Computational Methods (practice) - Lecture 4

Peter Boyle (BNL, Edinburgh)

- Monte Carlo Integration
- Euclidean path integral and HMC
- Pseudofermions
- Writing and running an HMC
- Odd flavours

Monte Carlo Integration

- Integration

$$\int_U f(U)dU = Vol \times \langle f \rangle \qquad ; \qquad Vol = \int_U dU$$

- Monte Carlo Integration (x_i uniform over compact domain)

$$\langle f \rangle = \frac{1}{N} \sum_i f(x_i)$$

- Importance sampling: draw x_i with positive normalised probability density $P(x_i)$

$$\langle f \rangle = \frac{1}{N} \sum_i \frac{f(x_i)}{P(x_i)}$$

- If $|f(x_i)| \propto P(x_i)$ this may converge better.
  NB: analogy to removing bias from fixing machine learned MC integrators
- Variance reduction: if $\tilde{f}$ is a good, cheap approximation for f

$$\langle f \rangle = \frac{1}{N \times M} \sum_i \frac{\tilde{f}(x_i)}{P(x_i)} + \frac{1}{N} \sum_j \frac{f(x_j) - \tilde{f}(x_j)}{P(x_j)}$$

Euclidean Path Integral

- Pure gauge path integral

$$\frac{1}{Z}\int_U e^{-S_G[U]}\mathcal{O}(U)dU$$

- Importance sample: seek to distribute gluon configuratoins according to

$$P(U) = \frac{e^{-S_G[U]}}{\int_U e^{-S_G[U]}dU}$$

- Calculate observables on each *configuration*

$$\langle\mathcal{O}\rangle = \frac{1}{N}\sum_i \mathcal{O}(U_i)$$

- $\Rightarrow$ Markov chain monte carlo:
  - 10^{10} degrees of freedom(!)
  - Sharply probability weight
  - Variance of $\mathcal{O}(U)$ determines how many samples are required.
  - 100-2000 samples typically good for 1% scale statistical errors
- This is observable dependent...

Markov chains

- Sequence of states generated by *transition probability* $M(X \to X')$ from X to X'
  Rule depends only on X.
- Usually composed of proposal and acceptance probablities

$$M(X \to X') = P_p(X \to X')P_{acc}(X \to X')$$

- Design rule $M(X \to X')$ to yield *desired* equilibrium probability distribution after many transitions$P_{eq}(X)$
- P_{eq} must map to itself under of the transition rule:

$$P_{eq}(X') = \sum_X P_{eq}(X)M(X \to X')$$

- An ergodic update satisfying this *and* is a contration mapping and Markov transitions converge on the desired equilibrium.

(Clear pedagogical review: Anthony Kennedy Nara lectures 2006)

Metropolis algorithms

- Detailed balance property:

$$P_{eq}(X)M(X \to X') = P_{eq}(X')M(X' \to X)$$

- Sum over X to obtain

$$\sum_X P_{eq}(X)M(X \to X') = \sum_X P_{eq}(X')M(X' \to X) = P_{eq}(X')$$

- So P_{eq} is a *fixed point* of the Markov process!
- We can sample any probability distribution we desire with such an update.

Metropolis algorithms

- Make the update combine proposal and acceptance probablities

$$M(X \to X') = P_p(X \to X')P_{acc}(X \to X')$$

- detailed balance

$$P_{eq}(X)P_p(X \to X')P_{acc}(X \to X') = P_{eq}(X')P_p(X' \to X)P_{acc}(X' \to X),$$

- is satisfied with the Metropolis acceptance probability,

$$P_{acc}(X \to X') = \mathrm{Min}(1, \frac{P_{eq}(X')P_p(X' \to X)}{P_{eq}(X)P_p(X \to X')})$$

- either $P_{acc}(X \to X') = 1$, or $P_{acc}(X' \to X)$; considering cases leads to trivial proof.
- Simplifies if $P_p(X' \to X) = P_p(X \to X')$ (reversible, area preserving constraint)

Basis of most Markov Chain Monte Carlo

- Aspects of this might be of interest to the numerical integration / ML / journal club (?)

QCD path integral

- Partition function becomes a real, statistical mechanical probability weight

$$Z = \int d\bar{\psi} d\psi dU e^{-S_G[U] - S_F[\bar{\psi}, \psi, U]}$$

- Dirac differential operator represented via discrete derivative approximations: sparse matrix
- Use pseudofermion approach to replace with Gaussian integral $\sqrt{\pi\lambda} = \int dt e^{-t^2/\lambda}$

$$\int \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-\bar{\psi}(x) A_{xy} \psi(y)} = \det A$$

$$\pi\lambda = \int d\phi_r e^{-\phi_r \frac{1}{\lambda} \phi_r} \int d\phi_i e^{-\phi_i \frac{1}{\lambda} \phi_i} = \int d\phi^* d\phi e^{-\phi^* \frac{1}{\lambda} \phi}$$

- replace two flavour determinant with a two flavour *pseudofermion* integral

$$(\det M)^2 = (\det \gamma_5 M)^2 = \det M^\dagger M = \int \mathcal{D}\phi^* \mathcal{D}\phi e^{-\phi^*(x)(M^\dagger M)^{-1} \phi(y)}$$

Hybrid Monte Carlo

- Auxiliary Gaussian integral over conjugate momentum field $\int d\pi e^{\frac{-\pi^2}{2}}$
  Lives in Lie algbra; serves only to move U round the group Manifold

$$\int d\pi \int d\phi \int dU \quad e^{-\frac{\pi^2}{2}} e^{-S_G[U]} e^{-\phi^*(M^\dagger M)^{-1}\phi}$$

- Outer Metropolis Monte Carlo algorithm
  - Draw momenta
  - Draw pseudofermion as gaussian $\eta = M^{-1}\phi$
  - Metropolis acceptance step
- Metropolis proposal includes inner molecular dynamics at constant Hamiltonian:

$$H = \frac{\pi^2}{2} + S_G[U] + \phi^*(M^\dagger M)^{-1}\phi$$

$$\dot{U} = i\pi U \qquad ; \qquad i\dot{\pi} = (U\nabla_U S)_{TA}$$

- Must invert $M^\dagger M$ at each timestep of evolution in MD force

$$\delta(M^\dagger M)^{-1} = -(M^\dagger M)^{-1}[(\delta M^\dagger)M + M(\delta M)](M^\dagger M)^{-1}$$

Observables

Importance sampling has reduced:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_U e^{-S_G[U]} \mathcal{O}(U) dU \rightarrow \frac{1}{N} \sum_i \mathcal{O}(U_i)$$

- Zero momentum pion, kaon or B meson two point function

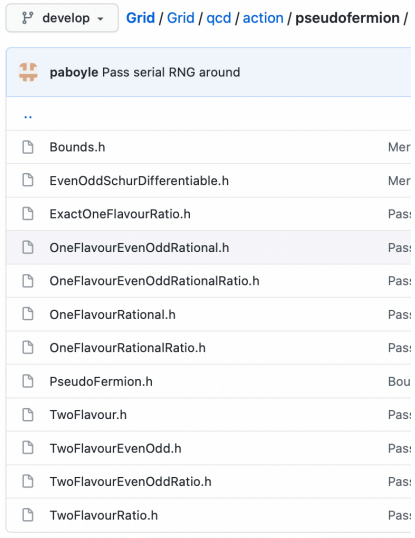
$$\sum_x \langle \bar{u} \gamma_0 \gamma_5 d(x,t) \bar{d} \gamma_0 \gamma_5 u(0,0) \rangle = \frac{1}{N} \sum_i \mathrm{trace}\{ \gamma_0 \gamma_5 M_d^{-1}(x,t;0,0) \gamma_0 \gamma_5 M_u^{-1}(0,0;x,t) \}$$

- Euclidean space $\propto Ae^{-mt}$
- Tune bare mass until interacting meson mass is correct, prefactor gives pion, kaon, B meson decay constant
- etc..

Pseudofermion options

https://github.com/paboyle/Grid/tree/develop/Grid/qcd/action/pseudofermion

- Recall $\det M = \det M_{pc} \det M_{ee}$
- Require symmetric positive definite Gaussian integral (*not* just positive $\det M$)
- Two degenerate flavours is easy: $\phi^\dagger M^\dagger M \phi$
- Odd flavours harder: take square root of $\phi^\dagger M^\dagger M \phi$ in HPD fashion
- Polynomial HMC (Chebyshev) and Rational HMC (c.f. num rep)
- *Require positivity of one flavour determinant*
  - Guaranteed for DWF with positive mass, but not for Wilson (expected for sufficiently large mass, exceptional configurations are light mass)
  - https://arxiv.org/abs/2003.13359 : *In the simulation of QCD with 2+1 flavors of Wilson fermions, the positivity of the fermion determinant is generally assumed. We present evidence that this assumption is in general not justified and discuss the consequences of this finding.*
  - For DWF exact one flavour algorithm also
- RHMC efficient due to *multi-shift solvers*



Integrators

- Integrators should be area preserving to keep phase space density same $\Rightarrow$ symplectic integrators
- Integrators can be nested (Sexton-Weingarten) to integrate different action fragments on different timescales
  - e.g. Gauge force is nearly free to evaluate
- Integrators can be nested (Sexton-Weingarten) to integrate different action fragments on different timescales
- Leapfrog, Omelyan, Force Gradient give different orders of integration error in δt
- Peak determinant force can be reduced using a series of *Hasenbusch determinant ratios*
- Tuning determinant factoring and timesteps is laborious and empirical
- Practical recommendation:
  - Factor determinants and place all on same timescale, use Force Gradient
  - Balance forces between pseudofermion factors
  - Increase fermion timestep until acceptance drops to 90%
  - Integrate gauge action on a sufficiently fine resolution that delta Hamiltonian is independent of gauge timestep

Exercise

- Quenched simulation of your choice
- Create a corresponding Grid HMC
- Run it on your laptop on 8^4 and check you get close to the same plaquette

Examples:
https://github.com/paboyle/Grid/blob/develop/HMC/Mobius2p1fRHMC.cc
https://github.com/paboyle/Grid/tree/develop/tests/hmc