Fluctuations in lattice Monte Carlo simulations

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Consider a quantum-mechanical lattice theory at finite temperature and fixed volume. We show that for the energy the standard deviation of the energy (or energy-density) estimator (in the "primitive algorithm") grows as the number of sites in the system. An estimator based on the virial theorem is proposed which is well behaved.

The Monte Carlo algorithm[1-3] has become an important method for computer simulations. In the particle-physics sphere, these techniques are often used to probe lattice gauge theories, particularly their phase structure[4-8] and mass content.[6,7,9,10]

The expectation value of an order parameter is often sought to signal a symmetry breakdown or a change in phase. However, one is also interested in bulk thermodynamic properties, like the expectation value of the energy, the specific heat, and the susceptibility; these cannot be determined from the decay of correlation functions. Such properties have been explored in computer simulation of free field theories[11] and SU(2)[12-17] and SU(3)[14,17-23] lattice gauge theories.

One *might* expect that increasing the number of lattice sites (thereby decreasing the lattice spacing) at fixed volume would increase the accuracy of the simulation by reducing the statistical error in the quantities averaged. We consider a quantum lattice theory (the Klein-Gordon model) at positive temperature and fixed volume. For (momentum-dependent) thermodynamic quantities like the energy or the energy density, in the "primitive algorithm," the error (standard deviation divided by the square root of the number of statistically independent passes averaged minus one) grows as the square root of (number of sites in the system)/(number of passes). Although the system might seem to settle in on an average value for the energy (density), the fluctuations in that value may be severe enough to render it inaccurate. This would then necessitate long running times. In some of the latent-heat and energy-density studies there are found increasing error bars and worsening of the base values as the number of sites along the time axis increases. We offer then one possible explanation and indicate a problem which will eventually occur, in any event, for sufficiently large lattices. An energy estimator based on the virial theorem is offered which is shown to be well behaved.[24]

Consider a system with Hamiltonian H at inverse temperature β. The partition function

$$Z=\mathrm{Tr}\exp(-\beta H) \tag{1}$$

has an associated position-space density matrix

$$\rho(\phi(x),\phi(y);\beta/N_t)=\langle\phi(x)|\exp(-\beta H/N_t)|\phi(y)\rangle \tag{2}$$

where the lattice time axis has been divided into N_t intervals with spacing $\epsilon=\beta/N_t$ and where locality of the interaction forces $\rho=0$ for x and y sufficiently separated; the fields in the theory are generically indicated by ϕ. The partition function can be written as

$$Z=\int[d\phi]\prod_{x,y}\rho(\phi(x),\phi(y);\beta/N_t) \tag{3}$$

with the product over interacting points x,y in space-time (similarly for fields living on links). Since the expectation value of the energy is given by

$$\langle E\rangle=-\frac{\partial}{\partial\beta}\ln Z\ , \tag{4}$$

an estimator for the energy in field configuration $\{\phi\}$ is

$$\varepsilon(\{\phi\})=-\sum_{x,y}\frac{\partial}{\partial\beta}\ln\rho(\phi(x),\phi(y);\beta/N_t)\ . \tag{5}$$

We call this the primitive algorithm.

Proceeding to a Monte Carlo simulation, one samples configurations of the fields weighted by the probability $\exp(-\beta H)$ (after equilibration), determines $\varepsilon(i)$ for a statistically independent pass i through the lattice, and gets an average by dividing by the total number, M, of such configurations averaged:

$$\langle E\rangle=\frac{1}{M}\sum_{i=1}^{M}\varepsilon(i)\ . \tag{6}$$

The fluctuations in this quantity are given by the standard deviation

$$\sigma=\langle\delta\varepsilon^2\rangle^{1/2}=\left[\frac{1}{M}\sum_{i=1}^{M}[\varepsilon^2(i)-\langle E\rangle^2]\right]^{1/2} \tag{7}$$

with error

$$\delta(E)=\sigma/(M-1)^{1/2}\ . \tag{8}$$

For a simple case (at fixed volume) we will compute $\delta(E)$ and show it goes as $(n/M)^{1/2}$, where n is the number of sites in the lattice, so that increasing the number of lattice points requires a proportional increase in the number of passes through the lattice to maintain the same error. Subsequently, another estimator is proposed which does not suffer from this problem.

Note that the specific heat

$$C=\beta^2\frac{\partial^2\ln Z}{\partial\beta^2}\neq\beta^2\langle\delta\varepsilon^2\rangle \tag{9}$$

does *not* diverge with N_t. Substitution of (3) in (9) gives an estimator for C different from the fluctuations in the energy estimator, hence the inequality in Eq. (9). However, the estimator for C also has error bars which grow as $n^{1/2}$.

Consider the Klein-Gordon theory on a hypercubical lattice. The Hamiltonian density is

$$\mathscr{H}=\tfrac{1}{2}(\pi^2+|\vec{\nabla}\phi|^2+m^2\phi^2)\,, \tag{10}$$

so that (in the short-time approximation)

$$Z=\int[d\pi][d\phi]\exp\left[a^3\epsilon\left\{\sum_t\sum_{\vec{x}} i\pi(\vec{x},t)\frac{\phi(\vec{x},t+\varepsilon)-\phi(\vec{x},t)}{\varepsilon}-\frac{1}{2}\left[\pi^2+\sum_{l=1}^{3}\left[\frac{\phi(\vec{x}+a\hat{l},t)-\phi(\vec{x},t)}{a}\right]^2+m^2\phi^2\right]\right\}\right], \tag{11}$$

where a is the spatial lattice spacing and $N_S a=L$ for L the length of a spatial edge; $n=N_S{}^3N_t$. The integral is taken with $\phi(\vec{x},\beta)=\phi(\vec{x},0)$ because the field is bosonic. Doing the momentum integration yields

$$Z=\left[\frac{N_t}{\beta a^3}\right]^{n/2}\int[d\phi]\exp\left[-\tfrac{1}{2}\sum_t\sum_{\vec{x}}\left[a^3\frac{N_t}{\beta}(\Delta_t\phi)^2+a\frac{\beta}{N_t}\sum_l(\Delta_l\phi)^2+a^3\frac{\beta}{N_t}m^2\phi^2\right]\right], \tag{12}$$

where $\Delta_\mu\phi(x)=\phi(x+\eta\hat{\mu})-\phi(x)$ with $\eta=\epsilon$ if $\mu=4$ and $\eta=a$ for $\mu=1,2,3$. The appearance of the β-dependent prefactor is crucial; this normalization constant cannot be avoided in a finite-temperature analysis.[25] Next, Fourier transform in three-space (we tacitly rescale the fields):

$$Z=\prod_{\vec{k}}\left[\frac{N_t}{\beta a^3}\right]^{N_t/2}\int[d\phi]\exp\left\{-\tfrac{1}{2}\sum_t\left[\frac{N_t}{\beta a^3}(\Delta_t\phi)^2+\frac{\beta}{a^3N_t}\left[\frac{G_1(\vec{k})}{a^2}+m^2\right]\phi(\vec{k},t)\phi(-\vec{k},t)\right]\right\}, \tag{13}$$

where

$$G_h(\vec{k})=2h^2\sum_{l=1}^{3}(1-\cos ak_l)\,, \tag{14}$$

$$\sum_{\vec{k}}\equiv\sum_{k_1}\sum_{k_2}\sum_{k_3}\,,\quad k_i=2\pi p/aN_s,\quad p=0,1,\ldots,N_s-1\,. \tag{15}$$

The energy estimator, Eq. (5), is

$$\varepsilon=\frac{n}{2\beta}-\gamma\,, \tag{16}$$

where

$$\gamma=\alpha-\lambda\,, \tag{17}$$

$$\alpha=\frac{N_t}{2\beta^2a^3}\sum_{\vec{k}}\sum_t(\Delta_t\phi)^2\,, \tag{18}$$

$$\lambda=\frac{1}{2a^3N_t}\sum_{\vec{k}}\sum_t\left[\frac{G_1(\vec{k})}{a^2}+m^2\right]\phi^2 \equiv\sum_{\vec{k}}\sum_t V(\phi(\vec{k},t))\,. \tag{19}$$

We wish to examine the behavior of the expectation values of these quantities and their fluctuations. The integration in time can be done exactly, so we may write the partition function as[3,26,27]

$$\ln Z(\beta,m,h,a)=\sum_{\vec{k}}\ln\frac{f^{N_t/2}}{f^{N_t}-1}\,, \tag{20}$$

where

$$f=1+\tfrac{1}{2}R^2+\tfrac{1}{2}R(4+R^2)^{1/2}\,, \tag{21}$$

$$R=\frac{\beta}{N_t}\left[\frac{G_h(\vec{k})}{a^2}+m^2\right]^{1/2}. \tag{22}$$

As an example, we determine $\langle\gamma\rangle$ and $\langle\delta\gamma^2\rangle$. Define the characteristic function of the distribution function of γ:[28]

$$P(s)=\langle\exp(-s\delta)\rangle\,. \tag{23}$$

Using Eq. (13) allows us to express $P(s)$ in terms of the partition function with rescaled parameters:

$$P(s)=\left[\frac{\beta}{\beta+s}\right]^{n/2}Z\left[\beta,\left[\frac{\beta-s}{\beta+s}\right]^{1/2}m,\left[\frac{\beta-s}{\beta+s}\right]^{1/2}h,\left[\frac{\beta}{\beta+s}\right]^{1/3}a\right]. \tag{24}$$

Now we have

$$\langle\gamma\rangle=\left.\frac{-\partial\ln P}{\partial s}\right|_{\substack{s=0\\h=1}}=\frac{n}{2\beta}-\langle E\rangle\,, \tag{25}$$

$$\langle\delta\gamma^2\rangle=\left.\frac{\partial^2\ln P}{\partial s^2}\right|_{\substack{s=0\\h=1}}=\frac{n}{2\beta^2}+\langle\delta E^2\rangle-\frac{\langle E\rangle}{\beta}\,, \tag{26}$$

where the exact expectation values of the energies, as the

Monte Carlo simulation would sample, are found from (20) and

$$\langle E\rangle = -\frac{\partial}{\partial\beta}\ln Z(\beta,m,1,a)\ , \tag{27}$$

$$\langle \delta E^2\rangle = T^2C = \frac{\partial^2}{\partial\beta^2}\ln Z(\beta,m,1,a)\ . \tag{28}$$

Similarly, one may obtain

$$\langle\alpha\rangle = \frac{n}{2\beta} - \tfrac{1}{2}\langle E\rangle\ , \tag{29}$$

$$\langle\delta\alpha^2\rangle = \frac{n}{2\beta^2} + \tfrac{1}{4}\langle\delta E^2\rangle - \frac{3}{4}\frac{\langle E\rangle}{\beta}\ , \tag{30}$$

$$\langle\lambda\rangle = \tfrac{1}{2}\langle E\rangle\ , \tag{31}$$

$$\langle\delta\lambda^2\rangle = \tfrac{1}{4}\langle E^2\rangle + \frac{1}{4}\frac{\langle E\rangle}{\beta}\ . \tag{32}$$

Since (16) gives $\langle\delta\varepsilon^2\rangle = \langle\delta\gamma^2\rangle$, the fluctuations in the energy estimator are given by (26). These are the *same* fluctuations as for γ, the energy *without* the $n/2\beta$ addend ($n = N_S{}^3N_t$). $\langle\delta E^2\rangle$ (the specific heat) and $\langle E\rangle$ are independent of n for $n\to\infty$,[28] so that the error in the energy estimator (as for the kinetic energy $\varepsilon-\lambda$) grows as $(n/M)^{1/2}$. This is an estimator that becomes less reliable as the number of lattice sites is increased. Making use of the virial theorem allows us to write down an energy estimator whose error goes as $1/M^{1/2}$:

Consider [see (19)]

$$\varepsilon^v \equiv \sum_{\vec{k}}\sum_{t}\left[V(\phi(\vec{k},t)) + \tfrac{1}{2}\phi(\vec{k},t)\frac{\partial V}{\partial\phi}\right]\ . \tag{33}$$

We show that this is a well-behaved energy estimator.[28] Let $U=\alpha+\lambda$ so that

$$Z = \left[\frac{N_t}{\beta a^3}\right]^{n/2}\int[d\phi]\exp(-\beta U)\ . \tag{34}$$

By performing an integration by parts, one easily finds

$$\left\langle\sum_{\vec{k},t}\phi\frac{\partial U}{\partial\phi}\right\rangle = \left\langle\sum\phi\frac{\partial\alpha}{\partial\phi}\right\rangle + \left\langle\sum\phi\frac{\partial\lambda}{\partial\phi}\right\rangle = \frac{n}{\beta}\ . \tag{35}$$

Using Euler's theorem, the first term in (35) is $\langle 2\alpha\rangle$, so

$$\left\langle\frac{n}{2\beta}-\alpha\right\rangle = \left\langle\tfrac{1}{2}\sum_{\vec{k},t}\phi\frac{\partial V}{\partial\phi}\right\rangle\ . \tag{36}$$

With (16) and (17), we see $\langle\varepsilon\rangle = \langle\varepsilon^v\rangle$ so that ε^v is an energy estimator. In our example $\varepsilon^v = 2\lambda$; but, by (32), $\langle\delta\lambda^2\rangle$ is well behaved.[29] Similarly, a good estimator for the kinetic energy is

$$k^v = \tfrac{1}{2}\sum\phi\frac{\partial v}{\partial\phi}\ . \tag{37}$$

Monte Carlo simulations were carried out in Ref. 28 for the $(0+1)$-dimensional theory (harmonic oscillator), and agreement with the fluctuations predicted here was obtained.

We have indicated here a possible explanation for fluctuations in the energy and other thermodynamic quantities which increase with the number of lattice sites (at fixed volume). There are other effects which may have been dominant[30] in studies done so far. However, the effect we describe here cannot be avoided for sufficiently large lattices.

In conclusion, the primitive algorithm gives fluctuations in the energy (or energy density) with the error growing as the number of sites in the system. In the virial estimator, the error is independent of this as the sites increase in number.

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[29]While this may be a possible solution, G. Jaccuci (report and private communication) has pointed out that the virial estimator may lead to increased correlation times.

[30]It is unclear if the effect we are discussing here is dominant yet because running times may have varied with the different lattice sizes. In the case where hopping-parameter expansions were used, more terms are needed as N_t increases. And, for a finite-temperature simulation, one ideally has $N_S \gg N_t$.