

An R Implementation for Correlated Pseudo Marginal Monte Carlo Methods

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Abstract

This document briefly summarises the statistical methodology underlying the `cpmmc` package, located at <https://github.com/JTT94/cpmmc>. In particular, this paper looks at the Correlated Pseudo Marginal Markov Chain theory introduced by Deligiannidis et al. (2015) and application to the random effect model.

1 Background

The Metropolis-Hastings (MH) algorithm, detailed fully by Roberts and Rosenthal (2004), is a particular Markov Chain Monte Carlo (MCMC) procedure used to sample asymptotically from a target distribution, π in order to compute expectations with respect to the target distribution. This and similar MCMC procedures are often employed when it is difficult to sample π directly. The outline of MH is that one builds a markov chain with states $\theta_t; t \in \mathbb{N}$, and stationary distribution π , coinciding with the desired target distribution. At each time, t , the state is updated stochastically via an accept/ reject probability on a proposal state, θ' , generated from some transitional kernel, K with density q . The acceptance probability is defined as $\alpha_E(\theta_{t-1}, \theta') = \min \left\{ 1, \frac{\pi(\theta')q(\theta', \theta_{t-1})}{\pi(\theta_{t-1})q(\theta_{t-1}, \theta')} \right\}$. Provided certain ergodic conditions given by Roberts and Rosenthal (2004) hold, the arithmetic average of accepted states in the generated Markov Chain will approach the desired expectation with respect to π .

In a Bayesian context, MH is often used to sample from a posterior distribution of some parameter of interest. Given observations $y_{1:t}$, and parameter of interest, θ , with prior distribution $p \theta \sim p$, the target distribution will be of form $\pi(\theta) = p(\theta y_{1:t}) \propto p(y|\theta)p(\theta)$.

In order to implement MH for Bayesian inference, one would need to be able to evaluate $p(y|\theta)p(\theta)$ in order to perform the accept/ reject step in building the Markov chain. For many applications such as with latent variable models, the likelihood, $p(y|\theta)$, is often intractable thus making MH difficult to implement.

The pseudo-marginal (PM) algorithm follows the same procedure as the idealised MH, however introduces an estimator for the intractable likelihood to replace the true likelihood ratio required for the acceptance probability. This reduces the requirement of being able to compute likelihood $p(y|\theta)$, to only being required to be able to compute a non-negative, unbiased, unnormalised Monte Carlo estimate of this likelihood.

The correlated pseudo-marginal (CPM) algorithm is a development of the PM algorithm and shall be the focus of this document. The CPM correlates the estimators for the likelihood to reduce the variance of the resulting likelihood ratio in order to improve efficiency in implementing the scheme. In Deligiannidis et al. (2015), correlated auxiliary variables are introduced in the calculation of the likelihood estimate to encourage correlation in the estimates.

The main contributions of Deligiannidis et al. (2015), in addition to introducing this correlation approach, are: providing theoretical results on the benefits, guidance on tuning parameters and demonstrated applications in state space and random effect models. This document shall focus on the high-level CPM theory, random effect model and a simulation study to demonstrate some properties empirically.

2 Methodology

Let $p(y|\theta)$ denote the likelihood for the T observations $y_{1:T}$, and let $p(\theta)$ be the prior density for the parameter $\theta \in \Theta \subseteq \mathbb{R}^d$. The Bayesian posterior density of interest can be written as $\pi(\theta) \propto p(y|\theta)p(\theta)$. To further abuse notation, denote $x \sim p$ to be that value x is a realised random variable sampled from distribution with density p .

2.1 Metropolis-Hastings

In a Bayesian setting, the MH algorithm is as detailed below, and the acceptance probability can be rewritten from $\alpha_E(\theta_{t-1}, \theta') = \min \left\{ 1, \frac{\pi(\theta')q(\theta', \theta_{t-1})}{\pi(\theta_{t-1})q(\theta_{t-1}, \theta')} \right\}$ to $\alpha_E(\theta_{t-1}, \theta') = \min \left\{ 1, \frac{p(y_{1:T}|\theta')q(\theta', \theta_{t-1})p(\theta')}{p(y_{1:T}|\theta_{t-1})q(\theta_{t-1}, \theta')p(\theta_{t-1})} \right\}$.

Algorithm 1 Idealised Metropolis Hastings

- 1: Initialise θ_0 :
 Sample from prior $\theta_0 \sim p$
 - 2: At each iteration $t > 0$:
 - 3: Sample proposal: $\theta' \sim q(\theta_{t-1}, \cdot)$
 - 4: Calculate accept/ reject probability: $\alpha_E(\theta_{t-1}, \theta') :$

$$\alpha_E(\theta_{t-1}, \theta') = \min \left\{ 1, \frac{p(y_{1:T}|\theta')q(\theta', \theta_{t-1})p(\theta')}{p(y_{1:T}|\theta_{t-1})q(\theta_{t-1}, \theta')p(\theta_{t-1})} \right\}$$
 - 5: With probability: $\alpha_E(\theta_{t-1}, \theta')$
 Set $\theta_t \leftarrow \theta'$ else $\theta_t \leftarrow \theta_{t-1}$
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2.2 Correlated Pseudo-Marginal Algorithm

To target π , the CPM first augments the state from θ to (θ, U) , with joint density $\bar{\pi}$. By simulating a Markov chain to target $\bar{\pi}$, one can record only the θ values in order to target π . Given that $\hat{p}(y_{1:T}|\theta, U)$ is unbiased, we have that $\pi(\theta)$ is a marginal density of $\bar{\pi}(\theta, u)$, as $\int \bar{\pi}(\theta, u)du = \pi(\theta)$.

$$\bar{\pi}(\theta, u) = \pi(\theta)m(u) \frac{\hat{p}(y_{1:T}|\theta, u)}{p(y_{1:T}|\theta)}$$

Assumptions:

- $\hat{p}(y_{1:T}|\theta, U)$ is a non-negative, unbiased estimator of likelihood $p(y_{1:T}|\theta)$
- $U \sim m$
- K is a transition kernel admitting an m-reversible Markov chain

$$m(u)K(u, u') = m(u')K(u', u)$$

The Correlated Pseudo Marginal algorithm, detailed below, uses the above assumptions and the Metropolis Hastings algorithm to target $\bar{\pi}$ with a choice of transition kernel K to induce correlated U proposals. This framework allows for running MH without having to compute $p(y_{1:T}|\theta)$. The primary difference to the idealised MH algorithm is swapping the likelihood ratio, $\frac{p(y_{1:T}|\theta, U')}{p(y_{1:T}|\theta, U)}$, with its estimator $\frac{\hat{p}(y_{1:T}|\theta, U')}{\hat{p}(y_{1:T}|\theta, U)}$ in the acceptance probability at each iteration.

Informally, the intuition behind the CPM, and in particular the correlation aspect, is as follows. Providing $\hat{p}(y_{1:T}|\cdot, \cdot)$ as a function of (θ, U) is sufficiently "nice" and θ is close to θ' , correlation amongst U and U' will induce correlation amongst $\hat{p}(y_{1:T}|\theta, U)$ and $\hat{p}(y_{1:T}|\theta', U')$. This correlation lowers the variance of the ratio seen in the acceptance probability, $\frac{\hat{p}(y_{1:T}|\theta, U')}{\hat{p}(y_{1:T}|\theta, U)}$. Hence, the algorithm will be "more similar" to the idealised MH algorithm, and reduce the inefficiency introduced by taking using likelihood estimates rather than computing exact values of the likelihood.

Algorithm 2 Correlated Pseudo Marginal Algorithm

- 1: Initialise :

$$\theta_0 \sim p_\theta$$

$$U_0 \sim p_U$$
 - 2: At each iteration $t > 0$:
 - 3: Sample proposal: $\theta' \sim q(\theta_{t-1}, \cdot)$
 - 4: Sample auxiliary variables: $\epsilon \sim \mathcal{N}(0_M, I_M)$
 Set $U' = \rho U_{t-1} + \sqrt{1 - \rho^2} \epsilon$
 - 5: Compute estimator $\hat{p}(y_{1:T}|\theta', U')$ of $p(y_{1:T}|\theta', U')$
 - 6: Calculate accept/ reject probability: $\alpha_E(\theta_{t-1}, \theta') :$

$$\alpha_E\{(\theta_{t-1}, U_{t-1}), (\theta', U')\} = \min \left\{ 1, \frac{\hat{p}(y_{1:T}|\theta', U')q(\theta', \theta_{t-1})p(\theta')}{\hat{p}(y_{1:T}|\theta_{t-1}, U_{t-1})q(\theta_{t-1}, \theta')p(\theta_{t-1})} \right\}$$
 - 7: With probabiliy: $\alpha_E\{(\theta_{t-1}, U_{t-1}), (\theta', U')\}$
 Set $(\theta_t, U_t) \leftarrow (\theta', U')$ else $(\theta_t, U_t) \leftarrow (\theta_{t-1}, U_{t-1})$
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2.3 Random Effect Model

Define the model as follows:

$$x \sim f_\theta(\cdot)$$

$$Y_t|X_t \sim g_\theta(\cdot|X_t)$$

where $t \in \mathbb{N}$ and $\{X_t; t > 0\}$ are \mathbb{R}^k - *valued* latent variables and $\{Y_t; t > 0\}$ are \mathcal{Y} - *valued* observations.

For observed data $Y_{1:T} = y_{1:T}$, the likelihood satisfies:

$$p(y_{1:T}) = \prod_{t=1}^T p(y_t|\theta)$$

$$p(y_t|\theta) = \int g_\theta(y_t|x_t, \theta) f_\theta(x_t) dx_t$$

If the integral for $p(y_t|\theta)$ is intractable, one can use teh CPM algorithm with importance sampling to form an unbiased estimator $\hat{p}(y_t|\theta)$, where N is the number of proposal samples.

Let:

$$\hat{p}(y_{1:T}|\theta, U) = \prod_{t=1}^T \hat{p}(y_t|\theta, U_t)$$

$$\hat{p}(y_t|\theta, U_t) = \frac{1}{N} \sum_{i=1}^N w(y_t, U_{t,i}; \theta)$$

$$w(y_t, U_{t,i}) = \frac{g_\theta(y_t|X_{t,i})f_\theta(X_{t,i})}{q_\theta(X_{t,i}|y_t)}$$

assuming a deterministic map $\Xi : \mathbb{R}^p \times \Theta \rightarrow \mathbb{R}^k$ where $X_{t,i} = \Xi(U_{t,i}, \theta) \sim q_\theta(\cdot|y_t)$ and $U_{t,i} \sim \mathcal{N}(0_p, I_p)$

2.4 Key Results on Parameter Tuning

Other than introducing the approach, the primary theoretic contributions of Deligiannidis et al. (2015) are in specifying the distributions of the loglikelihood error, $Z_T(\theta)$, and loglikelihood error ratio, $R_T(\theta, \theta')$ under correlated U proposals and under non-correlated for comparison of CPM with the PM algorithm.

The significance of these results lies in using them to inform choice of parameters ρ and N which controls the correlation and number of Monte Carlo samples in the unbiased estimator respectively.

$$Z_T(\theta) = \log(\hat{p}(Y_{1:T}|\theta, U)) - \log(p(Y_{1:T}|\theta))$$

$$R_T(\theta, \theta') = \log \frac{\hat{p}(Y_{1:T}|\theta', U')}{\hat{p}(Y_{1:T}|\theta, U)} - \log \frac{p(Y_{1:T}|\theta')}{p(Y_{1:T}|\theta)}$$

In the interest of brevity, the theorems of Deligiannidis et al. (2015) are not stated below. However, the key results were that one should find $\beta > 0, \psi > 0$ and set the CPM parameters such that:

$$N_T = \beta T^{\frac{1}{2}}$$

$$\rho = \exp(-\psi \beta T^{-\frac{1}{2}}) = \exp(-\psi \frac{N_T}{T})$$

Deligiannidis et al. (2015) then provides a heuristic to find these parameters, however due to the involved nature, it has been excluded from this document.

2.5 Discussion

- Higher dimension, size of $M = pTN$
- Difficulties when estimator is not "nice" i.e. continuous
- Implementation weak points, inefficiencies, have to loop through each data point and sample N for each point

3 Application

3.1 Simulation Study

4 Conclusion

References

- George Deligiannidis, Arnaud Doucet, and Michael K Pitt. The correlated pseudo-marginal method. *arXiv preprint arXiv:1511.04992*, 2015.
- Gareth O. Roberts and Jeffrey S. Rosenthal. General state space markov chains and mcmc algorithms. *Probab. Surveys*, 1:20–71, 2004. doi: 10.1214/154957804100000024. URL <https://doi.org/10.1214/154957804100000024>.