Algorithms

MITP - Summer school

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J. Finkenrath

Outline - Part 0

- Part 0
  - Markov Chain Monte Carlo
  - Hybrid Monte Carlo algorithm
- Part 1
  - Linear solvers, Krylov subspace solvers
  - Preconditioners, smoothers and coarse grid
- Part 3
  - Fermions in simulations

Parts of the talk is based on Mattia Della Brida's constribution from 2021

Goal: Evaluation of pathintegral

Compute

$$< O >= \frac{1}{Z} \int D\phi e^{-S(\phi)} O(\phi) \qquad D\phi = \prod_{i=1}^{M} d\phi_i \quad e.g. \quad \phi = U, \overline{\psi}, \psi$$

- Deterministic integration methods not feasible!

  Current lattice QCD simulations can have $M = O(10^9)$

- Monte Carlo: evaluates integral by sampling the integrand at points selected via probability under the integration measure

Basic idea

1. Generate sequence of field configurations with probability

$$P(\phi^{(t)}) = \frac{1}{Z} e^{-S(\phi^t)}$$

1. Evaluate

$$\overline{O} = \frac{1}{N} \sum_{t=1}^{N} O(\phi^{(t)})$$

Monte Carlo integration

Consider: an integral of dimension d

$$\langle f \rangle = \int_D dx\, f(x) \qquad x = (x_1, \dots, x_d) \quad D = [0,1]^d :$$

Compute: An estimate is given by

$$\bar{f}_N = \frac{1}{N} \sum_{k=1}^{N} f(x^{(k)}) \qquad x^{(k)} = (x_1^{(k)}, \dots x_d^{(k)})$$

where $x_i^{(k)}$ are random numbers uniformly distributed within $[0,1]$. This requires a solid random number generator.

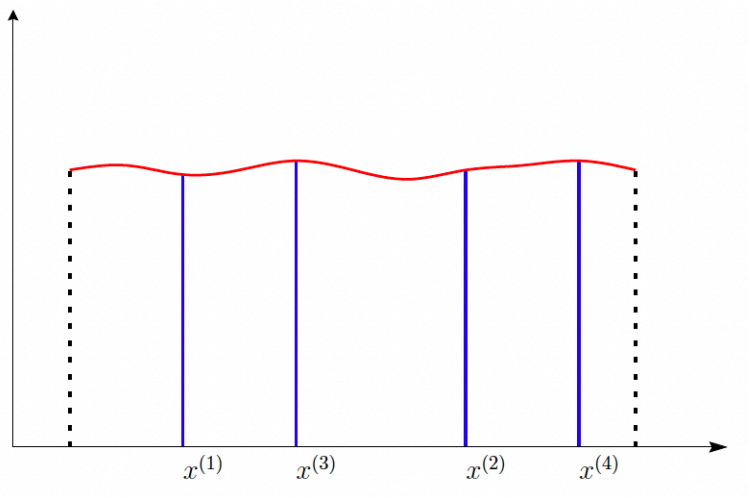
Central limit theorem:

$$P(\bar{f}_N) \overset{N\to\infty}{\propto} exp\left[-\frac{1}{2}\frac{(\bar{f}_N - \langle f \rangle)^2}{var(f)/N}\right] \quad with \quad var(f) = \langle (f - \langle f \rangle)^2 \rangle$$

with $\bar{f}_N - \langle f \rangle = (O)(1/\sqrt{N})$

- Uncertainty is of statistical nature and rather not systematic
- Error scales as $1/\sqrt{N}$ independently of the dimension d (not the case for other integral approximations like Simpson-rule)
- Rate of convergence depends on $var(f)$

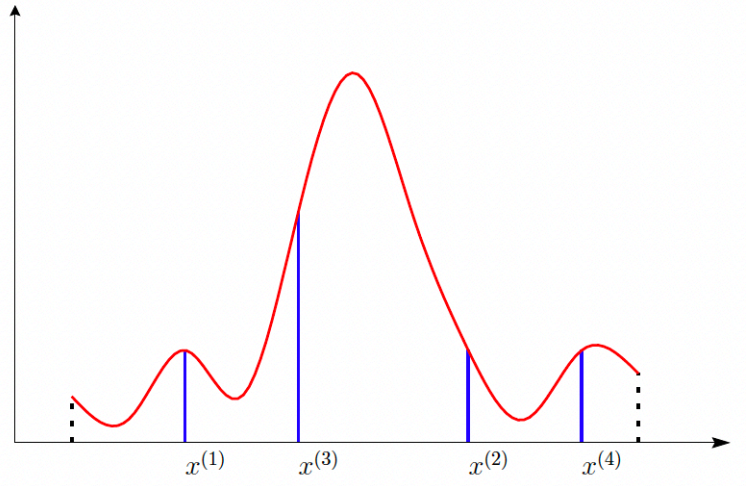
Monte Carlo integration



Uniformly sampling is effective

for approximately constant functions;

here: $var(f)$ is small



in contrast:

Sampling of more complicated functions is more difficult

here:

Using uniformly distributed random numbers can easily require large values of N to reach a good precision.

Importance sampling

Consider: adding a distribution $p(x)$ which can be sampled

$$\langle f \rangle = \int_D dx\, p(x) \left[\frac{f(x)}{p(x)} \right] = \langle g \rangle_p \qquad with \quad p(x) > 0 \quad and \quad \int_D dx\, p(x) = 1$$

with

$$g(x) = \frac{f(x)}{p(x)}$$

Compute

$$\overline{g}_N = \frac{1}{N} \sum_{k=1}^{N} g(x(k)) \qquad x^{(k)} = (x_1^{(k)}, \dots x_d^{(k)})$$

with $x^{(k)}$ random vectors distributed according to $p(x)$

Importance sampling

Central limit theorem: is modified ($\bar{f}_N \to \bar{g}_N$ and $var(f) \to var(g)$)

$$P(\bar{g}_N) \overset{N\to\infty}{\propto} exp\left[-\frac{1}{2}\frac{(\bar{g}_N - \langle f\rangle)^2}{var(g)/N}\right] \quad with \quad var(f) = \langle (g - \langle f\rangle)^2\rangle_p$$

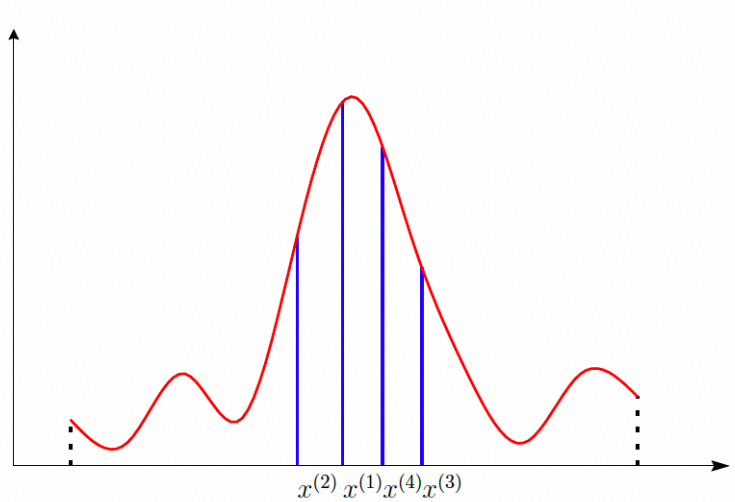
with

$$\langle f\rangle = \bar{g}_N \pm \sigma(\bar{g}_N) \qquad and \qquad \sigma(\bar{g}_N) = \sqrt{var(g)/N}$$

Choice of $p(x)$ can signicantly affect convergence:

- however optimal $p(x) = f(x)$ would solve the integral (trivial)
- Mostly relatively simple distributions $p(x)$ can be directly sampled via inverse transform or hit-and-miss, which decrease efficiency

Importance sampling

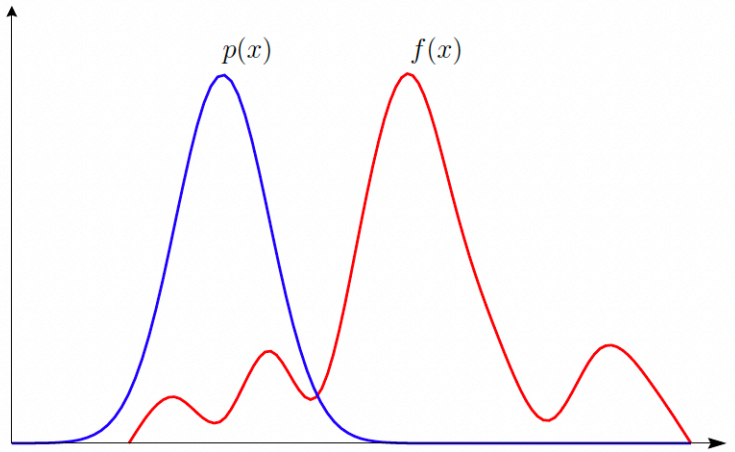


Effective

A better sampling distribution allows for

sampling more frequently the regions with larger contribution to the integral

$\Rightarrow$ faster convergence



However

If the sampling distribution and the function to integrate have little overlap,

there is an overlap problem

$\Rightarrow$ very ineffective sampling

Importance sampling

Application to lattice field theory:

$$\langle O \rangle = \int D\phi \, P_S(\phi) O(\phi) \qquad P_S(\phi) = \frac{1}{Z} e^{-S(\phi)}$$

- Sharply peaked around configurations of minimal action
- Far too **complicated distribution** for a direct sampling (large dimensionality, complex action S, normalisation unknown)

Require a method which can handle relative probabilities

- to avoid computation of partion function Z / normalization
- Usually done independently of $O(x)$ but is not necessarily optimal for all cases
  - could result in some large variances
- Using Monte Carlo method requires $S(\phi)$ to be real (and bounded)
  - Otherwise results in sign-problem (unknown to solve without an overlap problem)

Markov Chain Monte Carlo

To build a method with relative probabilities: (discrete) Markov chain is a sequence of random variables

$$\phi^{(0)} \to \phi^{(1)} \to \cdots \to \phi^{(t)} \to \cdots \cdots \to \phi^{(N)} \qquad \phi(t) \in \Omega \leftarrow \textit{state space}$$

which probability of extraction is given by a transition probability $T(\phi \to \phi')$ (t is referred to as Markov time)

Properties

1. **Markovian**

$$T(\phi \to \phi') \quad \textit{only depends on the current } (\phi) \textit{ and future } (\phi') \textit{ state}$$

2. **Time-homogeneous**

$$T(\phi \to \phi') \quad \textit{is constant along the chain, i.e. t–independent}$$

3. **Probability (density)**

$$\int D\phi'\, T(\phi \to \phi') = 1 \quad \text{and} \quad T(\phi \to \phi') >= 0$$

4. **Ergodic (& irreducible)**

$$T(\phi \to \phi') > 0 \quad \forall \phi, \phi' \in \Omega$$

A chain is completely specified by the starting distribution $P_0(\phi^{(0)})$ and transition probability $T(\phi \to \phi')$

Why Markov chains ?

Now we can define a stability condition:

$$P_{n+1}(\phi') = (TP_n)(\phi') = \int D\phi\, P_n(\phi) T(\phi \to \phi')$$

with $P^{(n)} \in P_\Omega$ where T is a linear map: $T : H \to H$ and H is the linear space of real functions on Ω.

Equilibrium distribution:

Given an ergodic Markov chain with transition probability T, the limit

$$\lim_{t\to\infty} P^{(t)} = \lim_{t\to\infty} T^t P^{(0)} = \Pi \in P_\Omega$$

exits, is unique and independent on $P^{(0)}$ in P_Ω. In particular, Π is the unique fixed point of the chain, i.e. $(TP) = P \Leftrightarrow P = \Pi$.

Remark:

This is the consequence that T has a unique eigenvalue $\lambda_0 = 1$ and

$$\lambda_0 > |\lambda_1| \geqslant |\lambda_2| \geqslant \dots, \; where\; T v_n = \lambda_n v_n \; and \; v_0 = \Pi$$

$$P^{(t)} = \Pi + \sum_{n>0} c_{t,n} (\lambda_n)^n v_n \overset{t\to\infty}{=} \Pi + O(e^{-t/\tau^{exp}}) \quad \tau^{exp} = 1/ln|\lambda_1|$$

Detailed balance condition

How can we find a T that has the desired distribution Π as equilibrium distribution ?

If T is ergodic, a sufficient (but not necessary) condition is **detailed balance**

$$\Pi(\phi')T(\phi' \to \phi) = \Pi(\phi)T(\phi \to \phi')$$

Proof: Integrate both sides over ϕ and use $\int D\phi\, T(\phi' \to \phi) = 1$.

This gives the stability or fix point condition

$$\Pi(\phi') = (T\Pi)(\phi')$$

Since T is ergodic, its fixed point is unique and corresponds to its equilibrium distribution

Remarks:

- If T satisfies detailed balance or stability but is not ergodic, the convergence for large t is not guaranteed
- Transition probabilities can be combined:

  $$T = T_1 \circ T_2 \circ \dots,$$

  with T_i not ergodic but satisfies detailed balance and such that T is ergodic. T will automatically satisfy the stability condition and converge to Π.

Metropolis-Hastings algorithm

A simple way to satisfy detailed balance is given by

$$T(\phi \to \phi') = P_C(\phi \to \phi') P_A(\phi \to \phi')$$

- A candidate ϕ' is proposed from ϕ with probability P_C
- ϕ' is accepted as the next step in the chain with probability P_A
- If ϕ' is rejected, ϕ is the next element (repeated in the chain)

Acceptance probability: We can ensure detailed balance for any choice of P_C by taking

$$P_A(\phi \to \phi') = min\left[1, \frac{\Pi(\phi') P_C(\phi' \to \phi)}{\Pi(\phi) P_C(\phi \to \phi')}\right]$$

If $P_C(\phi \to \phi') = P_C(\phi' \to \phi)$ *(symmetric proposal)*

$$P_A(\phi \to \phi') = min\left[1, \frac{\Pi(\phi')}{\Pi(\phi)}\right]$$

Other definitions of P_A are in principle possible but have lower acceptance.

Metropolis-Hastings algorithm

Remarks:

- only the relative probabilities $\Pi(\phi')/\Pi(\phi)$ are needed to construct T

  $\Rightarrow$ no need for normalization of Π

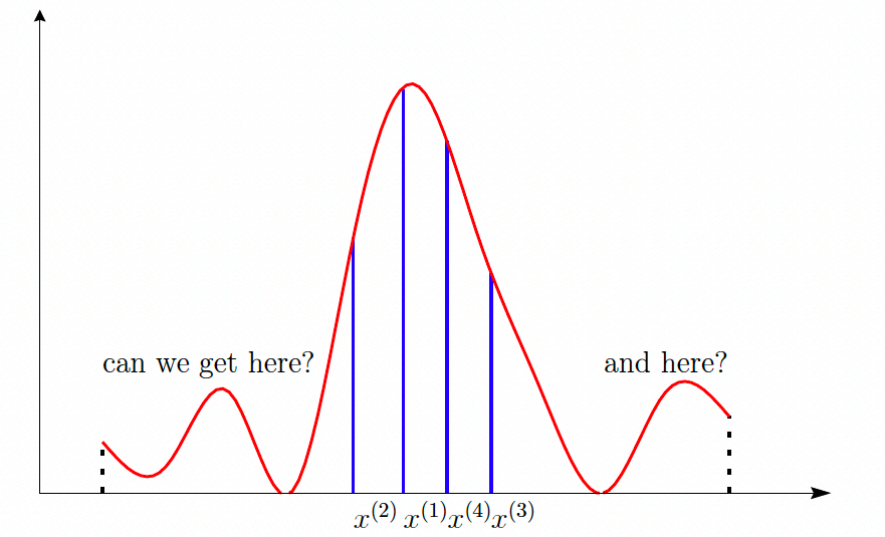
- We cannot use Markov chains to compute integrals directly, only ratios

$$\langle O \rangle = \frac{\int D\phi\, \Pi(\phi) O(\phi)}{\int D\phi\, \Pi(\phi)}$$

In practice there are challenges

in assuring that T is ergodic

$\longrightarrow$ this can lead to improper sampling and biased results



Simulating lattice ϕ^4-theory

Action

$$S = \sum_x \left[\sum_{\mu=0}^{D-1} \frac{1}{2} \left(\frac{\phi(x+\hat{\mu}) - \phi(x)}{a} \right) + \frac{m_0^2}{2} \phi^2(x) + \frac{g_0}{4!} \phi^4(x) \right]$$

Accept-reject step

1. Set $\phi(x) = \phi_0(x)$
2. Propose $\Delta > 0,\ r \in [0, 1)$ and $\phi'(x) = \phi(x) + \Delta(r - \frac{1}{2})$
3. Accept ϕ' or keep ϕ according to

   $P_A = min\left[1, e^{-\delta S}\right] \quad where \quad \delta S = S(\phi') - S(\phi) \quad only\ involves \quad \phi'(x), \phi(x), \phi(x \pm \hat{\mu})$
4. Repeat 2. & 3. for all points x, which defines a **sweep**
5. Skip k sweeps (thermalization) so that

$$P(\phi^{(t)}) \propto e^{-S(\phi^{(t)})} \quad \Rightarrow \overline{O} = \frac{1}{N} \sum_{t=k+1}^{N+k} O(\phi^{(t)}) \quad \Rightarrow \overline{O} = \langle O \rangle + O(1/\sqrt{N})$$

Autocorrelations

Subsequent states in a Markov chain are correlated

$$\langle\langle O^{(k)} O^{(l)} \rangle\rangle \neq \langle\langle O^{(k)} \rangle\rangle \langle\langle O^{(l)} \rangle\rangle \qquad O \equiv O(\phi^{(k)}) \qquad \langle\langle \cdot \rangle\rangle \equiv \text{avg. indep. chains}$$

The error on time-averages

$$\sigma^2(\overline{O}) = \langle\langle (\overline{O} - \langle O \rangle)^2 \rangle\rangle = \frac{1}{N^2} \sum_{k,l=1}^{N} \langle\langle O^{(k)} O^{(l)} \rangle\rangle - \langle O \rangle^2 \qquad [\langle\langle O^{(k)} \rangle\rangle = \langle O \rangle]$$

$$\text{can be written as} \qquad \sigma^2(\overline{O}) = \frac{2\tau^{int,O} var(O)}{N} \qquad \text{with} \quad var(O) = \langle O^2 \rangle - \langle O \rangle^2$$

Integrated autocorrelation time is given by

$$\tau^{int,O} = \frac{1}{2}\left[1 + 2\sum_{t=1}^{N-1} \frac{\Gamma^{(O)}(t)}{\Gamma^{(O)}(0)}\right]$$

and the **autocorrelation function** $\Gamma^{(O(t))} = \langle\langle O^{(t+i)} O^{(i)} \rangle\rangle - \langle O \rangle^2$

- Error scales via $N/2\tau^{int}$
- for time-homogeneous chains the function only depends on the distance in Markov time

Autocorrelations

Spectral decomposition

$$\Gamma^{(O)}(t) = \sum_{n>0} b_{n,O} e^{-t/\tau_n} \qquad \tau_n = -1/\ln|\lambda_n| \qquad [\lambda \text{ eignv. of } T]$$

- τ_n only depends on the properties of the Markov chain $\Rightarrow$ $\tau^{exp} = \tau_1$ is the "slowest" mode to decorrelate
- $b_{n,O}$ determines the coupling of O to the n-th mode $\Rightarrow$ it can vary significantly among observables

Estimate of the autocorrelation function

$$\overline{\Gamma}^{(O)}(t) = \frac{1}{N-t} \sum_{i=1}^{N-t} [(O^{(i+t)} - \overline{O})(O^{(i)} - \overline{O})]$$

Estimate of the integrated autocorrelation time

Relative error on the autocorrelation function grows exponentially $\longrightarrow$ we must choose a cutoff W

$$\tau^{int,O,W} = \frac{1}{2}\left[1 + 2\sum_{t=1}^{W} \frac{\Gamma^{(O)}(t)}{\Gamma^{(O)}(0)}\right]$$

and find a compromise between statistical and systematic error

Autocorrelations

- Autocorrelations (AC) are unavoidable in Markov Chain Monte Carlo (MCMC)
- A proper estimate of AC is curical
  - no proper AC estimate $\longrightarrow$ no proper error $\longrightarrow$ no proper result

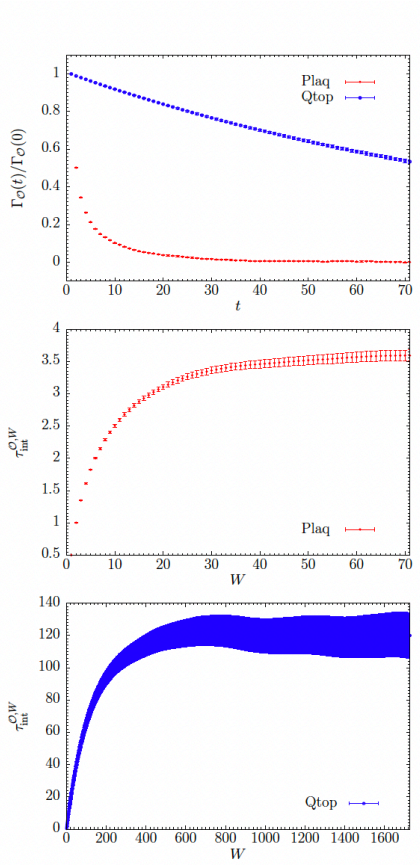
Ideal:

- Length of simulation $> O(100) * \tau^{exp}$
  - For thermalization $O(10) * \tau^{exp}$

but resources are compute and time limited

Risks: incomplete thermalization:

- wrong sampling and a biased result
- wrong estimation of AC, underestimation of errors



Estimation of τ^{exp}:

Look for the observable O^{slow} with the largest AC, i.e. is very sensitive to slow modes: take $\tau^{exp} \sim \tau^{int,O^{slow}}$

Simulating Lattice QCD

Feynman Pathintegral

$$\langle O \rangle = \frac{1}{Z} \int DU \, D\overline{\psi} \, D\psi \, e^{-Sg[U]} e^{-\overline{\psi} D[u] \psi} \cdot O[U, \overline{\psi}, \psi]$$

$$= \frac{1}{Z} \int DU e^{-Sg[U]} det(D[U]) \cdot O[U, \overline{\psi}, \psi]$$

- pure gauge theory: quenched simulation with $detD = 1$
- Action local : requires $O(1)$ operations for a single link U update
  - Heat-bath
  - Overrelaxation
- Action non-local: requires O(V) operations for a single link update
  - Global update
- Global update must be **coherent** otherwise

$$\delta S \propto V \qquad \Longrightarrow \qquad P_A \propto exp(-\delta S) \sim 0$$

Hybrid Monte Carlo

Add auxiliarry momentas:

$$\pi(x,\mu) = T^a \pi^a(x,\mu) \in su(3) \qquad (\pi,\pi) = \sum_{x,\mu,a} |\pi^a(x,\mu)|^2$$

Hamiltonian system:

$$\langle O \rangle = \frac{1}{Z} \int DU D\pi \, e^{-S[U]} e^{-(\pi,\pi)/2} \qquad with \qquad \int D\pi e^{-(\pi,\pi)/2} = 1$$

$$= \frac{1}{Z} \int DU D\pi \, e^{-H[\pi,U]} \qquad with \qquad H = \frac{1}{2}(\pi,\pi) + S[U]$$

Now, we can use Molecular dynamics to update:

$$U(x,\mu) \to U(x,\mu)(t) \qquad \pi(x,\mu) \to \pi(x,\mu)(t)$$

using Hamiltons equations: $\partial_t U(x,t) = \pi(x,\mu)U(x,\mu)$ and $\partial_t \pi(x,\mu) = -F(x,\mu)$ with

$$F(x,\mu)^a = \partial_{x,\mu} S[U] \qquad and \qquad [\partial^a{}_{x,\mu} U(y,\nu) = \delta_{xy}\delta_{\mu\nu} T^a U(x,\mu)]$$

Note that $P_H \propto exp[-H]$ and $P_S \propto exp[-S]$ are *equivalent* for sampling $O(U)$

Ideal HMC algorithm

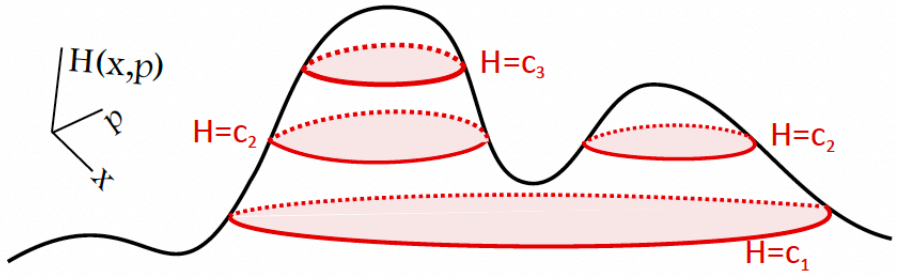
1. Start from a gauge-field $U(0)$
2. Sample a momentum field $P(0)$ from the Gaussian distribution

$$P_\pi = e^{(\pi,\pi)/2}/Z$$

3. Solver Hamilton equations for a time τ

$$(\pi(0), U(0)) \rightarrow (\pi(\tau), U(\tau))$$

4. Repeat 2. and 3. taking $U(0) = U(t)$



Hybrid Monte Carlo

Ergodicity:

First step is given by a heat-bath for the momenta's

$$P_\pi P_H = P_H$$

but the step is not ergodic in the total phase-space (only in the momentum part)

Second step is given by the Hamilton evolution

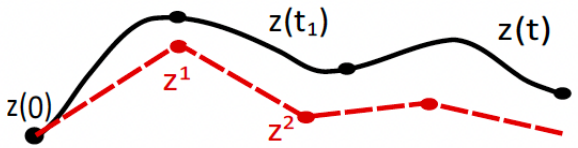
$$P_{MD}((\pi, U) \to (\pi', U')) = \delta(\pi' - \pi(\tau))\delta(U' - U(\tau))$$

it follows $P_{MD}P_H = P_H$ but is also not ergodic $(H = const.)$

However, the combination of first and second step is assumed to be ergodic $T = (P_{MD}P_\pi)$ has a fixed point and P_H is equilibrium distribution

In practice

- Hamilton equations can not be solved exactly (use numerical integration)
- H is not conserved (bias in equilibrium distribution)



Hybrid Monte Carlo on the computer

HMC algorithm *[Duane et al. 87]*

1. Start from a gauge-field $U(0)$
2. Sample a momentum field $P(0)$ from the Gaussian distribution

$$P_\pi = e^{(\pi,\pi)/2}/Z$$

3. Solve Hamilton equations numerically for a time t

$$(\pi^{(i)}, U^{(i)}) = (\pi(0), U(0)) \rightarrow (\pi(\tau), U(\tau)) = (\pi^{(f)}, U^{(f)})$$

4. Accept the configuration $U' = U(t)$ with probability

$$P_A = \min[1, e^{\delta H}] \quad with \quad \delta H \equiv H(\pi^{(f)}, U^{(f)}) - H(\pi^{(i)}, U^{(i)})$$

   If reject: continue from the initial state with $U' = U(0)$

5. Repeat 2. - 4. taking $U(i) = U'$ and iterate

Hybrid Monte Carlo on the computer

- The numerical solution of Hamilton equations is used as a proposal in a Metropolis step
- the accept-reject step guarantees that PH is the equilibrium distribution, even if

$$\delta H \neq 0$$

- For the correctness of the HMC, the numerical integrator must preserve two **key properties** of Hamilton dynamics
  - *Time-reversibility*

$$P_{MD}((\pi, U) \to (\pi', U')) = P_{MD}((-\pi', U') \to (-\pi, U))$$

  this guarantes a symmetric proposal

  - *Phase-space measure preservation*

$$D\pi(0)\, DU(0) = D\pi(\tau) DU(\tau)$$

  otherwise change of measure has to be taken into account.

  In conjuction with time reversibility this guarantes *detailed balance*

Molecular Dynamics integration

Integrable steps: with time evolution operators involving $\widehat{T} = T' \frac{\partial}{\partial q}$ and $\widehat{S} = -S' \frac{\partial}{\partial p}$

$$e^{\tau \widehat{T}} : f(p, q) \to f(p, q + \tau T'(p))$$

$$e^{\tau \widehat{S}} : f(p, q) \to f(p - \tau S'(q), q)$$

Measure preserving/Volume preserving

$$J(e^{\tau \widehat{T}}) = \frac{\partial e^{\tau \widehat{T}}(p, q)}{\partial (p, q)} = \det \begin{bmatrix} 1 & \tau T''(p) \\ 0 & 1 \end{bmatrix} = 1$$

$$J(e^{\tau \widehat{S}}) = \frac{\partial e^{\tau \widehat{S}}(p, q)}{\partial (p, q)} = \det \begin{bmatrix} 1 & 0 \\ -\tau S''(q) & 1 \end{bmatrix} = 1$$

- $exp(\tau \widehat{T})$ and $exp(\tau \widehat{S})$ are exactly integrable for any τ
- can be combined to built symplectic integrators i.e. time-reversible and measure preserving

Leap Frog: $[I_{LPFR}(h)]^n = \left(e^{\frac{h}{2} \widehat{S}} e^{h \widehat{T}} e^{\frac{h}{2} \widehat{S}} \right)^n$ which is reversible by construction and volume preserving

Integration error of symplectic integrators

Using **Baker-Campbell-Hausdorff (BCH)** formula

$$\ln(e^A e^B) = (A + B) + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] - [B, [A, B]]) + ...$$

the first error terms can be calculated:

$$[I_{LPFR}(h)]^n = \left(exp[(\hat{T} + \hat{S})h - \frac{1}{24}([\hat{S}, [\hat{S}, \hat{T}]] + 2[\hat{T}, [\hat{S}, \hat{T}]])h^3 + O(h^5)] \right)^\tau / h$$

$$= \left(exp[\tau((\hat{T} + \hat{S}) - \frac{1}{24}([\hat{S}, [\hat{S}, \hat{T}]] + 2[\hat{T}, [\hat{S}, \hat{T}]])h^2 + O(h^4))] \right)$$

$$\equiv exp(\tau\tilde{H}) = exp(\tau(\hat{T} + \hat{S}) + O(h^2))$$

Higher order integrators can be contructed:

- by adding more terms with parameters and eliminating higher oder terms $O(h^n)$
- usually fourth order sufficient
- higher order integrator become more unstable and due to that not effective in regions with $P^{acc} \sim 90$

Shadow Hamiltonian

Shadow Hamiltonian of Leap frog : stays invariant under integration

$$\Delta H_{LPFR} = \frac{1}{24}[(S,(S,T))_p + 2(T,(S,T))_p]h^2 + O(h^4)$$

$$= -\frac{1}{24}(S'^2(q) - 2p^2 S''(q))h^2 + O(h^4)$$

with

$$S'^2(q) = F^2 \quad \text{and} \quad S''(q) = F'$$

Remarks:

- existence of a conserved Hamiltonian $\tilde{H}$ along the trajectory means

$$\delta H = (H^{(f)} - \tilde{H}^{(f)}) - (H^{(i)} - \tilde{H}^{(i)}) = (\Delta H^{(f)} - \Delta H^{(i)}) = O(h^2)$$

  δH is independent from the trajectory length τ

Generalization of MD integrators

Second minimal norm scheme (OMF2)

$$I_{\mathrm{OMF2}}(h) = e^{\lambda h \hat{S}} e^{h/2 \hat{T}} e^{(1-2\lambda) h \hat{S}} e^{h/2 \hat{T}} e^{\lambda h \hat{S}}$$

with

$$\Delta H_{\mathrm{OMF2}} = (c_1(\lambda)(S,(S,T))_p + c_2(\lambda)(T,(S,T))_p)h^2 + O(h^4)$$

Minimizing $c_1^2 + c_2^2$ gives $\lambda \approx 0.19$

Fourth order integrator (OMF4) with 11 stages

$$I_{\mathrm{OMF4}}(h) = e^{r_0 h \hat{S}} \cdots e^{r_0 h \hat{S}} \qquad \text{and} \qquad \Delta H_{\mathrm{OMF4}} = O(h^4)$$

Remarks

- Measuring $\mathrm{var}(\Delta H)$ in simulations and minimizing it allows for a systematic optimization *[Clark et al. 11]*
- higher order integrator can be defined utilizing the force-gradient term $(S,(S,T))$
- variants are implemented in *openQCD*, see *[Schaefers, J.F. et al. 2024]*

Multiple time-scale integration

Multiple actions

$$H(p,q) = \frac{1}{2}p^2 + S_1(q) + S_2(q) \qquad \|F_2\| \ll \|F_1\|$$

If $\mathrm{Cost}(F_2) \gg \mathrm{Cost}(F_1)$ it may be convenient to use different step sizes h

Nested integrators *[Sexton, Weingarten 92]*

$$I(h) = e^{\frac{h}{2}\hat{S}_2}\left(e^{\frac{h}{2m}\hat{S}_1}e^{\frac{h}{m}\hat{T}}e^{\frac{h}{2m}\hat{S}_1}\right)^m e^{\frac{h}{2}\hat{S}_2}$$

Shadow Hamiltonian

$$\Delta H = [\alpha F_2^2 + \beta F_2' + \beta F_1 F_2 + \frac{1}{m^2}(\alpha F_1^2 + \beta F_1')]h^2 + O(h^4)$$

Remarks

- Correlation term between F_1 and F_2 is not suppressed by $m \rightarrow$ efficiency depends on correlation between forces
- in lattice QCD, $\|F_G\| \gg \|F_{F,1}\|$ but it opposite for their cost $\longrightarrow$ natural cost ordering

Some Remarks on MD integration

Gauge group integration

$$e^{h\hat{T}} : U(x,\mu) \to e^{h\pi(x,\mu)} U(x,\mu) \qquad \text{and} \qquad \pi(x,\mu) \to \pi(x,\mu)$$

$$e^{h\hat{S}} : U(x,\mu) \to U(x,\mu) \qquad \text{and} \qquad \pi(x,\mu) \to \pi(x,\mu) - hF(x,\mu)$$

Measure preservation:

$$\langle e^{-\delta H} \rangle = 1 \quad \delta H = H^{(f)} - H^{(i)}$$

Reversibility:

$$\Delta = \|U' - U\| \quad (\pi', U') = F \circ [I(h)]^n \circ F \circ [I(h)]^n (\pi, U)$$

with

$$F(\pi, U) = (-\pi, U)$$

is violated by rounding errors.

Remarks on MD integration

Acceptance probability:

$$P^{acc} = \langle \min[1, e^{-\delta H}] \rangle \overset{V\to\infty}{=} \operatorname{erfc}(\sqrt{\sigma^2(\delta H)/8})$$

With

$$\sigma^2(\delta H) = \langle (\delta H)^2 \rangle - \langle \delta H \rangle^2 \propto V h^{2n}$$

To tune the algorithm:

- Select stable integrator, see *[Schaefers, J.F. et al. 2025]*
- Minimize cost per trajectory at constant acceptance rate
  - Requires stable integrator

$$P^{acc} = \text{const.} \quad \Longrightarrow \quad \sigma^2 = \text{const.} \quad \Longrightarrow \quad h \propto V^{-1/2n}$$

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References

- Part of the lecture is based on Mattia Della Brida's Lattice Practice Contribution of 2021

Other references:

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Molecular Dynamics integration

Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 + S(q) = T(p) + S(q)$$

Time-evolution operator

$$exp\left(\tau\frac{d}{dt}\right) f(p(t),q(t)) = f(p(t+\tau),q(t+\tau))$$

(taylor expansion). We can write

$$exp\left(\tau\frac{d}{dt}\right) = exp\left(\tau\left[\frac{dp}{dt}\frac{\partial}{\partial t} + \frac{dq}{dt}\frac{\partial}{\partial t}\right]\right) = exp\left(\tau\left[-\frac{\partial H}{\partial q}\frac{\partial}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial}{\partial t}\right]\right) \equiv exp\left(\tau\hat{H}\right)$$

Hamiltonian vector field

$$\hat{H} = \left[\frac{\partial H}{\partial p}\frac{\partial}{\partial t} - \frac{\partial H}{\partial q}\frac{\partial}{\partial t}\right] = \hat{T} + \hat{S}$$

It follows

$$exp(\tau\hat{H})H = H \quad \Rightarrow \quad \partial_t H = 0 \qquad and \qquad \hat{T} = T'\frac{\partial}{\partial q} \quad and \quad \hat{S} = -S'\frac{\partial}{\partial p}$$

Shadow Hamiltonian

The commutator of two Hamiltonian vector fields is a Hamiltonian vector field

$$\tilde{H} = \frac{\partial \tilde{H}}{\partial p}\frac{\partial}{\partial q} - \frac{\partial \tilde{H}}{\partial q}\frac{\partial}{\partial p}$$

Symplectic intergrators exactly conserve a shadow Hamiltonian

It holds

$$[\hat{H}_1, \hat{H}_2] = \hat{H}_3$$

and its follows

$$H_3 = (H_1, H_2)_p = \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial q} - \frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial p}$$

Now to find the shadow Hamiltonian, replace the commutators with Poisson brackets

Shadow Hamiltonian of Leap frog : stays invariant under integration

$$\Delta H_{LPFR} = \frac{1}{24}[(S,(S,T))_p + 2(T,(S,T))_p]h^2 + O(h^4)$$