The Multiple-Try Method and Local Optimization in Metropolis Sampling

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This article describes a new Metropolis-like transition rule, the *multiple-try Metropolis*, for Markov chain Monte Carlo (MCMC) simulations. By using this transition rule together with adaptive direction sampling, we propose a novel method for incorporating local optimization steps into a MCMC sampler in continuous state-space. Numerical studies show that the new method performs significantly better than the traditional Metropolis–Hastings (M–H) sampler. With minor tailoring in using the rule, the multiple-try method can also be exploited to achieve the effect of a griddy Gibbs sampler without having to bear with griddy approximations, and the effect of a hit-and-run algorithm without having to figure out the required conditional distribution in a random direction.

KEY WORDS: Adaptive direction sampling; Conjugate gradient; Damped sinusoidal; Gibbs sampling; Griddy Gibbs sampler; Hit-and-run algorithm; Markov chain Monte Carlo; Metropolis algorithm; Mixture model; Orientational bias Monte Carlo.

1. INTRODUCTION

Monte Carlo simulation methods have increasingly been recognized by scientists as indispensable tools for difficult computational problems. These methods have also been central to many recent developments in statistical modeling, computation, and general practice. A common feature of methods for simulating from a complex probability distribution, say $\pi(\mathbf{x})$, is their reliance on cumulative evolutions of small, albeit random, changes. A fundamental construction that enables such "local-search" methods is the Markov transition function proposed by Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller (1953) and modified by Hastings (1970). Briefly, suppose that we currently have obtained $\mathbf{x}_t$; MH suggest that one can use a rather arbitrary Markov transition function T to generate a proposal $\mathbf{y} \sim T(\mathbf{x}_t, \cdot)$, and then "thin it down" by letting the next state $\mathbf{x}_{t+1} = \mathbf{y}$ with probability

$$r = \min\left\{1, \frac{\pi(\mathbf{y})T(\mathbf{y}, \mathbf{x}_t)}{\pi(\mathbf{x}_t)T(\mathbf{x}_t, \mathbf{y})}\right\}, \tag{1}$$

and letting $\mathbf{x}_{t+1} = \mathbf{x}_t$ with the remaining probability. We call r the M–H ratio.

The Metropolis-type local move allows one to break a complex task into a series of manageable pieces. On the other hand, however, these local moves often lead to slow-converging algorithms that are easily trapped in a local mode. A brute-force way of being "less local" is to directly increase the "searching region" of each M–H step characterized by $T(\mathbf{x}, \mathbf{y})$. But this approach often results in a very small M–H ratio and, therefore, an ineffective algorithm. The multiple-try Metropolis (MTM) algorithm described in this article tackles this "conflict of interest" by enabling one to propose multiple trial points from T, and thus allowing one to use those $T(\mathbf{x}, \mathbf{y})$ corresponding to a very large searching region.

As an alternative to the basic M–H construction, conditional sampling in some desirable subspaces or along certain directions as that in a Gibbs sampler (Geman and Geman 1984), in a multigrid Monte Carlo algorithm (Goodman and Sokal 1989), or in a hit-and-run (HR) algorithm (Chen and Schmeiser 1993) is often a powerful updating step in Markov chain Monte Carlo (MCMC). But an inherent difficulty with this approach is that the required conditional distributions are often difficult to deal with. The adaptive rejection method of Gilks and Wild (1992) is powerful for log-concave densities, but does not apply to others. Alternatively, one could draw from an approximation of the conditional distribution as in the griddy Gibbs sampler of Ritter and Tanner (1992). But when approximations are used, there will no longer be any guarantees of the existence of an equilibrium distribution, let alone an assessment of discrepancy between the Monte Carlo output and the target distribution. A remedy is to incorporate the M–H rule in using the approximate distribution. But a good approximation is usually too expensive to come by, and such approximations get worse very fast as dimension increases. The MTM method provides an effective way to conduct directional sampling without the shortcomings inherent in those previous approaches.

Another actively pursued direction for improving a MCMC sampler is via adaptation; roughly speaking, when one attempts to use information generated by the up-to-date iterations to guide for future simulations. A particularly interesting idea is the *adaptive direction sampling* (ADS) algorithm proposed by Gilks, Roberts, and George (1994), which suggests using multiple MCMC chains and adapting movements of one chain according to information from others. We describe a novel algorithm that combines the ADS framework with the MTM method. The main features of the new algorithm are (a) the local optimality information revealed by a deterministic local-search scheme is explicitly used for adaptation, and (b) the companion MTM allows

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for a very large step-size in searching along a "promising" direction. Our numerical examples show that the new sampler offers significant improvement over the traditional Metropolis sampler, especially in difficult problems.

This article is organized as follows. Section 2 introduces the basic MTM methodology and provides a simple proof for the correctness of the method. Section 3 discusses further extensions of the MTM and a few theoretical issues. Section 4 presents our new sampler, the *conjugate-gradient Monte Carlo*, and Section 5 shows two other variations in using the MTM. Section 6 demonstrates use of the method through several numerical examples, and Section 7 concludes with a brief discussion.

2. GENERAL METHODOLOGY OF MULTIPLE-TRY METROPOLIS

As in a standard M–H algorithm, we let $T(\mathbf{x}, \mathbf{y})$ be a proposal transition function that may or may not be symmetric. A modest requirement is that $T(\mathbf{x}, \mathbf{y}) > 0$ if and only if $T(\mathbf{y}, \mathbf{x}) > 0$. Furthermore, we define

$$w(\mathbf{x}, \mathbf{y}) = \pi(\mathbf{x}) T(\mathbf{x}, \mathbf{y}) \lambda(\mathbf{x}, \mathbf{y}), \qquad (2)$$

where $\lambda(\mathbf{x}, \mathbf{y})$ is a nonnegative symmetric function in $\mathbf{x}$ and $\mathbf{y}$ that can be chosen by the user. The only requirement is that $\lambda(\mathbf{x}, \mathbf{y}) > 0$ whenever $T(\mathbf{x}, \mathbf{y}) > 0$. We present a few choices of $\lambda(\mathbf{x}, \mathbf{y})$ in the latter part of this section. Suppose that the *current state* is $\mathbf{X}_t = \mathbf{x}$; then a MTM transition is defined as follows.

Multiple-try Metropolis

1. Draw k iid trial proposals, $\mathbf{y}_1, \ldots, \mathbf{y}_k$, from $T(\mathbf{x}, \cdot)$. Compute $w(\mathbf{y}_j, \mathbf{x})$ for $j = 1, \ldots, k$.

2. Select $\mathbf{Y} = \mathbf{y}$ among the trial set $\{\mathbf{y}_1, \ldots, \mathbf{y}_k\}$ with probability proportional to $w(\mathbf{y}_j, \mathbf{x}), j = 1, \ldots, k$. Then draw $\mathbf{x}_1^*, \ldots, \mathbf{x}_{k-1}^*$ from the distribution $T(\mathbf{y}, \cdot)$, and let $\mathbf{x}_k^* = \mathbf{x}$.

3. Accept $\mathbf{y}$ with probability

$$r_g = \min\left\{1, \frac{w(\mathbf{y}_1, \mathbf{x}) + \cdots + w(\mathbf{y}_k, \mathbf{x})}{w(\mathbf{x}_1^*, \mathbf{y}) + \cdots + w(\mathbf{x}_k^*, \mathbf{y})}\right\} \qquad (3)$$

and reject it with probability $1 - r_g$. The quantity r_g is called the *generalized M–H ratio*.

Theorem 1. The MTM transition rule described earlier satisfies the detailed balance condition and hence induces a reversible Markov chain with π as its invariant distribution.

Proof. Let $A(\mathbf{x}, \mathbf{y})$ be the actual transition probability for moving from $\mathbf{x}$ to $\mathbf{y}$ in a MTM sampler. Suppose that $\mathbf{x} \neq \mathbf{y}$, and let I indicate which of $\mathbf{y}_j$ has been selected. Because $w(\mathbf{y}, \mathbf{x}) = \pi(\mathbf{y}) T(\mathbf{y}, \mathbf{x}) \lambda(\mathbf{y}, \mathbf{x})$ and the $\mathbf{y}_j$ are exchangeable, we have

$$\pi(\mathbf{x}) A(\mathbf{x}, \mathbf{y})$$

$$= \pi(\mathbf{x}) P\left[\bigcup_{j=1}^{k} \{(\mathbf{Y}_j = \mathbf{y}) \cap (I = j)\} | \mathbf{x}\right]$$

$$= k\pi(\mathbf{x}) P[(\mathbf{Y}_k = \mathbf{y}) \cap (I = k) | \mathbf{x}]$$

$$= k\pi(\mathbf{x}) \int \cdots \int T(\mathbf{x}, \mathbf{y}) T(\mathbf{x}, \mathbf{y}_1) \cdots T(\mathbf{x}, \mathbf{y}_{k-1})$$

$$\times \frac{w(\mathbf{y}, \mathbf{x})}{w(\mathbf{y}, \mathbf{x}) + \sum_{j=1}^{k-1} w(\mathbf{y}_j, \mathbf{x})}$$

$$\times \min\left\{1, \frac{w(\mathbf{y}, \mathbf{x}) + \sum_{j=1}^{k-1} w(\mathbf{y}_j, \mathbf{x})}{w(\mathbf{x}, \mathbf{y}) + \sum_{j=1}^{k-1} w(\mathbf{x}_j^*, \mathbf{y})}\right\}$$

$$\times T(\mathbf{y}, \mathbf{x}_1^*) \cdots T(\mathbf{y}, \mathbf{x}_{k-1}^*) \, d\mathbf{y}_1 \cdots d\mathbf{y}_{k-1} \, d\mathbf{x}_1^* \cdots d\mathbf{x}_{k-1}^*$$

$$= k\frac{w(\mathbf{x}, \mathbf{y}) w(\mathbf{y}, \mathbf{x})}{\lambda(\mathbf{y}, \mathbf{x})} \int \cdots \int \min$$

$$\times \left\{\frac{1}{w(\mathbf{y}, \mathbf{x}) + \sum_j w(\mathbf{y}_j, \mathbf{x})}, \frac{1}{w(\mathbf{x}, \mathbf{y}) + \sum_j w(\mathbf{x}_j^*, \mathbf{y})}\right\}$$

$$\times T(\mathbf{x}, \mathbf{y}_1) \cdots T(\mathbf{x}, \mathbf{y}_{k-1}) T(\mathbf{y}, \mathbf{x}_1^*) \cdots T(\mathbf{y}, \mathbf{x}_{k-1}^*)$$

$$\times d\mathbf{y}_1 \cdots d\mathbf{y}_{k-1} \, d\mathbf{x}_1^* \cdots d\mathbf{x}_{k-1}^*. \qquad (4)$$

The expression (4) is symmetric in $\mathbf{x}$ and $\mathbf{y}$ because $\lambda(\mathbf{x}, \mathbf{y}) = \lambda(\mathbf{y}, \mathbf{x})$. Thus we proved that $\pi(\mathbf{x}) A(\mathbf{x}, \mathbf{y}) = \pi(\mathbf{y}) A(\mathbf{y}, \mathbf{x})$, which is the detailed balance condition.

The simplest choice of the symmetric function in the MTM sampler is $\lambda(\mathbf{x}, \mathbf{y}) \equiv 1$, and we call the resulting algorithm MTM (I). Another choice is

$$\lambda(\mathbf{x}, \mathbf{y}) = \left(\frac{T(\mathbf{x}, \mathbf{y}) + T(\mathbf{y}, \mathbf{x})}{2}\right)^{-1}. \qquad (5)$$

When $T(\mathbf{x}, \mathbf{y})$ is symmetric, (5) leads to the following MTM (II) algorithm:

1. Draw k trials $\mathbf{y}_1, \ldots, \mathbf{y}_k$ from a *symmetric* proposal distribution $T(\mathbf{x}, \cdot)$.

2. Select $\mathbf{Y} = \mathbf{y}$ among $\{\mathbf{y}_1, \ldots, \mathbf{y}_k\}$ with probability proportional to $\pi(\mathbf{y}_j), j = 1, \ldots, k$. Then draw $\mathbf{x}_1^*, \ldots, \mathbf{x}_{k-1}^*$ from the distribution $T(\mathbf{y}, \mathbf{x}^*)$. Denote $\mathbf{x}_k^* = \mathbf{x}$.

3. Accept $\mathbf{y}$ with probability

$$\min\left\{1, \frac{\pi(\mathbf{y}_1) + \cdots + \pi(\mathbf{y}_k)}{\pi(\mathbf{x}_1^*) + \cdots + \pi(\mathbf{x}_k^*)}\right\}$$

and reject with the remaining probability.

MTM (II) corresponds to the method of "orientational-biased Monte Carlo" described by Frenkel and Smit (1996, sec. 13.1), in which a specialized proof in the context of molecular structure simulation is also provided. The idea of utilizing multiple trial proposals to "bias" the local sampling in a Metropolis algorithm seems to have first been advanced by Mezei (1980), whose method is in fact very similar to a local griddy Gibbs. Cracknell, Nicholson, Parsonage, and Evans (1990) described a more general version of Mezei's method and applied it to the simulation of fluids (e.g., water, benzene) and other structured particles. However, Mezei's method differs substantially from MTM (II) because of its approximate nature.

Another sensible choice of λ is

$$\lambda(\mathbf{x}, \mathbf{y}) = \{T(\mathbf{x}, \mathbf{y}) T(\mathbf{y}, \mathbf{x})\}^{-\alpha}, \qquad (6)$$

defined in the region $\{(\mathbf{x}, \mathbf{y}): T(\mathbf{x}, \mathbf{y}) > 0\}$. When $\alpha = 1$, function $w(\mathbf{x}, \mathbf{y})$ corresponds to the importance weight of $\mathbf{x}$ as though the sampling distribution is $T(\mathbf{y}, \mathbf{x})$ and the target is $\pi(\mathbf{x})$. This seems to be an appealing feature. From our limited numerical experiences, we found that the performance of an MTM sampler is insensitive to the choice of $\lambda(\mathbf{x}, \mathbf{y})$, although the form (6) with α close to 1 worked the best in a few cases and MTM (II) was robust in all of our examples. It is still an open question whether and how we can find an optimal $\lambda(\mathbf{x}, \mathbf{y})$ for a particular problem.

The MTM transition allows one to explore more thoroughly in the "neighboring region" defined by $T(\mathbf{x}, \mathbf{y})$. This is especially useful when such a region (or direction) is obtained from a relatively expensive adaptation method.

3. SOME THEORETICAL DISCUSSIONS ON THE MULTIPLE-TRY METROPOLIS

3.1 Further Generalizations

From the proof of Theorem 1, we observe that the k trial proposals $\mathbf{y}_1, \ldots, \mathbf{y}_k$ need not be independent draws from $T(\mathbf{x}, \cdot)$. For example, if the transition function depends on another random variable $\mathbf{e}$ whose sampling distribution is $f_{\mathbf{x}}(\mathbf{e})$—that is, $T(\mathbf{x}, \mathbf{y}) = \int T_{\mathbf{e}}(\mathbf{x}, \mathbf{y}) f_{\mathbf{x}}(\mathbf{e}) \, d\mathbf{e}$—then we can first draw $\mathbf{e}$ and then draw the trial set $\{\mathbf{y}_1, \ldots, \mathbf{y}_k\}$ from $T_{\mathbf{e}}(\mathbf{x}, \cdot)$. In this case, the $\mathbf{y}$'s are no longer independently distributed but are still exchangeable. The MTM rule can be modified accordingly. More precisely, by defining that

$$w_{\mathbf{e}}(\mathbf{x}, \mathbf{y}) = \pi(\mathbf{x}) f_{\mathbf{x}}(\mathbf{e}) T_{\mathbf{e}}(\mathbf{x}, \mathbf{y}) \lambda_{\mathbf{e}}(\mathbf{x}, \mathbf{y}), \tag{7}$$

where $\lambda_{\mathbf{e}}(\mathbf{x}, \mathbf{y})$ is a positive symmetric function in $\mathbf{x}$ and $\mathbf{y}$, we can implement a modified MTM as follows: (a) choose $\mathbf{Y} = \mathbf{y}$ among $\{\mathbf{y}_1, \ldots, \mathbf{y}_k\}$ with probability proportional to $w_{\mathbf{e}}(\mathbf{x}, \mathbf{y}_j)$; (b) generate $\mathbf{x}_1^*, \ldots, \mathbf{x}_{k-1}^*$ from $T_{\mathbf{e}}(\mathbf{y}, \cdot)$; and (c) accept $\mathbf{y}$ with the generalized Metropolis ratio

$$\min \left\{ 1, \frac{w_{\mathbf{e}}(\mathbf{y}, \mathbf{x}) + \sum_{j=1}^{k-1} w_{\mathbf{e}}(\mathbf{y}_j, \mathbf{x})}{w_{\mathbf{e}}(\mathbf{x}, \mathbf{y}) + \sum_{j=1}^{k-1} w_{\mathbf{e}}(\mathbf{x}_j^*, \mathbf{y})} \right\}. \tag{8}$$

One can easily show that this scheme satisfies the detailed balance. When the sampling distribution of $\mathbf{e}$ is independent of the location $\mathbf{x}$ or $\mathbf{y}$, the generalized Metropolis ratio (8) can be further simplified by ignoring $f_{\mathbf{x}}(\mathbf{e})$ in the definition of $w_{\mathbf{e}}(\mathbf{x}, \mathbf{y})$; that is, by using $w_{\mathbf{e}}(\mathbf{x}, \mathbf{y}) = \pi(\mathbf{x}) T_{\mathbf{e}}(\mathbf{x}, \mathbf{y}) \lambda_{\mathbf{e}}(\mathbf{x}, \mathbf{y})$.

Some other generalizations of the basic MTM algorithm are also possible. For example, the trial set $\{\mathbf{y}_1, \ldots, \mathbf{y}_k\}$ can be generated from a Markov chain (or even deterministically) in which case the balance set $\{\mathbf{x}_1^*, \ldots, \mathbf{x}_{k-1}^*\}$ has to be generated differently. The effectiveness of these algorithms is currently under investigation.

3.2 Limiting Behavior of Multiple-Try Metropolis

It is of interest to know the limiting behavior of the MTM sampler as the number of trial proposals k becomes large. Let

$$\rho(\mathbf{x}, \mathbf{y}) = T(\mathbf{x}, \mathbf{y}) T(\mathbf{y}, \mathbf{x}) \lambda(\mathbf{x}, \mathbf{y}), \tag{9}$$

and define $M(\mathbf{x}) = E_{\pi}[\rho(\mathbf{x}, \mathbf{Y})]$. Then, by the weak law of large numbers (WLLN),

$$\frac{1}{k} \{w(\mathbf{y}_1, \mathbf{x}) + \cdots + w(\mathbf{y}_k, \mathbf{x})\} \overset{k \to \infty}{\Longrightarrow} M(\mathbf{x}) \quad \text{in probability}$$

if and only if $M(\mathbf{x}) < \infty$. Similarly, $\{w(\mathbf{y}, \mathbf{x}_1^*) + \cdots + w(\mathbf{y}, \mathbf{x}_k^*)\}/k \to M(\mathbf{y})$. To ensure a robust performance of MTM, we may want to impose the condition $\text{var}_{y|x} \{w(\mathbf{Y}, \mathbf{x})\} < \infty$ so that the strong law holds.

Under the limiting situation, the proposal distribution of $\mathbf{y}$ is, therefore,

$$p(\mathbf{y}|\mathbf{x}) = \frac{\pi(\mathbf{y}) \rho(\mathbf{x}, \mathbf{y})}{M(\mathbf{x})}.$$

Intuitively, the proposal transition function $T(\mathbf{x}, \mathbf{y})$ is first "symmetrized" and then applied. If we choose $\lambda(\mathbf{x}, \mathbf{y})$ as in (6) with $\alpha = 1$ in the region $A_{\mathbf{x}} = \{\mathbf{y} : T(\mathbf{x}, \mathbf{y}) > 0\}$, then we would have $\rho(\mathbf{x}, \mathbf{y}) = 1$ in $A_{\mathbf{x}}$, $M(\mathbf{x}) = \pi(A_{\mathbf{x}})$, and $p(\mathbf{y}|\mathbf{x}) \propto \pi(\mathbf{y})$ with $\mathbf{y} \in A_{\mathbf{x}}$. If $T(\mathbf{x}, \cdot)$ is restricted to be uniform in a region A regardless of $\mathbf{x}$, then each MTM step converges to an exact draw from $\pi(\mathbf{x})$ conditioned on that $\mathbf{x} \in A$. This is essentially a Gibbs sampling update.

Realistically, the efficiency of a MTM sampler relies on the calibration between the proposal step size, the number of multiple trials k, and the landscape of the target density π. A further theoretical understanding on these issues is desirable.

3.3 Multiple-Try Metropolis and the General Formulation of Reversible Markov Chains

A general way of producing a reversible Markov chain with π as its invariant distribution is to let the actual transition function from $\mathbf{x}$ to $\mathbf{y}$(for $\mathbf{y} \neq \mathbf{x}$) be of the form

$$A(\mathbf{x}, \mathbf{y}) = \pi(\mathbf{y}) \delta(\mathbf{x}, \mathbf{y}), \tag{10}$$

where $\delta(\mathbf{x}, \mathbf{y})$ is any suitable (nonnegative) symmetric function in $\mathbf{x}$ and $\mathbf{y}$ (C. Stein, personal communication). One can easily verify that $A(\mathbf{x}, \mathbf{y})$ given by (10) satisfies the detailed balance condition. However, the choice of $\delta(\mathbf{x}, \mathbf{y})$ is far from arbitrary because of the constraint that

$$\int_{\mathbf{y} \neq \mathbf{x}} A(\mathbf{x}, \mathbf{y}) \, d\mathbf{y} \leq 1, \quad \text{for almost all } \mathbf{x}.$$

In contrast, the choice of $\lambda(\mathbf{x}, \mathbf{y})$ in a MTM sampler is nearly arbitrary. Clearly, function $A(\mathbf{x}, \mathbf{y})$ in a M–H algorithm is of the form $\pi(\mathbf{y}) \delta_{\text{MH}}(\mathbf{x}, \mathbf{y})$ with

$$\delta_{\text{MH}}(\mathbf{x}, \mathbf{y}) = \min \left\{ \frac{T(\mathbf{x}, \mathbf{y})}{\pi(\mathbf{y})}, \frac{T(\mathbf{y}, \mathbf{x})}{\pi(\mathbf{x})} \right\},$$

which is apparently symmetric in $\mathbf{x}$ and $\mathbf{y}$. In contrast, the limiting transition function of MTM corresponds to

$$\delta_{\text{MTM}}(\mathbf{x}, \mathbf{y}) = \rho(\mathbf{x}, \mathbf{y}) \min\{M^{-1}(\mathbf{x}), M^{-1}(\mathbf{y})\},$$

with ρ defined in (9). This form might be useful in comparing different choices of $\lambda(\mathbf{x}, \mathbf{y})$ in MTM. Because $M(\mathbf{x})$ is obtained by averaging π over a "neighborhood" of $\mathbf{x}$, the resulting transition makes it more likely to move away from

x. Because of the construction of MTM, the asymptotic convergence property of the sampler is similar to that of a M–H sampler. (See Roberts and Tweedie 1996 for methods of analyzing such a chain.)

4. USING LOCAL OPTIMIZATION FOR ADAPTATION IN MARKOV CHAIN MONTE CARLO

In this section we show how to combine the MTM with the ADS method of Gilks et al. (1994) to produce a better sampler. The ADS method resembles the HR algorithm (see Sec. 4.1) but has its sampled direction, e_t, determined by other previously sampled points. Another distinctive feature of the method is that it attempts to use information across multiple chains.

4.1 Adaptive Direction Sampling

At each iteration of the ADS (or snooker algorithm), one has a population of samples, say $\mathcal{S}_t = \{\mathbf{X}_t^{(1)}, \dots, \mathbf{X}_t^{(m)}\}$, of size m. Each of the $\mathbf{X}_t^{(j)}$ is also called a "stream." Then the next generation $\mathcal{S}_{t+1}$ is generated as follows: (a) select a member $\mathbf{X}_t^{(c)}$ from $\mathcal{S}_t$ at random; (b) generate a random direction e_t as $e_t = (\mathbf{X}_t^{(c)} - \mathbf{X}_t^{(a)})/\|\mathbf{X}_t^{(c)} - \mathbf{X}_t^{(a)}\|$, where the anchor point $\mathbf{X}_t^{(a)}$ is chosen at random from $\mathcal{S}_t \setminus \{\mathbf{X}_t^{(c)}\}$; (c) generate a scalar r_t from an appropriate distribution $f(r)$; and finally, (d) update $\mathbf{X}_{t+1}^{(c)} = \mathbf{X}_t^{(a)} + r_t e_t$ and $\mathbf{X}_{t+1}^{(j)} = \mathbf{X}_t^{(j)}$ for $j \neq c$.

Gilks et al. (1994) and Roberts and Gilks (1994) showed that $f(r)$ should be of the form

$$f(r) \propto |r|^{d-1} \pi(\mathbf{X}_t^{(a)} + r e_t),$$

where d is the dimensionality of the state space. They also gave a more general form of this algorithm and provided cautionary advice on the use of their algorithm. They noted particularly that the adaptation may or may not improve the performance of the algorithm.

The ADS is a powerful formulation, but it leaves several issues unsettled. One question is how one can select a meaningful direction e_t. In the following, we demonstrate that if the choice of e_t is guided by a local optimization search, the resulting algorithm can be more effective. The second unanswered question, as we mentioned in Section 1, is how to sample from $f(r)$ effectively. We tackle this problem by using the MTM.

4.2 Local Optimization-Based Multiple-Try Metropolis

We follow the ADS approach of evolving a population of samples, say, $\mathcal{S}_t = \{\mathbf{X}_t^{(1)}, \dots, \mathbf{X}_t^{(m)}\}$, at each iteration. To update one of the samples, say $\mathbf{X}_t^{(c)}$, we use the other samples to construct a good reference point $\mathbf{Y}_t$, and then update $\mathbf{X}_t^{(c)}$ by an MTM transition along the direction defined by $\mathbf{X}_t^{(c)}$ and $\mathbf{Y}_t$. With the theory established by Roberts and Gilks (1994), one can see that essentially *any* way of choosing the reference point $\mathbf{Y}_t$ is appropriate provided that $\mathbf{Y}_t$ is indepnedent of $\mathbf{X}_t^{(c)}$ and that the distribution along the line, $f(r)$, is properly adjusted. For example, we can use a

conjugate gradient search to construct the reference point. The algorithm is then specified as follows.

Conjugate-Gradient Monte Carlo (CGMC)

Suppose that at time t we have a population of samples $\mathcal{S}_t = \{\mathbf{X}_t^{(1)}, \dots, \mathbf{X}_t^{(m)}\}$. AT time $t + 1$:

1. Choose $\mathbf{X}_t^{(r)} \in \mathcal{S}_t$ at random. Obtain either the gradient of $\log \pi(\mathbf{x})$ at $\mathbf{X}_t^{(r)}$ or the conjugate gradient formed by two gradient steps started from $\mathbf{X}_t^{(r)}$. Denote this direction by $\mathbf{u}_t$ and conduct a *deterministic* search to find the mode (anchor point), $\mathbf{A}_t$, of π along $\mathbf{X}_t^{(r)} + r\mathbf{u}_t$.

2. Choose another member $\mathbf{X}_t^{(c)} \neq \mathbf{X}_t^{(r)}$ from $\mathcal{S}_t$ at random.

3. Let $e_t = (\mathbf{A}_t - \mathbf{X}_t^{(c)})/\|\mathbf{A}_t - \mathbf{X}_t^{(c)}\|$, and sample along the line $\mathbf{A}_t + r e_t$ by the MTM method, with the target distribution for $r \in (-\infty, \infty)$ being

$$f(r) \propto |r|^{d-1} \pi(\mathbf{A}_t + r e_t), \tag{11}$$

where d is the dimensionality of the state space.

The gradient/conjugate gradient procedure in step 1 can be iterated for any number of times and can also be replaced by *any* effective local optimization method, such as the iterative conditional maximization or a few EM steps. In all of our examples, we have used the conjugate gradient directional method coupled with a one-dimensional minimization algorithm of Press, Tenkolsky, Vetterling, and Flannery (1996, p. 418). In steps 2 and 3 of CGMC, one can choose any number of chains in $\mathcal{S}_t \setminus \{\mathbf{X}_t^{(r)}\}$ to move toward anchor point A_t simultaneously. This modification sometimes can improve the performance of CGMC.

The population size m need not be too large. In fact, we found that having $m = 2$ to 5 was good enough for all of our examples. However, it should be a worthwhile topic to study the effect of m on the convergence of the algorithm. The following theorem shows that CGMC is indeed a proper transition. Our proof is modeled after that of Roberts and Gilks (1994).

Theorem 2. If we have population $\mathcal{S}_t = \{\mathbf{x}_t^{(1)}, \dots, \mathbf{x}_t^{(m)}\}$ in a CGMC setting, then the invariant distribution of $\mathcal{S}_t$ under the CGMC move is $\pi(\mathbf{x}_t^{(1)}) \times \cdots \times \pi(\mathbf{x}_t^{(m)})$.

Proof. Suppose that at time t, the distribution of $\mathcal{S}$ is

$$\pi^*(\mathcal{S}) = \pi(\mathbf{x}_t^{(1)}) \times \cdots \times \pi(\mathbf{x}_t^{(m)}).$$

Without loss of generality, we assume that in the next step $\mathbf{x}_t^{(1)}$ is chosen to be updated, and a_t is the anchor point obtained by a local optimization step started from $\mathbf{x}_t^{(m)}$, say. Because the local optimization step can be viewed as a function of $\mathbf{x}_t^{(m)}$, we can write $a_t = g(\mathbf{x}_t^{(m)})$. Because $\mathbf{x}_t^{(m)}$ follows π and is independent of $\mathbf{x}_t^{(1)}$, the anchor point a_t must also be independent of $\mathbf{x}_t^{(1)}$. The theorem then follows from the following lemma, which is a slightly more general version of lemma 3.1 of Roberts and Gilks (1994).

Lemma 1. Suppose that $\mathbf{x} \sim \pi$ and $\mathbf{y}$ is any fixed point in a d-dimensional space. Let $\mathbf{e} = (\mathbf{x} - \mathbf{y})/\|\mathbf{x} - \mathbf{y}\|$ be a unit vector. If r is drawn from distribution $f(r) \propto |r|^{d-1}\pi(\mathbf{y} + r\mathbf{e})$, then $\mathbf{x}' = \mathbf{y} + r\mathbf{e}$ follows distribution π. If $\mathbf{y}$ is generated from a distribution $D(\mathbf{y})$ independent of $\mathbf{x}$, then $\mathbf{x}'$ is independent of $\mathbf{y}$ and has density $\pi(\mathbf{x}')$.

Proof. Without loss of generality, we can let $\mathbf{y}$ be the origin. Then $\mathbf{e} = \mathbf{x}/\|\mathbf{x}\|$. If scalar r is drawn from $f(r) \propto |r|^{d-1}\pi(r\mathbf{x}/\|\mathbf{x}\|)$, $\mathbf{x}$ is drawn from $\pi(\cdot)$, and $\mathbf{x}' = r\mathbf{e}$, then for any measurable function $h(\mathbf{x})$,

$$E\{h(\mathbf{x}')\} = E[E\{h(\mathbf{x}')|\mathbf{x}\}]$$

$$= \int \int h(r\mathbf{x}/\|\mathbf{x}\|)\frac{|r|^{d-1}\pi(r\mathbf{x}/\|\mathbf{x}\|)}{\int |r'|^{d-1}\pi(r'\mathbf{x}/\|\mathbf{x}\|)\,dr'}\,dr$$

$$\times \pi(\mathbf{x})\,dr\,d\mathbf{x}.$$

By letting $s = r/\|\mathbf{x}\|$, we can rewrite the foregoing equation as

$$E\{h(\mathbf{x}')\} = \int \int h(s\mathbf{x})\frac{|s|^{d-1}\pi(s\mathbf{x})}{\int |s'|^{d-1}\pi(s'\mathbf{x})\,ds'}\pi(\mathbf{x})\,ds\,d\mathbf{x}.$$

Let $g(\mathbf{x}) = \int |s'|^{d-1}\pi(s'\mathbf{x})\,ds'$. Then $g(\mathbf{x})$ has the property that $g(t\mathbf{x}) = |t|^{-d}g(\mathbf{x})$. Letting $\mathbf{z} = s\mathbf{x}$, we obtain that

$$E\{h(\mathbf{x}')\} = \int \int h(\mathbf{z})\pi(\mathbf{z})|s|^{-1}\pi(s^{-1}\mathbf{z})/g(s^{-1}\mathbf{z})\,ds\,d\mathbf{z}$$

$$= \int h(\mathbf{z})\pi(\mathbf{z})/g(\mathbf{z})\int |s|^{-d-1}\pi(s^{-1}\mathbf{z})\,ds\,d\mathbf{z}$$

$$= \int h(\mathbf{z})\pi(\mathbf{z})\,d\mathbf{z} = E_\pi\{h(\mathbf{x})\}.$$

The second to last equality follows because $\int |s|^{-d-1}\pi(s^{-1}\mathbf{z})\,ds = \int |u|^{d-1}\pi(u\mathbf{z})\,du = g(\mathbf{z})$. Thus the updated sample $\mathbf{x}'$ follows distribution π. Because the expectation $E\{h(\mathbf{x}')\}$ does not depend on a particular value of $\mathbf{y}$, the independence between $\mathbf{x}'$ and $\mathbf{y}$ is apparent.

5. OTHER VARIATIONS OF MULTIPLE-TRY METROPOLIS

In this section we describe two other ways of using MTM in MCMC sampling. The first method is closely related to the HR algorithm of Chen and Schmeiser (1993); the second to the griddy Gibbs sampler (Ritter and Tanner 1992).

5.1 Random-Ray Monte Carlo

Hit-and-Run Algorithm. For a given current sample $\mathbf{X}_t$, one does the following: (a) uniformly select a random direction $\mathbf{e}_t$, (b) sample a scalar r_t from density $f(r) \propto \pi(\mathbf{X}_t + r\mathbf{e}_t)$, and (c) update $\mathbf{X}_{t+1} = \mathbf{X}_t + r_t\mathbf{e}_t$. This algorithm behaves like a random-direction Gibbs sampler, and it tends to be very helpful if the probability landscape of π consists of distinctive modes along noncoordinate directions.

A main difficulty in implementing the HR algorithm, however, is that sampling from $f(r)$ is rarely feasible in practice; one often ends up using only a single step of a Metropolis-type update (Chen and Schmeiser 1993). The MTM method combats this limitation by using a relatively flat and long-tailed proposal transition $T(r_1, r_2)$ (along direction $\mathbf{e}_t$) that corresponds to a very large searching range. As discussed in Section 3.2, as $k \to \infty$ and when T diverges

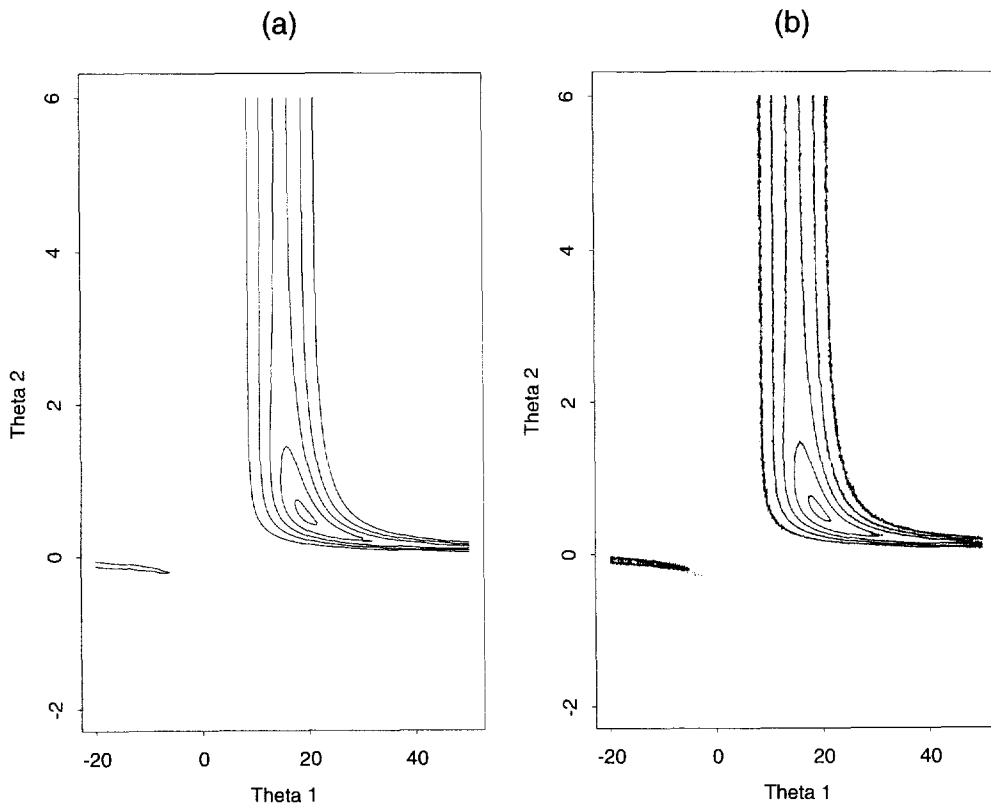(a)   (b)

Figure 1. Comparison of (a) the Exact Contour Plots With (b) the Plots Estimated by the MTM-Gibbs Samples (b).

to a uniform distribution, the resulting algorithm is exactly an HR sampler. Suppose that the current state is $\mathbf{X}_t = \mathbf{x}$, the random-ray algorithm executes the following update:

1. Randomly generates a direction (a unit vector) e.
2. Draws $\mathbf{y}_1, \ldots, \mathbf{y}_k$ from the proposal transition $T_{\mathbf{e}}(\mathbf{x}, \cdot)$ along the direction e. A generic choice is to draw iid samples $r_1, \ldots, r_k$ from $N(0, \sigma^2)$, where σ can be chosen rather large and set $\mathbf{y}_j = \mathbf{x} + r_j \mathbf{e}$. Another possibility is to draw $r_j \sim \text{Unif}[-\sigma, \sigma]$.
3. Conducts the MTM, as described in Section 3.1.

In our experience, a much larger σ, than that in an HR with single Metropolis update can be used, resulting in a higher acceptance rate for the same computational time.

5.2 Griddy Gibbs Multiple-Try Metropolis

The Gibbs sampler differs from the Metropolis algorithm in its emphasis on the use of conditional distributions. When sampling from a certain conditional distribution is not analtyically achievable, Ritter and Tanner (1992) proposed an approximate method—the griddy Gibbs sampler—as an alternative. The method has been successfully applied to several statistical problems (Barnard, McCullough, and Meng 1998), but its approximate nature still prevents it from being widely used. Using the MTM method, we can design a sampler, the MTM-Gibbs, that resembles the griddy Gibbs in both form and performance but is *exact* in the sense that π is invariant under the sampler's transition. The computation effort required by the new sampler is at most twice that of the original griddy Gibbs. Suppose that $\mathbf{x} = (x(1), \ldots, x(d))$ and that it is of interest to draw from

$\pi(\mathbf{x})$. With the current state $\mathbf{X}_t = \mathbf{x}$, the transition rule of the MTM-Gibbs is as follows:

1. Pick any component, say $x(i)$. Draw $y_1, \ldots, y_k$ iid from a transition $T(x(i), \cdot)$ along the axis of $x(i)$, and evaluate

$$w(y_j, x(i)) = \pi(x(1), \ldots, x(i-1), y_j, x(i+1), \ldots, x(d))$$

$$T(y_j, x(i))\lambda(y_j, x(i)).$$

for $j = 1, 2, \ldots, k$. The transition T is allowed to depend on $x[-i]$. The simplest such choice is $T(x(i), y) \equiv c$; that is, uniform in the range of $x(i)$ when the range is finite. Altneratively, one often chooses $t = x(i) + \varepsilon$ with $\varepsilon \sim N(0, \sigma^2)$.

2. Choose $y = y_j$ with probability proportional to $w(y_j, x(i))$. Draw $k - 1$ iid samples from $T(y, \cdot)$, say $s_1, \ldots, s_{k-1}$. Name $s_k = x(i)$.

3. Compute the generalized Metropolis ratio r_g as in (3); accept y with probability r_g and reject with $1 - r_g$.

We applied the foregoing algorithm to an example of Ritter and Tanner (1992, sec. 6.1) in which they fitted a nonlinear model,

$$y = \theta_1(1 - \exp(-\theta_2 x)) + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2),$$

to a real dataset. The prior of σ^2 was chosen to be flat on $(0, \infty)$, and the prior of (θ_1, θ_2) was uniform in the region $[-20, 50] \times [-2, 6]$. Note that the posterior would have been improper had a flat improper prior for (θ_1, θ_2) been chosen.

With $k = 10$, we let the proposal of a MTM-Gibbs be $N(\theta, 25^2)$ in the θ_1 direction and $N(\theta, 3^2)$ in the θ_2 direction. The starting point was randomly drawn from the unit
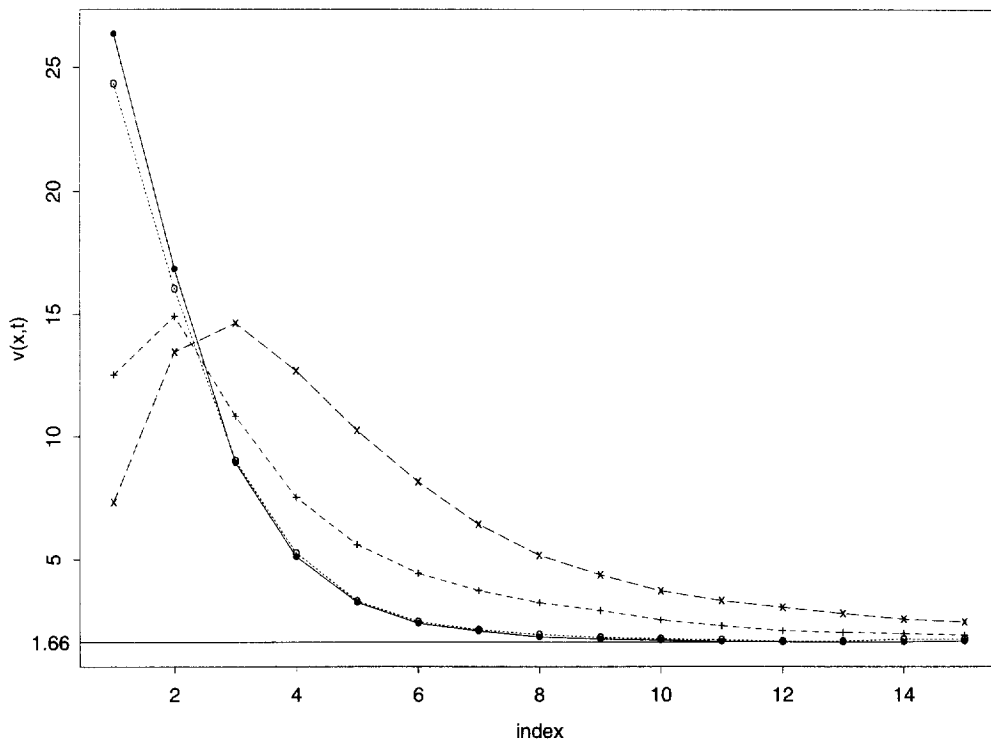

Figure 2. Comparison of the MTM scheme [•, MTM (I); ○, MTM (II)] with the Metropolis (×) and Langevin—Euler (+) schemes. The curves have been adjusted for computational costs; that is, those points with the same index value correspond to the same computing time (instead of iterations).

Histogram of Metropolis samples

Histogram of CGMC samples

Autocorrelation: Metropolis
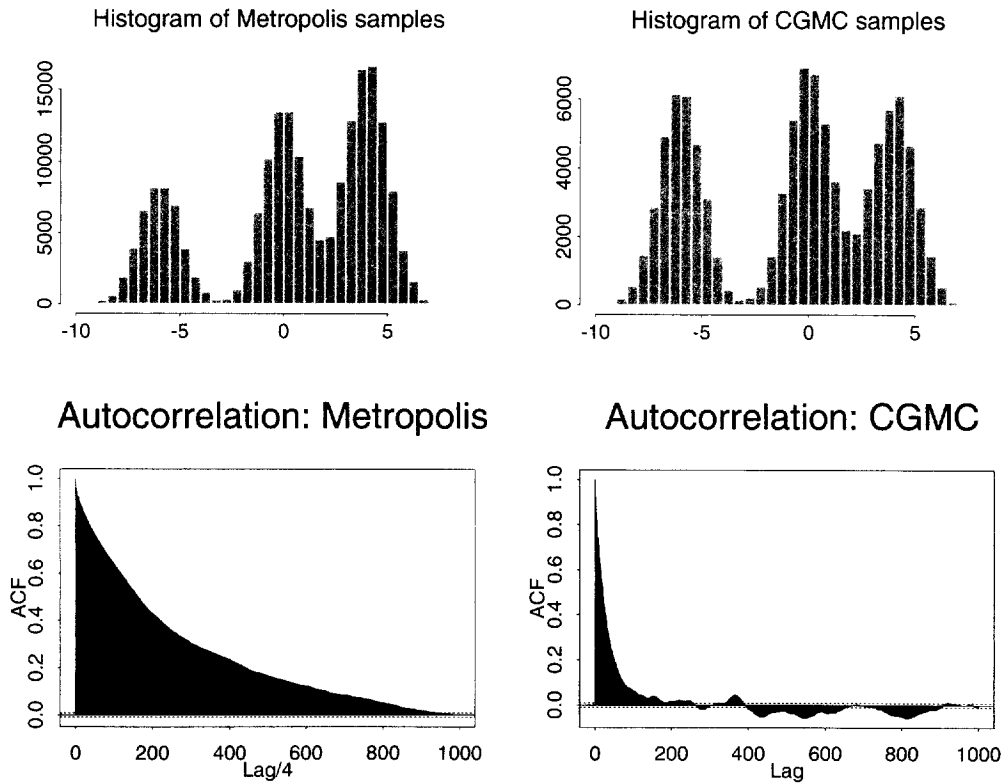
Autocorrelation: CGMC

Figure 3. Comparison of Results Obtained by the Metropolis Sampler and by the CGMC. The autocorrelation plot of the Metropolis samples has taken the computational cost into account.

square. We ran a total of 4.0e+7 MTM-Gibbs iterations and used the resulting MC samples to estimate the contour lines corresponding to 85%, 90%, 95%, 99% and 99.9% of the mass. Figure 1(a) shows the true contour lines (from a theoretical evaluation), and Figure 1(b) shows the estimated ones. Even though the mass of the second mode is
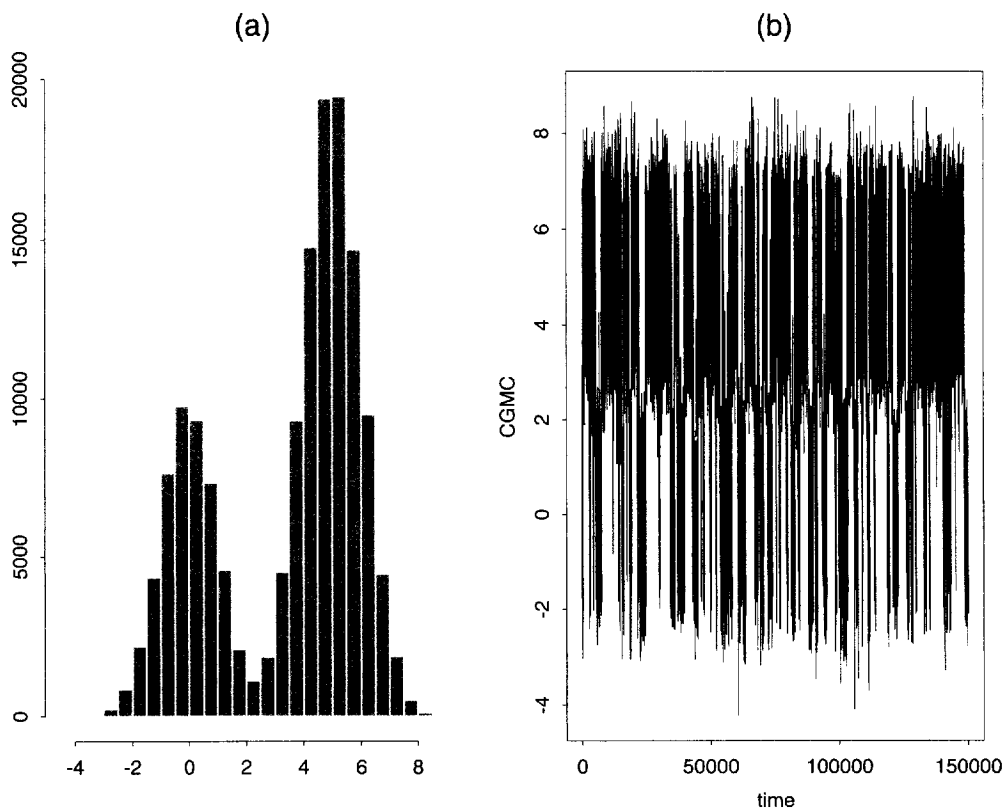
(a)

(b)

Figure 4. The Mixing Result of the CGMC Samples: (a) Marginal Histogram of the Sample; (b) Time Series Plot of One Stream of the CGMC.

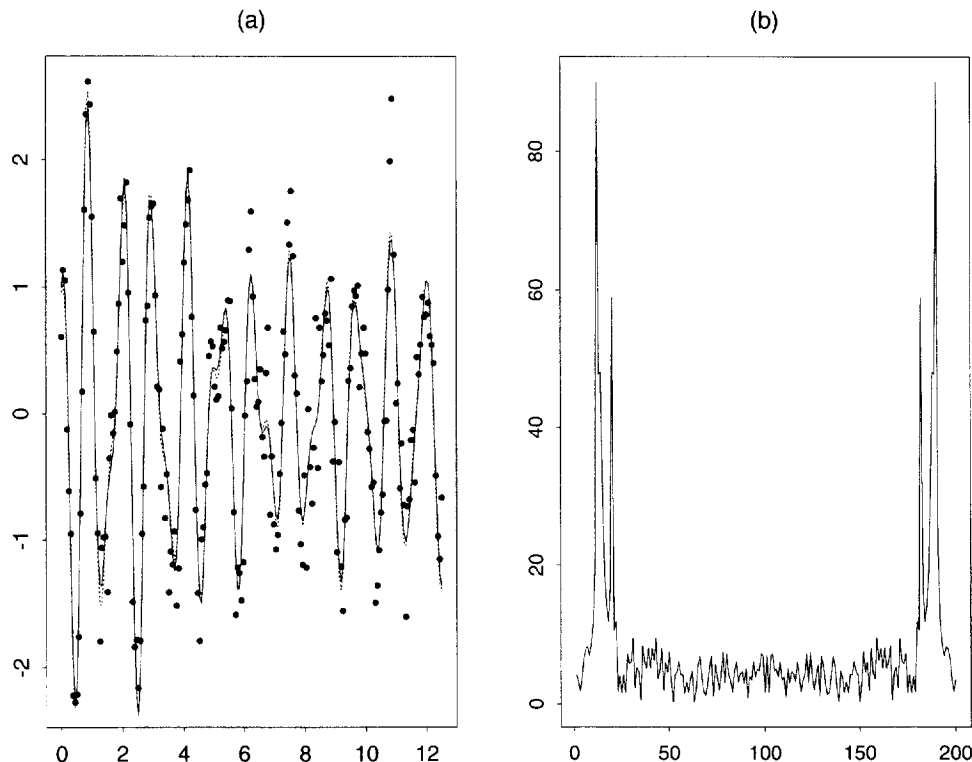(a)   (b)

Figure 5.   (a) The Simulated Sinusoidal Data and the Fitted Curve –, Original Data; —, True Curve; ···, Fitted Curve, and (b) the Fourier Transform of the Data.

very small (approximately .32%), the sampler gave us a fairly accurate estimate, .31%. The CGMC algorithm was also applied to the example with the number of streams $m = 3$ and the number of multiple tries $k = 10$. The proposal function for the line search was $N(x, 25^2)$, and that for the local Metropolis was unif$[-4, 4]$ along a randomly chosen direction. We observed that the CGMC produced about 50% more effective samples than the griddy Gibbs in one unit of computing time.

6.   NUMERICAL EXAMPLES

6.1   A Simple Unimodal Example for Comparisons

We first applied the MTM algorithm to sample from a simple t distribution with 5 degrees of freedom. The main purpose of this exercise is to compare the performance of the MTM sampler with that of a Metropolis sampler and a Langevin–Euler sampler for a smooth, but long-tailed target distribution. The Langevin–Euler scheme can be understood as a special M–H algorithm. Identical to the setting of Stramer and Tweedie (1998), we used the proposal function $T(x, \cdot) = N(x, 1)$ for the Metropolis algorithm, and used the proposal function

$$T(x, \cdot) = N\left(x + \frac{1}{2}h\nabla \log \pi(x), h\right) \qquad (12)$$

with $h = 1$ for the Langevin–Euler scheme. A scheme like this tends to perform well when the target distribution is smooth, but the type of move is far too "local" when the target distribution has a rough landscape.

Following Stramer and Tweedie (1998), we let all of the competing samplers start from $x = 9$ and monitored $v(x, t)$ (computed by averaging over 5,000 replications), the mean estimation of the variance of π, by using the first t consecutive MCMC samples (see Stramer and Tweedie 1998 for more details). As $t \to \infty, v(x, t)$ should converge to 1.66. We applied both MTM (I) and MTM (II) with $k = 5$ to this problem. For MTM (I), the proposal function is $T(x, \cdot) = N(x, \sigma_x^2)$, where $\sigma_x = \max\{10, |x|\}$. For MTM (II), the symmetric proposal is $N(x, 10^2)$. Figure 2 shows that the two MTM schemes performed rather similarly and that both outperformed the Metropolis and the Langevin–Euler schemes (after taking into consideration the extra computational cost). More important, we note that the MTM strategy can be applied in combination with all of the advanced M–H–type algorithms (including the Langevin-type and the self-targeting–type algorithms) to achieve better performance.

6.2   A Multimodal Example

Consider simulating from a two-dimensional mixture Gaussian distribution $\pi(x)$

$$.34 \times N_2(\mathbf{0}, I_2) + .33 \times N_2\left\{\begin{pmatrix} -6 \\ -6 \end{pmatrix}, \begin{pmatrix} 1 & .9 \\ .9 & 1 \end{pmatrix}\right\}$$

$$+ .33 \times N_2\left\{\begin{pmatrix} 4 \\ 4 \end{pmatrix}, \begin{pmatrix} 1 & -.9 \\ -.9 & 1 \end{pmatrix}\right\}.$$

Here the covariance matrices in the three components are identical to those of Gilks, Roberts, and Sahu (1998), but

the mean vectors are separated by a larger distance in each dimension.

We started two independent Metropolis samplers with starting points drawn from $\text{unif}[-.5, .5]^2$. A spherical proposal function was used: A direction was generated uniformly, and then the radius drawn from $\text{unif}[0, a]$, where a ($= 4$ in our case) was calibrated so that the Metropolis sampler had an acceptance rate of about .23 (Gelman, Roberts, and Gilks 1996). A total of 200,000 iterations of the Metropolis step was conducted for each sampler, which took about 28 seconds of CPU time on a Sun Ultra 2 workstation. Figure 3 plots the histograms and autocorrelations for one of the variables (left panels). It is seen that the Metropolis sampler moves very slowly due to the low-probability barriers between the modes, and the mixture proportions were very poorly estimated.

The CGMC method was applied to this problem with $m = 2$ streams and 20,000 iterations for each. Each iteration consists of two Metropolis steps and one adaptation step. So a total of 100,000 random draws from π, which took about 27 seconds of CPU time from the same computer, were produced as the program ended. The proposal function for the Metropolis step was the same spherical distribution as in the previous case but with a narrower range for the radius: $[0, 2.5]$ (corresponding to an acceptance rate of .37). For the CGMC, a small Metropolis step is beneficial for the purpose of exploring local features. The line sampling proposal was a univariate Gaussian with variance $= 10^2$ and the number of tries $k = 5$. This corresponds to an acceptance rate of .47. Our experience shows that an acceptance rate between .4 and .5 for the multiple-try step is appropriate. Figure 3 plots the histograms and autocorrelations for one of the variables in one stream.

Using the heuristic of *integrated autocorrelation time* (IAT), which equals to the sum of all-lag autocorrelations, we can estimate that with the *same* amount of CPU time, the IAT for the Metropolis algorithm is about 249 after adjusting for the computational cost (4 to 1 ratio), whereas for each stream of the CGMC, the integrated autocorrelation time is about 34. This translates to a sevenfold improvement.

To push the limit, we also tested the CGMC on a five-dimensional mixture Gaussian

$$\pi(\mathbf{x}) = \frac{1}{3}\, N_5(\mathbf{0}, I_5) + \frac{2}{3}\, N_5(\mathbf{5}, I_5),$$

where $\mathbf{0} = (0, \ldots, 0)$ and $\mathbf{5} = (5, \ldots, 5)$. (The distance between the two modes is $5\sqrt{5} = 11.2$.) We applied both the Metropolis algorithm (with proposal $N(x, 1.5^2)$) and the Langevin–Euler scheme (12) to this distribution and they performed similarly. In all of the 70 million iterations, the Langevin–Euler scheme with $h = 2.8$ (acceptance rate .247) was not able to escape from the mode in which it was started.

We started the CGMC with $m = 2$ streams and the initial values drawn from $\text{unif}[-.5, .5]^5$ (e.g., both streams were started from the first mode). Each iteration of the CGMC algorithm comprises two Metropolis steps and one gradient line-sampling step. The line-sampling step uses a Gaussian proposal with std $= 20$ and $k = 10$ multiple tries (the resulting acceptance rate was about .44). The Metropolis step
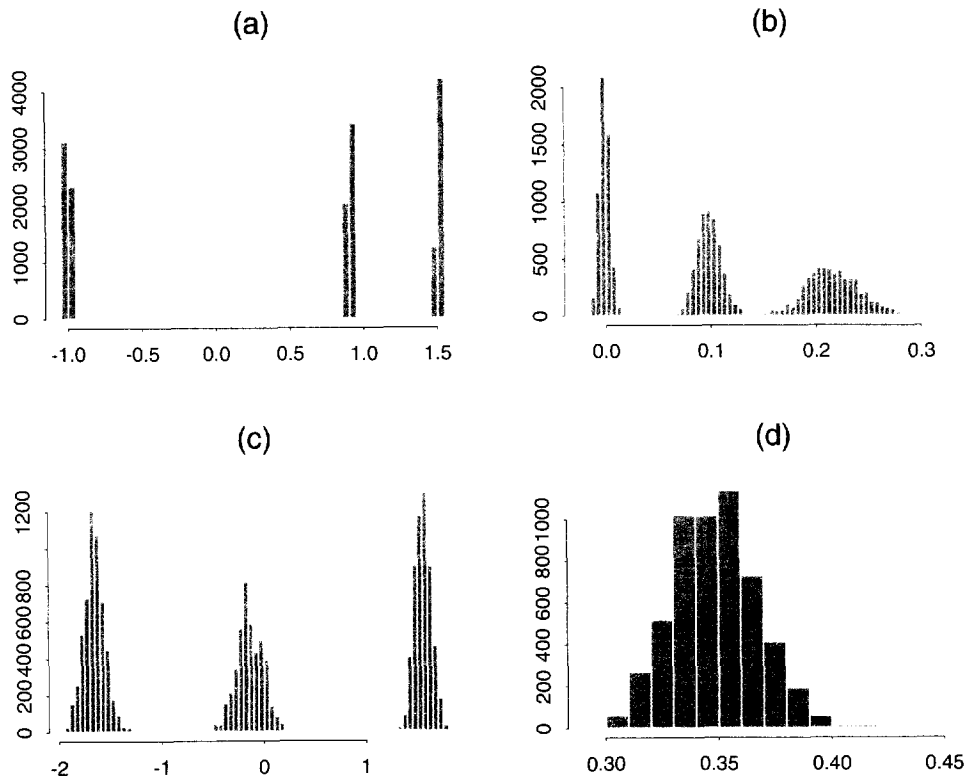
(a)

(b)

(c)

(d)

Figure 6. Using Monte Carlo Samples Produced by the CGMC, Histograms of (a) Three Frequencies (True Values c_j = .9, 1, and 1.5), (b) Three Damping Coefficients (True Values b_j = 0, .1, and .2), (c) Three Phases (True Values d_j = −1.57, 0, and 1.57), and (d) the Error Standard Deviation (True Value σ = .3).

uses a spherical distribution, which is uniform in the polar coordinates with radius $\in (0, 1.5)$ (acceptance rate $= .36$). We tested a large number of different proposal step sizes, ranging from 5 to 25. The results were insensitive to the choice of step size in this range. Two general guidelines are that (a) the step size for the line sampling should be reasonably large, that is, with a resulting acceptance rate in the range of $(.35, .55)$; and (b) the proposal step size for the Metropolis should give an acceptance rate in the range of $(.35, .5)$.

With 100,000 iterations, the CGMC algorithm produced a total of 300,000 random draws from π in about 300 seconds of CPU time. The estimates of mixing proportion, marginal means, variances, and even cdf's based on these 300,000 samples are rather accurate (i.e., they differ from the true values in the second decimal place). Figure 4 plots the histogram and the time series of the first coordinate of x in one of the two streams (of size 150,1347). The IAT for this time series in the range of 400–550, which leaves us an effective sample size of about 600 with two streams.

A random-ray sampler (Sec. 4.1) was also applied to the problem with $k = 8$ and the proposal STD $= 12$. It performed rather well for this problem. With the same CPU time, it can produce about 300 effective samples, slightly worse than the CGMC. This similarity in performance between the two methods is understandable; because the two modes are essentially unconnected, the gradient information in this example provides little help for the CGMC. The reason why both methods work is the effectiveness of line sampling.

6.3 Damped Sinusoidal Fitting

In this experiment we simulated $n = 200$ observations from the model

$$y_i = \sum_{j=1}^{J} e^{-a_j - b_j x_i} \cos(c_j x_i + d_j) + \varepsilon_i,$$

where $\varepsilon_i \sim N(0, \sigma^2)$. The true signal in this model has three sinusoidal components $(J = 3)$, where each component is characterized by its weights, e^{-a_j}; damping constant, b_j; angular frequency, c_j; and phase, d_j. In our simulation the weight factor $a_j = 0, j = 1, 2, 3$, is assumed known. Thus there are a total of 10 unknown parameters, which can be summarized as $\theta = (\sigma; b_j, c_j, d_j, j = 1, \ldots, 3)$, with true values $(.3, 0, .9, 1.57, .2, 1, 0, .1, 1.5, -1.57)$. Note that the three different frequencies (c_j) are .9, 1.0, and 1.5. The likelihood function of θ can be written as

$$L(\theta | y_1, \ldots, y_n) \propto \frac{1}{\sigma^2}$$

$$\exp\left\{-\frac{\sum_{i=1}^{n}(y_i - \sum_{j=1}^{3} e^{-a_j - b_j x_i} \cos(c_j x_i + d_j))^2}{2\sigma^2}\right\}, \quad (13)$$

which can also be treated as a posterior distribution of θ with a flat prior. To avoid improper posterior distribution, we restricted b_j, c_j, and d_j in a bounded region $[-1, 1] \times [-3, 3] \times [-3, 3]$.

A fast Fourier transform (FFT) was first applied to the data. Two major frequencies were easily recognized, but the third frequency component was not detectable. Moreover, Fourier analysis has difficulties in resolving the damping coefficients [Fig. 5(b)]. These suggest that, although it is computationally more demanding, a brute-force curve-
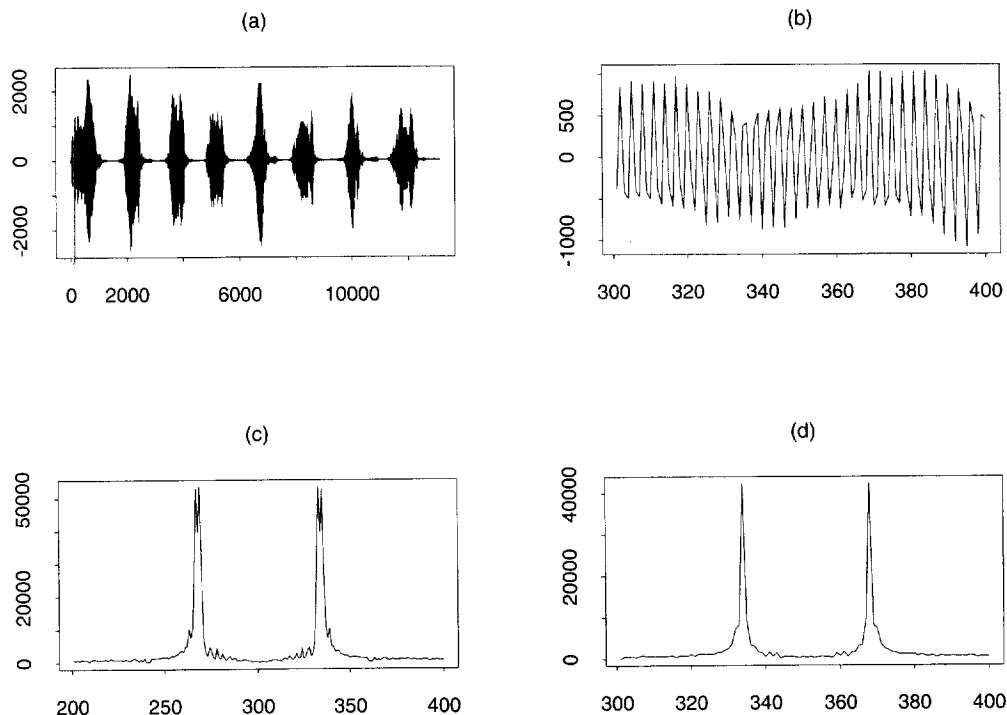

(a)

(b)

(c)

(d)

Figure 7. (a) Plot of the Bird Chirp Sequence; (b) Plot of a Segment ([301:400]) of the Original Sound Signal Sequence; (c) the FFT of Data Segment [201:400]; and (d) the FFT of Segment [301:400].

fitting method can sometimes help gain more information on the finer structure of a sinusoidal signal than can a fast Fourier analysis.

We applied both the Metropolis and the CGMC method to find the maximum likelihood fit of the data. We ran the CGMC with $m = 5$ streams for 14.5 minutes, producing 1,200 iterations (with each iteration consisting of one step of line sampling and 20 steps of Metropolis). We ran the Metropolis for the same amount of time (five independent streams, each with 2.000×20 Metropolis steps in each iteration). We monitored the change of likelihood as the iterations proceeded. The Metropolis found the modal region (the best out of five streams) six times out of 20 repeated runs (about 30%). In contrast, the CGMC found the modal region 14 times in 20 trials (about 70%). Interestingly, the deterministic conjugate gradient method, which is routinely used for nonlinear least squares fitting, failed in this problem. The best fit of the data is shown by dotted lines in Figure 5(a). Posteriors of the unknown quantities, based on histograms obtained from one CGMC run with $m = 5$ chains, are shown in Figure 6.

We also applied this Bayesian curve-fitting procedure to analyze the recording of bird chirps contained in the standard MATLAB 4.2 demo folder. The whole data file comprises 13,129 digital signals, as plotted in Figure 7(a). We took a segment of length 100 (segment [301: 400]) from it for analysis [plotted in Fig. 7(b)]. Two related Fourier transforms (of two segments) are shown in in Figure 7(c) and (d). As one can see, the FFT of the data segment [201:400] revealed two distinct frequency peaks, whereas only one frequency appeared when FFT was applied to seg-

ment [301:400]. Even with extensive zero padding, we still could not see the two distinct frequencies.

In contrast, our Bayesian curve-fitting procedure (with $J = 3$) found the two major frequency components at 4.22 and 2.14, which correspond well to the two components revealed by the Fourier analysis of the longer data segment [201:400]. We also found another minor frequency at 1.95 with a large damping coefficient. The three components are plotted in Figure 8. The fitted value (solid line) agreed very well with the original data.

6.4 Fitting Mixture Models

Suppose that $y_1, \ldots, y_n$ are iid samples from a mixture distribution with three Gaussian components with unknown means, variances, and proportions. It is easy to write the likelihood as

$$L(\boldsymbol{\theta}|y_1, \ldots, y_n) = \prod_{i=1}^{n} \left\{ p_1 \phi \left(\frac{y_i - \mu_1}{\sigma_1} \right) \right.$$
$$\left. + p_2 \phi \left(\frac{y_i - \mu_2}{\sigma_2} \right) + p_3 \phi \left(\frac{y_i - \mu_3}{\sigma_3} \right) \right\},$$

where $p_3 = 1 - p_1 - p_2$ and $\phi(\cdot)$ is the standard Gaussian density. For technical reasons, we performed a parameter transformation $u_1 = \log p_1$ and $u_2 = \log p_2$, and let our sampler operate on $\boldsymbol{\theta} = (u_1, u_2; \mu_i, \log \sigma_i, i = 1, 2, 3)$. With a flat prior on $(\log \sigma_i, \mu_i; i = 1, 2, 3)$ in a bounded region $[-4, 4]^3 \times [-10, 10]^3$ and a prior $p(u_1, u_2) \propto (1 - e^{u_1} - e^{u_2})_+$ with $(u_1, u_2) \in [-10, 0] \times [-10, 0]$, we obtained an expression for the posterior distribution of these parameters, up to a normalizing constant. To cope with the nonidentifiability problem, we imposed the constraint that $\mu_1 \geq \mu_2 \geq \mu_3$.
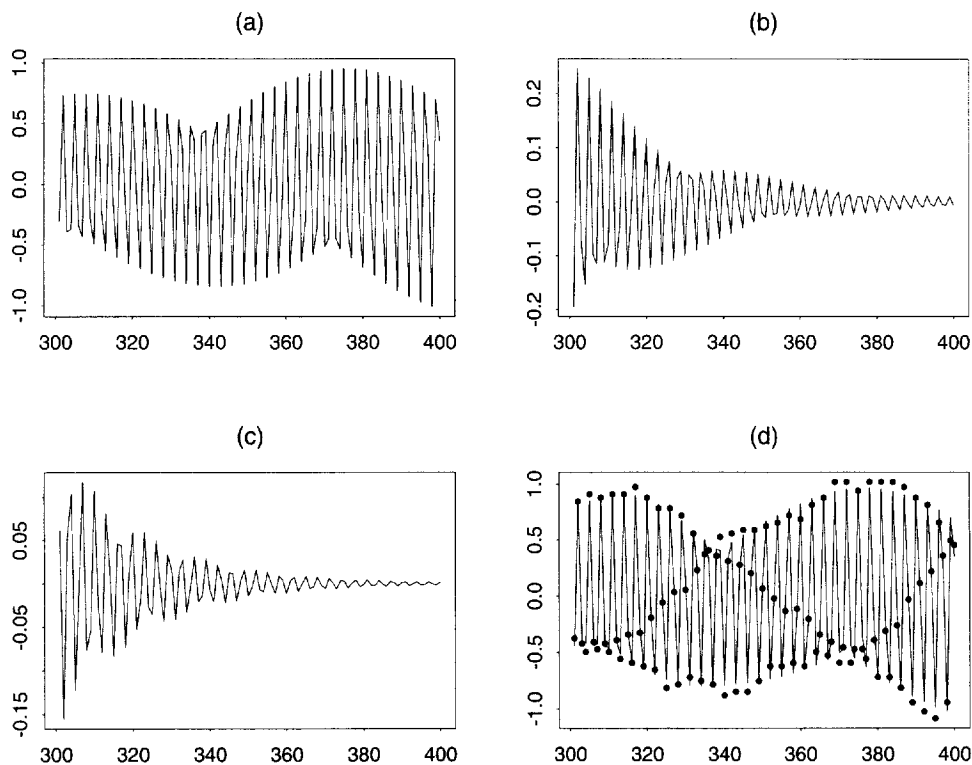

Figure 8. Results From CGMC Fitting. (a) The first fitted component; (b) the second fitted component; (c) the third fitted component; (d) the fitted value versus original data. The dots in (d) correspond to the original signals, plotted in Figure 7(b), after rescaling.
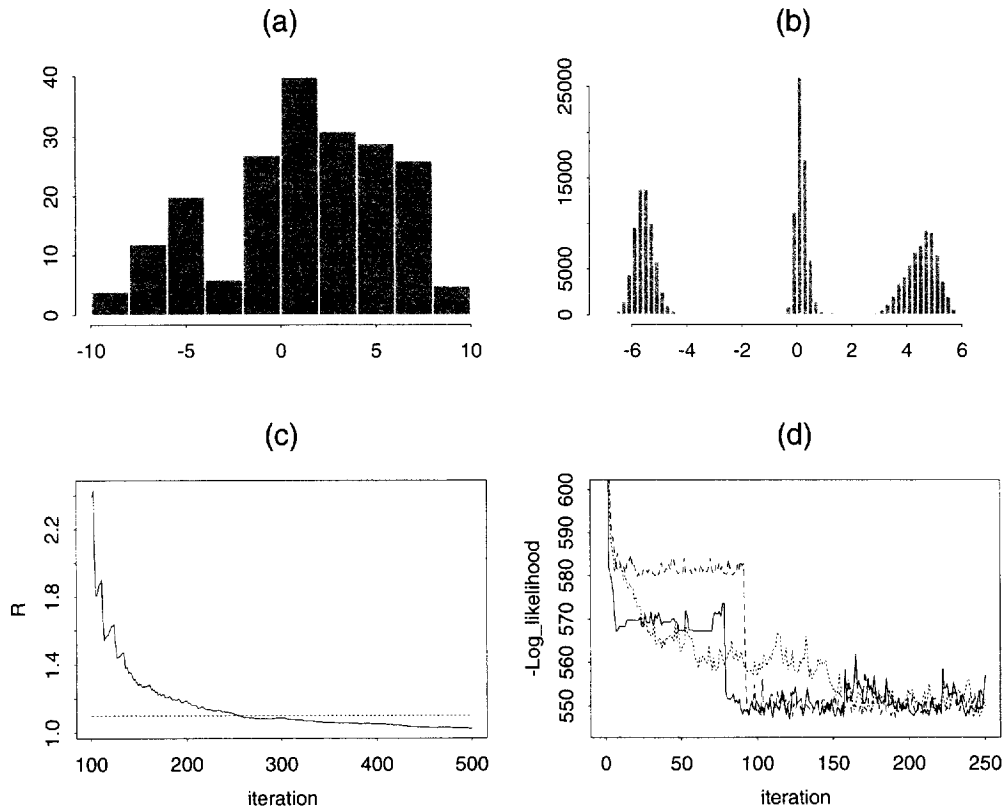
(a)   (b)

(c)   (d)

Figure 9. (a) Histogram of the Data; (b) Posterior Distribution of the μ_j, With the Samples Obtained from the CGMC; (c) Gelman—Rubin Convergence Criterion $\hat{R}$; and (d) Time Series Plot of the Four Streams in the CGMC (——, Stream 1; · · ·, Stream 2; – – –, Stream 3; — — —, Stream 4). Every iteration unit in both (c) and (d) corresponds to one step of line sampling and 20 steps of Metropolis in simulation.

We simulated a dataset with $n = 200; p_1 = .2, p_2 = .3; \mu_1 = -5, \mu_2 = 0, \mu_3 = 5$; and $\sigma_1 = 2, \sigma_2 = 1, \sigma_3 = 2$. The histogram of this dataset is shown in Figure 9(a). A

Gibbs sampler can be designed for this problem with the introduction of a set of latent component-indicator variables (Chen and Liu 1996; Diebolt and Robert 1994). Instead of

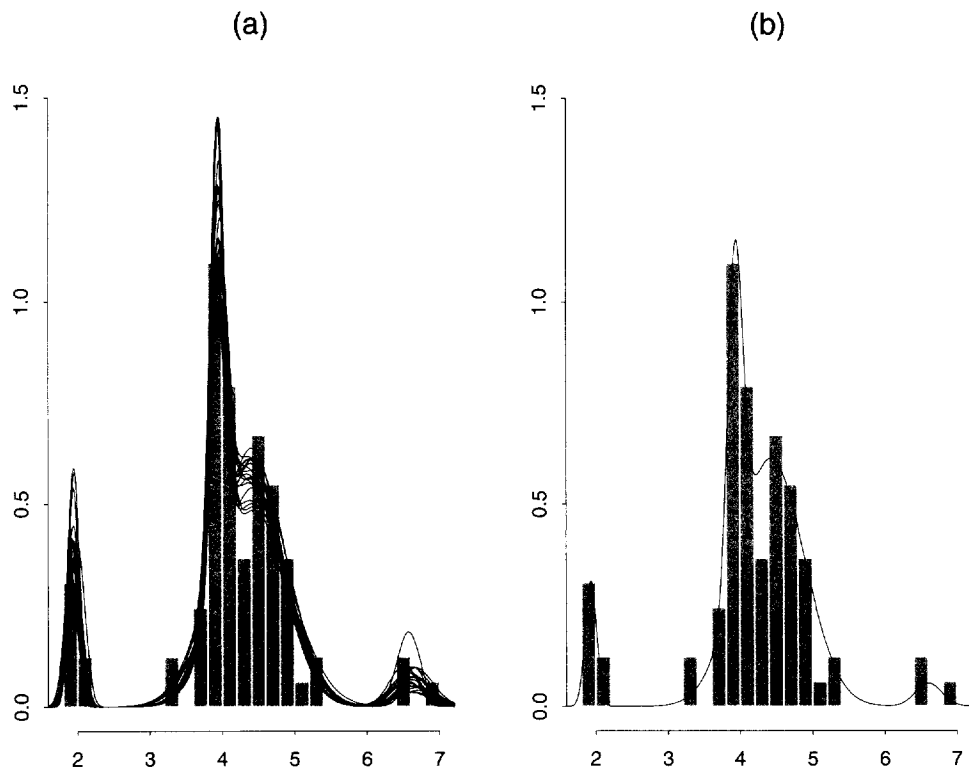## (a)   (b)

Figure 10. (a) Random Draws of the Posterior Predictive Densities for the Galaxy Data of Roeder and Wasserman (1997) and (b) Maximum a posteriori Estimate of the Predictive Density.

taking the latent variable approach, we can also attempt to simulate from the joint posterior distribution of θ directly by a Metropolis sampler.

Clearly, the efficiency of a Metropolis sampler running on the space of θ depends strongly on its proposal distribution. In the test example, we used a generic proposal: uniformly choosing a direction in the θ space, and then sampling a distance from $\text{unif}[0, a]$, where a is adjusted so that the overall acceptance rate is about .25. For our example, $a = .3$ was suitable. This choice of the proposal was apparently unfavorable for the simulation because it put all of the parameters in a common scale (e.g., it treats $\log p_i$, μ_j, and $\log \sigma_k$ indiscriminately). Although we understand that a more sophisticated choice of the proposal distribution can increase efficiency of the sampler, we believe that it would be a more convincing illustration to use a generic proposal without entertaining any special property of the problem. The CGMC will also use a similar proposal—by which we hope to show that a brute force approach is also a viable choice.

We independently started 100 Metropolis chains with random starting points and monitored their log-likelihood values. With 21,000 Metropolis steps, we observed that 33 of the 100 chains were stuck in local modes, whereas the remainder successfully settled down in the modal region (i.e., log-likelihood ≥ -555).

We applied the CGMC to the same problem, with one-step conjugate-gradient local optimization, a radius of 8 for the line-sampling, and $k = 20$ multiple tries. The total number of streams was kept at $m = 4$. Between every line sampling, 20 Metropolis steps were inserted. Thus, "one-iteration" in this algorithm consisted of a line sampling and 20 Metropolis steps. The computational cost of one step of line sampling is roughly the same as 10 steps of the standard Metropolis moves. We did 10 independent runs of the CGMC on this problem, which produced a total of 40 chains. We found that all but three chains settled in the modal region within 500 iterations (equivalent of 7,500 Metropolis steps). Figure 9(d) shows the time series plot of the log-likelihood for the four streams of a randomly chosen CGMC run.

A byproduct of the CGMC sampler is that a convergence-diagnostic statistic can be produced based on the multiple streams of a single CGMC run. In this example, the time series plot [Fig. 9(d)] together with the Gelman–Rubin statistic $\hat{R}$ [Fig. 9(c)] served convergence diagnosis purposes very well; an $\hat{R} < 1.2$ computed with $m = 4$ chains always indicated that stationarity was reached. Although a large $\hat{R}$ does indicate nonconvergence, caution is needed when claiming convergence; because the multiple streams used in the CGMC are not completely independent before they reach equilibrium, the resulting $\hat{R}$ is not as reliable an indicator as that from independent runs. A quick remedy is to execute a small number (2 to 5) of independent CGMC runs for computing the Gelman-Rubin statistic.

The foregoing mixture model-fitting procedure was applied to the galaxy dataset analyzed by Roeder and Wasserman (1997). The original data were first rescaled by 5,000 and then fitted by a four-component Gaussian mixture model. Figure 10(a) shows the overlay plot of 20 sampled predictive densities for the galaxy dataset, and Figure 10(b) shows the overlay plot of the maximum a posteriori predictive density.

7. DISCUSSION

We have proposed two novel ideas and their variations: a new transition rule applicable to all MCMC algorithms and a way to utilize local optimization in Monte Carlo simulation. Necessary theoretical foundations have been provided to justify these ideas, and their usefulness has been carefully examined through several numerical examples. Generally speaking, the MTM enables us to make large step-size transitions in a MCMC sampler. It is particularly useful when one is able to identify certain directions of interest but then has difficulty implementing a Gibbs sampling–type move because of unfavorable conditional distributions.

It has been suggested by some researchers that Monte Carlo efficiency might be improved by first doing mode-finding and then adjusting the proposal function accordingly (Gelman and Rubin 1992). But to the best of our knowledge, there is no effective and general purpose means for putting mode-finding steps into a proper MCMC framework. Lemma 1 shows that any anchor point that is independent of the current state can be used effectively in a MCMC sampler to direct future draws. Thus one can either apply deterministic mode finders in advance to locate some modes as anchor points, or apply these deterministic procedures adaptively as in our CGMC sampler. Further analysis along this direction is of interest.

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