorithm to an IMHwG algorithm the mixing and convergence properties of the chain do deteriorate to the extent that $\boldsymbol{\theta}$ and $\mathbf{y}_{1:n}$ are dependent in the posterior. In practice this can often be solved by reparameterizing the model, e.g. using a non-centered parameterization (Gelfand et al., 1995; Roberts and Sahu, 1997; Van Dyk and Meng, 2001; Bernardo et al., 2003).

4 Spatially Modeling County Population Estimates

The American Community Survey (ACS) provides 5-year period estimates of county populations as recently as 2014. In 2014 there were 3,142 counties in the United States, including the District of Columbia and counties in Alaska and Hawaii. We use two separate data models in order to illustrate when both the joint and global conditional Laplace approximations work well. The first is a Poisson data model, i.e., $Z_i \sim \text{Poisson}(\lambda_i)$ where $\lambda_i = \exp(Y_i)$. Through visual inspection of a histogram, it was determined that log county populations look approximately normally distributed, so our second data model is $\log Z_i \sim N(\mu_i, \phi^2)$, where $\mu_i = Y_i$.

The process model in both cases is a reduced rank spatial model $Y = \mathbf{X}\boldsymbol{\beta} + \mathbf{S}\boldsymbol{\delta}$, where $\mathbf{X}\boldsymbol{\beta}$ represents the process mean at each county and $\mathbf{S}\boldsymbol{\delta}$ implies the spatial correlation across counties. The spatial correlation term consists of a set of r basis functions evaluated at each of the $n = 3,142$ counties, denoted by the $n \times r$ matrix \mathbf{S} , and a common random effect $\boldsymbol{\delta}$. We assume that $\boldsymbol{\delta}$ is r -dimensional with $r \ll n$ so that the model is reduced rank. Any set of spatial basis functions could be used for \mathbf{S} but we use the Moran's I (MI) basis set, described below, but see Hughes and Haran (2013), Porter et al. (2015), Bradley et al. (2015) and references therein for additional discussion. Another possibility is to define a reduced rank model for a point-level spatial process using a basis function expansion and compute the implied set of basis functions for each of the census tracts by integrating the point level basis functions appropriately. See Sections 2.1, 3.1, and 4 of Bradley et al. (2016) for details.

The MI basis functions are defined through the orthogonal projection matrix $\mathbf{P}_\mathbf{X} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$. Let \mathbf{A} denote the binary adjacency matrix with $a_{ij} = 1$ if counties i and j are neighbors, $a_{ij} = 0$ otherwise, and $a_{ii} = 0$ along the diagonal, and define the MI operator \mathbf{G} as

$$\mathbf{G} = (\mathbf{I}_n - \mathbf{P}_\mathbf{X})\mathbf{A}(\mathbf{I}_n - \mathbf{P}_\mathbf{X})$$

where \mathbf{I}_n is the $n \times n$ identity matrix. The spectral decomposition of \mathbf{G} is $\mathbf{G} = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}'$. To use a reduced rank version of the MI basis functions we truncate the basis function expansion and take \mathbf{S} to be the $n \times r$ matrix formed by the r columns of $\boldsymbol{\Phi}$ corresponding to the r largest in magnitude eigenvalues of \mathbf{G} . The random effect $\boldsymbol{\delta}$ is further modeled as $\boldsymbol{\delta} \sim N(\mathbf{0}_r, \boldsymbol{\Sigma}(\boldsymbol{\theta}))$ where $\mathbf{0}_r$ denotes an r -dimensional vector of zeroes and $\boldsymbol{\Sigma}(\boldsymbol{\theta})$ is an unknown covariance matrix that depends on the parameter $\boldsymbol{\theta}$. The covariance matrix of $\mathbf{S}\boldsymbol{\delta}$ is then $\mathbf{S}\boldsymbol{\Sigma}(\boldsymbol{\theta})\mathbf{S}'$.

The process model depends on choices for \mathbf{X} and r . In practice r can be chosen using a sensitivity analysis. Since our goal is to illustrate computational methods, we will elide

choosing r in a principled way and instead use several values for r in order to illustrate when the parameter space becomes too high dimensional for our method to be advantageous. For simplicity we choose an intercept only model, but all derivations for the model here and in Appendix A assume that \mathbf{X} is $n \times p$.

Finally, we consider two extreme parameterizations of $\Sigma(\theta)$ — the iid parameterization where $\Sigma = \sigma^2 \mathbf{I}_r$ and the full parameterization where Σ is fully parameterized. In the iid parameterization we assume that $\sigma^2 \sim IG(a_\sigma, b_\sigma)$ in the prior, while in the full parameterization we assume that $\Sigma \sim IW(d, \mathbf{E})$. The prior for β in all models is $\beta \sim N(\mathbf{b}, v^2 \mathbf{I}_p)$, and in the lognormal models the prior for ϕ^2 is $\phi^2 \sim IG(a_\phi, b_\phi)$. We assume that the parameters β , Σ , and when applicable ϕ^2 are mutually independent in the prior. For our examples we assume that $a_\sigma = a_\phi = b_\sigma = b_\phi = 1$, $\mathbf{b} = \mathbf{0}_p$, $v = 10$, $d = r + 1$ and $\mathbf{E} = \mathbf{I}_p$. Often a more complicated prior is appropriate on variance or covariance matrix parameters so that the marginal posterior is not sensitive to arbitrary choices in the prior (Gelman, 2006). We use these conditionally conjugate priors because they allow for a fair comparison between MCMC algorithms — most alternatives will complicate alternative Gibbs samplers with extra steps or necessitate Metropolis steps making IMH or IMHwG relatively more attractive.

Between the two possible parameterizations of Σ and the two choices for the data model we consider four possible classes of models. Both for implementing PSO algorithms to find the Laplace approximations and for running the IMH and IMHwG algorithms, we reparameterize the variance and covariance matrix parameters so that they have support on an unconstrained space. For σ^2 and ϕ^2 we use the log transformation, and for Σ we use the Cholesky factorization of Σ^{-1} allowing the diagonal elements to be negative. See Appendix A for details about the posterior distributions, including this transformation and relevant full conditionals.

5 Predicting the 1988 presidential election

Gelman and Hill (2006, Chapter 14) describes a model used to predict state-level opinions about the 1988 presidential candidates from national polls in order to predict the outcome of the election. They model the responses to a series of seven polls conducted by CBS News during the week before the 1988 presidential election. The variable of interest is binary: $Z_i = 1$ if the i th respondent said they supported the Republican candidate and $Z_i = 0$ if they said they supported the Democratic candidate, with undecideds being excluded. Focusing on the last poll, they ultimately estimate a logistic regression model with fixed effects for race (whether the respondent was African American or not), sex, and $\text{race} \times \text{sex}$, and random effects for four age categories, four education categories, and 16 $\text{age} \times \text{education}$ categories, as well as for the respondent's state of residence (including District of Columbia). The mean of the state random effect distribution is one of five region random effects plus the proportion of the state that voted republican in the last election times a slope coefficient.

The model is somewhat overparameterized since it has age, education, and $\text{age} \times \text{education}$ random effects, so we reduce its size by omitting the age and education random effects. In our model the $\text{age} \times \text{education}$ random effects now represent the random effects for each $\text{age} \times \text{education}$ category rather than an interaction term. The single poll data model is

$$P(Z_i = 1) = \theta_i, \quad \theta_i = \exp(Y_i) / \{1 + \exp(Y_i)\},$$

$$Y_i = \beta_0 + f_i\beta_f + b_i\beta_b + f_i b_i \beta_{fb} + \alpha_{ae}[ae_i] + \alpha_s[s_i] \quad (\text{single poll data model}),$$

where f_i indicates whether respondent i identified as female, b_i indicates whether respondent i identified as African American, ae_i indicates respondent i 's $\text{age} \times \text{education}$ category, and s_i indicates respondent i 's state of residence. Here we use $\alpha_s[k]$ to denote the k th element of the vector α_s , so α_{ae} contains 16 elements, and α_s contains 51 elements (50 states plus

the District of Columbia). The single poll process model is

$$\begin{aligned}\alpha_s[k] &\stackrel{iid}{\sim} N(\alpha_r[r_k] + prev_k \beta_{prev}, \sigma_s^2) \text{ for } k = 1, 2, \dots, 51, \\ \alpha_{ae}[k] &\stackrel{iid}{\sim} N(0, \sigma_{ae}^2) \text{ for } k = 1, 2, \dots, 16, \\ \alpha_r[k] &\stackrel{iid}{\sim} N(0, \sigma_r^2) \text{ for } k = 1, 2, \dots, 5 \quad (\text{single poll process model}),\end{aligned}$$

where $\alpha_r[r_k]$ denotes the region containing state k and $prev_k$ denotes the average vote share for the Republicans in the previous three presidential elections. This model expands the class of models discussed in Section 2 by allowing the mean of δ to depend on random effects that are further modeled, but adding a level to the hierarchy does not fundamentally change the applicability of the Laplace approximations.

The last poll had 2,015 respondents, but together all seven polls have 11,566 respondents. Using each poll with a minimal number of additional parameters to account for poll to poll variability should increase the quality of the model and result in a posterior with better Laplace approximations since there is so much more data. We analyze a model for all of the polls using the following data model

$$\begin{aligned}P(Z_i = 1) &= \theta_i, \quad \theta_i = \exp(Y_i) / \{1 + \exp(Y_i)\}, \\ Y_i &= \beta_0 + f_i \beta_f + b_i \beta_b + f_i b_i \beta_{fb} + \alpha_{ae}[ae_i] + \alpha_s[s_i] + \alpha_p[p_i] \quad (\text{all polls data model}),\end{aligned}$$

where p_i denotes which poll respondent i was surveyed in. The process model is given by

$$\begin{aligned}\alpha_s[k] &\stackrel{iid}{\sim} N(\alpha_r[r_k] + prev_k \beta_{prev}, \sigma_s^2) \text{ for } k = 1, 2, \dots, 51, \\ \alpha_{ae}[k] &\stackrel{iid}{\sim} N(0, \sigma_{ae}^2) \text{ for } k = 1, 2, \dots, 16, \\ \alpha_r[k] &\stackrel{iid}{\sim} N(0, \sigma_r^2) \text{ for } k = 1, 2, \dots, 5, \\ \alpha_p[k] &\stackrel{iid}{\sim} N(0, \sigma_p^2) \text{ for } k = 1, 2, \dots, 7 \quad (\text{all polls process model}).\end{aligned}$$

In both models we assume each of the β s have independent $N(0, 1000)$ priors, and each of the σ^2 s have $IG(1, 1)$ priors. Including the random effects the single poll model contains

80 parameters while the all polls model contains 89 parameters. Writing down the log posteriors and deriving the Hessians is straightforward but tedious for these models, so we omit these steps, though note that for both the PSO and IMH algorithms the variances should be transformed to the log scale. For MCMC algorithms with multiple Gibbs steps, in single poll model of Section 5, we draw $(\beta_0, \beta_f, \beta_b, \boldsymbol{\alpha}_s, \boldsymbol{\alpha}_{ae})$ in the Metropolis step, while in the all polls model we draw all of those parameters and additionally $\boldsymbol{\alpha}_p$ in the Metropolis step. Then for both models there are two additional Gibbs steps — one where each random effect variance is drawn, and one where $(\beta_{prev}, \boldsymbol{\alpha}_r)$ is drawn. These full conditionals are straightforward to derive, so we do not reproduce them here. [SHOULD WE ADD THESE DETAILS INTO AN APPENDIX?]

6 Discussion

References

- Berliner, L. M. (1996). “Hierarchical Bayesian time series models.” In *Maximum entropy and Bayesian methods*, 15–22. Springer.
- Bernardo, J., Bayarri, M., Berger, J., Dawid, A., Heckerman, D., Smith, A., and West, M. (2003). “Non-centered Parameterisations for Hierarchical Models and Data Augmentation.” In *Bayesian Statistics 7: Proceedings of the Seventh Valencia International Meeting*, 307–326. London: Oxford University Press.
- Bradley, J. R., Holan, S. H., and Wikle, C. K. (2015). “Multivariate spatio-temporal models for high-dimensional areal data with application to longitudinal employer-household dynamics.” *Annals of Applied Statistics*, 9, 4, 1761–1791.
- Bradley, J. R., Wikle, C. K., and Holan, S. H. (2016). “Regionalization of multiscale spatial processes by using a criterion for spatial aggregation error.” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*.
- Gelfand, A. E., Sahu, S. K., and Carlin, B. P. (1995). “Efficient Parametrisations for Normal Linear Mixed Models.” *Biometrika*, 82, 3, 479–488.
- Gelman, A. (2006). “Prior Distributions for Variance Parameters in Hierarchical Models (Comment on Article by Browne and Draper).” *Bayesian analysis*, 1, 3, 515–534.
- Gelman, A. and Hill, J. (2006). *Data analysis using regression and multilevel/hierarchical models*. Cambridge University Press.
- Hughes, J. and Haran, M. (2013). “Dimension reduction and alleviation of confounding for spatial generalized linear mixed models.” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 75, 1, 139–159.

- Porter, A. T., Holan, S. H., and Wikle, C. K. (2015). “Bayesian semiparametric hierarchical empirical likelihood spatial models.” *Journal of Statistical Planning and Inference*, 165, 78–90.
- Robert, C. and Casella, G. (2013). *Monte Carlo statistical methods*. 2nd ed. Springer Science & Business Media.
- Roberts, G. O. and Sahu, S. K. (1997). “Updating Schemes, Correlation Structure, Blocking and Parameterization for the Gibbs Sampler.” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 59, 2, 291–317.
- Schervish, M. J. (1997). *Theory of statistics*. Springer Science & Business Media.
- Stroup, W. W. (2012). *Generalized linear mixed models: modern concepts, methods and applications*. CRC press.
- Tanner, M. A. and Wong, W. H. (1987). “The calculation of posterior distributions by data augmentation.” *Journal of the American statistical Association*, 82, 398, 528–540.
- Van Dyk, D. and Meng, X.-L. (2001). “The Art of Data Augmentation.” *Journal of Computational and Graphical Statistics*, 10, 1, 1–50.
- Wikle, C. K. et al. (2003). “Hierarchical Models in Environmental Science.” *International Statistical Review*, 71, 2, 181–199.

Supplemental Web Material for Independent Metropolis-Hastings Steps for Generalized Linear Models with Latent Gaussian Processes via Global Conditional Laplace Approximations

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A County Population Model Details

We consider two possible data models, Poisson and lognormal, and two possible random effect distributions, iid normal and normal with a fully correlated covariance matrix. The posterior distributions for the models with iid random effects can be written as

$$\begin{aligned}
p(\boldsymbol{\beta}, \sigma^2, \boldsymbol{\delta}, \phi^2 | \mathbf{z}, \mathbf{X}, \mathbf{S}) &\propto (\phi^2)^{-n/2-a_\phi-1} \exp \left[-\frac{1}{\phi^2} \left\{ \frac{(\log \mathbf{z} - \mathbf{y})'(\log \mathbf{z} - \mathbf{y})}{2} + b_\phi \right\} \right] \\
&\times (\sigma^2)^{-\frac{r}{2}-a_\sigma-1} \exp \left\{ -\frac{1}{\sigma^2} \left(\frac{\boldsymbol{\delta}'\boldsymbol{\delta}}{2} + b_\sigma \right) \right\} \exp \left\{ -\frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{2v} \right\} \quad (\text{iid lognormal}), \\
p(\boldsymbol{\beta}, \sigma^2, \boldsymbol{\delta} | \mathbf{z}, \mathbf{X}, \mathbf{S}) &\propto \prod_{i=1}^n \frac{\exp\{-\exp(y_i)\} \exp(y_i z_i)}{z_i!} \\
&\times (\sigma^2)^{-\frac{r}{2}-a_\sigma-1} \exp \left\{ -\frac{1}{\sigma^2} \left(\frac{\boldsymbol{\delta}'\boldsymbol{\delta}}{2} + b_\sigma \right) \right\} \exp \left\{ -\frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{2v} \right\} \quad (\text{iid Poisson}).
\end{aligned}$$

For fully parameterized $\boldsymbol{\Sigma}$ we write the posteriors in terms of the precision matrix $\boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1}$, yielding

$$\begin{aligned}
p(\boldsymbol{\beta}, \boldsymbol{\Omega}, \boldsymbol{\delta}, \phi^2 | \mathbf{z}, \mathbf{X}, \mathbf{S}) &\propto (\phi^2)^{-n/2-a_\phi-1} \exp \left\{ -\frac{1}{\phi^2} \left(\frac{(\log \mathbf{z} - \mathbf{y})'(\log \mathbf{z} - \mathbf{y})}{2} + b_\phi \right) \right\} \\
&\times |\boldsymbol{\Omega}|^{(d-r)/2} \exp \left\{ -\frac{1}{2} \left(\boldsymbol{\delta}'\boldsymbol{\Omega}\boldsymbol{\delta} + \frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{v} + \text{tr}(\mathbf{E}\boldsymbol{\Omega}) \right) \right\} \quad (\text{full lognormal}), \\
p(\boldsymbol{\beta}, \boldsymbol{\Omega}, \boldsymbol{\delta} | \mathbf{z}, \mathbf{X}, \mathbf{S}) &\propto \prod_{i=1}^n \frac{\exp\{-\exp(y_i)\} \exp(y_i z_i)}{z_i!} \\
&\times |\boldsymbol{\Omega}|^{(d-r)/2} \exp \left\{ -\frac{1}{2} \left(\boldsymbol{\delta}'\boldsymbol{\Omega}\boldsymbol{\delta} + \frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{v} + \text{tr}(\mathbf{E}\boldsymbol{\Omega}) \right) \right\} \quad (\text{full Poisson})
\end{aligned}$$

where $\text{tr}(\cdot)$ denotes the trace operator. For the PSO algorithm and some MCMC algorithms it will be easier to work with the Cholesky decomposition of $\boldsymbol{\Omega}$ given by $\mathbf{L}\mathbf{L}' = \boldsymbol{\Omega}$ where \mathbf{L} is lower triangular. It is often more convenient to put the prior distribution directly on \mathbf{L} rather than on $\boldsymbol{\Omega}$ or $\boldsymbol{\Omega}^{-1}$ and solving for the Jacobian, but this depends in part on which MCMC algorithm is used to fit the model. So while we use the prior distribution on \mathbf{L} implied by a Wishart prior on $\boldsymbol{\Omega}$, in practice it is advantageous to use one of the priors suggested by Chen and Dunson (2003) or Frühwirth-Schnatter and Tüchler (2008). We allow the diagonal

entries of \mathbf{L} to be negative in the PSO and IMH algorithms, so \mathbf{L} is not strictly speaking a Cholesky decomposition. The determinant of the Jacobian is the same in both cases up to a proportionality constant. The signs of the elements of \mathbf{L} are not identified, therefore care needs to be taken when interpreting the results of MCMC, but transforming back to the precision matrix in a post processing step is sufficient. Let ℓ_{ij} denote the (i, j) th element of \mathbf{L} . Then the Jacobian of $\mathbf{\Omega} \rightarrow \mathbf{L}$ is given by

$$|J(\mathbf{\Omega} \rightarrow \mathbf{L})| \propto \prod_{k=1}^r |\ell_{kk}|^{r+1-k}$$

where $\mathbf{\Omega}$ is $r \times r$. Under this parameterization the full posteriors can be written as

$$\begin{aligned} p(\boldsymbol{\beta}, \mathbf{L}, \boldsymbol{\delta}, \phi^2 | \mathbf{z}, \mathbf{X}, \mathbf{S}) &\propto (\phi^2)^{-n/2 - a_\phi - 1} \exp \left[-\frac{1}{\phi^2} \left\{ \frac{(\log \mathbf{z} - \mathbf{y})'(\log \mathbf{z} - \mathbf{y})}{2} + b_\phi \right\} \right] \\ &\quad \times \prod_{k=1}^r (\ell_{kk}^2)^{(d-k+1)/2} \\ &\quad \times \exp \left[-\frac{1}{2} \left\{ \boldsymbol{\delta}' \mathbf{L} \mathbf{L}' \boldsymbol{\delta} + \frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{v} + \text{tr}(\mathbf{E} \mathbf{L} \mathbf{L}') \right\} \right] \quad (\text{full lognormal}), \\ p(\boldsymbol{\beta}, \mathbf{L}, \boldsymbol{\delta} | \mathbf{z}, \mathbf{X}, \mathbf{S}) &\propto \prod_{i=1}^n \frac{\exp\{-\exp(y_i)\} \exp(y_i z_i)}{z_i!} \times \prod_{k=1}^r (\ell_{kk}^2)^{(d-k+1)/2} \\ &\quad \times \exp \left[-\frac{1}{2} \left\{ \boldsymbol{\delta}' \mathbf{L} \mathbf{L}' \boldsymbol{\delta} + \frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{v} + \text{tr}(\mathbf{E} \mathbf{L} \mathbf{L}') \right\} \right] \quad (\text{full Poisson}). \end{aligned}$$

In Appendix A.2 we derive the Hessian for the fully parameterized Poisson model. The other models are analogous, though the variances in the iid models and in the lognormal models should be transformed to the log scale first.

A.1 Full conditionals for MCMC

We consider several alternative Gibbs sampling algorithms, detailed in Appendix B, which draw the covariance matrix from its full conditional distribution. When the covariance matrix is fully parameterized the full conditional distribution of the precision matrix $\mathbf{\Omega}$ is Wishart, that is $\mathbf{\Omega} \sim W(\tilde{d}, \tilde{\mathbf{E}})$. This draw is usually accomplished via the Bartlett decomposition

(Smith and Hocking, 1972). Let $\tilde{\mathbf{C}}$ be the lower triangular Cholesky decomposition of $\tilde{\mathbf{E}}$. Then let \mathbf{A} be an $r \times r$ random lower triangular matrix with independent elements $\{a_{ij} : 0 < i \leq j \leq r\}$ where $a_{ii} \sim \sqrt{\chi_{\tilde{d}-i+1}^2}$ for $i = 1, 2, \dots, r$ and $a_{ij} \sim N(0, 1)$ for $0 < i \leq j \leq r$. Then $\mathbf{\Omega} = \mathbf{L}\mathbf{L}' \sim W(\tilde{d}, \tilde{\mathbf{E}})$ where $\mathbf{L} = \tilde{\mathbf{C}}\mathbf{A}$. In the process of drawing $\mathbf{\Omega}$ we must first draw \mathbf{L} , so we construct our Gibbs samplers in terms of \mathbf{L} instead of $\mathbf{\Omega}$.

IMH applies straightforwardly to each of these models, though see Appendix A.2 for a detailed derivation of the Hessian for the county population models with a fully parameterized covariance matrix associated. To apply IMHwG in the county population models, we draw $(\boldsymbol{\beta}, \boldsymbol{\delta})$ in the Metropolis step and σ^2 , \mathbf{L} , and/or ϕ^2 in the conditionally conjugate step, depending on the model. The full conditional distribution of σ^2 in both iid models is $IG(a_\sigma + r/2, b_\sigma + \boldsymbol{\delta}'\boldsymbol{\delta}/2)$. The full conditional distribution of $\mathbf{\Omega}$ in both fully correlated models is $W\{r + 1, (\mathbf{E} + \boldsymbol{\delta}\boldsymbol{\delta}')^{-1}\}$. Then a draw from the full conditional distribution of \mathbf{L} can be obtained via the Bartlett decomposition as described in the previous paragraph. In the lognormal models the full conditional distribution of ϕ^2 is $IG\{a_\phi + n/2, b_\phi + (\log \mathbf{z} - \mathbf{X}\boldsymbol{\beta} - \mathbf{S}\boldsymbol{\delta})'(\log \mathbf{z} - \mathbf{X}\boldsymbol{\beta} - \mathbf{S}\boldsymbol{\delta})/2\}$.

A.2 Deriving the Hessian

The log posterior in the fully parameterized Poisson case can be written as

$$\begin{aligned} \log p(\boldsymbol{\beta}, \mathbf{L}, \boldsymbol{\delta} | \mathbf{z}, \mathbf{X}, \mathbf{S}) &= \text{constant} + \sum_{i=1}^n (y_i z_i - \exp(y_i)) + \sum_{k=1}^r \frac{d - k + 1}{2} \log \ell_{kk}^2 \\ &\quad - \frac{1}{2} \left\{ \boldsymbol{\delta}' \mathbf{L} \mathbf{L}' \boldsymbol{\delta} + \frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{v^2} + \text{tr}(\mathbf{E} \mathbf{L} \mathbf{L}') \right\} \\ &= \text{constant} + \sum_{i=1}^n \{z_i y_i - \exp(y_i)\} + \frac{1}{2} \mathbf{R}_r \text{vech}(\log \mathbf{L}^2) \\ &\quad - \frac{1}{2} \left[\text{vech}(\mathbf{L})' \mathbf{M}_r \{ \mathbf{K}_r' (\boldsymbol{\delta} \boldsymbol{\delta}' \otimes \mathbf{I}_r) \mathbf{K}_r + (\mathbf{I}_r \otimes \mathbf{E}) \} \mathbf{M}_r' \text{vech}(\mathbf{L}) + \frac{(\boldsymbol{\beta} - \mathbf{b})'(\boldsymbol{\beta} - \mathbf{b})}{v^2} \right] \end{aligned}$$

where $y_i = \mathbf{x}_i' \boldsymbol{\beta} + \mathbf{s}_i' \boldsymbol{\delta}$, \otimes is the Kronecker product, \mathbf{I}_r is the $r \times r$ identity matrix, and \mathbf{R}_r is an $r(r+1)/2 \times r(r+1)/2$ matrix of zeroes except the $(r+1)k - k(k+1)/2 + k - \text{rst}$ diagonal

element is equal to $d - k + 1$ for $k = 1, 2, \dots, r$, corresponding to locations in $\text{vech}(\mathbf{L})$ that store the diagonal elements of \mathbf{L} . In $\text{vech}(\log \mathbf{L}^2)$ the log and power are applied element-wise. The expansions of $\boldsymbol{\delta}' \mathbf{L} \mathbf{L}' \boldsymbol{\delta}$ and $\text{tr}(\mathbf{E} \mathbf{L} \mathbf{L}')$ can be derived from the properties of the trace operator, Kronecker products, and the following identities.

$$\begin{aligned}\boldsymbol{\delta}' \mathbf{L} \mathbf{L}' \boldsymbol{\delta} &= \text{vec}(\mathbf{L}' \boldsymbol{\delta})' \text{vec}(\mathbf{L}' \boldsymbol{\delta}), \\ \text{vec}(\mathbf{L}' \boldsymbol{\delta}) &= (\boldsymbol{\delta}' \otimes \mathbf{I}_r) \text{vec}(\mathbf{L}'), \\ \text{vec}(\mathbf{L}') &= \mathbf{K}_r \text{vec}(\mathbf{L}) = \mathbf{K}_r \mathbf{M}_r' \text{vech}(\mathbf{L}),\end{aligned}$$

and assuming $\mathbf{E} = \mathbf{C} \mathbf{C}'$, then $\text{tr}(\mathbf{L}' \mathbf{C} \mathbf{C}' \mathbf{L}) = \text{vec}(\mathbf{C}' \mathbf{L})' \text{vec}(\mathbf{C}' \mathbf{L})$ where $\text{vec}(\cdot)$ is the vectorization operation which stacks each column of its argument on top of each other into a single column vector, $\text{vech}(\cdot)$ is the half-vectorization operator which is similar but omits elements above the diagonal, tr is the trace operator, \mathbf{K}_r is the $r^2 \times r^2$ commutation matrix such that for any $r \times r$ matrix \mathbf{L} , $\text{vec}(\mathbf{L}') = \mathbf{K}_r \text{vec}(\mathbf{L})$, \mathbf{M}_r is the $r^2 \times r(r+1)/2$ elimination matrix such that for $\text{vech}(\mathbf{L}) = \mathbf{M}_r \text{vec}(\mathbf{L})$ and if additionally \mathbf{L} is lower triangular, $\text{vec}(\mathbf{L}) = \mathbf{M}_r' \text{vech}(\mathbf{L})$ (Magnus and Neudecker, 1980; Magnus, 1988). Let \mathbf{E}_{ij} be an $r \times r$ matrix of zeroes with a one in only its (i, j) th position, $\mathbf{u}_{ij} = \text{vech}(\mathbf{E}_{ij})$, and \mathbf{e}_i be a r -dimensional column vector of zeroes with a one in the i th row. Then \mathbf{K}_r and \mathbf{M}_r can be written as

$$\mathbf{K}_r = \sum_{i=1}^r \sum_{j=1}^r \mathbf{E}_{ij} \otimes \mathbf{E}_{ij}' \quad \text{and} \quad \mathbf{M}_r = \sum_{i \geq j}^r \mathbf{u}_{ij} \otimes \mathbf{e}_j' \otimes \mathbf{e}_i'.$$

Now the first derivatives of the log posterior are given by

$$\begin{aligned}\frac{\partial \log p}{\partial \boldsymbol{\beta}} &= \sum_{i=1}^n (z_i - e^{y_i}) \mathbf{x}_i' - \frac{(\boldsymbol{\beta} - \mathbf{b})'}{v^2}, \\ \frac{\partial \log p}{\partial \boldsymbol{\delta}} &= \sum_{i=1}^n (z_i - e^{y_i}) \mathbf{s}_i' - \boldsymbol{\delta}' \mathbf{L} \mathbf{L}', \\ \frac{\partial \log p}{\partial \text{vech}(\mathbf{L})} &= - \text{vech}(\mathbf{L})' \mathbf{M}_r [\mathbf{K}_r' (\boldsymbol{\delta} \boldsymbol{\delta}' \otimes \mathbf{I}_r) \mathbf{K}_r + (\mathbf{I}_r \otimes \mathbf{E})] \mathbf{M}_r' + \mathbf{R}_r \text{vech}(1/\mathbf{L}),\end{aligned}$$

where in $\text{vech}(1/\mathbf{L})$ the division is applied element-wise. Next the second derivatives are

$$\begin{aligned}
\frac{\partial^2 \log p}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}'} &= - \sum_{i=1}^n e^{y_i} \mathbf{x}_i \mathbf{x}_i' - \frac{1}{v^2} \mathbf{I}_p \\
\frac{\partial^2 \log p}{\partial \boldsymbol{\delta} \partial \boldsymbol{\delta}'} &= - \sum_{i=1}^n e^{y_i} \mathbf{s}_i \mathbf{s}_i' - \mathbf{L} \mathbf{L}' \\
\frac{\partial^2 \log p}{\partial \text{vech}(\mathbf{L}) \partial \text{vech}(\mathbf{L})'} &= - \mathbf{M}_r [\mathbf{K}_r' (\boldsymbol{\delta} \boldsymbol{\delta}' \otimes \mathbf{I}_r) \mathbf{K}_r + (\mathbf{I}_r \otimes \mathbf{E})] \mathbf{M}_r' - \mathbf{R}_r \text{diag}(\text{vech}(\mathbf{L})^{-2}) \\
\frac{\partial^2 \log p}{\partial \boldsymbol{\beta} \partial \boldsymbol{\delta}'} &= - \sum_{i=1}^n e^{y_i} \mathbf{s}_i \mathbf{x}_i' \\
\frac{\partial^2 \log p}{\partial \boldsymbol{\beta} \partial \text{vech}(\mathbf{L})'} &= \mathbf{0}_{p \times r(r+1)/2} \\
\frac{\partial^2 \log p}{\partial \boldsymbol{\delta} \partial \text{vech}(\mathbf{L})'} &= - \frac{\partial \boldsymbol{\delta}' \mathbf{L} \mathbf{L}'}{\partial \text{vech}(\mathbf{L})'} = -(\boldsymbol{\delta}' \otimes \mathbf{I}_r)(\mathbf{I}_{r^2} + \mathbf{K}_r)(\mathbf{L} \otimes \mathbf{I}_r) \mathbf{M}_r',
\end{aligned}$$

where $\text{diag}(\text{vech}(\mathbf{L})^{-2})$ is a diagonal matrix with the elements of $\text{vech}(\mathbf{L})$ raised to the power -2 along the diagonal. The last second derivative matrix can be derived using repeated application of the chain rule and from the following facts for any $r \times r$ matrix \mathbf{A} (Magnus and Neudecker, 2005):

$$\begin{aligned}
\frac{\partial \text{vec}(\mathbf{A} \mathbf{A}')}{\partial \text{vec}(\mathbf{A})} &= (\mathbf{I}_{r^2} + \mathbf{K}_r)(\mathbf{A} \otimes \mathbf{I}_r) \\
\frac{\partial \mathbf{A} \boldsymbol{\delta}}{\partial \text{vec}(\mathbf{A})} &= \boldsymbol{\delta}' \otimes \mathbf{I}_r.
\end{aligned}$$

Then, using the chain rule for lower triangular \mathbf{L} we have

$$\begin{aligned}
\frac{\partial \boldsymbol{\delta}' \mathbf{L} \mathbf{L}'}{\partial \text{vech}(\mathbf{L})'} &= \frac{\partial \boldsymbol{\delta}' \mathbf{L} \mathbf{L}'}{\partial \mathbf{L} \mathbf{L}' \boldsymbol{\delta}} \frac{\partial \mathbf{L} \mathbf{L}' \boldsymbol{\delta}}{\partial \text{vec}(\mathbf{L} \mathbf{L}')} \frac{\partial \text{vec}(\mathbf{L} \mathbf{L}')}{\partial \text{vec}(\mathbf{L})} \frac{\partial \text{vec}(\mathbf{L})}{\partial \text{vech}(\mathbf{L})} \frac{\partial \text{vech}(\mathbf{L})}{\partial \text{vech}(\mathbf{L})'} \\
&= \mathbf{I}_r \frac{\partial \mathbf{L} \mathbf{L}' \boldsymbol{\delta}}{\partial \text{vec}(\mathbf{L} \mathbf{L}')} \frac{\partial \text{vec}(\mathbf{L} \mathbf{L}')}{\partial \text{vec}(\mathbf{L})} \mathbf{M}_r' \mathbf{I}_{r(r+1)/2} \\
&= (\boldsymbol{\delta}' \otimes \mathbf{I}_r)(\mathbf{I}_{r^2} + \mathbf{K}_r)(\mathbf{L} \otimes \mathbf{I}_r) \mathbf{M}_r'.
\end{aligned}$$

Finally, the Hessian is

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 \log p}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}'} & \frac{\partial^2 \log p}{\partial \boldsymbol{\beta} \partial \boldsymbol{\delta}'} & \frac{\partial^2 \log p}{\partial \boldsymbol{\beta} \partial \text{vech}(\mathbf{L})'} \\ \frac{\partial^2 \log p}{\partial \boldsymbol{\delta} \partial \boldsymbol{\beta}'} & \frac{\partial^2 \log p}{\partial \boldsymbol{\delta} \partial \boldsymbol{\delta}'} & \frac{\partial^2 \log p}{\partial \boldsymbol{\delta} \partial \text{vech}(\mathbf{L})'} \\ \frac{\partial^2 \log p}{\partial \text{vech}(\mathbf{L}) \partial \boldsymbol{\beta}'} & \frac{\partial^2 \log p}{\partial \text{vech}(\mathbf{L}) \partial \boldsymbol{\delta}'} & \frac{\partial^2 \log p}{\partial \text{vech}(\mathbf{L}) \partial \text{vech}(\mathbf{L})'} \end{bmatrix}.$$

B Alternative MCMC algorithms

[CURRENTLY THIS SECTION ONLY HAS GENERIC VERSIONS OF THE ALGORITHMS. DETAILS FOR OUR CASES?] This section describes the alternative MCMC algorithms used for comparisons with PSO assisted Metropolis-Hastings algorithms. In particular, we use two types of adaptive random walk Metropolis within Gibbs algorithms. In the generic problem, suppose we wish to sample from the posterior distribution $p(\boldsymbol{\theta}|\mathbf{y})$ using MCMC methods. Suppose that $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and that the full conditional $p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2, \mathbf{y})$ can be sampled from easily while the full conditional for $\boldsymbol{\theta}_2$ may be intractable. Then a single move random walk Metropolis within Gibbs (RWwG) algorithm for this problem is as follows.

Algorithm B.1 (Single move random walk Metropolis within Gibbs) *Given target posterior $p(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2|\mathbf{y})$ where $\boldsymbol{\theta}_2 = (\theta_{21}, \theta_{22}, \dots, \theta_{2n})$, it is easy to sample from $p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2, \mathbf{y})$, and given that the support of $p(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1, \mathbf{y})$ is \mathbb{R}^n , iteration $t + 1$ is obtained from iteration t via*

1. Draw $\boldsymbol{\theta}_1^{(t+1)} \sim p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2^{(t)}, \mathbf{y})$

2. For $k = 1, 2, \dots, n$

Draw $\theta_{2k}^{(prop)} \sim N(\theta_{2k}^{(t)}, \eta_k)$ and form the Metropolis acceptance ratio

$$a_k^{(t)} = \frac{p(\theta_{2k}^{(prop)}|\boldsymbol{\theta}_1^{(t+1)}, \theta_{21}^{(t+1)}, \dots, \theta_{2k-1}^{(t+1)}, \theta_{2k+1}^{(t)}, \dots, \theta_{2n}^{(t)}, \mathbf{y})}{p(\theta_{2k}^{(t)}|\boldsymbol{\theta}_1^{(t+1)}, \theta_{21}^{(t+1)}, \dots, \theta_{2k-1}^{(t+1)}, \theta_{2k+1}^{(t)}, \dots, \theta_{2n}^{(t)}, \mathbf{y})}.$$

Then set $\theta_{2k}^{(t+1)} = \theta_{2k}^{(prop)}$ with probability $r_k^{(t)} = \min(a_k, 1)$ and otherwise set $\theta_{2k}^{(t+1)} = \theta_{2k}^{(t)}$

A major problem with this algorithm is that the η_k s must be selected so that the algorithm Metropolis steps accept a reasonable amount of time. According to Gelman et al. (1996) the optimal acceptance rate in a narrow set of problems is 0.44 for a single dimensional random walk, though this is often used as a guideline for more complex problems. We

adaptively tune η_k during the burn-in period of the chain in a manner discussed in Andrieu and Thoms (2008). The computed Metropolis acceptance probability for θ_{2k} is denoted by $r_k^{(t)} = \min(a_k^{(t)}, 1)$; let r^* denote the target acceptance probability. Then we evolve η_k over time via

$$\log \eta_k^{(t+1)} = \log \eta_k^{(t)} + \gamma^{(t+1)}(r_k^{(t)} - r^*)$$

where $\gamma^{(t)}$ is a fixed sequence decreasing to zero fast enough to enough that the algorithm converges. The intuition here is that if the acceptance rate is too high, we can increase the effective search space by increasing the random walk standard deviation, while if it is too low, we can decrease the effective search space by decreasing the random walk standard deviation. We use $r^* = 0.44$. A tuning method such as this implies that $(\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \dots)$ is no longer a Markov chain, and additional conditions are required to ensure convergence to the target posterior distribution. So in practice our RWwG algorithms run Algorithm B.1 with the tuning method described above until convergence and until the η_k s settle into a rough equilibrium, then we use Algorithm B.1 without tuning but using the last known values of the η_k s. In practice this is equivalent setting $\gamma^{(t)} = 0$ after the burn-in period. During the burn-in we set $\gamma^{(t)} = 1$ and we initialize at $\eta_k^{(0)} = 1$ for all k .

An alternative to RWwG algorithms are block random walk Metropolis within Gibbs algorithms (B-RWwG). Suppose we have an estimate of the covariance structure between the elements of $\boldsymbol{\theta}_2$ in the posterior. Then

Algorithm B.2 (Block random walk Metropolis within Gibbs) *Given target posterior $p(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2 | \mathbf{y})$ where it is easy to sample from $p(\boldsymbol{\theta}_1 | \boldsymbol{\theta}_2, \mathbf{y})$, the support of $p(\boldsymbol{\theta}_2 | \boldsymbol{\theta}_1, \mathbf{y})$ is \mathbb{R}^n , and given an estimate $\boldsymbol{\Sigma}$ of $\text{cov}(\boldsymbol{\theta}_2 | \mathbf{y})$, iteration $t + 1$ is obtained from iteration t via*

1. Draw $\boldsymbol{\theta}_1^{(t+1)} \sim p(\boldsymbol{\theta}_1 | \boldsymbol{\theta}_2^{(t)}, \mathbf{y})$

2. Draw $\boldsymbol{\theta}_2^{(prop)} \sim N(\boldsymbol{\theta}_2^{(t)}, \eta \boldsymbol{\Sigma})$ and form the Metropolis acceptance ratio

$$a = \frac{p(\boldsymbol{\theta}_2^{(prop)} | \boldsymbol{\theta}_1^{(t+1)}, \mathbf{y})}{p(\boldsymbol{\theta}_2^{(t)} | \boldsymbol{\theta}_1^{(t+1)}, \mathbf{y})}.$$

Then set $\boldsymbol{\theta}_2^{(t+1)} = \boldsymbol{\theta}_2^{(prop)}$ with probability $\min(a, 1)$ and otherwise set $\boldsymbol{\theta}_2^{(t+1)} = \boldsymbol{\theta}_2^{(t)}$.

We make this algorithm adaptive as well by tuning η in the same fashion as the η_k s above. The main difference is that this algorithm must be initialized with a crude estimate of $\boldsymbol{\Sigma}$ by running another algorithm, e.g. Algorithm B.1, or Algorithm B.2 with $\boldsymbol{\Sigma}$ chosen to be diagonal and manually tuned.

References

- Andrieu, C. and Thoms, J. (2008). “A tutorial on adaptive MCMC.” *Statistics and Computing*, 18, 4, 343–373.
- Chen, Z. and Dunson, D. B. (2003). “Random effects selection in linear mixed models.” *Biometrics*, 59, 4, 762–769.
- Frühwirth-Schnatter, S. and Tüchler, R. (2008). “Bayesian parsimonious covariance estimation for hierarchical linear mixed models.” *Statistics and Computing*, 18, 1, 1–13.
- Gelman, A., Roberts, G., and Gilks, W. (1996). “Efficient Metropolis jumping rules.” *Bayesian statistics*, 5, 599-608, 42.
- Magnus, J. R. (1988). *Linear structures*. No. 42 in Griffin’s Statistical Monographs and Courses. New York: Oxford University Press.
- Magnus, J. R. and Neudecker, H. (1980). “The elimination matrix: some lemmas and applications.” *SIAM Journal on Algebraic Discrete Methods*, 1, 4, 422–449.
- (2005). *Matrix differential calculus with applications in statistics and econometrics*. 3rd ed. New York: John Wiley & Sons.
- Smith, W. and Hocking, R. (1972). “Algorithm AS 53: Wishart variate generator.” *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, 21, 3, 341–345.