Comparing the $R$ algorithm and RHMC for staggered fermions

M. A. Clark, B. Joó and A. D. Kennedy
School of Physics, The University of Edinburgh, Edinburgh, EH9 3JZ, UK

The $R$ algorithm is widely used for simulating two flavours of dynamical staggered fermions. We give a simple proof that the algorithm converges to the desired probability distribution to within $O(\delta \tau^2)$ errors, but show that the relevant expansion parameter is $(\delta \tau/m)^2$, $m$ being the quark mass. The Rational Hybrid Monte Carlo (RHMC) algorithm provides an exact (i.e., has no step size errors) alternative for simulating the square root of the staggered Dirac operator. We propose using it to test the validity of the $R$ algorithm for simulations carried out with $\delta \tau \approx m$.

1. Introduction

The motivation for this work is the need to decide which lattice action to use in the future, to allow dynamical fermion simulations using as light a quark mass as possible. Recent UKQCD research has been performed using Wilson fermions, but the computational cost of producing ensembles is too great for $m_{\pi}/m_{\rho} < 0.4$. One alternative conclusion is to use two flavours of improved staggered fermions, since the cost appears to scale significantly better for small masses.

Clearly, it is important to verify that the $R$ algorithm is correct for small quark masses; this is the subject of this investigation. The other possible failings of two flavour staggered fermions will not be addressed here.

2. Deriving the $R$ Algorithm

2.1. The $\Phi$ Algorithm

We start with the probability distribution for gauge field $U$ and pseudofermion field $\Phi$,

$$ P(U, \Phi) = \frac{1}{Z} e^{-[S_W(U) + \Phi^* (\mathcal{M}^4 \mathcal{M})^{-1}] + \Phi} = e^{-S_{\text{eff}}}. $$

The staggered Dirac operator is $\mathcal{M}$ with the pseudofermion field only defined on even sites.

The $\Phi$ algorithm [1] is a Hybrid Molecular Dynamics (HMD) algorithm for 4 flavours of staggered fermions. It iterates a composite Markov step, which is ergodic and has a fixed point distribution close to the desired one. We introduce conjugate momenta $\pi$ in order to define a Hamiltonian $H$,

$$ P(U, \Phi, \pi) = \frac{1}{Z} e^{-\frac{1}{2} \pi^2 + S_{\text{eff}}} = \frac{1}{Z} e^{-H(U, \Phi, \pi)}. $$

The action $S_{\text{eff}}$ takes the role of the potential in the Hamiltonian. The gauge fields $U$ can then be allowed to evolve for a time $\tau$ by integrating Hamilton’s equations, using a Molecular Dynamics (MD) integration scheme. Each MD trajectory consists of a momentum refreshment heat-bath using Gaussian noise, a pseudofermion heat-bath using Gaussian noise, and finally an MD trajectory consisting of $\tau/\delta \tau$ steps.

Typically a $QPQ$ symmetric symplectic integrator is used, that is one which evolves $U$ by half a step, $\pi$ by a step and finally $U$ by a half step. This does not conserve energy, having $\delta H = O(\delta \tau^2)$ for any trajectory length.

For $\delta \tau > 0$, the fixed point distribution of the MD step and the momentum refreshment heat-bath do not coincide. We must find the actual equilibrium distribution of the composite of these two steps. Since we discard the new momenta and pseudofermions after each step we consider the full Markov step as an update of $U$ alone, integrating out the auxiliary fields $\pi$ and $\Phi$. Let $V(\tau)$ represent the evolution operator for the MD step $V(\tau) : (U, \pi) \mapsto (U'', \pi'')$ and $e^{-(S + \Delta S)}$ denote the fixed point distribution of the full Markov step, where $\Delta S$ measures the deviation from the desired distribution. This must satisfy

$$ e^{-[S(U'') + \Delta S(U'')] + \pi''} = \int dU d\pi e^{-H(U, \pi) - \Delta S(U)} \delta(U' - U''). $$
The coefficient of \((1 - \pi^2)\delta \tau^2\) is proportional to the variance of the estimated force and will only vanish if the force is computed exactly. Since the momentum average is not Gaussian after many leapfrog steps, the leading order term is not cancelled as it would be if we only did one MD step per trajectory. Thus over an entire trajectory \(\delta H \sim O(\delta \tau)\) and the leading error of \(R_0\) is \(\Delta S \sim O(\delta \tau)\).

2.4. The \(R\) algorithm

The only difference between \(\chi\) and \(R_0\) is that in the former the pseudofermion field is calculated at the beginning of every MD step, and in the latter the noisy field (effectively pseudofermions) is calculated in the middle of each MD step. \(\chi\) has \(O(\delta \tau^2)\) errors for \(n = 1\) multiplets, whereas \(R_0\) has errors \(O(\delta \tau)\). However for \(n = 0\) (i.e., no fermions) both are identical and have errors of \(O(\delta \tau^2)\). We expect that the leading error has a linear dependence on the time the pseudofermions are refreshed and on the number of multiplets, so if we refresh the pseudofermion field at \(t = (1 - n)\delta \tau / 2\), an \(O(\delta \tau^2)\) algorithm for \(0 \leq n \leq 1\) fermion multiplets should be obtained. For two flavours of staggered fermions, this means evaluating the pseudofermion field a quarter way through each MD update. This leads to an algorithm that is neither reversible nor area preserving and so cannot be made exact (unlike the previous algorithms which could be made exact through the inclusion of an accept/reject step).

The argument leading to Equation (1) may be generalised to give

\[
\langle e^{-(\delta + \delta)(H + \Delta S) - \text{tr ln } V_\tau} \rangle_\pi = 1, \tag{2}
\]

where \(\delta\) measures lack of “energy” conservation, \(\delta\) measures lack of reversibility \(\delta : \Omega \mapsto \Omega \circ [V(\tau)^{-1} - F \circ V \circ F]\) and \(\text{tr ln } V_\tau \equiv \ln \det \frac{\partial(U''')}{\partial(U, \pi)}\) measures lack of area preservation. Considering a single step of the \(R\) algorithm, where the auxiliary field \(\chi\) is computed at a time \(t = (1 - \alpha)\delta \tau / 2\) where \(\alpha\) is some parameter to be determined, and expanding Equation (2) in \(\delta \tau\) we find

\[
\langle e^{-(\delta + \delta)(H + \Delta S) - \text{tr ln } V_\tau} \rangle_\pi = 1 - A\delta \tau^2 + O(\delta \tau^3), \tag{3}
\]

where \(A\) is proportional to \((n - \alpha)\). If \(\alpha = n\) the leading term cancels, and thus the leading error
is $O(\delta \tau^2)$ for the entire trajectory. Therefore, as claimed $R$ is an $O(\delta \tau^2)$ algorithm, and thus so is $\chi$ (i.e., $R$ with $n = 1$).

3. A Source of Inaccuracy

The staggered fermion kernel is

$$\mathcal{M} = 2m\delta_{i,j} + \sum_{\mu} \eta_{i,\mu}(U_{i,\mu}\delta_{i,j-\mu} - U_{i,-\mu,\mu}\delta_{i,j+\mu}),$$

where $m$ is the fermion mass and $U_{i,\mu}$ is the gauge field link matrix at site $i$ in direction $\mu$ and $\eta_{i,\mu}$ are the staggered fermion phase factors. The $\delta \tau^3$ term in Equation (3) should have a coefficient that behaves as $[(\mathcal{M}^\dagger \mathcal{M})^{-1} \frac{\partial}{\partial \mathcal{M}}(\mathcal{M}^\dagger \mathcal{M})]^3$, thus for light modes this term could be expected to behave as $O(m^{-3})$. This presents no problems, as long as $\delta \tau$ is small compared to the mass. If $\delta \tau \approx m$, then the $\delta \tau$ expansion breaks down. For an exact algorithm, the accept/reject step would have corrected for this, however with an inexact algorithm $\Delta S \sim O((\delta \tau/m)^2) = O(1)$, so we would be simulating an action $S + \delta S$ which differs from $S$ by terms which are not small.

When short distance observables (e.g., the plaquette) are measured with $\delta \tau \approx m$ (typical of light fermion simulations) there is the expected $\delta \tau^2$ scaling, with no indication of the inaccuracy just highlighted. However the $m^{-3}$ behaviour would only be expected to be true for the lightest fermion modes, and since bosonic observables do not couple strongly to these modes; we do not expect the $m^{-3}$ behaviour to be observable here.

Instantons correspond to zero modes of the Dirac operator in the massless limit, and are crucial for physical dynamical quark effects, such as the $\eta'$ mass. An error $\Delta S \sim O(1)$ for the lightest modes would thus most likely affect the instanton sector, and thus one may get the most interesting light dynamical quark physics wrong. Unfortunately accurate measurement of such effects is notoriously hard.

4. The RHMC algorithm

The RHMC is an exact algorithm which can be used to to simulate two flavours of staggered fermions. It is like HMC with two extra ingredients: a fairly cheap but very accurate force computation and a cheap noisy accept/reject step\[2\][3].

We now write the fermion action as $S_F = \chi^\dagger (\mathcal{M}^\dagger \mathcal{M})^{-1/2} \chi$. The inverse square root of the Dirac operator, can be approximated using an optimal Chebyshev rational approximation. The advantage of rational approximations is that the error in the approximation falls as $e^{n/\ln m}$ where $n$ is the degree of the rational function used and $m$ is the fermion mass. This accuracy is maintained over the entire spectrum of the Dirac operator.

The noisy part of the accept/reject step corrects the errors in the approximation of the square-root, the $\delta \tau$ errors being corrected exactly.

5. Testing the $R$ algorithm

We propose to test $R$ by comparing it against RHMC. Initially RHMC will be used to generate thermalised ensembles which will then be evolved using $R$. Changes in observables and/or autocorrelation lengths would signal $R$ does not get the correct distribution.

Initial work has begun on the testing, although it is still too early to reach any conclusions.

6. Acknowledgments

Our thanks go to Robert Edwards, Ivan Horváth, Stefan Sint and Urs Wenger for discussions and for providing the RHMC code in the SZIN software system\[3\].

Work supported by the European Community’s Human potential programme under HPRN-CT-2000-00145 Hadrons/LatticeQCD.

REFERENCES

1. S. Gottlieb, D. T. W. Liu, R. L. Renken, and R. L. Sugar, Phys. Rev. D 35, 2531 (1987).
2. I. Horváth, A. D. Kennedy, and S. Sint, Nuclear Physics B (Proc. Suppl.) 73, 834 (1998), hep-ph/9809092.
3. JLQCD Collaboration, K-I. Ishikawa et al., Talk given at Lattice 2002 (2002), hep-lat/0208058.
4. http://www.jlab.org/edwards/szin.html.