An improvement to the linear accept/reject algorithm

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We study the improvement of Kennedy-Kuti’s linear accept/reject algorithm with different ordering criterion and modified Bhanot-Kennedy estimator of $e^{\Delta H}$ to reduce probability-bound violation. A new stochastic Monte Carlo algorithm to accommodate the probability-bound violation is proposed.

1. Introduction

Sometime ago, Kennedy and Kuti\cite{1} proposed a Monte Carlo algorithm which admits stochastically estimated transition probabilities as long as they are unbiased. This opens up the door to solving problems where it is feasible to estimate the transition probabilities but intractable or impractical to calculate them exactly.

The acceptance probability (denoted as $P_a$ from now on) in Kennedy-Kuti’s linear algorithm is

$$P_a(U_1 \rightarrow U_2) = \lambda^+ + \lambda^- e^{\Delta H}$$

if $f(U_1) > f(U_2)$, \hfill (1)

$$P_a(U_1 \rightarrow U_2) = \lambda^- + \lambda^+ e^{\Delta H}$$

if $f(U_1) \leq f(U_2)$, \hfill (2)

where $\lambda^\pm$ are tunable real parameters ranging from 0 to 1, $\hat{r}$ denotes an unbiased estimate of $r$ and $\Delta H = H(U_1) - H(U_2)$. $U_1$ denotes the old configuration and $U_2$ the new (or proposed) configuration. $f(U)$ is some observable of the gauge configuration $U$ adopted for ordering between $U_1$ and $U_2$. Detailed balance can be proven to be satisfied.

But there is a major problem with the linear algorithm. The value of $P_a$ can violate the probability bound $[0,1]$ since it is estimated stochastically. Once the probability bound restriction is not respected, detailed balance is destroyed and systematic bias will show up. Hopefully, if the bound violation occurs very rarely (e.g. once every one million times), then the systematic bias might be very small and the expectation values of various quantities can still be correct within statistical errors\cite{1}.

Within the framework of the linear algorithm, there are at least three ways to reduce the probability of bound violations:

(1) In general, the two tunable parameters $\lambda^\pm$ can be parameterized as

$$\lambda^+ = 0.0, \quad \lambda^- = \frac{1}{1 + \epsilon}$$ \hfill (3)

where $0 \leq \epsilon < \infty$. So $e^{\Delta H}$ is allowed to fluctuate between 0 and $1 + \epsilon$. If we increase $\epsilon$, then the allowed range of $e^{\Delta H}$ will be larger and the probability of bound violations can be reduced (although the intrinsic acceptance rate will be reduced simultaneously).

(2) One can choose a better ordering criterion to reduce the bound violation. One can imagine that when the ordering criterion is uncorrelated with $\Delta H$, then the upper bound will be violated quite frequently (about 50% of the time for $\lambda^- = 1$). Thus, we believe the “ideal” ordering criterion is $\Delta H$ itself. However, we cannot calculate $\Delta H$ exactly (otherwise we would not need the stochastic estimator): the best we can do is to estimate $\Delta H$ stochastically (without bias). We will obtain a number (denoted as $x_0$) which can be made reasonably close to the true value of $\Delta H$, and use it as the ordering criterion. This should greatly reduce the probability of upper-bound violations.
(3) Most importantly, one can reduce the variance of the estimated acceptance probability either by brute force or by constructing a better (unbiased) stochastic estimator. This will help reduce the probability of lower-bound violations and further reduce upper-bound violations as well.

Although one can improve the performance of the linear algorithm with these techniques, there are still problems inherent to the algorithm which are impossible to eradicate. First of all, if we assume that the estimator of the acceptance probability has a Gaussian distribution (which should be a reasonable assumption), then no matter how hard we work, we will never completely exclude the bound violations since the two long tails of the Gaussian distribution always exist. Secondly, the linear algorithm with a stochastic estimator is a volume-squared algorithm. This can be easily seen by the following consideration. The variance of the estimated acceptance probability is roughly proportional to $\delta^2/N$ where $\delta^2$ is the intrinsic variance and $N$ is the number of hits. (This proportionality relation is true no matter what unbiased estimator we choose.) The intrinsic variance $\delta^2$ is proportional to the lattice size. Therefore, if we want to keep the bound violations under very tight control, we need to work harder and harder (i.e. $N$ should become larger and larger) so that the lattice size grows. So $N$ should grow as the first power of the volume $V$, and the cost will be proportional to $V^2$ since the cost of the stochastic estimator is usually proportional to $V$. In real simulations on lattice QCD with dynamical fermions, to lessen the probability bound violation in this way could be very costly.

In order to completely remove any systematic bias coming from bound violations, and to reduce the cost of simulation on larger lattices, we need to go beyond the linear algorithm and come up with some new method. In the next section, we propose a new algorithm which will achieve these goals. We will see that the new algorithm eliminates the upper bound violation and absorbs the negative sign of the lower bound violation into the observables by introducing some auxiliary fields and going back to the Metropolis accept/reject.

2. The New Algorithm

The first step toward the new algorithm is to transform the “noise” (coming from the stochastic estimator) into “auxiliary fields”, just as pseudofermion fields are introduced as auxiliary fields. Therefore, the configuration space is enlarged, and the updating and the accept/reject will be carried out in this enlarged space. To be more precise, the partition function $Z$ is

\[
Z = \int [DU] e^{-S_G(U)} e^{-S_F(U)}
\]

\[
= \int [DU] [Dp] e^{-H(U,p)} e^{-S_F(U)}
\]

\[
= \int [DU] [Dp] [D\xi] P_\xi(\xi) e^{-H(U,p)} f(U,\xi),
\]

where $U$ represents the original field (not necessarily the link variable), $p$’s are the conjugate momenta introduced in the Hybrid Monte Carlo (HMC) algorithm in case the molecular dynamics is used for updating. $H(U,p) = \frac{p^2}{2} + S_G(U)$ is the hamiltonian and $\xi$’s are the auxiliary fields “representing” the stochastic fields. $P_\xi$ is the probability distribution for $\xi$’s. The function $f(U,\xi)$ is any function which satisfies

\[
e^{-S_F(U)} = \int [D\xi] P_\xi(\xi) f(U,\xi),
\]

i.e. $f(U,\xi)$ is an unbiased estimate of $e^{-S_F(U)}$ for noise $\xi$.

This completes the first step toward the new algorithm. The space is indeed enlarged. Originally, we had a configuration space of the $U$’s. HMC enlarges the space to $(U,p)$. Now it is further enlarged to $(U,p,\xi)$ with the inclusion of the stochastic field $\xi$. This first step actually sets up the platform for performing updates in the enlarged space. So from now on, when we specify a state, we are specifying a state in this enlarged space.

One should also notice that everything is general so far. We have not written down a specific functional form for $f(U,\xi)$ yet, nor have we decided what $P_\xi$ should be. So this means the new algorithm can be applied to a general class of problems. It is not restricted to a specific type
of problem. The auxiliary fields can have arbitrary distributions (e.g. Gaussian, \( Z_2 \) etc.)

The second step of this new algorithm is to observe that
\[
f(U, \xi) = \text{sign}(f) |f(U, \xi)|. \tag{6}
\]
Therefore sign(f), which means the sign of the function f, is a state function. We then can do the following:
\[
\langle A \rangle = \int [DU][DP][D\xi] P_\xi(\xi) A(U) \text{sign}(f) e^{-H(U,p)} |f(U, \xi)|, \tag{7}
\]
where \( A \) is the quantity we want to measure.

We now reinterpret \(|f|\), which is positive definite, as part of the probability distribution. So we are measuring the quantity \( A(U)|\text{sign}(f)\) under the probability distribution \( e^{-H(U,p)} |f(U, \eta, \rho)| \) and the partition function \( Z = \langle \text{sign}(f) \rangle \). This in principle takes care of the lower-probability-bound violations. (Actually they are is replaced with a potential sign problem.) Notice that this reinterpretation is possible because the sign of \( f(U, \eta, \rho) \) is a state function. In the linear accept/reject, one calculates the transition probability directly (and stochastically). There, the transition probability is not a state function. When we obtain a minus sign there, it can not be swept into the observable as in Eq. \( \[8\] \).

The third part of the new algorithm is to go back to Metropolis to do the accept/reject. There are two accept/reject steps. The first one is to propose updating of \( U \) and \( p \) in the usual way, e.g. molecular dynamics evolution while keeping the stochastic field \( \xi \) fixed. The acceptance probability \( P_a \) is
\[
P_a(U_1, p_1, \xi_1 \rightarrow U_2, p_2, \xi_2) = 
\min \left( 1, \frac{e^{-H(U_2,p_2)} |f(U_2, \xi)|}{e^{-H(U_1,p_1)} |f(U_1, \xi)|} \right). \tag{8}
\]

The second accept/reject step refreshes the stochastic field \( \xi \) according to the probability distribution \( P_\xi(\xi) \) while keeping \( U \) and \( p \) fixed. The acceptance probability in then
\[
P_a(U, p, \xi_1 \rightarrow U, p, \xi_2) = 
\min \left( 1, \frac{|f(U, \xi_2)|}{|f(U, \xi_1)|} \right). \tag{9}
\]

Obviously, there is no probability-bound violation in either of these Metropolis accept/reject steps.

Detailed balance can be proven to be satisfied. It is obvious that all the techniques for reducing the variance of the estimator developed before can be applied here.

We have tested the new algorithm on a very simple 5-state model. (This is the same model used in \[1\] for demonstration.) We calculated the average energy with the linear algorithm and the new algorithm. Some data are presented in table 1. (The exact value is 0.180086.)

We see that as the intrinsic variance of the estimator grows, the linear algorithm introduces a systematic error (mostly due to upper-bound violations). The new algorithm, however, still gives the correct value within errors.

To apply this new algorithm to the dynamical fermion problem, we note that the fermion determinant can be calculated stochastically as a random walk process \[1\]
\[
e^{Tr \ln M} = 1 + Tr \ln M (1 + \frac{Tr \ln M}{2}) (1 + \frac{Tr \ln M}{3}) \ldots,
\]
which can in turn be written in the following integral
\[
e^{Tr \ln M} = \int \prod_{i=1}^{\infty} D\eta_i \delta(|\eta_i| - 1) \int_0^1 \prod_{n=1}^{\infty} D\rho_n [1 + \eta_i^2 \ln M \eta_1 (1 + \theta(\rho_2 - 1/2)) \eta_2^3 \ln M \eta_3 (1 + \theta(\rho_3 - 2/3)]
\]
This sequence terminates stochastically in finite time and only the seeds from the pseudo-random

| \( \delta^2 \) | Linear | New |
|---|---|---|
| 1.0 | 0.18009(14) | 0.17994(14) |
| 3.0 | 0.18127(14) | 0.17999(14) |
| 6.0 | 0.18216(14) | 0.18014(14) |
| 10.0 | 0.18257(14) | 0.18005(14) |
| 20.0 | 0.18342(14) | 0.17995(14) |
number generator need to be stored in practice. Comparing this to Eq. (2), the function $f(U, \eta, \rho)$ (the $\xi$ in Eq. (2) is represented by two stochastic fields $\eta$ and $\rho$ here) can be defined for the fermion determinant. One can then use the efficient Padé-$Z_2$ algorithm [3] to calculate $f(U, \eta, \rho)$.

While we are in the process of applying this algorithm to QCD, we have considered how efficiently the HMC with pseudofermions is as far as updating $Tr \ln M$ is concerned. To this end, we have run the HMC with pseudofermions on an $8^3 \times 18$ lattice at $\beta = 5.6$ and $\kappa = 0.154$. 40 steps are taken with step size of 0.025 in 170 molecular dynamics trajectories. We calculated the correlation between the change of $Tr \ln M$ and the change of the pseudofermion action $S_F$ along a trajectory. The latter is designed to emulate the former. We find the normalized correlation is

$$\langle \Delta Tr \ln M \Delta S_F \rangle = 0.053 \pm 0.133,$$

which is quite small. This raises a question as to how efficient the HMC with pseudofermions might be in updating the fermion determinant. Further study of the autocorrelation of $Tr \ln M$ is needed to answer this question.

3. Summary and Discussion

In summary, the new algorithm solves the problem of probability-bound violations which has been troubling the linear accept/reject algorithm. The upper-bound violation problem is solved by going back to the Metropolis accept/reject (in the enlarged space). The lower-bound violation problem is solved by grouping the sign with the observable. With the probability bound violation problem solved, we do not have to have an extremely small variance in the stochastic estimation. So, in principle, the volume-squared behaviour of the algorithm is less severe and hopefully can be put under control.

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