

# Markov Chains of Infinite Order and Asymptotic Satisfaction of Balance: Application to the Adaptive Integration Method<sup>†</sup>

David J. Earl and Michael W. Deem\*

Departments of Bioengineering and Physics & Astronomy, Rice University, 6100 Main Street—MS 142, Houston, Texas 77005-1892

Received: October 3, 2004; In Final Form: November 17, 2004

Adaptive Monte Carlo methods can be viewed as implementations of Markov chains with infinite memory. We derive a general condition for the convergence of a Monte Carlo method whose history dependence is contained within the simulated density distribution. In convergent cases, our result implies that the balance condition need only be satisfied asymptotically. As an example, we show that the adaptive integration method converges.

## 1. Introduction

Adaptive Monte Carlo methods that change the sampling strategy based upon statistics collected on the fly have been shown to be very powerful in a number of interesting applications.<sup>1–5</sup> Typically these adaptive methods use the statistics collected during a run to construct an importance sampling potential that is intended to remove the most significant barriers to sampling in the problem. These methods, however, have been criticized by various authors due to their lack of satisfying detailed balance. Although the use of adaptive simulation methods is growing, and their success has been demonstrated in a number of cases,<sup>4</sup> widespread acceptance of the correctness of the approach within the simulation community has been hampered by these questions of detailed balance and so of convergence of the simulated distribution in phase space. In most of these methods, it is clear that there is at least one fixed point of the distribution, the Boltzmann, possibly modified by an importance sampling factor that is itself a functional of the Boltzmann distribution. As the Monte Carlo algorithm will be started from an arbitrary initial condition, it is of interest to know whether these algorithms will converge to the Boltzmann, or any other, fixed point. Such fixed point analysis has not been performed for this class of algorithms and is the subject of this paper.

As an archetypal example of these adaptive Monte Carlo methods, we consider the adaptive integration scheme of Fasnacht, Swendsen, and Rosenberg.<sup>6</sup> In this method, we focus on one order parameter,  $\lambda$ , of the system that leads to the most significant barriers. We construct an estimate of the probability distribution of  $\lambda$ , and we use the inverse of this probability as the importance sampling function:

$$P(\lambda_0) = \langle \delta(\lambda(\mathbf{x}) - \lambda_0) \rangle = \frac{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \delta(\lambda(\mathbf{x}) - \lambda_0)}{\int d\mathbf{x} e^{-\beta U(\mathbf{x})}} \quad (1)$$

where  $\beta$  is the inverse temperature, and  $\mathbf{x}$  is a vector in  $3n$  dimensions. We define

$$e^{-\beta F(\lambda_0)} = \int d\mathbf{x} e^{-\beta U(\mathbf{x})} \delta(\lambda(\mathbf{x}) - \lambda_0) \quad (2)$$

Then the probability distribution is given by

$$P(\lambda_0) = \frac{e^{-\beta F(\lambda_0)}}{Z} \quad (3)$$

where the configurational integral is  $Z = \int d\mathbf{x} e^{-\beta U(\mathbf{x})}$ . Now, consider

$$\begin{aligned} \frac{d(\ln P(\lambda_0))}{d\lambda_0} &= \frac{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \frac{d}{d\lambda_0} \delta(\lambda(\mathbf{x}) - \lambda_0)}{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \delta(\lambda(\mathbf{x}) - \lambda_0)} \\ &= \frac{\int d\mathbf{x} \delta(\lambda(\mathbf{x}) - \lambda_0) \frac{d}{d\lambda_0} e^{-\beta U(\mathbf{x})}}{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \delta(\lambda(\mathbf{x}) - \lambda_0)} \\ &= -\beta \frac{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \frac{dU}{d\lambda_0} \delta(\lambda(\mathbf{x}) - \lambda_0)}{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \delta(\lambda(\mathbf{x}) - \lambda_0)} \\ &= -\beta \left\langle \frac{dU}{d\lambda_0} \right\rangle_{\lambda_0} \end{aligned} \quad (4)$$

where we have used the fact that both  $\lambda$  and  $U$  are functions of  $\mathbf{x}$ , and  $dU/d\lambda$  really means  $\nabla U \cdot d\mathbf{x}/d\lambda$ . Thus, we come to the thermodynamic integration formula for the free energy as a function of  $\lambda$ :

$$\begin{aligned} F(\lambda_0) &= \int d\lambda \left\langle \frac{dU}{d\lambda} \right\rangle \\ &= \int_{\lambda_{\min}}^{\lambda_0} d\lambda' \frac{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \frac{dU}{d\lambda'} \delta(\lambda(\mathbf{x}) - \lambda')}{\int d\mathbf{x} e^{-\beta U(\mathbf{x})} \delta(\lambda(\mathbf{x}) - \lambda')} \end{aligned} \quad (5)$$

We desire the observed distribution in the Monte Carlo scheme to be

$$\rho(\mathbf{x}) = (\text{const}) e^{-\beta U(\mathbf{x})} / P(\lambda(\mathbf{x})) = (\text{const}) e^{-\beta U(\mathbf{x}) + \beta F(\mathbf{x})} \quad (6)$$

\* Corresponding author. E-mail: mwdeem@rice.edu. Fax: 713-348-5811.

<sup>†</sup> Part of the special issue “David Chandler Festschrift”.

As the simulation is performed, the estimated value of the importance sampling free energy,  $\hat{F}(\lambda)$ , is constructed from eq 6 and used in eq 5. For example, if the distribution to date is  $\rho(\mathbf{x})$ , then we have

$$\hat{F}(\lambda_0) = \int_{\lambda_{\min}}^{\lambda_0} d\lambda' \frac{\int d\mathbf{x} \rho(\mathbf{x}) \frac{dU}{d\lambda} \delta(\lambda(\mathbf{x}) - \lambda')}{\int d\mathbf{x} \rho(\mathbf{x}) \delta(\lambda(\mathbf{x}) - \lambda')} \quad (7)$$

In the context of a Metropolis algorithm, the acceptance criterion would be

$$\text{acc}(o \rightarrow n) = \min\{1, e^{-\beta U(\mathbf{x}^n) + \beta U(\mathbf{x}^o) + \beta \hat{F}(\lambda(\mathbf{x}^n)) - \beta \hat{F}(\lambda(\mathbf{x}^o))}\} \quad (8)$$

Although we have written transition probabilities that satisfy detailed balance in eq 8, our analysis is equally applicable to transition probabilities that satisfy only balance.<sup>7</sup> Since the importance sampling function is changing with step number, due to the updates to density and so to  $\hat{F}$ , this adaptive algorithm does not satisfy detailed balance. It is clear, however, that if the density has converged to the Boltzmann,  $\rho(\mathbf{x}) = (\text{const})e^{-\beta U(\mathbf{x}) + \beta F}$ , then the estimation in eq 7 is exact, and the acceptance criterion in eq 8 is exact and constant for future steps. Thus, the desired exact answer, eq 6, is a fixed point of this algorithm. We also note that if the observed density distribution is not exact, but if  $\rho(\mathbf{x})/\rho(\mathbf{y}) = e^{-\beta U(\mathbf{x}) + \beta U(\mathbf{y})}$  whenever  $\lambda(\mathbf{x}) = \lambda(\mathbf{y})$ , then the estimated importance sampling function, eq 7, is also exact. This property will prove to be useful.

The Markov process underlying a Monte Carlo algorithm with acceptance probabilities such as eq 8 has memory, because the process depends on all past states through the observed density distribution  $\rho(\mathbf{x})$ . Technically, this is a Markov chain of infinite order.<sup>8</sup> Markov chains of infinite order have a solid body of convergence results when the dependence on the past, essentially, decays exponentially fast (technically, when they are continuous with respect to the past).<sup>9</sup> The Markov process in adaptive integration is dramatically discontinuous with respect to the past: the first point observed is just as important as the most recent point observed in the measured density distribution.

We here consider the infinite order Markov process that occurs in adaptive Monte Carlo. In section 2, we derive a general condition on the transition matrices for adaptive Monte Carlo that guarantees convergence to a unique distribution. Although we often use continuous notation, technically we limit discussion to finite, discrete spaces, in the belief that the continuous limit exists as the grid spacing goes to zero. In section 3, we examine the special case of adaptive integration Monte Carlo, showing convergence to a unique distribution occurs. We discuss our findings in section 4.

## 2. Theory

We wish to find the conditions under which a Markov chain of infinite order converges to a unique limiting distribution. We consider the chain to possess a transition probability that depends on the current and future state and on the density constructed from all previously observed states, as in eqs 7 and 8. We assume that the transition probabilities satisfy a generalization of the irreducibility condition: we assume there is a  $c > 0$  such that

$$\text{Prob}[\mathbf{x}(t), \rho(t) \rightarrow \mathbf{y}(t+m)] > c \quad (9)$$

for all  $\mathbf{x}, \mathbf{y}, \rho$ , and  $t$  for some fixed  $m$ . This is a precise statement of our desire that the process be ergodic, with mixing time  $m$ . Thus, we have  $\text{Prob}[\mathbf{x}(t)] > c$  for all times  $t > m$ , because we

can apply eq 9 to each of the initial states  $1, \dots, m-1$ , and then iterate to conclude  $\text{Prob}[\mathbf{x}(m' + m)] = \sum_{\mathbf{x}'} \text{Prob}[\mathbf{x}'(m'), \rho(m') \rightarrow \mathbf{x}(m + m')]\text{Prob}[\mathbf{x}'(m')] \geq c \sum_{\mathbf{x}'} \text{Prob}[\mathbf{x}'(m')] = c$ . In fact, we consider a larger value of  $m$ , so that any given Markov chain has an observed density that equals the expected probability distribution to  $O(1/\sqrt{m})$ .<sup>10</sup> Now consider a Markov chain that has run for  $M$  Monte Carlo steps,  $M \gg m$ . For this process, it will be true that

$$\rho(M+m) = \rho(M) + O(m/M) \cong \rho(M) \quad (10)$$

Thus, the transition matrix  $A[\rho(M)]$  will be roughly constant during this time interval, since the density itself is not changing much, and assuming the transition matrix depends smoothly on the density. The distribution of new states during this time period will converge to

$$\begin{aligned} \text{Prob}[\mathbf{x}(M+m)] &= A[\rho(M+m-1)]A[\rho(M+m-2)] \dots \\ &\quad A[\rho(M)]\rho(M) \\ &= A[\rho(M)]^m \rho(M) + O(m^2/M) \\ &= \rho^*[\rho(M)] + O(r^m, m^2/M) \end{aligned} \quad (11)$$

Here  $r < 1$  is the second largest generalized eigenvalue of  $A[\rho(M)]$ .<sup>11</sup> The probability distribution is driven to the limiting distribution of the transition matrix for large  $m$ :  $\text{Prob}[\mathbf{x}(M+m)] \rightarrow \rho^*[\rho(M)]$ . By the Frobenius–Perron theorem,<sup>11</sup> this limiting distribution depends on the measured density, but not on the state at  $M$ :  $\rho^* = \lim_{m \rightarrow \infty} A^m[\rho(M)]\rho(M) = \lim_{m \rightarrow \infty} A^m[\rho(M)]\rho$  for any  $\rho$ . By the central limit theorem of Markov processes,<sup>10</sup> any likely instance of this probability distribution will be accurate to  $O(1/\sqrt{m})$ . Thus, the contribution of these  $m$  steps to the history-dependent density is

$$\begin{aligned} \rho(M+m) &= \frac{M}{M+m} \rho(M) + \frac{m}{M+m} \rho^*[\rho(M)] + \\ &\quad \frac{m}{M+m} O\left(\frac{m^2}{M}, r^m, 1/\sqrt{m}\right) \end{aligned} \quad (12)$$

Since we consider the limit of  $1 \ll m^2 \ll M$ , we may drop the error terms. We let  $u = m/(M+m)$ . Then by the contraction mapping theorem on compact spaces<sup>12</sup> there will be a fixed point to eq 12 if there is a metric,  $D$ , such that

$$D[(1-u)\rho_1 + u\rho^*[\rho_1], (1-u)\rho_2 + u\rho^*[\rho_2]] \quad (13)$$

is initially decreasing as  $u$  increases from 0, for any arbitrary  $\rho_1$  and  $\rho_2$ . If this condition is satisfied, the fixed point exists and is unique for our finite, discrete system.<sup>12</sup> We note that if the following is satisfied for arbitrary  $\rho_1$  and  $\rho_2$ , then eq 13 is automatically satisfied for small  $u$ :

$$D[\rho^*[\rho_1], \rho^*[\rho_2]] < D[\rho_1, \rho_2] \quad (14)$$

Alternatively, we can consider the uniqueness and existence of the mapping  $\rho_{n+1} = \rho^*[\rho_n]$  for arbitrary  $\rho_0$ .

## 3. Application to Adaptive Monte Carlo

The general condition, eq 13, seems difficult to check for an arbitrary functional dependence on the measured density,  $\rho^*[\rho]$ .

We, thus, specialize consideration to the adaptive integration method. We rewrite eq 12 as

$$\rho(t + \Delta t) = \left(1 - \frac{\Delta t}{t}\right)\rho + \frac{\Delta t}{t}\rho^*[\rho(t)] \quad (15)$$

where  $\Delta t = m$ . Assuming that this difference equation is well-approximated by a differential equation, we find

$$\frac{d\rho}{dt}\Delta t = -\frac{\Delta t\rho}{t} + \frac{\Delta t}{t}\rho^*[\rho] \quad (16)$$

$$\frac{d\rho}{dt} = \frac{1}{t}(\rho^*[\rho] - \rho) \quad (17)$$

$$\frac{d\rho}{d(\ln t)} = \rho^*[\rho] - \rho \quad (18)$$

Letting  $\alpha = \ln t$

$$\frac{d\rho}{d\alpha} = \rho^*[\rho] - \rho \quad (19)$$

We note that for  $\rho < \rho^*$ ,  $\rho$  increases, whereas for  $\rho > \rho^*$ ,  $\rho$  decreases. Therefore,  $\rho = \rho^*$  informally appears to be a stable fixed point.

We now consider more carefully the function  $\rho^*[\rho]$ . Letting  $t \gg M$ , we find

$$\rho(t) = \frac{M}{t}(\text{arbitrary initial } \rho) + \left(1 - \frac{M}{t}\right) \sum_{i=M/m}^{t/m} \frac{\rho_i}{(t - M)/m} \quad (20)$$

where the density at time  $t = i\Delta t$ ,  $\rho_i = \rho^*_i = e^{-\beta U/P_i(\lambda)}$ , is correct for a given  $\lambda$ ,  $\rho_i(\mathbf{x})/\rho_i(\mathbf{y}) = e^{-\beta U(\mathbf{x}) + \beta U(\mathbf{y})}$ , but for which  $P_i(\lambda)$  has not converged to eq 1. This result for the ratio of the density follows from eqs 6–8. Thus, for a given  $\lambda$ ,

$$\rho(t)(\mathbf{x}) = (\text{const})\exp^{-\beta U(\mathbf{x})} + O\left(\frac{M}{t}\right) \quad (21)$$

Equations 6–8 in the limit  $1 \ll m^2 \ll M \ll t$  thus imply that  $\hat{F}$  and  $\rho$  are becoming exact:

$$\begin{aligned} \rho^*[\rho] &= \rho^* + \frac{\delta\rho^*}{\delta\rho}\delta\rho \\ &= \rho^* + O(M/t) \end{aligned} \quad (22)$$

Thus, eq 19 becomes

$$\begin{aligned} \frac{d\rho}{d\alpha} &= \rho^*[\rho^* + \delta\rho] - \rho + O(M/t, m^2/t, r^m, 1/\sqrt{m}) \\ &= \rho^* - \rho + O(Me^{-\alpha}, m^2e^{-\alpha}, r^m, 1/\sqrt{m}) \end{aligned} \quad (23)$$

where we have reinserted the additional error terms from eq 12. Thus

$$\rho \rightarrow \rho^* + O(Me^{-\alpha}, m^2e^{-\alpha}, r^m, 1/\sqrt{m}) \quad (24)$$

exponentially fast in  $\alpha$ . Thus, in the limit  $1 \ll m^2 \ll M \ll t$ , we find

$$\rho(t) \rightarrow \rho^* + O(M/t, m^2/t, r^m, 1/\sqrt{m}, 1/t) \quad (25)$$

as  $t \rightarrow \infty$ , where the errors in eq 25 are respectively from the error on  $\hat{F}$ , the change of the density during  $\Delta t$ , the Monte Carlo

convergence for a given  $\hat{F}$ , the stochastic convergence of the density to the distribution, and the convergence of the differential equation.

#### 4. Discussion

Our analysis of the convergence of the adaptive integration Monte Carlo scheme gives insight into why the convergence of the method is so rapid. That is, the adaptive method converges as fast as the underlying Monte Carlo method converges for density distributions with a given value of  $\lambda$ . Once these estimates have converged, then the sampling over different values of  $\lambda$  is typically exponentially accelerated by the importance sampling bias introduced by the  $P(\lambda)$  factors in eq 6, so that a simple random walk in the  $\lambda$  order parameter may be achieved without any barriers to sampling. Thus, if the most significant barriers in the problem are fully captured by the  $\lambda$  order parameter, then the adaptive integration dramatically speeds up the convergence of the underlying Monte Carlo algorithm. In the context of the above analysis, an improved importance sampling estimate dramatically reduces the number of steps,  $m$ , that it takes to reach equilibrium for a given value of  $\lambda$ .

In the above analysis, full convergence was shown. That is, convergence of both the density distribution for a given value of  $\lambda$  and the distribution of  $\lambda$  was shown. Since adaptive integration Monte Carlo is a form of iteration, we see the linear convergence, as  $O(1/t)$ , in eq 25. In the analysis of the Monte Carlo data, we will remove the bias introduced by the  $P(\lambda)$ . That is, we will adjust the observed densities, scaling out the  $P(\lambda)$  dependence by histogram reweighting. Incidentally, we note from eq 20, that when reweighting the histograms, one should use the average of the calculated importance sampling factors,  $\langle 1/P_i(\lambda) \rangle$ , rather than the instantaneous importance sampling factor,  $1/P_i(\lambda)$ . Such a reweighting procedure implies by eqs 6 and 7 that once the simulated density has converged within a given value of  $\lambda$  (in  $O(m)$  steps), the reweighted density has also converged for all  $\lambda$ . So, the slow linear convergence observed in eq 25 is actually not a great concern. Conversely, our major algorithmic interest is in the exponential reduction of the sampling time,  $m$ , within a given value of  $\lambda$ , which is already induced by an only roughly converged importance sampling bias,  $P(\lambda)$ .

In conclusion, detailed balance, or balance,<sup>7</sup> need not be satisfied at all times in a Monte Carlo simulation. Balance need only be satisfied asymptotically. Indeed, the desire to maintain balance comes only from the Markov chain theory that shows such an approach converges to a unique limiting distribution. Any Monte Carlo method that converges to the specified unique limiting distribution will be equally valid. Given the success of the adaptive Monte Carlo methods, it would appear that the importance of detailed balance is overrated.

**Acknowledgment.** The authors thank David J. Aldous for pointing out the relevance of the contraction condition, eq 13. This work was supported by the U.S. Department of Energy Office of Basic Energy Sciences.

#### References and Notes

- (1) Mezei, M. *J. Comput. Phys.* **1987**, *68*, 237–248.
- (2) Smith, G. R.; Bruce, A. D. *J. Phys. A* **1995**, *28*, 6623–6643.
- (3) Engkvist, O.; Karlstrom, G. *Chem. Phys.* **1996**, *213*, 63–76.
- (4) Wang, F.; Landau, D. P. *Phys. Rev. Lett.* **2001**, *86*, 2050–2053.
- (5) Wang, J. S.; Swendsen, R. H. *J. Stat. Phys.* **2002**, *106*, 245–285.

- (6) Fasnacht, M.; Swendsen, R. H.; Rosenberg, J. M. *Phys. Rev. E* **2004**, 69, 056704.
- (7) Manousiouthakis, V. I.; Deem, M. W. *J. Chem. Phys.* **1999**, 110, 2753–2756.
- (8) Harris, T. E. *Pacific J. Math.* **1955**, 5, 707–724.
- (9) Fernández, R.; Maillard, G. *Electron. J. Probab.* **2004**, 9, 145–176.
- (10) Norris, J. R. *Markov Chains*; Cambridge University Press: New York, 1997. Convergence in every possible state may require m much larger than the total number of states.
- (11) Gantmacher, F. R. *Matrix Theory*; volume 1 Chelsea: New York, 1959.
- (12) Lax, P. D. *Functional Analysis*; John Wiley & Sons: New York, 2002.