Tuning HMC using Poisson Brackets

M. A. Clark\textsuperscript{1}, A. D. Kennedy\textsuperscript{2}, and P. J. Silva\textsuperscript{3}

We demonstrate how measurement of the average values of the contributions to the Poisson brackets \(\{S, \{S, T\}\}\) and \[\{T, \{S, T\}\}\] allows us to optimize the integrators used for generating dynamical fermion configurations.

Theory

**Symplectic Integrators**

We are interested in finding the classical trajectory in phase space of a system described by the Hamiltonian \(H(q, p) = T(q) + S(q)\), which is the idea of a symplectic integrator to write the evolution operator as \[\exp\left(-i\frac{\delta\tau}{\hbar} \hat{H}\right) = \exp\left(-i\frac{\delta\tau}{\hbar} \hat{H}_{\text{kin}}\right) \exp\left(-i\frac{\delta\tau}{\hbar} \hat{H}_{\text{pot}}\right)\].

Since the kinetic energy \(T\) is a function only of \(p\) and the potential energy \(S\) is a function only of \(q\), it follows that the action \[\delta^2 S = f(q, p) \to f(q, p - \delta q; p)\] and \[\delta^2 T = f(q, p) \to f(q, p + \delta p; p)\]

are just translations of the appropriate variables.

We now make use of the Baker-Campbell-Hausdorff (BCH) formula, which tells us that the product of exponentials in any associative algebra can be written as \[\exp(A)\exp(B) = \exp(A + [A, B] + \frac{1}{2}[A, [A, B]] + \cdots)\]. This is the fundamental result we use to define a Hamiltonian vector field \(\tilde{A}\). By doing this, we need to use some differential geometry. The following table summarizes the difference between the formulation on flat space that we have discussed up to now and the formulation on a group manifold. To do this, we need to use some differential geometry.

<table>
<thead>
<tr>
<th>Symplectic Integrator</th>
<th>Flat Manifold</th>
<th>General</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hamiltonian vector field</td>
<td>(H = \frac{d}{dt} }</td>
<td>(H = \frac{d}{dt} } + \frac{1}{2} {H, M}</td>
</tr>
<tr>
<td>Equations of motion</td>
<td>(q = \frac{\partial H}{\partial p} )</td>
<td>(q = \frac{\partial H}{\partial p} ) + (\frac{1}{2} {q, {H, M}} )</td>
</tr>
<tr>
<td>Poisson bracket</td>
<td>({A, B} = -\frac{1}{2} {A, {B, {A, B}}} )</td>
<td>({A, B} = -\frac{1}{2} {A, {B, {A, B}}} )</td>
</tr>
</tbody>
</table>

Poisson Brackets

A Hamiltonian of the form \(H = T + S\) we find that the leading Poisson brackets that appear in the shadow Hamiltonian for a symplectic symmetric integrator are \(\{S, \{S, T\}\}\) and \(\{T, \{S, T\}\}\). The idea of a symplectic integrator is to optimize the integrator (by adjusting the step sizes, order of the integration scheme, integrator parameters, number of numerical fields, etc.) to minimize the cost. This is possible because the acceptance rate and instabilities are completely determined by \(H = H_T\). As a very simple example consider the minimum norm Poisson integrator \(U_{\text{PQM}}(S, T) = \exp\left(-i\frac{\delta\tau}{\hbar} \{\hat{S}, \hat{T}\} \right)\). This is the usual way to write the classical trajectory in phase space of a system described by the Hamiltonian \(H = H_T + H_S\). One way of optimizing this integrator is to minimize \(|\Delta H_T|\) with respect to \(\alpha\), the average being taken with respect to the equilibrium distribution \(e^{-\beta H}\); this makes \(\alpha\) as close to the conserved \(H\) as possible. Another option is to minimize \(|\Delta H_T|\) with respect to \(\alpha\), the average being taken with respect to the equilibrium distribution \(e^{-\beta H}\); this makes \(\alpha\) as close to the conserved \(H\) as possible. Another option is to minimize \(|\Delta H_T|\) with respect to \(\alpha\), the average being taken with respect to the equilibrium distribution \(e^{-\beta H}\); this makes \(\alpha\) as close to the conserved \(H\) as possible.

**Nest Integrators**

If it is much cheaper to evaluate the force for one part of the action, such as the pure gauge part, we can use a nested integrator with a very small step size for the “inner” cheap part. One might expect that one could then tune the “outer” parameter without reference to the cheap part, but this is not the case. Let the Hamiltonian be \(H = H_T + S + T\), with \(S \in [S, \{S, T\}]\) and \(T \in [T, \{S, T\}]\), a composite step of the form \(H = H_T + S + T\), and \(\dot{q} = \frac{\partial H}{\partial p}\). For the inner integrator the BCH formula tells us that \(\exp(-i\delta\tau \{\hat{S}, \hat{T}\})\) may be written as \[\exp(-i\delta\tau \{\{\hat{S}, \hat{T}\}\})\] and the potential energy \(\tilde{S}\) depends on the cheap action \(S\) but is not suppressed by any inverse power of \(\alpha\); it is therefore necessary to measure this quantity in order to optimize the integrator.

Acknowledgements & References

P. J. Silva acknowledges support from FCT via grant SFRH/BPD/90998/2014. This work was supported in part by NSF grant PHY-0427646 and PPARC/STFC grant PP/D000238/1.

