A New Exact Method for Dynamical Fermion Computations with Non-Local Actions

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We introduce a new algorithm which we call the \textit{Rational Hybrid Monte Carlo} Algorithm (RHMC). This method uses a rational approximation to the fermionic kernel together with a noisy (Kennedy–Kuti \textsuperscript{[1]}) acceptance step to give an efficient algorithm with no molecular dynamics integration step-size errors.

1. Introduction

The RHMC algorithm is an exact method for generating lattice configurations distributed according to some non-local action. Both the terms ‘non-local’ and ‘exact’ require some explanation.

By a non-local action we mean one which is constructed from some continuous function of a local kernel, for example \( \bar{\psi} \sqrt{M} \psi \) where \( M \) is the usual staggered kernel; we do not mean an action with complicated long-range interactions and many coupling constants such as a ‘perfect’ action. Two examples of interesting non-local actions are two flavours of staggered fermions, and solutions of the Ginsparg–Wilson relation such as Neuberger’s action \textsuperscript{[2–4]}. Our goal is not to consider the virtues or otherwise of such actions, but only to discuss how they might be efficiently simulated.

‘Exact’ algorithms in our sense are ones which do not require a zero integration step-size extrapolation. This is important in the case of two flavours of staggered fermions in order to determine the order of phase transitions, for example.

2. Ideas underlying the algorithm

Our method is a Hybrid Monte Carlo (HMC) algorithm with two new ingredients, a cheap accept/reject step, and a cheap force computation.

For the accept/reject step, which is needed to make the algorithm exact, the problem is that it is too expensive to compute the change in energy \( \delta H \) exactly. We therefore apply the Kennedy–Kuti method \textsuperscript{[1]} and use a linear accept/reject step by defining an ordering of the fields independent of the estimator of the action. The number of violations of \( 0 \leq \text{P}_{\text{acc}} \leq 1 \) can be counted explicitly and easily be made negligibly small by a suitable choice of algorithmic parameters. In order to produce an unbiased stochastic estimate of \( \exp \text{tr} \ln M \), we sum the series expansions for \( e^x \) and \( \ln(1-x) \) stochastically \textsuperscript{[5]}.

2.1. Noisy Force

The computation of the force needed for the molecular dynamics (MD) evolution is also prohibitively expensive for non-local actions, and we first investigated modifying the Hybrid Molecular Dynamics (HMD) \( R_0 \) algorithm by adding an accept/reject step to make it exact. This did not lead to a feasible algorithm because the integration errors grow as \( \delta H \propto V \delta \tau \), and thus the cost grows as \( V(V \delta \tau)(\xi/\delta \tau) = V^2 \xi \) where \( \delta \tau \) is the integration step size, \( \xi \) is the correlation length in units of MD time and \( V \) is the lattice volume. This cannot be improved using higher-order integration schemes because the errors are intrinsi-
cally due to the noise. The $R$ algorithm \cite{6} is not area-preserving or reversible so cannot be made exact in any obvious fashion.

2.2. Polynomial Force

Instead of using a noisy force we then observed that the HMC algorithm does not require that we integrate the classical equations of motion for the Hamiltonian corresponding to the action we are interested in: any area-preserving reversible mapping on phase space suffices to give a valid algorithm. Using an MD Hamiltonian which approximates the desired one sufficiently well to give a good acceptance rate is a good choice, and following Lüscher \cite{7} we can do this using a polynomial in $M$ with a minimax error over the compact spectrum of $M$ which falls exponentially with the degree of the polynomial.

The existence of such optimal polynomials was shown by Chebyshev, and a truncated expansion in Chebyshev polynomials is usually very good, although in general not optimal. The optimal polynomials can be computed easily using the Remez algorithm. It is not obvious that the minimax norm is the best for our purposes, indeed Montvay uses an $L^2$ norm instead, but it seems to be a safe and adequate choice.

Such polynomial actions have been used before \cite{8–10}, but not in combination with a noisy acceptance step for non-local actions. The major difficulty with using such high-degree polynomial actions is that they can be very sensitive to rounding errors in numerical computation, and much work has gone into choosing orderings of the roots of the polynomial which minimise these difficulties \cite{11}.

2.3. Rational Force

It is well-known in the numerical analysis literature that rational function approximations not only share the exponential convergence property of polynomial approximations, but also usually reach a sufficiently small minimax error for much lower degree. The existence of optimal rational approximations is easily established using Chebyshev’s arguments, but in this case we must use an iterative method such as the Remez algorithm to find the optimal approximation. If we choose to use a diagonal rational approximation, that is one in which the numerator and denominator are polynomials of equal degree, then it turns out that the roots of both are all real and negative. An example of such an approximation is

$$
\frac{1}{\sqrt{x}} \approx 0.3904603901 \times \frac{(x+2.3475661045)(x+0.104834460)(x+0.0073063814)}{(x+0.4105999971)(x+0.0286165446)(x+0.0012779193)}
$$

The evaluation of such a rational approximation for a matrix requires several conjugate gradient inversions with increasing masses. Figure \ref{fig:1} illustrates the quality of the minimax approximations.

3. Numerical results

The results of our numerical tests of the RHMC algorithm are shown in Figure \ref{fig:2} for the case of four flavours of staggered fermions, where the results may be compared with a conventional HMC computation, and in Figure \ref{fig:3} for the case of two staggered flavours, where there is no other exact

\footnote{We are also investigating using a partial fraction expansion of the rational function and using a multiple mass solver.}
method available for comparison.

Each of these figures is composed of four graphs: the top one shows the mean acceptance rate, which for our choice of parameters should be exactly 70%; the second one shows the number of violations, when this is zero the method is exact; the third one shows the mean plaquette; and the bottom one the largest eigenvalue of the staggered Dirac operator. The solid circles are results using a [3,3] rational approximation for the force and the open ones are for a [32,0] polynomial approximation. The lines are the results from a conventional HMC computation when this was possible.

Results are shown both for the algorithm with the noisy accept/reject step (indicated by the suffix N) and for an inexact version without the accept/reject step (indicated by the suffix D). The δτ² step size errors in the latter are evident, as are the difficulties in carrying out an accurate zero step size extrapolation.

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