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Note on Monte Carlo Methods Without Necessary Detailed Balance

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Simple criteria for convergence of Monte Carlo algorithms not necessarily requiring detailed balance for any specified transition probability are derived and it is shown that it is possible to view the algorithm as a superimposition of a Brownian motion on configurational space coupled to the transition probabilities. As such, the error contributions due to a particular Monte Carlo algorithm and the integration limits in configuration space must be distinguished from those due to the nonuniform sampling of the Brownian motion, and criteria related to the number of steps required to distinguish these errors are provided for the simplest cases involving one dimension and symmetrical probability distributions.

KEY WORDS: Monte Carlo methods; detail balance.

The normal Monte Carlo (MC) procedures use the pivotal condition of detail balance[1,2] coupled with linear master equations with a normalized probability of states that appear to incorporate a type of random walk within the transition probabilities,[1] although the algorithm can call points randomly in configurational space. In the M(RT)^2 procedure[1,2] the transition probabilities are written in standard notation[1] as

$$\left.\begin{aligned} P_{jk} &= A_{jk}, \qquad U_k \leqslant U_j \\ &= A_{jk} \exp[-(U_k - U_j)/kT]; \qquad U_k > U_j \end{aligned}\right\} \quad k \neq j \tag{1}$$

with

$$P_{jj} = 1 - \sum_{k \neq j} P_{jk} \tag{2}$$

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where (2) is the defined normalization condition, A_{jk} is the space factor defined as $A_{jk} = 1/8N\delta^3$ for all j, k during the perturbation of coordinates, $|x_j - x_k| < \delta$, and $A_{jk} = 0$ otherwise[1]; δ is the 'grid size' of the configuration space and thus the algorithm does not preclude a uniform calling of any point in configuration space which is then represented by the weight given by the above transition probabilities. Usually, however, the points are picked beforehand[3] in a defined δ neighborhood of the previous points, so it is not so clear what the equivalence of this method is to that where the transition probabilities incorporate the above space factor,[1] but where the points are randomly chosen, as assumed in the theory. Here we suggest an equivalence based on the random walk. Ergodicity is supposed to prevail to ensure a stationary distribution in the limit of large numbers.[1] Practically all routine Monte Carlo runs are based on the prevailing condition of detailed balance,[2] but recently there have appeared suggestions[4] that some systems (e.g., spin system phase transitions) do not exhibit detailed balance, but where, under appropriate conditions, the cited algorithms for statistical simulations may still be utilized. To extend the method to cases where detailed balance and normalization may or may not be directly applicable requires simple and general criteria which are provided here. For a system uniformly sampled by an algorithm in configuration space Ω which specifies transition probabilities P_{ij} such that the number of times a state is visited is proportional to the probability density,[5] consider the case when the configuration space Ω is divided into a countable set of states represented by grids of arbitrary size dx, and which has probability P_i of occupying state i [where in the continuous case $P_i \sim f(x_i)\, dx$, with f the probability density]. For N states, the probability of choosing state j from i is $P_{rc}(i, j) \sim 1/N$. Hence the number of times any state j is called from i in the entire run of the algorithm is approximately constant, $\sim n_{\text{trans}}$. Since the MC method is concerned only with relative probability weights, we get

$$P_j/P_i \approx n_{\text{trans}} \sum_{i \neq j} [P_{ij} + (1 - P_{ji})]/n_{\text{trans}} \sum_{q \neq i} [P_{qi} + (1 - P_{iq})]$$

or (3)

$$P_j/P_i = \lim_{N \to \infty} \left(\sum_{i \neq j}^{N} [P_{ij} + (1 - P_{ji})] \Big/ \sum_{q \neq i}^{N} [P_{qi} + (1 - P_{iq})] \right)$$

Furthermore, since the number of systems is conserved, we must also have for $N \to \infty$, for all indices q, r,

$$\lim_{N \to \infty} \left(\sum_{j=1}^{N} P_{qj} \Big/ \sum_{j=1}^{N} P_{rj} \right) = 1 \tag{4}$$

Conditions (3) and (4) taken together ensure the workability of any MC algorithm with the defined transition probabilities not necessarily exhibiting detailed balance. It can be shown that the typical MC transition probabilities obeying detailed balance (including $P_{ij}=P_j$, where the detailed balance condition $P_iP_{ij}=P_jP_{ji}$ is fulfilled trivially as $P_jP_i=P_jP_i$) fulfills both (3) and (4). Regarding the superimposition of a random walk in configuration space with the specified MC transition probabilities, the description below is for one dimension using symmetrical probability distributions throughout, but which can be generalized in some cases to higher orders. In practice, multidimensional spaces which do not possess symmetry in the occupation of states and which require integration to infinite limits are often explored, so that personal experience, familiarity, trial and error, and comparision with other techniques and experiment are the usual criteria for confidence in MC methods, rather than reliance on mathematical formulas for specifying convergence. However, a rough indication of the minimum number of steps N to achieve an approximately uniform sampling of Ω even for simple symmetrical functions of configurational space occupancy is useful. If a number below the minimum number of steps leads to values deemed to be those for converged results, then one can argue that the coincidence is fortuituous, and did not arise from the uniform sampling of the configuration space, but from the combined effects of nonuniform sampling coupled with the probability distribution used to compute the transition probabilities.

For a general MC method with the background configuration space chosen not randomly but via a random walk with mean step size Δx, then if Δx is "small", the probability distribution of the random walk particle coordinate approximates the (Brownian motion) Gaussian function with variance $\sigma^2=(\Delta x)^2 t$, where t is the length of the run N.[6] As a rough measure, we suppose that over ~ 1 standard deviation of the random walk σ, the configuration space is uniform (for refinement, a smaller interval may be chosen and the subsequent equation modified by substituting $q\sigma$ for σ, where $q<1$). If the actual probability density is $P_{ac}(x)$, and if the actual points x are chosen with frequency weighted according to P_{ac}, then standard theory[5] gives

$$\bar{A}=\int_{-\infty}^{\infty} A(x)\,P_{ac}(x)\,dx \approx \left[\sum_{i=1}^{N} A(x_i)\right]\Big/N$$

and the accuracy of the integral can be estimated. Assume P_{ac} is symmetrically distributed about an origin with standard deviation σ_d and that $A(x)$ is bounded, where $\int_{-n\sigma_d}^{n\sigma_d} P_{ac}(x)\,dx=\delta$ (and $\delta\sim 1$, n being an integer which must be specified). Since it is not possible to sample to infinite limits, the

value of the integral is relative to the specified limits $\pm n\sigma_d$. Denote the states covered by the range (approximately $\pm n\sigma_d$) as $\{i, j, k, ..., n\}$. Then to first order, where the primed quantities are the apparent probabilities of the states generated by the approximately "uniformly" distributed random walk x values over approximately $\pm 1\sigma$,

$$P'_i : P'_j : P'_k \cdots P'_m \cdots \sim P_i : P_j : \cdots P_m \cdots$$

and $P'_j \neq P_j$ in general for the same j state (σ is the standard deviation of the random walk distribution). Hence, following this approximation,

$$\int_\Omega P'(x)\, dx = k \int_{-n\sigma_d}^{n\sigma_d} P_{ac}\, dx = 1 \qquad (k \geqslant 1) \tag{5}$$

where $P'(x)$ is any arbitrary distribution which approximates the P'_j states. Let $\varepsilon = \{\max |A(x)|, |x| \geqslant n\sigma_d\}$, $\sqrt{N} = n\sigma_d/\Delta x = L$, and $k\delta = 1$ [from (5)]. Since $n\sigma_d = \Delta x \sqrt{N}$, for $\varepsilon(1-\delta) \ll 1$, a heuristic criterion for the error % P in the integral $\bar{A}$ is given for large enough N (as $N \to \infty$) by

$$\begin{aligned} P &\sim 100\varepsilon(1-\delta) N \Big/ \left[\sum_{i=1}^{N} A(x_i) \right] \\ &= 100\varepsilon(k-1)\, L^2 \Big/ \left[k \sum_{i=1}^{L^2} A(x) \right] \end{aligned} \tag{6}$$

Thus Δx and N may be chosen to reduce the error by an arbitrary amount. We emphasize that (6) represents the estimate of the absolute error of the integral, due to the truncation of the limits at $\pm n\sigma_d$ of the integral, which must be distinguished from the MC error due to fluctuations. The latter are normally computed by dividing the number of moves into intervals and calculating the desired quantity $\bar{A}$ for each of the intervals; one derives a measure for the error of $\bar{A}$ from the different $\bar{A}$ values from these intervals.

Regarding an estimate of the minimal run number N_t to achieve a uniform sampling of the configuration space, we observe that this occurs when $\sigma = n\sigma_d$ and $N = N_t$, where

$$N_t \sim (n\sigma_d/\Delta x)^2 \tag{7}$$

For values of $N \gg N_t$, the errors in the integral will be due to the particular characteristics of the MC method and the limits of Ω space, and are not due to the distortion of the configuration space due to the random walk. Lastly, the equivalence of the above, where the points in configuration space are chosen with fixed step size in each step, to the method

described by (1) and (2), where the points in configuration space are chosen randomly, comes from noting that the probability of moving in the space with limits $\pm L$ is $\delta/2L$ with mean step size $\delta/2$. The mean number of steps before a move is $2L/\delta$, and so the effective step variable is $N' = N\delta/2L$. For $L = n\sigma_d$, the minimal number of N_t steps required for uniform sampling is

$$N_t \sim 8(n\sigma_d)^2/\delta^3 \tag{8}$$

and any value of $N \gg N_t$ will ensure that the errors are largely attributable to the MC rate of convergence and the limits rather than nonuniformity of sampling Ω space.

The conclusion of this note is that it is possible to provide simple criteria for the convergence of MC algorithms without necessary detailed balance and the errors involved if a nonuniform random walk is superimposed on the configuration space without immediate recourse to Markov chains and linear master equations.

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REFERENCES

1. W. W. Wood and F. R. Barker, *J. Chem. Phys.* **27**(3), 720 (1957).
2. M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods, Vol. I: Basics* (Wiley, New York, 1986), esp. Section 3.7, p. 73.
3. A. A. Barker, *Aust. J. Phys.* **18**:119 (1964).
4. M. Katori and N. Konno, *J. Magn. Magn. Mat.* **104–107**(1):267 (1992).
5. D. W. Heermann, *Computer Simulation Methods in Theoretical Physics* (Springer-Verlag, Berlin, 1986), esp. Eqs. (4.28) and (4.35).
6. Y. A. Razanov, *Probability Theory: A Concise Course* (Dover, New York, 1969), p. 64.