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Y. Fan
University of New South Wales

D. S. Leslie
University of Bristol

M. P. Wand
University of Wollongong, mwand@uow.edu.au

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Y. Fan, D. S. Leslie and Matt P. Wand

Centre for Statistical & Survey Methodology, University of Wollongong, Wollongong NSW 2522. Phone +61 2 4221 5435, Fax +61 2 4221 4845. Email: anica@uow.edu.au

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BY Y. FAN
School of Mathematics and Statistics,
University of New South Wales, Sydney 2052, AUSTRALIA

D.S. LESLIE
School of Mathematics, University of Bristol, University Walk, Bristol, BS8 1TW,
UNITED KINGDOM

AND M.P. WAND
School of Mathematics and Applied Statistics,
University of Wollongong, Wollongong 2522, AUSTRALIA

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ABSTRACT

We present a sequential Monte Carlo algorithm for the Bayesian analysis of generalised linear mixed models (GLMMs). These models support an extraordinary variety of interesting regression-type analyses, but performing inference is often extremely difficult, even when using the Bayesian approach combined with Markov chain Monte Carlo (MCMC). Sequential Monte Carlo (SMC) is a new and general method for producing samples from posterior distributions. In this article we demonstrate use of the SMC method for performing inference for GLMMs. We demonstrate the effectiveness of the method on both simulated and real data, and find that sequential Monte Carlo is a competitive alternative to the available MCMC techniques.

Keywords: generalised additive models; longitudinal data analysis; nonparametric regression; sequential Monte Carlo.

1 Introduction

Effective strategies for generalised linear mixed model (GLMM) analysis continues to be a vibrant research area. Reasons include:

- GLMMs have become an indispensable vehicle for analysing a significant portion of contemporary complex data sets.
- GLMMs are inherently difficult to fit compared with ordinary linear mixed models and generalised linear models.

- Existing strategies involve a number of trade-offs concerning, for example, approximation accuracy, computational times and Markov chain convergence.

Overviews of the usefulness and difficulties of GLMM-based analysis may be found in, for example, McCulloch & Searle (2000), Ruppert, Wand & Carroll (2003) and Skrondal & Rabe-Hesketh (2004).

Most practical GLMM methodology falls into two categories: analytic approximations (e.g. Breslow & Clayton, 1993) and Monte Carlo methods (e.g. Clayton, 1996). Monte Carlo methods have the advantage of providing direct approximations to quantities of interest (Besag, Green, Higdon & Mengersen, 1995). On the other hand, analytic approximations, such as Laplace approximation, are indirect and prone to substantial bias (e.g. Breslow & Lin, 1995). The most common Monte Carlo approach is Markov Chain Monte Carlo (MCMC), where approximation accuracy is associated with Markov chain convergence.

Zhao, Staudenmayer, Coull & Wand (2006) is a recent example of research concerned with practical GLMM analysis via Markov chain Monte Carlo. Those authors explored use of the MCMC computing package `WinBUGS` and showed it to exhibit good performance for a number of examples.

One of the major difficulties associated with using MCMC is the need to assess convergence. While theoretical results bounding the difference between the simulation result and the true distribution have been developed (e.g. Rosenthal, 1995, Cowles & Rosenthal, 1998), their applications remain limited to special cases. Hence popular methods for convergence assessment rely on the comparison of multiple sample output (see Cowles & Carlin, 1996 for a comparative review). These methods can invariably fail to detect a lack of convergence and one needs to be cautious when taking such an approach. Another major drawback of MCMC is the difficulty in designing efficient samplers. The need for such algorithms is more apparent for complex problems. Various methods have been proposed in the literature, (see Frigessi, 2003), however most have limited applicability.

Both problems associated with MCMC discussed above are inherently due to the reliance on a Markov chain. The need for convergence assessment is a by-product of the reliance on the single Markov chain, while the consequent discarding of burn-in can be unreliable and wasteful. The necessity for more efficient samplers often stem from the slow mixing suffered by MCMC samplers due to the Markovian nature of the sampler, and the attempts in overcoming this problem is again restricted by the need to preserve the stationary distributions of the Markov chain. Sequential Monte Carlo methods are a class of very flexible Monte Carlo samplers that extend the well known importance sampling method. In this article we show that sequential Monte Carlo methods provide a simple and effective means of Bayesian GLMM analysis. These methods produce weighted samples from the target distribution without the need to assess convergence of a Markov chain. We provide a general yet simple framework for efficient design of the sampler, and demonstrate that this approach is a viable alternative to MCMC.

Section 2 contains a brief summary of Bayesian approaches to generalised linear mixed models. In Section 3 we provide details on analysis for such models via sequential Monte Carlo sampling. In Section 4 we present two examples. In a simulated Poisson regression example, we compare the efficiencies of SMC with alternative Monte Carlo methods, and then demonstrate the effectiveness of SMC in a binary logistic regression example involv-

ing real data. Some concluding remarks are given in Section 5.

2 Bayesian Generalised Linear Mixed Models

GLMMs for canonical one-parameter exponential families (e.g. Poisson, logistic) and Gaussian random effects take the general form

$$[\mathbf{y}|\boldsymbol{\beta}, \mathbf{u}, \mathbf{G}] = \exp\{\mathbf{y}^T(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}) - \mathbf{1}^T b(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}) + \mathbf{1}^T c(\mathbf{y})\}, \tag{1}$$

$$[\mathbf{u}|\mathbf{G}] \sim N(\mathbf{0}, \mathbf{G}) \tag{2}$$

where here, and throughout, the distribution of a random vector $\mathbf{x}$ is denoted by $[\mathbf{x}]$ and the conditional distribution of $\mathbf{y}$ given $\mathbf{x}$ is denoted by $[\mathbf{y}|\mathbf{x}]$. In the Poisson case $b(x) = e^x$, while in the logistic case $b(x) = \log(1 + e^x)$. An important special case of (1)-(2) is the variance components model

$$\begin{aligned} [\mathbf{y}|\boldsymbol{\beta}, \mathbf{u}, \sigma^2_{u1}, \ldots, \sigma^2_{uL}] &= \exp\{\mathbf{y}^T(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}) - \mathbf{1}^T b(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}) + \mathbf{1}^T c(\mathbf{y})\}, \\ \mathbf{u} &= \begin{bmatrix} \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_L \end{bmatrix}, \qquad [\mathbf{u}|\sigma^2_{u1}, \ldots, \sigma^2_{uL}] \sim N(\mathbf{0}, \text{blockdiag}_{1\le\ell\le L}(\sigma^2_{u\ell}\mathbf{I}_{q_\ell})). \end{aligned} \tag{3}$$

where q_ℓ is the number of elements in $\mathbf{u}_\ell$. While (3) is not as general as (1)-(2) it still handles many important situations such as random intercepts and generalised additive models (Zhao *et al.*, 2006). With simplicity in mind, we will focus on this GLMM for the remainder of the paper.

The prior on $\boldsymbol{\beta}$ will be taken to be a diffuse Gaussian:

$$\boldsymbol{\beta} \sim N(\mathbf{0}, \sigma^2_\beta \mathbf{I}) \tag{4}$$

for some large $\sigma^2_\beta > 0$. The prior for $(\sigma^2_{u1}, \ldots, \sigma^2_{uL})$ is assumed to have independent components; i.e.

$$[\sigma^2_{u1}, \ldots, \sigma^2_{uL}] = [\sigma^2_{u1}] \cdots [\sigma^2_{uL}].$$

A number of possibilities for $[\sigma^2_{u\ell}]$ could be considered (Gelman 2006). These include an inverse gamma distribution, a uniform distribution, and a folded Cauchy distribution. However in this paper we use a conditionally conjugate inverse gamma distribution:

$$[\sigma^2_{u\ell}] = \frac{A^{A_{u\ell}}_{u\ell}}{\Gamma(A_{u\ell})}(\sigma^2_{u\ell})^{-A_{u\ell}-1} e^{-A_{u\ell}/\sigma^2_{u\ell}}, \quad \sigma^2_{u\ell} > 0 \ . \tag{5}$$

This prior distribution was advocated by Zhao *et al* (2006) for $A_{u\ell} = 0.01$. The prior is therefore fairly non-informative, yet results in a slightly simpler sampling procedure; the method generalises easily to the other prior distributions.

It will be convenient to introduce some additional notation to enable the model to be described more succinctly. We start by writing

$$\mathbf{C} = [\mathbf{X}\ \mathbf{Z}] \quad \text{and} \quad \boldsymbol{\nu} = \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u} \end{bmatrix}.$$

We also write q_β for the number of elements in β, and

$$\mathbf{V} = \text{blockdiag}(\sigma_\beta^2 \mathbf{I}_{q_\beta}, \sigma_{u1}^2 \mathbf{I}_{q_1}, \ldots, \sigma_{uL}^2 \mathbf{I}_{q_L})$$

for the prior covariance of $\boldsymbol{\nu}$. Writing $\boldsymbol{\sigma}^2$ for $(\sigma_{u1}^2, \ldots, \sigma_{uL}^2)$, we can then combine (3), (4) and (5) to give the joint density of all parameters and data:

$$[\mathbf{y}, \boldsymbol{\nu}, \boldsymbol{\sigma}^2] = \exp\Big[\mathbf{y}^T\mathbf{C}\boldsymbol{\nu} - \mathbf{1}^T b(\mathbf{C}\boldsymbol{\nu}) + \mathbf{1}^T c(\mathbf{y}) - \tfrac{1}{2}\boldsymbol{\nu}^T\mathbf{V}^{-1}\boldsymbol{\nu} - \sum_{\ell=1}^{L} \tfrac{q_\ell}{2}\log(\sigma_{u\ell}^2)$$
$$+ \sum_{\ell=1}^{L}\left\{A_{u\ell}\log(A_{u\ell}) - \log\Gamma(A_{u\ell}) - (A_{u\ell}+1)\log(\sigma_{u\ell}^2) - A_{u\ell}/\sigma_{u\ell}^2\right\}\Big].$$

From this, and noting that $\boldsymbol{\nu}^T\mathbf{V}^{-1}\boldsymbol{\nu} = \|\boldsymbol{\beta}\|^2/\sigma_\beta^2 + \sum_{\ell=1}^{L}\|\mathbf{u}_\ell\|^2/\sigma_{u\ell}^2$, it is clear that the posterior distribution of the parameters is simply proportional to the function

$$\begin{aligned}\pi(\boldsymbol{\nu}, \boldsymbol{\sigma}^2) \;\; = \;\; & \exp\Big[\mathbf{y}^T\mathbf{C}\boldsymbol{\nu} - \mathbf{1}^T b(\mathbf{C}\boldsymbol{\nu}) - \frac{1}{2\sigma_\beta^2}\|\boldsymbol{\beta}\|^2 \\ & - \sum_{\ell=1}^{L}\left\{(A_{u\ell} + \tfrac{q_\ell}{2} + 1)\log(\sigma_{u\ell}^2) + (A_{u\ell} + \|\mathbf{u}_\ell\|^2)/\sigma_{u\ell}^2\right\}\Big]. \qquad (6)\end{aligned}$$

In Section 3, we will develop a sequential Monte Carlo sampler to produce samples from the distribution proportional to π.

3 Sequential Monte Carlo Sampling

The Monte Carlo approach to GLMM analysis performs inference by drawing samples from the joint posterior distribution of the parameters $\boldsymbol{\theta} = (\boldsymbol{\beta}, \mathbf{u}, \sigma_{u1}^2, \ldots, \sigma_{uL}^2)$. We write $\pi(\boldsymbol{\theta})$ for the (unnormalised) density of this posterior distribution. Instead of using a Markov chain with π as its stationary distribution to produce these samples, the sequential Monte Carlo (SMC) method is a generalisation of importance sampling that produces a weighted sample from π while retaining some of the benefits of MCMC analysis (Del Moral, Doucet & Jasra, 2006).

The use of SMC for static problems (as opposed to particle filters for dynamic problems; Doucet, Godsill & Andrieu, 2000) requires the introduction of auxiliary distributions π_0, π_1,..., π_{S-1}. At stage s of the sampler we use a (weighted) sample from the previous distribution π_{s-1} to produce a (weighted) sample from π_s. We set $\pi_S = \pi$ so that after S stages we have a sample from the posterior distribution of interest. The auxiliary distributions can be constructed in several ways: Chopin (2002) introduces the observations incrementally to evolve the distribution from the prior to the posterior; Fearnhead (2004) uses a similar technique, but increases the size of the state space as more observations are added; Del Moral *et al.* (2006) use

$$\begin{aligned}\pi_s \;\; & \propto \;\; \pi_0^{1-\gamma_s}\pi^{\gamma_s}, \quad \text{where} \qquad (7) \\ 0 \;\; & = \;\; \gamma_0 \le \gamma_1 \le \cdots \le \gamma_S = 1\end{aligned}$$

and π_0 is chosen to be the prior distribution for the parameters. In this article, due to the diffuse nature of the prior distribution, the initial distribution π_0 is instead chosen to be a multivariate Normal distribution with mean and covariance matrix chosen based on estimates obtained using classical methods for fitting GLMMs.

The SMC algorithm starts by sampling N samples, termed "particles", from the initial distribution π_0. Denote by $\boldsymbol{\theta}_i^0$ the ith particle at initial stage $s = 0$, and allocate weight $w_i^0 \equiv 1$ to each of the N particles, so that $\{\boldsymbol{\theta}_i^0, w_i^0\}$ is a weighted sample from π_0.

The SMC technique uses the weighted particles from distribution π_{s-1} to produce particles from distribution π_s through moving, reweighting and (possibly) resampling; see Del Moral *et al.* (2006). For simplicity, the formulation we use is that described in detail in Section 3.3.2.3 of that paper, which essentially results in the resample–move algorithm used by Chopin (2002) and Gilks & Berzuini (2001). This is also similar to the annealed importance sampling method of Neal (2001), but the use of resampling within the algorithm greatly improves the efficiency of the method. Writing $\boldsymbol{\theta}_i^s$ for the ith particle at stage s, at each stage $0 < s \leq S$ of the algorithm we perform the following steps:

Reweight Given N weighted particles $\{\boldsymbol{\theta}_i^{s-1}, w_i^{s-1}\}$ from π_{s-1}, set

$$w_i^s = w_i^{s-1} \frac{\pi_s(\boldsymbol{\theta}_i^{s-1})}{\pi_{s-1}(\boldsymbol{\theta}_i^{s-1})}.$$

$\{\boldsymbol{\theta}_i^{s-1}, w_i^s\}$ is now a weighted sample from π_s.

Resample If the effective sample size (ESS), defined as $(\sum_{i=1}^N w_i^s)^2 / \sum_{i=1}^N (w_i^s)^2$, is less than kN, where k is some constant typically taken to be $1/2$, then we perform stratified resampling (Kitagawa, 1996). ESS estimates the equivalent number of random samples required to obtain an estimate, such that its Monte Carlo variation is equal to that of the N weighted particles. Resampling then discards particles with low weights and multiplies particles with high weights. Finally, resampled particle weights are reset to $\{w_i^s\} \equiv 1$.

Move Let $\{\boldsymbol{\theta}_s, w_i^s\}, i = 1, \ldots, N$ denote samples from at the current distribution π_s after reweighting and (possibly) resampling. To increase particle diversity we replace each sample according to

$$\boldsymbol{\theta}_i^s \sim K_s(\boldsymbol{\theta}_i^s, \cdot)$$

where K_s is an MCMC transition kernel that admits π_s as stationary distribution. Gamerman (1997) provides detail on MCMC transition kernels.

It is known that this particular formulation of the SMC algorithm is suboptimal, especially if the distributions on consecutive stages are too far apart. However it is one of the easiest SMC algorithms to implement, and for the static problem we have here it is easy to ensure that the difference between π_{s-1} and π_s is small. (Contrast this situation with that of an SMC algorithm for a dynamic problem, or the technique of Chopin (2002) where data arrive over time and there is no control over the distance between π_{s-1} and π_s.)

The "parameters" of the algorithm that must be chosen when implementing this sampler are therefore:

- the initial distribution π_0,
- the sequence of values γ_s that govern the rate of transition from the initial distribution π_0 to the posterior distribution π,
- the transition kernels K_s, used to move the particles within the distribution proportional to π_s, and
- the number of particles N.

Specific choices of these parameters used in this paper are discussed in the following subsections. We give a more algorithmic description of our method in the Appendix.

3.1 Initial distribution π_0

As previously observed, using the prior distribution as an initial distribution is flawed in this case, since the prior is highly diffuse. Instead we use the penalised quasi-likelihood (PQL) method (Breslow & Clayton 1993) to obtain an approximate fit of the model. Let $\widehat{\boldsymbol{\nu}}_{\text{PQL}}$ and $\widehat{\boldsymbol{\sigma}}^2_{\text{PQL}}$ be the estimate of $\boldsymbol{\nu}$ and $\boldsymbol{\sigma}^2$ obtained using PQL. We will calculate a normal approximation of the posterior distribution of $\boldsymbol{\nu}$ centred at this approximate maximum likelihood estimate, which can then be used to construct an initial distribution π_0 for the SMC procedure. Note from (6) that

$$\pi(\boldsymbol{\nu}, \boldsymbol{\sigma}^2) = \exp\left\{\mathbf{y}^T\mathbf{C}\boldsymbol{\nu} - \mathbf{1}^T b(\mathbf{C}\boldsymbol{\nu}) - \tfrac{1}{2}\boldsymbol{\nu}^T\mathbf{V}^{-1}\boldsymbol{\nu} + f(\boldsymbol{\sigma}^2)\right\},$$

where f is some function that does not depend on $\boldsymbol{\nu}$. It is a simple calculation to see that the matrix of second derivatives with respect to components of $\boldsymbol{\nu}$ is $-\mathbf{C}^T\text{diag}\{b''(\mathbf{C}\boldsymbol{\nu})\}\mathbf{C} - \mathbf{V}^{-1}$; we therefore initialise our algorithm by taking a normal distribution for $\boldsymbol{\nu}$ with mean $\widehat{\boldsymbol{\nu}}_{\text{PQL}}$ and covariance matrix

$$\boldsymbol{\Sigma} = \left[\mathbf{C}^T\text{diag}\left\{b''(\mathbf{C}\widehat{\boldsymbol{\nu}}_{\text{PQL}})\right\}\mathbf{C} + \widehat{\mathbf{V}}^{-1}_{\text{PQL}}\right]^{-1}, \tag{8}$$

where the entries in $\widehat{\mathbf{V}}_{\text{PQL}}$ are taken from $\widehat{\boldsymbol{\sigma}}^2_{\text{PQL}}$.

It remains to specify a distribution for the variance vector $\boldsymbol{\sigma}^2$. We have found it convenient to specify this conditional on $\boldsymbol{\nu}$, and of a form that is consistent with the posterior distribution π. We take

$$\pi_0(\boldsymbol{\sigma}^2 \mid \boldsymbol{\nu}) \propto \prod_{\ell=1}^{L}(\sigma^2_{u\ell})^{-A_{u\ell}-q_\ell/2-1}e^{-(A_{u\ell}+\frac{1}{2}\|\mathbf{u}_\ell\|^2)/\sigma^2_{u\ell}}, \tag{9}$$

i.e. the $\sigma^2_{u\ell}$ are conditionally independent given $\boldsymbol{\nu}$, and each has an inverse gamma distribution depending on the corresponding components of $\mathbf{u}$. Hence, an initial sample from π_0 can easily be generated by first sampling from the normal distribution for $\boldsymbol{\nu}$ then sampling the $\sigma^2_{u\ell}$ from their conditional distributions. Furthermore, we will see in Sections 3.2 and 3.3 that this results in simple conditional distributions for $\sigma^2_{u\ell}$ at all stages of the sampler.

Putting together the initial distributions of $\boldsymbol{\nu}$ and $\boldsymbol{\sigma}^2$, we see that

$$\pi_0(\boldsymbol{\nu}, \boldsymbol{\sigma}^2) \propto \exp\Big[(\boldsymbol{\nu} - \widehat{\boldsymbol{\nu}}_{\text{PQL}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\nu} - \widehat{\boldsymbol{\nu}}_{\text{PQL}}) - \sum_{\ell=1}^{L} \big\{ (A_{u\ell} + \tfrac{q_\ell}{2} + 1) \log \sigma_{u\ell}^2 + (A_{u\ell} + \tfrac{1}{2}\|\mathbf{u}_\ell\|^2)/\sigma_{u\ell}^2 \big\} \Big]. \quad (10)$$

3.2 Sequence of intermediary distributions

In this section we describe the sequence of distributions used to transition from π_0 to $\pi_S = \pi$. Recall that we choose to use the formulation (7). Using (10) and (6) it is clear that the intermediate distributions are proportional to π_s where

$$\begin{aligned}
& \pi_s(\boldsymbol{\nu}, \boldsymbol{\sigma}^2) \\
= \; & \exp\Big[\gamma_s \big\{ \mathbf{y}^T \mathbf{C}\boldsymbol{\nu} - \mathbf{1}^T b(\mathbf{C}\boldsymbol{\nu}) - \frac{1}{2\sigma_\beta^2}\|\boldsymbol{\beta}\|^2 \\
& \qquad - \sum_{\ell=1}^{L} \big((A_{u\ell} + \tfrac{q_\ell}{2} + 1) \log(\sigma_{u\ell}^2) + (A_{u\ell} + \|\mathbf{u}_\ell\|^2)/\sigma_{u\ell}^2 \big) \big\} \\
& + (1 - \gamma_s) \big\{ (\boldsymbol{\nu} - \widehat{\boldsymbol{\nu}}_{\text{PQL}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\nu} - \widehat{\boldsymbol{\nu}}_{\text{PQL}}) \\
& \qquad - \sum_{\ell=1}^{L} \big((A_{u\ell} + \tfrac{q_\ell}{2} + 1) \log \sigma_{u\ell}^2 + (A_{u\ell} + \tfrac{1}{2}\|\mathbf{u}_\ell\|^2)/\sigma_{u\ell}^2 \big) \big\} \Big] \\
= \; & \exp\Big[\gamma_s \big\{ \mathbf{y}^T \mathbf{C}\boldsymbol{\nu} - \mathbf{1}^T b(\mathbf{C}\boldsymbol{\nu}) - \frac{1}{2\sigma_\beta^2}\|\boldsymbol{\beta}\|^2 \big\} \\
& \qquad + (1 - \gamma_s) \big\{ (\boldsymbol{\nu} - \widehat{\boldsymbol{\nu}}_{\text{PQL}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\nu} - \widehat{\boldsymbol{\nu}}_{\text{PQL}}) \big\} \\
& \qquad - \sum_{\ell=1}^{L} \big\{ (A_{u\ell} + \tfrac{q_\ell}{2} + 1) \log \sigma_{u\ell}^2 + (A_{u\ell} + \tfrac{1}{2}\|\mathbf{u}_\ell\|^2)/\sigma_{u\ell}^2 \big\} \Big]
\end{aligned} \quad (11)$$

In the absence of any additional information about the shapes of these distributions, it is difficult to specify a sensible generic sequence of γ_s values. Hence for the rest of the paper we choose to increase γ_s from $\gamma_0 = 0$ to $\gamma_{S-5} = 1$ in a linear fashion, that is, values of γ_s are sequentially incremented by the same amount. Additionally, we append $\gamma_{S-4} = \cdots = \gamma_S = 1$ to this sequence to give five stages at the end of the sampler on which the particles are not resampled. This means that the final sample is well spread out over the distribution π (it was found that if resampling happened too close to the end of the sampler then several samples might be identical, resulting in poor density estimates being produced using the standard techniques).

It is an interesting and open research question as to whether the sequence γ_s can be chosen in a more principled manner. One option would be to choose the sequence in advance using some properties of the distributions π_0 and π. An alternative would be to choose the next γ_s adaptively while the sampler proceeds through the sequence of distributions; however it is not straightforward to generalise the proofs of validity of the sampler in this case.

3.3 Transition kernels

For this paper we choose to use Metropolis-Hastings transition kernels for the parameters in $\boldsymbol{\nu}$. The choice of inverse gamma distributions for the components of $\boldsymbol{\sigma}^2$ within π_0 means that we can simply use Gibbs sampling steps to update those components. At each step s we use a Metropolis–Hastings transition kernels K_s. Since π_0 is an approximation to π, and π_s is in some sense between π_0 and π, we use the same proposal distributions at each step s. These proposal distributions are derived from π_0 as described in this section.

We form a partition $\{\mathcal{I}_1, \ldots, \mathcal{I}_J\}$ of $\{1, \ldots, P\}$ so that $[\mathbf{C}_{\mathcal{I}_1} \cdots \mathbf{C}_{\mathcal{I}_J}]$ is the matrix $\mathbf{C}$, but with columns possibly re-ordered; and

$$\begin{bmatrix} \boldsymbol{\nu}_{\mathcal{I}_1} \\ \vdots \\ \boldsymbol{\nu}_{\mathcal{I}_J} \end{bmatrix}$$

is the corresponding partition of $\boldsymbol{\nu}$. (The case $J = 1$ corresponds to no partitioning.) On each move step of the algorithm we move through the series of subsets $\mathcal{I}_j$, for $j = 1, \ldots, J$. We apply a Metropolis-Hastings transition kernel to the components $\boldsymbol{\nu}_{\mathcal{I}_j} = (\nu_i)_{i \in \mathcal{I}_j}$.

To describe the transitions we introduce the matrices $\boldsymbol{\Sigma}_{\mathcal{I}_j}$, where $\boldsymbol{\Sigma}_{\mathcal{I}_j}$ is the conditional covariance under π_0 of $\boldsymbol{\nu}_{\mathcal{I}_j}$ given the values of $\boldsymbol{\nu}_{-\mathcal{I}_j} = (\nu_i)_{i \notin \mathcal{I}_j}$. These can be calculated at the start of the algorithm. Recall that since π_0 is an approximation of π, the $\boldsymbol{\Sigma}_{\mathcal{I}_j}$ matrices therefore correspond to approximations of the conditional covariance of $\boldsymbol{\nu}_{\mathcal{I}_j}$ given $\boldsymbol{\nu}_{-\mathcal{I}_j}$ under the posterior distribution π.

The proposal distribution for $\boldsymbol{\nu}_{\mathcal{I}_j}$ is then a normal distribution centered on the current value of $\boldsymbol{\nu}_{\mathcal{I}_j}$ with covariance $\tau_j^{\nu} \boldsymbol{\Sigma}_{\mathcal{I}_j}$. The acceptance probability for the move, applied after reweighting to get a weighted distribution from π_s, is simply calculated from the ratio of π_s values for the proposed and current values.

The scaling parameters τ_j^{ν} are by default chosen to be $2.4/\sqrt{|\mathcal{I}_j|}$ following the heuristic of Roberts, Gelman and Gilks (1997). However in practise they are usually chosen, based on several runs of the algorithm, to ensure that the acceptance rates remain close to 0.23 (again following Roberts, Gelman and Gilks 1997). Details of specific choices used are given in the examples.

To update the variance parameters $\boldsymbol{\sigma}^2$, a Gibbs sampling step can be applied. Note from (11) that for each s the full conditional distribution of $\sigma_{u\ell}^2$ is simply an inverse gamma distribution, depending on the corresponding vector of regression coefficients $\mathbf{u}_\ell$. However if a different prior is used for $\boldsymbol{\sigma}^2$ then Gibbs sampling will not be available and a Metropolis–Hastings update should be performed for each $\sigma_{u\ell}^2$ in turn.

4 Examples

In this section we will demonstrate the methodology on two examples. The first example is a semiparametric Poisson regression model, with simulated data so that fair comparisons can be drawn with alternative MCMC approaches. The second example is a binary logistic regression involving respiratory infection in Indonesian children, with both a semiparametric component and random effects. All computation were carried out in the

R language (Venables & Ripley, 2005), using dual Opteron 2.0GHz CPU computational cluster node.

4.1 Semiparametric Poisson regression

In this section, we generate $n = 500$ Poisson random variables $y_i, i = 1, \ldots, n$ from

$$y_i \sim \text{Poisson}(\exp\{0.7x_{1i} + 2x_{2i} + \cos(4\pi x_{2i})\})$$

where x_{1i} is 0 or 1 with probability 0.5, and x_{2i} is uniformly sampled from the interval $[0, 1]$.

We fit model (3), with

$$b(x) = e^x, \qquad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{21} \\ 1 & x_{12} & x_{22} \\ \vdots & \vdots & \vdots \\ 1 & x_{1n} & x_{2n} \end{bmatrix}.$$

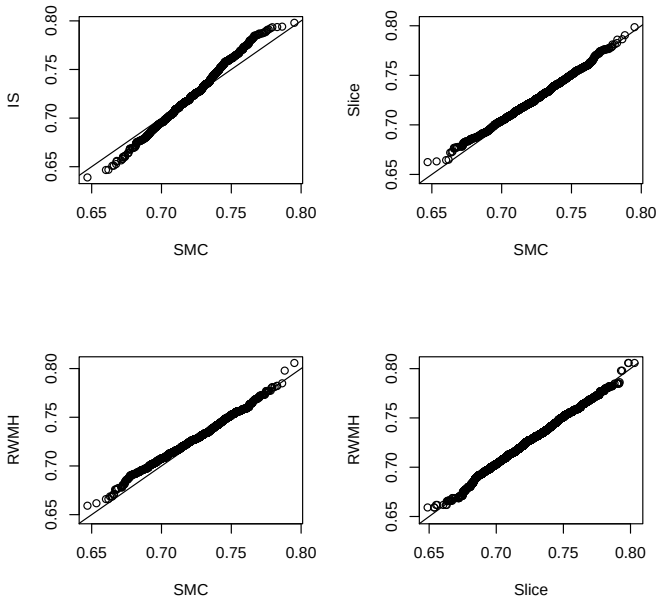
The radial cubic basis function is used to model the function $f(x_{2i}) = \cos(4\pi x_{2i})$. This implies modelling $f(x_{2i}) = \beta_{x_2} x_{2i} + \mathbf{Z}_{x_{2i}}\mathbf{u}$, where for knot points κ_k, chosen to be the $(\frac{k+1}{K+2})$th quantile of the unique predictor values, for $k = 1, \ldots, K, K = 10$,

$$\mathbf{u} = \begin{bmatrix} u_1 \\ \vdots \\ u_{10} \end{bmatrix}, \quad [\mathbf{u}|\sigma_u^2] \sim N(\mathbf{0}, \sigma_u^2\mathbf{I}), \quad \text{and} \quad \mathbf{Z}_{x_{2i}} = [|x_{2i} - \kappa_k|^3]_{1\le k\le 10}[|\kappa_{k'} - \kappa_k|^3]^{-1/2}_{1\le k,k'\le 10}$$

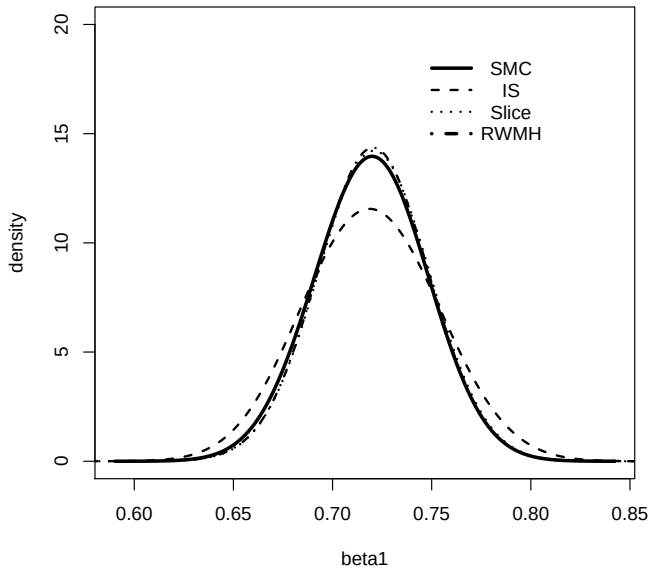
The `glmmPQL` method of the R statistical package gives an approximate MLE for the regression coefficients $\widehat{\boldsymbol{\nu}}_{\text{PQL}}$, and the variance parameters $\widehat{\boldsymbol{\sigma}}^2_{\text{PQL}}$.We follow the general algorithm given in Section 3. There are 13 regression coefficients to be estimated for this model, and one variance parameter. In a model of this size we can block update the regression coefficient $\boldsymbol{\nu}$ in a single random walk Metropolis-Hastings (RWMH) update. As with MCMC, the tuning of this kernel is crucial to the success of the algorithm; to achieve an acceptance rate in the MCMC step between 20–30% we set $\tau^{\nu}_{\mathcal{I}} = 1/3$. We also choose the number of steps $S = 105$ and the number of particles $N = 2000$ based on preliminary runs.

We compare the performance of the SMC simulations by monitoring the QQ-plots of samples from a simple importance sampler, a single-variable slice sampler which updates one parameter at a time and a standard RWMH sampler with the same transition kernels as used in the SMC algorithm (i.e. those described in Section 3.3). Figure 1(a) shows the QQ-plot for the β_1 parameter, and the corresponding density estimates for β_1 is given in (b). With the exception of the importance sampler, which can perform badly on different simulated data sets, the remaining samplers achieved good concordance. This required 2,000 particles with 100 steps for the SMC sampler. For comparison, we used 20,000 iterations of both slice sampler and RWMH MCMC scheme, with the first 10,000 discarded as burn-in. These took approximately 1394 and 580 seconds respectively, whereas the SMC sampler took approximately 422 seconds.

The nonparametric fits of the model, calculated using the estimated posterior mean of $\mathbf{u}$, are displayed in Figure 2. The model has successfully recovered the nonlinearity in the dependency on x_2 and fits the data well.



(a)



(b)

Figure 1: *QQ-plots of SMC output against simple importance sampler, the slice sampler and the RW Metropolis-Hastings sampler for β_1 (a). The corresponding density estimates (b).*

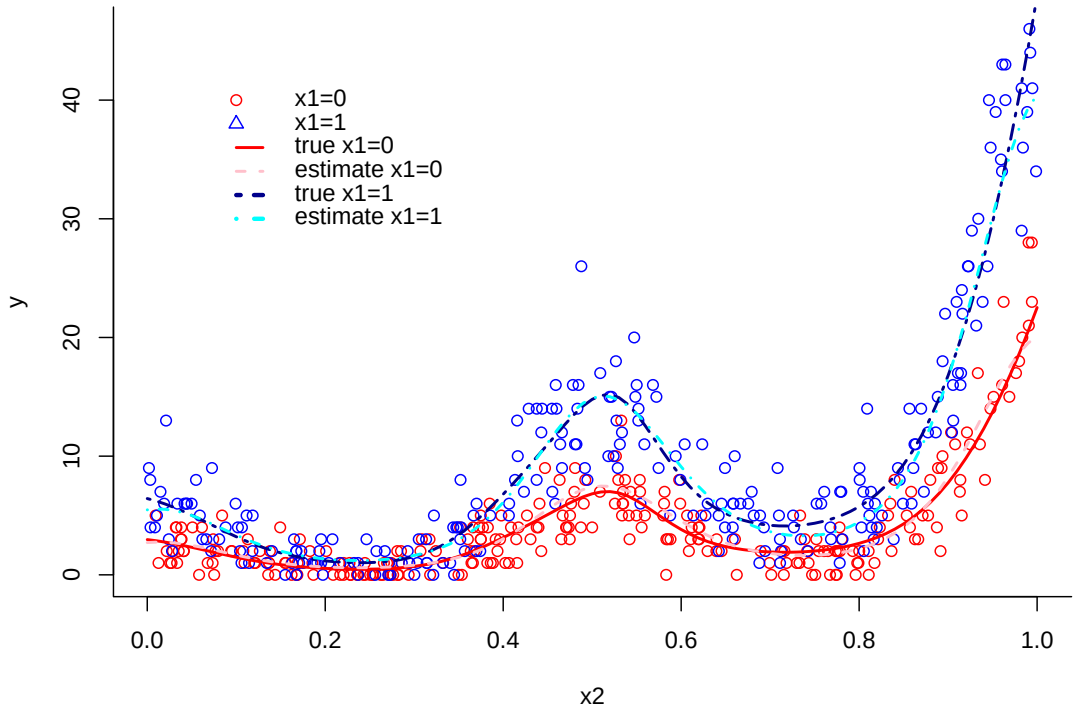


Figure 2: *The data, the true mean values, and the estimated mean values for the simulated Poisson example. The fit was based on a SMC run with 2000 particles, as described in the text.*

4.2 Example: Respiratory infection in Indonesian children

Here we apply sequential Monte Carlo algorithm to an example involving respiratory infection in Indonesian children (see Diggle, Liang & Zeger 1995, Lin & Carroll 2001). The data contain longitudinal measurements on 275 Indonesian children, where the indicator for respiratory infection is the binary response. The covariates include age, height, indicators for vitamin A deficiency, sex, stunting and visit numbers (one to six).

Previous analyses have shown the effect of age of the child to be non-linear, hence we use a logistic additive mixed model of the form

$$\text{logit}\{P(\text{respiratory infection}_{ij} = 1)\} = \beta_0 + U_i + \boldsymbol{\beta}^T x_{ij} + f(\text{age}_{ij})$$

for $1 \leq i \leq 275$ children and $1 \leq j \leq n_i$ repeated measures within a child. $U_i \overset{\text{i.i.d.}}{\sim} N(0, \sigma_U^2)$ is a random child effect, x_{ij} is the measurement on a vector of the remaining 9 covariates, and f is modelled using penalized splines with spline basis coefficients u_k i.i.d. $N(0, \sigma_u^2)$.

As recommended by Gelfand *el al.* (1995), we use hierarchical centering of random effects. All continuous covariates are standardised to have zero mean and unit standard deviation, so that the choices of hyperparameters can be independent of scale. Radial cubic basis functions are used to fit the covariate age, where

$$f(\text{age}) = \beta_{\text{age}}\text{age} + \mathbf{Z}_{\text{age}}\mathbf{u}$$

where

$$\mathbf{Z}_{\text{age}} = [|\text{age} - \underset{1\leq\kappa\leq K}{\kappa_k}|^3][|\underset{1\leq k,k'\leq K}{\kappa_k - \kappa_{k'}}|^3]^{-1/2} \quad \text{and} \quad \mathbf{u} \sim N(0, \sigma_u^2\mathbf{I})$$

with κ_k chosen to be the $(\frac{k+1}{K+2})$th quantile of the unique predictor values. We take $K = 20$ in this example.

We use a vague prior $N(0, 10^8)$ for the fixed effects. For both variance components, we use the conjugate Inverse Gamma prior IG$(0.01, 0.01)$. Other prior choices are available, see Zhao *et al.* (2006). Here, random walk Metropolis-hastings updates were carried out for each regression coefficient separately, with Gibbs sampling used for the variance parameters. We note that blocking highly correlated parameters together will probably improve the mixing properties of the sampler; in this work we choose instead to investigate the "vanilla" version of the SMC strategy. The tuning parameters $\tau^{\nu}_{\mathcal{I}_j}$ for the Metropolis-Hastings update are again chosen to achieve an acceptance rate in the MCMC step between 20–30%, we used $\tau^{\nu}_{\mathcal{I}_j} = 3$ for the fixed effect coefficients, $\tau^{\nu}_{\mathcal{I}_j} = 6$ for the random effect coefficients, and $\tau^{\nu}_{\mathcal{I}_j} = 5$ for the spline coefficients.

Figure **??** show the results from simulation, using 1000 particles and 55 intermediate steps. The Figure shows borderline positive effect of Vitamin A deficiency, sex and some visit numbers on respiratory infection. These results are in keeping with previous analyses. Figure **??** shows the nonlinear effect of age; **??** shows the effective sample size at each of 50 sequential steps of the simulation, vertical lines indicate the occurrence of resampling.

Again, we compare the performance of the SMC sampler with the importance sampler, slice sampler and RWMH sampler with the same transition kernel as Step 3 of the SMC algorithm. Results for 5,000 samples of the importance sampler, 1,000 SMC particles and 5,000 slice samples with 5,000 burn-in and 5,000 RWMH samples with 5,000 burn-in

are plotted in Figure **??**, good agreements are found between the SMC, slice and MCMC samplers. Moreover, the SMC sampler took approximately 1.6 hours to run, whereas the slice sampler took 2.8 hours and the RWMH took about 9 hours (similarly 9 hours was required in `WinBUGS`), so a substantial saving in computational time in achieved by using the SMC algorithm.

5 Conclusion

In this paper we presented a general sequential Monte Carlo algorithm to produce samples from the posterior distribution for Bayesian analysis of generalised linear mixed models. The algorithm is an alternative to the popular Markov chain Monte Carlo methods. We have demonstrated that the algorithm can handle high-dimensional problems, and it is generally simple to apply. We have also demonstrated that it can have substantial efficiency gains over traditional MCMC in both a simulated poisson example and a real data binomial example. Finally, perhaps the biggest advantage of SMC over MCMC samplers is the fact convergence of SMC samplers does not rely on convergence of Markov chains, which can be extremely slow in complex problems.

In implementing SMC, one has some degree of flexibility within the Markov chain Monte Carlo update. For example, one may consider a better choice of proposal distributions for the Metropolis-Hastings algorithm, by allowing the algorithm to automatically scale a proposal distribution, see for example Chopin, (2002). Here a major advantage over the traditional MCMC is that the algorithm does not suffer from the restrictions associated with a Markov chain, and information from previous samples can be freely used to obtain future samples. Finally, one is not restricted to only MCMC type of moves in this step, other move types are possible, see Del Moral, Doucet & Jasra (2006).

However, sequential Monte Carlo algorithms are not black-box algorithms, requiring a certain amount of tuning and user input. In particular, one needs to set the number of sequential distributions (S) the number of particles to sample (N) and tuning parameters for the Metropolis-Hastings kernels in the move step of the algorithm.

Acknowledgements

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Appendix: Algorithmic description of the SMC method for GLMMs

In this appendix we give a detailed description of how to use the SMC method to perform inference in GLMMs. We use the notation of Section 2; choices made in the implementation of the algorithm are explained in Section 3.

For any subset $\mathcal{I}$ of $\{1, \ldots, P\}$ we write $\mathbf{C}_{\mathcal{I}}$ for the submatrix of of the design matrix $\mathbf{C}$ consisting of columns in $\mathcal{I}$, $\mathbf{C}_{-\mathcal{I}}$ for the submatrix consisting of columns of $\mathbf{C}$ not in $\mathcal{I}$, $\boldsymbol{\nu}_{\mathcal{I}}$ and $\boldsymbol{\nu}_{-\mathcal{I}}$ for the analogously defined subvectors of $\boldsymbol{\nu}$. Also for any square matrix $\mathbf{Q}$ we write $\mathbf{Q}_{\mathcal{I}\mathcal{I}}$ for the square submatrix corresponding to rows and columns in $\mathcal{I}$, $\mathbf{Q}_{\mathcal{I},-\mathcal{I}}$ for the submatrix with rows in $\mathcal{I}$ and columns not in $\mathcal{I}$, $\mathbf{Q}_{-\mathcal{I},\mathcal{I}}$ for the submatrix with rows not in $\mathcal{I}$ and columns in $\mathcal{I}$, and $\mathbf{Q}_{-\mathcal{I},-\mathcal{I}}$ for the square submatrix with rows and columns not in $\mathcal{I}$.

Initialisation

- Set the number of particles N and the number of intermediary distributions S.
- Construct a vector $\boldsymbol{\gamma}$ with sth entry $\psi(s)$, $s = 0, 1, \ldots, S$, where $\psi : \{0, 1, \ldots, S\} \to [0, 1]$ is an increasing function such that $\psi(0) = 0$ and $\psi(S) = 1$. For the results in this paper we used $\psi(s) = \min\{1, s/(S-5)\}$.
- Construct subsets $\mathcal{I}_1, \ldots, \mathcal{I}_J$ of $\{1, \ldots, P\}$ such that $\bigcup_{j=1}^{J} \mathcal{I}_j = \{1, \ldots, P\}$. The case $J = 1$ corresponds to no blocking of variables for the move step.
- Set tuning parameters $\tau_j^{\nu} > 0$, $j = 1, \ldots, J$ for the Metropolis–Hastings updates. Usually these will be set based on preliminary runs of the algorithm, and convenient defaults are $\tau_j^{\nu} = 2.4/\sqrt{|\mathcal{I}_j|}$.
- Use the Breslow & Clayton (1993) penalised quasi-likelihood (PQL) algorithm to obtain initial estimates:

  $$\widehat{\boldsymbol{\nu}}_{\text{PQL}} \quad \text{and} \quad \widehat{\boldsymbol{\sigma}}^2_{\text{PQL}}.$$

  This is facilitated by software such as `glmmPQL()` in the `R` package `MASS` (Venables & Ripley, 2005). Use these estimates in (8) to calculate $\boldsymbol{\Sigma}$.
- For each $j = 1, \ldots, J$, calculate the conditional covariance under π_0 of $\boldsymbol{\nu}_{\mathcal{I}}$ conditional of $\boldsymbol{\nu}_{-\mathcal{I}}$. If $Q = \Sigma^{-1}$, then this conditional covariance is $\boldsymbol{\Sigma}_{\mathcal{I}_j} := (Q_{\mathcal{I}\mathcal{I}})^{-1}$.

Initial sample from π_0

- Produce a sample of size N from π_0: for each $i = 1, \ldots, N$ sample ν_i from the normal distribution with mean $\widehat{\boldsymbol{\nu}}_{\text{PQL}}$ and covariance $\boldsymbol{\Sigma}$, then sample $\boldsymbol{\sigma}_i^2$ from the conditional inverse gamma distributions (9).
- Set the weights $w_i = 1/N$ for each $i = 1, \ldots, N$.

Sequential sampling from each π_s

For each $s = 1, \ldots, S$ in turn,

Reweight For each $i = 1, \ldots, N$, update w_i according to

$$w_i \leftarrow w_i \frac{\pi_s(\nu_i, \boldsymbol{\sigma}_i^2)}{\pi_{s-1}(\nu_i, \boldsymbol{\sigma}_i^2)} = \left(\frac{\pi(\nu_i, \boldsymbol{\sigma}_i^2)}{\pi_0(\nu_i, \boldsymbol{\sigma}_i^2)} \right)^{\gamma_s - \gamma_{s-1}}$$

then normalise the weights by setting $w_i \leftarrow w_i / \sum_{j=1}^N w_j$. To avoid overflow and underflow problems it is recommended that logarithms be used in this step.

Resample Calculate the effective sample size (ESS) using

$$ESS = (\sum_{i=1}^N w_i)^2 / \sum_{i=1}^N (w_i)^2.$$

If $ESS < N/2$ (or if $s = \min\{s : \gamma_s = 1\}$) then resample the particles. The naive version of resampling, which introduces unnecessary Monte Carlo variation into the scheme, simply samples (with replacement) from the pool of particles, with particle i selected with probability w_i. However in our implementation we use stratified resampling (Kitagawa, 1996) to reduce the Monte Carlo variation. After resampling set $w_i = 1/N$ for all $i = 1, \ldots, N$.

Move

- For each $j = 1, \ldots, J$ and each $i = 1, \ldots, N$, generate proposals $(\tilde{\boldsymbol{\nu}}_i)_{\mathcal{I}_j} \sim N((\tilde{\boldsymbol{\nu}}_i)_{\mathcal{I}_j}, \tau_j^{\nu} \boldsymbol{\Sigma}_{\mathcal{I}_j})$, $1 \leq i \leq N$. With probability

$$\alpha^{(i)} = \max \left\{ 1, \frac{\pi_s((\tilde{\boldsymbol{\nu}}_i)_{\mathcal{I}_j} | (\boldsymbol{\nu}_i)_{-\mathcal{I}_j}, \boldsymbol{\sigma}_i^2)}{\pi_s(\boldsymbol{\nu}_i, \boldsymbol{\sigma}_i^2)} \right\}$$

  accept the proposal and set $(\boldsymbol{\nu}_i)_{\mathcal{I}_j} = (\tilde{\boldsymbol{\nu}}_i)_{\mathcal{I}_j}$. Otherwise reject the proposal and leave $(\boldsymbol{\nu}_i)_{\mathcal{I}_j}$ unchanged. Again, it is recommended that logarithms be used when calculating α to avoid overflow and underflow problems. Note that several parts of the ratio in the calculation of α are the same in both the numerator and denominator and need not be calculated.

- For each $\ell = 1, \ldots, L$, and for each $i = 1, \ldots, N$, sample $(\boldsymbol{\sigma}_i^2)_\ell$ from the inverse gamma distribution with shape $A_{u\ell} + q_\ell/2$ and rate $A_{u\ell} + \|\mathbf{u}_\ell\|^2/2$. Note that if inverse gamma distributions are not used as the prior distribution for $\boldsymbol{\sigma}^2$ then sampling from inverse gamma distributions here would not result in a transition kernel that admits π_s as a stationary distribution. Instead further Metropolis–Hastings can be used for each $\sigma_{u\ell}^2$ in turn.

Note that the decision to resample on the first step at which $\gamma_s = 1$ means that the final sample is an unweighted sample from π. Hence standard techniques for dealing with samples from posterior distributions can be used. However for plug-in density estimation techniques it was found that resampling close to step S resulted in poor choice of bandwidth, since some particles were identical. This is the reason that we generally set $\gamma_{S-5} = 1$ and finish with five applications of the transition kernel to the unweighted sample, resulting in a suitably diverse sample from π.

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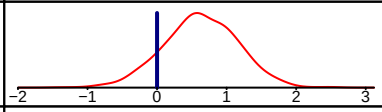
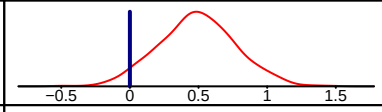
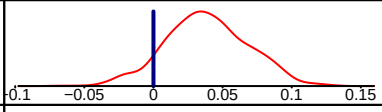
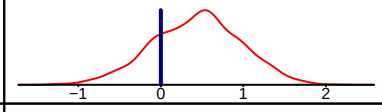
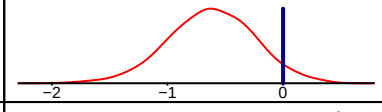
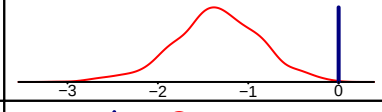
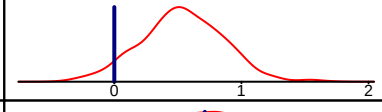
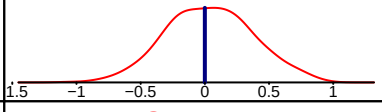
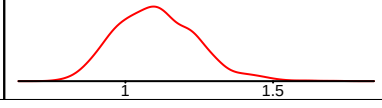
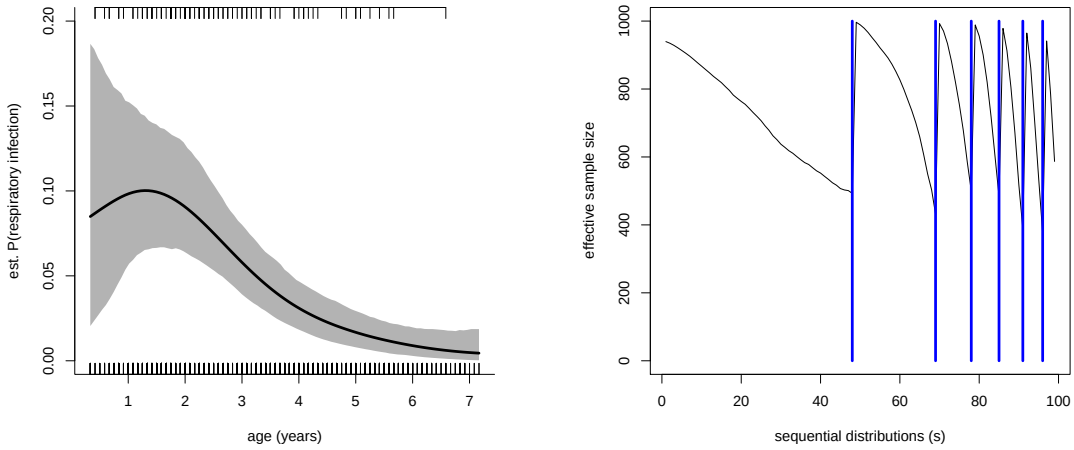
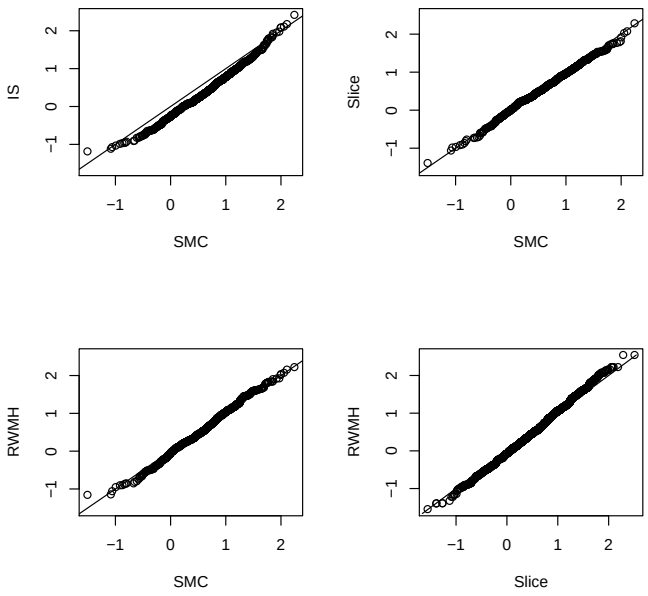
coefficient	density	summary
vitamin A deficit		posterior mean: 0.627 95% credible interval: (−0.442,1.65)
male		posterior mean: 0.49 95% credible interval: (−0.0509,1.05)
height		posterior mean: 0.0386 95% credible interval: (−0.0199,0.0947)
stunted		posterior mean: 0.434 95% credible interval: (−0.624,1.4)
visit 2		posterior mean: −1.2 95% credible interval: (−1.99,−0.49)
visit 3		posterior mean: −0.621 95% credible interval: (−1.38,0.102)
visit 4		posterior mean: −1.35 95% credible interval: (−2.39,−0.425)
visit 5		posterior mean: 0.536 95% credible interval: (−0.108,1.17)
visit 6		posterior mean: 0.0373 95% credible interval: (−0.603,0.709)
st.dev.(subject)		posterior mean: 1.11 95% credible interval: (0.873,1.41)

Figure 3: *Summary of coefficients in respiratory infections in Indonesian children example.*

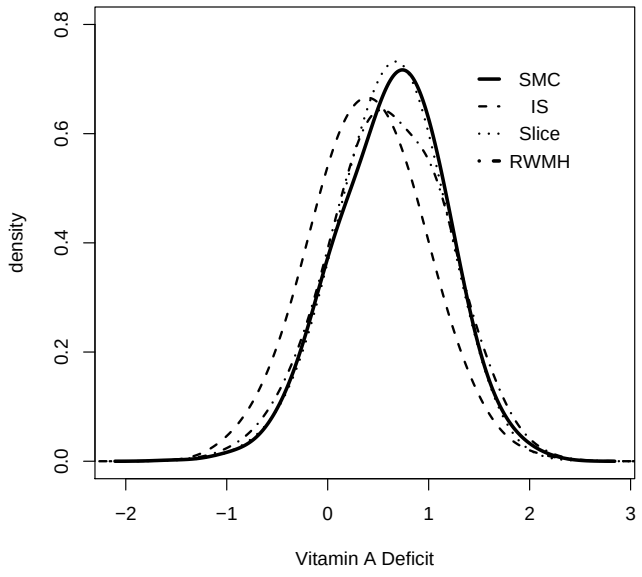


(a) (b)

Figure 4: *Respiratory infections in Indonesian children example. (a) Posterior mean of the estimated probability of respiratory infection $f(\texttt{age})$ with all other covariates set to their average values. (b) Effective sample size over 50 distributions, vertical lines indicate instances of resampling.*



(a)



(b)

Figure 5: *QQ-plots of SMC output against simple importance sampler, the slice sampler and the RW Metropolis-Hastings sampler for the coefficient of vitamin A deficiency (a). The corresponding density estimates (b).*