Numerical methods for lattice field theory

Mike Peardon

Trinity College Dublin

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Numerical methods - references

Monte Carlo integration of the path integral of QFTs

- The ergodic theorem tells us Markov chains can be used to perform importance sampling Monte Carlo. We have seen a few methods for building suitable Markov processes with a stationary state of our choice.

- Making predictions from the (Euclidean) path integral of a lattice quantum field theory is now possible.

\[ \langle F \rangle = \frac{1}{Z} \int D\phi \ F(\phi) e^{-S(\phi)} \]

- The (finite) lattice has made the path integral a high-dimensional “ordinary” integral, which we can estimate using Monte Carlo.

- The Boltzmann weight of configurations means only miniscule fractions of the configuration space contribute to the integral - it is crucial to use importance sampling.
Monte Carlo integration of the path integral of QFTs

- Start with bosonic fields. For a field $\phi$ representing a scalar boson on the lattice, we have

$$S(\phi) = \sum_{x,y} \phi_x M_{xy} \phi_y + \sum_x S_{\text{int}}(\phi_x)$$

- $M_{x,y}$ describes the Klein-Gordon operator, so we could discretise on a lattice with spacing $a$ using

$$M_{x,y} = (am)^2 \delta_{x,y} - \sum_{\mu} (\delta_{x+\hat{\mu},y} + \delta_{x-\hat{\mu},y} - 2\delta_{x,y})$$

- Since (usually) $S_{\text{int}}$ is local, Metropolis-Hasting with a change at a single site will often work well. A suitable proposal step might be

$$\phi'_x = \phi_x + \delta$$

with $\delta$ drawn from a normal distribution with mean 0. The variance of this distribution can be used to control the acceptance rate, and so the efficiency of the simulation.
Gauge bosons

- For the pure Yang-Mills theory, the Wilson gauge action is localised.
- A link appears in the action in just $2d$ plaquette terms.
- A local update (Gibbs sampler) is computationally efficient.

For a Gibbs sampler, the action break-up

$S_G = S_{\text{Gibbs}}(U_\mu(x) + \tilde{S}_\mu(x))$ becomes

$S_{\text{Gibbs}}[U_\mu(x)] = \text{ReTr} (U_\mu(x)\Sigma_\mu(x))$

with

$\Sigma_\mu(x) = \sum_{\nu \neq \mu} U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x) + U_\nu^\dagger(x + \hat{\mu} - \hat{\nu}) U_\mu^\dagger(x - \hat{\nu}) U_\nu(x - \hat{\nu})$
Gauge bosons

- Updating one link would require generating a group element from

\[ \mu(U) = \frac{\exp(-\beta \text{ReTr} \, U \Sigma)}{\int dU \exp(-\beta \text{ReTr} \, U \Sigma)} \]

- Creutz developed an algorithm for \( SU(2) \) (M. Creutz, Phys.Rev.D21 (1980) 2308-2315.)

- \( SU(2) \) has the useful property that \( \Sigma = k \bar{U}, \bar{U} \in SU(2) \). so re-write the problem in terms of \( U' = U \bar{U} \) and draw from

\[ \frac{1}{Z} \exp\left(\frac{1}{2} \beta k \text{Tr} \, U'\right) dU' \]

- For \( SU(2) \), we can parameterise \( U' \) in terms of 4 real numbers

\[ U = a_0 + i \sum_{k=1}^{3} a_k \sigma_k \]
Gauge bosons

- The group-invariant Haar measure (for this parameterisation) is
  \[ dU' = \frac{1}{2\pi^2} \delta(|a|^2 - 1) d^4a \]
  and changing to (three-dimensional) spherical polar co-ordinates deals with the constraint to give a distribution
  \[ d\Omega da_0 \frac{1}{2} \sqrt{1 - a_0^2} e^{\beta ka_0} \]
  which means \( a_0 \) and the direction of the three-vector \( a \) are independent (it has length \( \sqrt{1 - a_0^2} \)).

- \( a_0 \) is generated with the rejection method, first using \( e^{\beta ka_0} \), then accepting with probability \( \sqrt{1 - a_0^2} \).

- “We leave it to the interested reader to design his own scheme for randomly selecting the direction for \( a \)” (Creutz).

- Cabibbo and Marinari used this to make a “quasi-heatbath” method for general \( SU(N) \) by updating \( SU(2) \) subgroups. \( SU(2) \)
Fermions

- The lattice physicist’s complaint: “why are there no grassmann-valued variables in my computer?”
- While the algebra is simple to formulate, it is tricky to handle directly in a computer (it can be represented as a matrix algebra)

\[
\int \eta d\eta = 1, \quad \int 1 d\eta = 0
\]

- Direct representation of the algebra is avoided; integrate out a fermion bilinear to give an effective action.

\[
\int D\bar{\psi}D\psi e^{-\bar{\psi}M\psi} = \det M
\]

- “\(\gamma_5\)-hermiticity” \((M^\dagger = \gamma_5 M \gamma_5)\) implies \(\det M\) is real, but not that it is positive. Odd numbers of (mass-degenerate) fermions are potentially a problem: importance sampling need a +ve-definite weight.
- Use \(|\det M|\) with \(\text{sgn} \det M\) in the observables. This introduces a “sign problem”: variances of estimators can be prohibitively large.
Local Four-fermi (and more) interactions can be handled by introducing an auxiliary field. A simple example illustrates the idea:

\[ e^{\sigma \bar{\psi} \Gamma \psi - \sigma^2/2} = 1 + \sigma \bar{\psi} \Gamma \psi + \frac{\sigma^2}{2} (\bar{\psi} \Gamma \psi) (\bar{\psi} \Gamma \psi) \quad \text{if} \quad (\bar{\psi} \Gamma \psi)^3 = 0 \]

so

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} d\sigma \quad e^{\sigma \bar{\psi} \Gamma \psi - \sigma^2/2} = 1 + \frac{1}{2} (\bar{\psi} \Gamma \psi) (\bar{\psi} \Gamma \psi) = e^{\frac{1}{2}(\bar{\psi} \Gamma \psi)(\bar{\psi} \Gamma \psi)} \]

The four-fermi interaction at one site is then replaced by an interaction with a new (non-propagating!) field and a fermion bilinear.

We can now integrate out the fermion and put the auxiliary field on the computer.
Fermions (3)

- We have just postponed the problem of simulating fermions.
- Now we have a **non-local** function of the remaining (bosonic/gauge/auxiliary) fields that coupled to the fermions.
- Manipulating large determinants is computationally expensive. A “bosonisation” trick is commonly used: the pseudofermion field.
- For two flavours of fermions with a $\gamma_5$-hermian lattice representation of the Dirac matrix, we have

\[
\det M^2 = \det M^\dagger M = \frac{1}{\det [M^\dagger M]^{-1}}
\]

and this is represented as a gaussian integral;

\[
\frac{1}{\det [M^\dagger M]^{-1}} = \int D\phi D\phi^* \ e^{-\phi^* [M^\dagger M]^{-1} \phi}
\]

- The pseudofermions inherit the spin structure and colour charge.
- For (eg) quarks coupled to a gluon field, $M$ depends on the links.
With this machinery, Euclidean lattice QCD can be manipulated in a computer. An expression for an observable is:

$$\langle F \rangle = \int DUD\phi^*D\phi \ F[U] \ \mu(U, \phi^*, \phi)$$

where $\mu$ is the (importance sampling) weight

$$\mu(U, \phi^*, \phi) = \frac{1}{Z} \exp \left\{ -\beta S_G[U] - \phi^* \left( M^t[U]M[U] \right)^{-1} \phi \right\}$$

with $Z$ the path integral

$$Z = \int DUD\phi^*D\phi \ \exp \left\{ -\beta S_G[U] - \phi^* \left( M^t[U]M[U] \right)^{-1} \phi \right\}$$

So if a Markov chain of configurations can be generated with stationary state $\mu$ then the ergodic theorem gives us $\langle F \rangle = E[F(U)]_\mu$
Molecular dynamics

- Consider a bosonic theory with a (possibly non-local) action $S$. The importance sampling measure we want to draw from is

$$\mu[\phi] = \frac{1}{Z} e^{-S[\phi]}$$

- For every degree of freedom in $\phi$, add an independent partner, $\pi$. The joint probability distribution for this system is

$$\mu'[\phi, \pi] = \frac{1}{Z'} e^{-S[\phi] - T[\pi]}$$

$E[f(\phi)]$ is unchanged: the density is a separable product $e^{-S} \times e^{-T}$

- We’ll choose $T[\pi] = \frac{1}{2} \sum_x \pi^2$ so $\pi$ is normally distributed.

- Now the magic sleight-of-hand; write

$$\mathcal{H} = S + T$$

and pretend $\mathcal{H}$ is a (classical) hamiltonian, which defines equations of motion in a new fictitious time co-ordinate when $\pi$ is thought of as the momentum conjugate to $\phi$. 
...a word from my sponsors...

William Rowan Hamilton (1805-1865)

Andrews Professor of Astronomy
Trinity College Dublin
Molecular dynamics (2)

- These equations of motion define an **area-preserving (Liouville’s theorem) reversible mapping** on the phase space \( \{ \phi, \pi \} \).
- We can use this to define a Markov process suitable for importance sampling:
  1. Draw \( \pi \) from the normal distribution.
  2. Integrate the equations of motion for \( \mathcal{H} \) for some time interval, \( \tau \).
- The equations of motion are
  \[
  \dot{\phi}_i = \pi_i, \quad \dot{\pi}_i = -\frac{\partial S}{\partial \phi_i}
  \]
- but unfortunately it is usually impossible to write a simple expression that solves the equations of motion. We must use a numerical integrator and this will introduce a finite-step-size error.
- **Langevin dynamics** (stochastic differential equations) use a similar idea. The R-algorithm is adaptable to fractional powers of the fermion matrix, and is popular for staggered fermions.
Molecular dynamics (3)

- To avoid finite-step-size integrator errors for the equations of motion, a modified algorithm, **HMC** was proposed (S. Duane, A.D. Kennedy, B.J. Pendleton and D. Roweth, Phys.Lett.B195 (1987) 216-222.)
- Remember that the Metropolis-Hastings algorithm has two parts; a reversible, area-preserving proposal step followed by an accept-reject test and it obeys detailed balance for a given stationary state.
- Numerical integrators that exactly preserve $\mathcal{H}$ are hard to build, but ones that *almost* conserve $\mathcal{H}$ but retain the important properties (reversibility and area-preservation) can be found.
- The best-known integrators with these properties are called reversible **symplectic** integrators.

**The leap-frog integrator**

- Update $\phi : \phi_i(t + \frac{h}{2}) = \phi_i(t) + \frac{h}{2} \pi_i(t)$
- Update $\pi : \pi_i(t + h) = \pi_i(t) - h \frac{\partial S}{\partial \phi_i}(t + \frac{h}{2})$
- Update $\phi : \phi_i(t + h) = \phi_i(t + \frac{h}{2}) + \frac{h}{2} \pi_i(t)$
Hybrid Monte Carlo

1. Draw new conjugate momenta, $\pi$ from the normal distribution
2. Store the current field, $\phi$ and compute $\mathcal{H}(\pi, \phi)$
3. Integrate the equations of motion using a reversible, symplectic integrator with step-size $h$ (such as leap-frog) so $(\phi, \pi) \xrightarrow{\text{leapfrog}} (\phi', \pi')$
4. Compute $\mathcal{H}(\pi', \phi')$ and the change, $\Delta \mathcal{H}$
5. Accept $\phi'$ as the new entry in the Markov chain with probability

$$P_{\text{acc}} = \min \left[ 1, e^{-\Delta \mathcal{H}} \right]$$

if the new configuration is rejected, then make $\phi$ the new entry.

- As $h \to 0$, $\Delta \mathcal{H} \to 0$, so $P_{\text{acc}} \to 1$
- $E[e^{-\Delta \mathcal{H}}] = 1$ and $E[\Delta \mathcal{H}] = \frac{1}{2} E[(\Delta \mathcal{H})^2]$ for small $\Delta \mathcal{H}$
Molecular dynamics (4)

- For gauge theories, our degrees of freedom are constrained, so we need to define hamiltonian dynamics on curved manifolds.

- A Lie group $G$ (all continuous gauge groups) has particularly helpful properties. At all points, there is a well-defined, tangent space (the Lie algebra at the identity element) in which conjugate momenta naturally live.

- A useful definition for a momentum variable $p$ conjugate to a group element $U$ is

$$p = p_a T_a \text{ so } p \in \mathcal{L}(G)$$

with $T_a$ the (hermitian) generators of the group and define the equation of motion for $U$ to be

$$\dot{U} = ipU$$

- The extra appearance of $U$ shows we need to rotate the Lie algebra (where $p$ lives) to be tangent to $U$. The left multiplication is a convention (right works just as well).