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ACCEPTANCES AND AUTOCORRELATIONS IN HYBRID MONTE CARLO

A. D. KENNEDY

SCRI, Florida State University, Tallahassee, FL 32306-4052, USA

Brian PENDLETON

Physics Department, Edinburgh University, Edinburgh EH9 3JZ, Scotland

We present the results of an analytic study of the Hybrid Monte Carlo algorithm for free field theory. We calculate the acceptance rate and autocorrelation function as a function of lattice volume, integration step size, and (average) trajectory length. We show that the dynamical critical exponent z can be tuned to unity by a judicious choice of average trajectory length.

1. INTRODUCTION

In this paper we address the question: "How much does Hybrid Monte Carlo[1] really cost?" We calculate the HMC acceptance rate for free field theory as a function of the integration step-size $\delta\tau$ and the lattice volume V. Our result confirms and extends results obtained from general arguments and simple approximations[2, 3, 4]. Next we turn our attention to the autocorrelation function of the theory and present an explicit derivation of the anticipated result that the average HMC trajectory length should be chosen inversely proportional to the frequency of the slowest eigenmode of the system.[5]

2. ACCEPTANCE RATE FOR FREE FIELDS

2.1. Uncoupled Oscillators

We begin with a brief description of the calculation of the acceptance rate for Langevin Monte Carlo simulations of a system of N uncoupled oscillators with frequencies ω_j [6]. Using field theory notation, the Hamiltonian for evolution in fictitious time τ is

$$H = \frac{1}{2}\sum_{j=1}^{N}(\pi_j^2 + \omega_j^2\phi_j^2). \qquad (2.1)$$

The LMC algorithm consists of the following steps:

1. Generate a new set of momenta π_j from their equilibrium distribution: $P(\pi_j(0)) \propto \exp(-\frac{1}{2}\pi_j(0)^2)$.
2. Integrate the fields and momenta through one leapfrog iteration (of length $\delta\tau$):
$$\begin{aligned} \pi_j(\delta\tau/2) &= \pi_j(0) - \omega_j^2\phi_j(0)\,\delta\tau/2 \\ \phi_j(\delta\tau) &= \phi_j(0) + \pi_j(\delta\tau/2)\,\delta\tau \\ \pi_j(\delta\tau) &= \pi_j(\delta\tau/2) - \omega_j^2\phi_j(\delta\tau)\,\delta\tau/2 \end{aligned}$$
3. Accept the new fields and momenta with probability $\min[1, \exp(-\delta H)]$.

The acceptance rate is obtained by integrating over equilibrium configurations of the fields $\phi_j(0)$ and momenta $\pi_j(0)$. The equilibrium acceptance probability for Langevin Monte Carlo is thus

$$P_{\text{acc}} = \frac{1}{Z}\int d^N\phi\, d^N\pi\, e^{-H(\phi_j,\pi_j)}\min(1, e^{-\delta H}). \qquad (2.2)$$

with

$$\begin{aligned} \delta H &\equiv H(\delta\tau) - H(0) \\ &= \sum_j\Big\{\frac{1}{4}\omega_j^4\phi_j\pi_j\delta\tau^3 + \frac{1}{8}\omega_j^4(\pi_j^2 - \omega_j^2\phi_j^2)\delta\tau^4 \\ &\qquad - \frac{1}{8}\omega_j^6\phi_j\pi_j\delta\tau^5 + \frac{1}{32}\omega_j^8\phi_j^2\delta\tau^6\Big\}. \end{aligned}$$

To evaluate the integral in equation (2.2) we perform an asymptotic expansion to generate a power series in $1/N$ which is valid for all $\delta\tau \ll N$ [7]. To leading order we have[6, 7, 8]

$$P_{\text{acc}} = \text{erfc}\left(\frac{\delta\tau^3}{8}\sqrt{\frac{N\sigma_6}{2}}\right). \qquad (2.3)$$

where we have introduced the quantity $\sigma_8 \equiv \frac{1}{N}\sum_j \omega_j^8$.

2.2. Free Field Theory

For simplicity we consider a real free scalar field theory in one dimension. The Hamiltonian governing evolution in fictitious time is

$$H = \frac{1}{2}\sum_{x=1}^{N}\left\{\pi_x^2 + \phi_x(-\Delta^2 + m^2)\phi_x\right\}. \qquad (2.4)$$

The calculation of P_{acc} is most easily performed by Fourier transforming to "real momentum space" where

$$H = \frac{1}{2}\sum_{p=1}^{N}\left\{\pi_p^2 + \omega_p^2\phi_p^2\right\} \qquad (2.5)$$

The frequency spectrum is

$$\omega_p^2 \equiv m^2 + 4\sin^2\left(\frac{\pi p}{N}\right). \qquad (2.6)$$

Since the Jacobian for Fourier transformation is unity, we can use the result for uncoupled oscillators with impunity. The parameter σ_8 in the acceptance rate becomes

$$\begin{aligned}\sigma_8 &\equiv \frac{1}{N}\sum_{p=1}^{N}\omega_p^8 = \frac{1}{N}\sum_{p=1}^{N}\left[m^2 + 4\sin^2\left(\frac{\pi p}{N}\right)\right]^4 \\ &\to \int_0^{2\pi}\frac{d\tilde{p}}{2\pi}\left[m^2 + 4\sin^2\left(\frac{\tilde{p}}{2}\right)\right]^4 \qquad (2.7)\end{aligned}$$

as $N \to \infty$, with $\tilde{p} \equiv 2\pi p/N$. Hence the acceptance rate is given by equation (2.3) with $\sigma_8 = 70+18m^2+6m^4+m^6$. In higher dimensions we obtain the same result with an appropriate spectral sum σ_8.

2.3. Higher-Order Integration Scheme

One can construct a generalisation of the leapfrog integration scheme having single step errors which are $O(\delta\tau^5)$ [9]. The new scheme comprises a leapfrog step with step-size ϵ, a "backward" step of size $-\sqrt[3]{2}\epsilon$, followed by another forward step of size ϵ. To ensure that the higher order step moves the same distance as the leapfrog step requires $\varepsilon = \dfrac{\delta\tau}{2-\sqrt[3]{2}}$. The calculation of the acceptance rate is straightforward but tedious. The result is

$$P_{acc} \approx \operatorname{erfc}\left(1.2\frac{\delta\tau^5}{32}\sqrt{\frac{N\sigma_{10}}{2}}\right). \qquad (2.8)$$

with $\sigma \equiv \frac{1}{N}\sum_i \omega_i^{10}$. For free field theory on an infinite lattice we have $\sigma_{10} = 252+350m^2+200m^4+60m^6+10m^8+m^{10}$.

Comparing the results for the two discretisations we see that to keep a constant acceptance rate requires $\delta\tau \propto N^{-1/6}$ for leapfrog and $\delta\tau \propto N^{-1/10}$ for the higher order algorithm. However, since $\sigma_{10} \gg \sigma_8$ the higher order scheme wins only on large lattices. Assuming that the free field results carry over qualitatively to the interacting case for HMC, this might explain why leapfrog is hard to beat on present day lattices.[10]

2.4. Hybrid Monte Carlo

It is relatively straightforward to extend the LMC results to HMC with n leapfrog iterations between momentum refreshment and the Metropolis step. Once again free field theory in momentum space is a special case of the system of N uncoupled oscillators.

The crucial observation is that the leapfrog update is a linear map on phase space.

$$\begin{bmatrix}\phi_j(\delta\tau)\\ \pi_j(\delta\tau)\end{bmatrix} = \begin{bmatrix}1-\frac{1}{2}\omega_j^2\delta\tau^2 & \delta\tau \\ -\omega_j^2\delta\tau(1-\frac{1}{4}\omega_j^2\delta\tau^2) & 1-\frac{1}{2}\omega_j^2\delta\tau^2\end{bmatrix}\begin{bmatrix}\phi_j(0)\\ \pi_j(0)\end{bmatrix} \qquad (2.9)$$

Diagonalizing this matrix and performing an eigenvector expansion allows us to write down an exact expression for δH after n leapfrog steps. Writing $n = \tau_0/\delta\tau$, Taylor expanding δH through $O(\delta\tau^4)$, and performing the integral over equilibrium fields and momenta gives[7,8]

$$P_{acc} = \operatorname{erfc}\left(\frac{\delta\tau^2}{4}\sqrt{\frac{N\sigma_{hmc}}{2}}\right). \qquad (2.10)$$

where

$$\sigma_{hmc} \equiv \frac{1}{N}\sum_j \omega_j^4\left(\frac{1}{2}\sin\omega\tau_0\right)^2. \qquad (2.11)$$

Using the free field spectrum we get

$$\begin{aligned}\sigma_{hmc} &= \frac{1}{8N}\sum_{p=1}^{N}\left[m^2 + 4\sin^2\left(\frac{\pi p}{N}\right)\right]^2 \times \\ &\times\left[1-\cos\left(2\tau_0\sqrt{m^2+4\sin^2\left(\frac{\pi p}{N}\right)}\right)\right]\end{aligned}$$

For $m = 0$ and $N \to \infty$ we can evaluate σ_{hmc} exactly,

$$\begin{aligned}\sigma_{hmc} &= \frac{2}{\pi}\int_0^{\pi} dz\, \sin^4 z[1-\cos(4\tau_0\sin z)] \\ &= \frac{3}{4} - \frac{3}{4}J_0(4\tau_0) + J_2(4\tau_0) - \frac{1}{4}J_4(4\tau_0)\end{aligned}$$

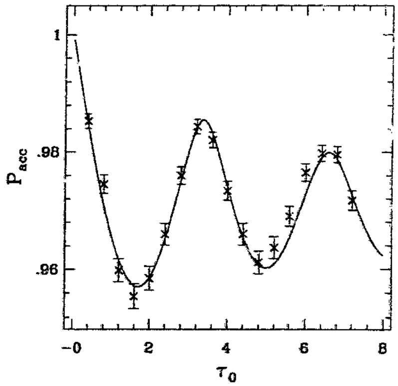

Figure 1: HMC acceptance rate P_{acc} as a function of trajectory length τ_0 for massless free field theory at $N = 20$ and $\delta\tau = 0.2$. The solid line is given by the analytic result of equations (2.10) and (2.11).

As expected, we find that we must tune $\delta\tau \propto N^{-1/4}$ to maintain a constant acceptance rate. Note that although the acceptance rates for LMC and HMC have the same functional form, σ_{hmc} cannot be obtained from σ_8 in any simple way. For $\tau_0 = \delta\tau$, expanding equation (2.10) gives the LMC result (2.3).

We have checked the analytic result against numerical simulations of free field theory for a variety of values of N and $\delta\tau$. Figure 1 shows the results obtained on a lattice of 20 sites at $\delta\tau = 0.2$.

3. AUTOCORRELATION FUNCTION

Another important issue for HMC is the question of what trajectory length one should employ. In reference 1 we tuned the trajectory length τ_0 to coincide with one of the peaks of the acceptance rate. However, as we shall see, this may turn out to be far from optimal due to an effect first pointed out by Mackenzie[11].

Let us define the autocorrelation function for the magnetisation

$$C(\tau) \equiv \frac{\sum_{j=1}^{N}\langle\phi_j(\tau)\phi_j(0)\rangle}{\sum_{j=1}^{N}\langle\phi_j^2(0)\rangle} = \frac{\sum_{p=1}^{N}\langle\phi_p(\tau)\phi_p(0)\rangle}{\sum_{p=1}^{N}\langle\phi_p^2(0)\rangle}. \tag{3.1}$$

Once again the properties of the Fourier transform allow us to perform the entire calculation in momentum space.

We shall consider here only the limit $\delta\tau \to 0$. The evolution of the field for classical dynamics is given by the solution of Newton's equations

$$\phi_p(\tau) = \phi_p(0)\cos(\omega_p\tau) + \frac{\pi_p(0)}{\omega_p}\sin(\omega_p\tau). \tag{3.2}$$

Now suppose that there are exactly n momentum refreshments at times $0 \le \tau_1 \le \cdots \le \tau_{n-1} \le \tau_n \equiv \tau$. Generalising equation (3.2) to the case of multiple trajectories and integrating over equilibrium distribution of the field $\phi_p(0)$ and of the refreshed momenta $\pi_p(\tau_i)$ gives the autocorrelation function

$$C_n(s_1,\ldots,s_n) \equiv \frac{1}{Z_C}\sum_{p=1}^{N}\frac{1}{\omega_p^2}\prod_{i=1}^{n}\cos(\omega_p s_i) \tag{3.3}$$

where $Z_C \equiv \sum_{p=1}^{N}\langle\phi_p^2(0)\rangle = \sum_{p=1}^{N}\omega_p^{-2}$ and $s_i \equiv \tau_i - \tau_{i-1}$ is the length of the ith trajectory.

It is simple to generalise equation (3.3) to the case of random trajectory lengths. Let $P_R(s)$ be the probability of choosing a trajectory of length s. The autocorrelation function is then

$$\begin{aligned} C(\tau) \;\equiv\; & \sum_{n=1}^{\infty}\int_0^\infty ds_1\cdots\int_0^\infty ds_n\, P_R(s_1)\cdots P_R(s_n) \\ & \times C_n(s_1,\ldots,s_n)\,\delta(\tau - \sum_{i=1}^{n}s_i). \end{aligned} \tag{3.4}$$

We can factorise this expression and thus sum the series by taking the Laplace transform

$$\begin{aligned} F(\beta) &\equiv \int_0^\infty d\tau\, C(\tau)\exp(-\beta\tau) \qquad (3.5)\\ &= \frac{1}{Z_c}\sum_{p=1}^{N}\frac{1}{\omega_p^2}\left[\frac{1}{1-G_p(\beta)} - 1\right] \qquad (3.6)\end{aligned}$$

where

$$G_p(\beta) \equiv \int_0^\infty ds P_R(s)\exp(-\beta s)\cos(\omega_p s). \tag{3.7}$$

For ergodic processes the autocorrelation function at large times will decay as

$$C(\tau) \sim \exp(-\tau/T) \tag{3.8}$$

where T is the exponential autocorrelation time. Hence, from equation (3.5) we see that $F(\beta)$ will have a pole at $\mathrm{Re}\,\beta_C = -1/T$ and this will be the rightmost pole.

Let us calculate T for the case of exponentially distributed trajectory lengths $P_R(s) = \exp(-s/\tau_0)/\tau_0$ as originally proposed by Duane[5]. This gives an average trajectory length $\langle s \rangle = \tau_0$. Performing the Laplace transform, we find poles in $F(\beta)$ for

$$\beta_p = \frac{1}{2\tau_0}\left[-1+\sqrt{1-(2\omega_p\tau_0)^2}\right]. \qquad (3.9)$$

We are interested in the slowest decaying exponential in $C(\tau)$, this occurs for the mode of the field with lowest frequency $\omega_{\min}$ as one might expect. More precisely, we find

$$T = \begin{cases} \frac{2\tau_0}{1-\sqrt{1-(2\omega_{\min}\tau_0)^2}} & \text{for } \tau_0 \le \frac{1}{2\omega_{\min}} \\ 2\tau_0 & \text{for } \tau_0 \ge \frac{1}{2\omega_{\min}} \end{cases} \qquad (3.10)$$

The optimal average trajectory length is clearly $\tau_0 = 1/(2\omega_{\min})$ which gives $T = 1/\omega_{\min}$.

Let us now consider the dynamical critical exponent z. The computer time T_{comp} required to generate a new independent configuration is proportional to $T/\delta\tau$. For stability of the leapfrog integration scheme, we must have $\omega_{\max}\delta\tau \le 1$. At $T = 1/\omega_{\min}$ we obtain

$$T_{\text{comp}} \propto \frac{\omega_{\max}}{\omega_{\min}} \propto \left(\frac{\xi}{a}\right)^z \qquad (3.11)$$

with $z = 1$, ξ being the correlation length and a the lattice spacing. This result was first suggested by Duane.[5, 12] A similar calculation for short trajectories ($\tau_0 \approx \delta\tau$) yields the value $z = 2$ expected from a local algorithm. Hence the non-local update generated by classical dynamics over a finite trajectory length has alleviated the problem of critical slowing down.

We can easily repeat the above analysis for fixed length trajectories $P_R(s) = \delta(s-\tau_0)$. We find

$$T = \max_p \frac{\tau_0}{\ln|\cos(\omega_p\tau_0)|}. \qquad (3.12)$$

Now, if $\tau_0 \approx n\pi/\omega_p$ for some ω_p, then $T \to \infty$ and the system never equilibrates.[11]

4. CONCLUSIONS

Our results show that the cost of simulating free field theory at fixed correlation length on an N-site lattice with Hybrid Monte Carlo is proportional to $N^{5/4}$, as has been widely anticipated. Furthermore, we can tune the average trajectory length in such a way that the system evolves via a guided random walk with dynamical critical exponent $z = 1$ and critical slowing down is much reduced.

Can we also alleviate critical slowing down in interacting field theories? If so, is the optimal average trajectory length for QCD proportional to the inverse of the pion mass? We shall report on numerical results in a future publication.

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