UNIVERSITÄT BONN

JÜLICH FORSCHUNGSZENTRUM

From Quarks and Gluons to Nuclear Forces and Structure

Lecture 5: Intro to Hybrid Monte Carlo

July 22, 2019 | Thomas Luu, IAS-4

Up till now we've been doing *local* updates!

"*Simulated Annealing*"

- Randomly select a degree of freedom (e.g. auxilliary field ϕ, link variable U_μ, or spin) on a particular site x
- Jiggle the degree of freedom using some random procedure
- Calculate the change of some quantity due to the change of the state, which is usually the change in the hamiltonian or action
- Accept/reject the change according to some predescribed procedure (e.g. Metropolis-Hastings algorithm)
- Repeat

- The whole accept/reject procedure depends on a single site x (or clusters of sites).
- If the interactions between sites are local, then the change of the action/hamiltonian can be easily calculated since it only depends on the sites near x. This can be fast and efficient. This is a *local update*.

WARNING! It can take a long time to sweep through all degrees of freedom in this manner. For large lattices, this algorithm scales *poorly*!

When do local updates fail?

We answer this question by posing more questions:

- What happens when interactions are no longer local? Not so easy to calculate the change in the state!
- What if there is a phase transition, and some correlation length ξ diverges? Local updates cannot capture such behavior. Indeed, slight pertubations near phase transitions can have large consequences!
  - Example: $D \geq 2$ Ising model
  - Example: Lattice QCD in the continuum limit (!)
- In these cases local updates have bad acceptance rates and cannot capture all relevant physical length scales. We encounter *critical slowing down*

Goal: global updates

We want to find an algorithm that allows us to update all degrees of freedom at the same time, and then do the accept/reject.

Some reminders in case you partied too hard over the weekend!

Definition (The partition function $\mathcal{Z}$)

$$\mathcal{Z} = \int \mathcal{D}[\phi] e^{-S[\phi]} \tag{1}$$

The integration metric is

$$\mathcal{D}[\phi] = \int \prod_i d\phi_i \,, \tag{2}$$

where the product i is over all degrees of freedom (e.g. sites, spins, color, flavor, etc. . .). Integrating over this metric is interpretated as the *path integral*.

Definition (Observable $\mathcal{O}$)

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\phi] e^{-S[\phi]} \mathcal{O}[\phi] = \int \mathcal{D}[\phi] P[\phi] \mathcal{O}[\phi] \tag{3}$$

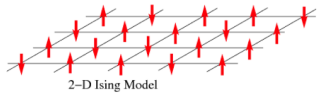
Example actions $S[\phi]$ you've encountered thus far in these lectures

- Example: QED
- Example: 1-D (an)Harmonic oscillator
- Example: pure SU(3) gauge theory (yes, I know, the code was VERY slow)
- Example: QCD (i.e. SU(3) gauge theory + fermions)
- Example: Hubbard model (ok, it was just a 1-site problem, but it had fermions!)
- NEW Example: Ising model

But why the Ising model?

- One of the goals of this lecture is to draw the connection between critical slowing down near phase transitions
- This motivates the need for *global* updates
- Easiest to see phase transitions (or *remnants* of phase transitions in finite volumes) and their consequences (e.g. diverging correlation lengths) using the 2D Ising model (IMO)
- General concepts are applicable to phase transitions in other systems (e.g. lattice QCD in the continuum limit, Hubbard model at critical coupling U (Mott-insulator phase transition))

So what is the Ising model?



- Collection of spins on an array of lattice sites
- Hamiltonian

$$H(s_1, \ldots, s_N) = -\sum_{i,j} s_i J_{ij} s_j + \sum_i h_i s_i \qquad \begin{cases} J_{ij} > 0 & \text{ferromagnetic} \\ J_{ij} < 0 & \text{anti-ferromagnetic} \end{cases}$$

- Partition function

$$\mathcal{Z} = \sum_{s_1,\ldots,s_N} e^{-\beta H(s_1,\ldots,s_N)}$$

- Expectation value of some operator O

$$\langle O \rangle = \sum_{s_1,\ldots,s_N} O(s_1, \ldots, s_N) \frac{e^{-\beta H(s_1,\ldots,s_N)}}{\mathcal{Z}}$$

Wait! Is this problem really that hard?

Answer: yes and no

No answer (assumes only nearest neighbor interactions):

- 1-D problem is analytically solved (Ising did this, but then he assumed too much!)
- 2-D problem is solved thanks to Onsager

Yes answer (for general interactions, NOT just nearest neighbor):

- For $D > 2$, answer not known
- Numerically, even in 2-D the problem is non-trivial. One would have to sum 2^N configurations (where N is the number of lattice sites), and this starts to hit the "*curse of dimensionality*"!

We are naturally interested in a numerical solution

But you've heard this story before!

- Even if we could sum over all states, we'd be wasting a lot of cpu time
  - Most states contribute almost zero weight to the sum (the Boltzmann weight suppresses them)
    $$\frac{e^{-\beta H(s_1,\ldots,s_N)}}{\mathcal{Z}}$$
  - Energy fluctuations scale as
    $$\frac{\langle H^2\rangle - \langle H\rangle^2}{\langle H\rangle^2} \propto \frac{1}{N}$$
  - This means that the number of configurations that contribute to the Boltzmann sum has zero weight in the thermodynamic limit $N \to \infty$!
- So we need to sample smart!

How would you sample in a smart fashion?

You know how to do this!

- Randomly choose a spin and flip it
- Calculate change in action ΔS
- Accept spin flip with probability

$$\mathbb{P}_{a/r} = \min\left(1, e^{-\Delta S}\right)$$

- Repeat

A couple things to note:

- Usually one does a “sweep” through all lattice sites before writing out a spin configuration
- We are working in a *discrete* space (have only spin up or down per site)
  - What are the implications of this?

You have access to a python script that does this

generateConfigs.py

```
for i in range(ncfg): # now take statistics...
    for j in range(nsweep):
        x,y=random.randint(0,nx-1),random.randint(0,ny-1)  # this routine randomly selects sites
        deltaS = action.calcDeltaS_2d(s,J,h,x,y,nx,ny)
        if random.uniform(0,1) <= math.exp(-deltaS): # accept!  (metropolis-hastings)
            s[x][y] *= -1
            prob=np.append(prob,1.)
        else:  # otherwise reject
            prob=np.append(prob,0.)
    m=np.append(m,s.mean())  # mean magnetization per site
    absm=np.append(absm,abs(s.mean()))  # absolute value of mean magnetization per site
    spins.append(s)
```

Included in the codes is `actions.py`, which uses the package `numba` (JIT compilation). Comment out this stuff if your code segfaults (or update `numba`)

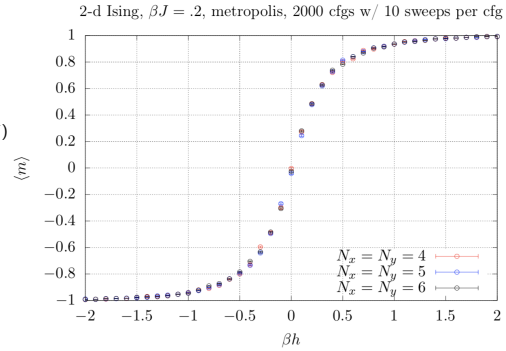
Some interesting observables

- Energy per site

$$\langle \epsilon \rangle = \frac{1}{N} \sum_{s_1,\ldots,s_N} H(s_1,\ldots,s_N) \frac{e^{-\beta H(s_1,\ldots,s_N)}}{\mathcal{Z}} = -\frac{1}{N} \frac{\partial}{\partial \beta} \log(\mathcal{Z})$$

- Net spin per site (magnetization)

$$\langle m \rangle = \frac{1}{N} \left\langle \sum_i s_i \right\rangle = \frac{1}{N\beta} \sum_i \frac{\partial}{\partial h_i} \log(\mathcal{Z})$$



The spin-spin correlator $g(r)$

The spin-spin correlator is defined as[1]

$$g(i,j) = \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle = \langle s_i s_j \rangle - \langle m \rangle^2$$

Translational invariance implies that the correlator is function of the relative distance between spin sites

$$g(r) = \langle s_i s_{i+\vec{r}} \rangle - \langle m \rangle^2 \sim e^{-r/\xi}$$

Here ξ is the spin-spin "correlation length".

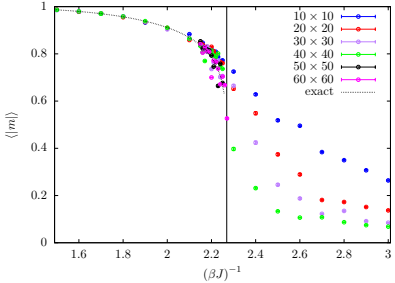
[1] For those who did the exercise on autocorrelation functions, this should look VERY familiar!

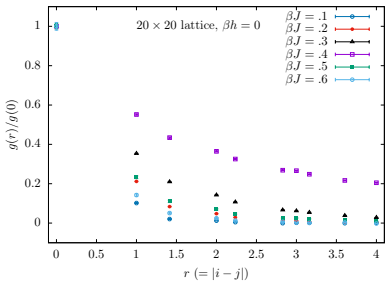
Near a phase transition

- For $D \geq 2$, the Ising model undergoes a phase transition at some critical value of βJ (here we assume $h = 0$)
  - For $D = 2$ have (thank you Onsager!)

$$(\beta J)_c^{-1} = \frac{2}{\ln(1+\sqrt{2})} = 2.26919\ldots$$

- Near phase transitions, correlation lengths diverge $\implies$ all length scales are relevant!





Near phase transitions, it takes longer and longer to obtain statistically independent results. Local updates cannot capture gross changes in the system and acceptance rates plummet. We have "critical slowing down". Need a way to do global updates before the accept/reject step.

Enter *Hybrid Monte Carlo (HMC)*

First step: multiply by $\mathbb{1}$!

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}[\phi] e^{-S[\phi]} \mathcal{O}[\phi]}{\int \mathcal{D}[\phi] e^{-S[\phi]}} = \frac{\int \mathcal{D}[p]\mathcal{D}[\phi] e^{-\frac{1}{2}\sum_i p_i^2 - S[\phi]} \mathcal{O}[\phi]}{\int \mathcal{D}[p]\mathcal{D}[\phi] e^{-\frac{1}{2}\sum_i p_i^2 - S[\phi]}} = \frac{\int \mathcal{D}[p]\mathcal{D}[\phi] e^{-\mathcal{H}[p,\phi]} \mathcal{O}[\phi]}{\int \mathcal{D}[p]\mathcal{D}[\phi] e^{-\mathcal{H}[p,\phi]}}$$

where

$$\mathcal{D}[p] = \prod_i dp_i$$

$$\mathcal{H}[p,\phi] = \frac{1}{2}\sum_i p_i^2 + S[\phi] \qquad \text{(artificial Hamiltonian)}$$

For each degree of freedom i, we essentially introduced a normalized gaussian variable p_i

And we can easily (numerically) perform these gaussian integrals since we have *fast* routines for sampling gaussians!

Equations of motion of $\mathcal{H}[p, \phi]$

The Euler-Lagrange equations of motions for p and ϕ that keep $\mathcal{H}[p, \phi]$ invariant:

$$\begin{aligned} \dot{\phi}_i &= \frac{\partial \mathcal{H}}{\partial p_i} = p_i \\ \dot{p}_i &= -\frac{\partial \mathcal{H}}{\partial \phi_i} = -\frac{\partial \mathcal{S}}{\partial \phi_i} \end{aligned}$$

Integrating these equations *exactly* tells us how to evolve

$$\begin{aligned} \phi &\rightarrow \phi' \\ p &\rightarrow p' \, , \end{aligned}$$

such that

$$\mathcal{H}[p, \phi] \rightarrow \mathcal{H}[p', \phi'] = \mathcal{H}[p, \phi] \, .$$

Any numerical integration of Euler-Lagrange equations:

$$\mathcal{H}[p, \phi] \rightarrow \mathcal{H}[p', \phi'] = \mathcal{H}[p, \phi] + \Delta\mathcal{H} \, .$$

The Hybrid Monte-Carlo Algorithm

1. Input: some ensemble of ϕ
2. Generate p_i from normal distribution (i.e. perform MC integration over p field)
3. Integrate EoM numerically for some trajectory length τ (molecular dynamics trajectory)
4. Calculate $\Delta\mathcal{H}$ and accept new phi' with probability

$$\min\{1, e^{-\Delta\mathcal{H}}\}$$

5. Go back to 2

Note: **ALL** fields ϕ were evolved at the same time to determine $\Delta\mathcal{H}$!

Why is this called *hybrid* MC?

- To perform the numerical integration of the EoMs, one uses a “molecular dynamics” integrator. So our routine involves both MC (gaussian) sampling/integration (e.g. quantum fluctuations) of conjugate variables and MD integration (to solve the EoMs). This is what is meant by *hybrid algorithm*.
- The ACCEPT/REJECT step at the end differentiates this problem as *hybrid MC*
- Note: there are certain constraints that must be enforced on the integrator!
  - *symplectic* (or area preserving): the integration scheme must leave the measure $\mathcal{D}[p]\mathcal{D}[\phi]$ invariant
  - *reversible*: integrating *backwards* from the new configuration should give the old configuration
  - These conditions are needed to ensure *detailed balance*
- Must ensure ergodicity in ϕ (come back to this later)

The *leap-frog* integrator

This integrator satisfies the conditions for *area preservation* and *reversibility*

3-step leap-frog integration of length $\tau = 2\epsilon$

$$\begin{array}{ccccccccc} p(0) & \to & p(\epsilon/2) & \longrightarrow & p(3\epsilon/2) & \longrightarrow & p(5\epsilon/2) & \to & p(3\epsilon) \\ \phi(0) & & \longrightarrow & \phi(\epsilon) & \longrightarrow & \phi(2\epsilon) & \longrightarrow & & \phi(3\epsilon) \end{array}$$

Here, for example

$$p\left(\frac{\epsilon}{2}\right) = p(0) - \frac{\epsilon}{2} \times \frac{\partial \mathcal{S}}{\partial \phi(0)}$$
$$\phi(\epsilon) = \phi(0) + \epsilon \times p\left(\frac{\epsilon}{2}\right)$$

Leap-frog is the limit of the more general *Omelyan* integrator

If one starts at $p(3\epsilon)$ and $\phi(3\epsilon)$, and sets $\epsilon \to -\epsilon$ in the leap-frog integrator, one arrives back at $p(0)$ and $\phi(0)$. This is the same for and n-step integration procedure. This demonstrates *reversibility*:

$$P_{md}(p', \phi'|p, \phi) = P_{md}(-p, \phi| - p', \phi') = P_{md}(p, \phi|p', \phi')$$

As one moves from $\phi \to \phi'$ and $p \to p'$, one must account for the change of variables

$$dpd\phi \to dp'd\phi' = \det\left[\frac{\partial(p', \phi')}{\partial(p, \phi)}\right] dpd\phi$$

Can be shown that Jacobian $\det\left[\frac{\partial(p', \phi')}{\partial(p, \phi)}\right] = 1 \implies$ *area preservation*.

(Outline of) Proof of detailed balance

We use these results to (quasi-) prove detailed balance

Probability of $\phi \to \phi'$

$$P(\phi'|\phi) = \int \mathcal{D}[p]\mathcal{D}[p'] P_{a/r}(p', \phi'|p, \phi) P_{md}(p', \phi'|p, \phi) e^{-p^2/2}$$

where

$$P_{a/r}(p', \phi'|p, \phi) = \min\left(1, \frac{\exp(-\mathcal{H}[p', \phi'])}{\exp(-\mathcal{H}[p, \phi])}\right)$$

Now can do the following manipulation:

$$
\begin{aligned}
P_{a/r}(p', \phi' | p, \phi) &= \min\left(1, \frac{\exp(-\mathcal{H}[p', \phi'])}{\exp(-\mathcal{H}[p, \phi])}\right) \\
&= e^{-\mathcal{H}[p', \phi'] + \mathcal{H}[p, \phi]} \min\left(\frac{\exp(-\mathcal{H}[p, \phi])}{\exp(-\mathcal{H}[p', \phi'])}, 1\right) \\
&= e^{-\mathcal{H}[p', \phi'] + \mathcal{H}[p, \phi]} P_{a/r}(p, \phi | p', \phi') \\
&= e^{-p'^2/2 - S[\phi'] + p^2/2 + S[\phi]} P_{a/r}(-p, \phi | -p', \phi')
\end{aligned}
$$

The last step relies on the fact that p and p' are *degrees of freedom*, i.e. they are quadratic in the action.

Detailed balance

Now plugging everything in and integrating over p and p' gives

$$
\begin{aligned}
P(\phi'|\phi) &= \int \mathcal{D}[p]\mathcal{D}[p'] e^{-p'^2/2 - S[\phi'] + p^2/2 + S[\phi]} P_{a/r}(-p, \phi| - p', \phi') P_{md}(p, \phi|p', \phi') e^{-p^2/2} \\
&= \int \mathcal{D}[p]\mathcal{D}[p'] e^{-p'^2/2 - S[\phi'] + S[\phi]} P_{a/r}(-p, \phi| - p', \phi') P_{md}(p, \phi|p', \phi') \\
&= \int \mathcal{D}[p]\mathcal{D}[p'] e^{-p'^2/2 - S[\phi'] + S[\phi]} P_{a/r}(-p, \phi| - p', \phi') P_{md}(-p, \phi| - p', \phi') \quad \text{(reversibility)} \\
&= \int \mathcal{D}[p]\mathcal{D}[p'] e^{-p'^2/2 - S[\phi'] + S[\phi]} P_{a/r}(p, \phi|p', \phi') P_{md}(p, \phi|p', \phi') \quad (p \to -p, p' \to -p') \\
&= e^{-S[\phi'] + S[\phi]} P(\phi|\phi')
\end{aligned}
$$

$$
\Longrightarrow \boxed{e^{-S[\phi]} P(\phi'|\phi) = e^{-S[\phi']} P(\phi|\phi')}
$$

So we have detailed balance!

HMC is *magical*!

Let's look at the last equation of the previous slide again:

$$P(\phi'|\phi) = \int \mathcal{D}[p]\mathcal{D}[p'] e^{-p'^2/2 - S[\phi'] + S[\phi]} P_{a/r}(p, \phi | p', \phi') P_{md}(p, \phi | p', \phi')$$

Assume we have an *exact* MD integrator. This implies that

$$P_{a/r}(p, \phi | p', \phi') = 1 \; \forall \; p', \phi' \qquad \text{(exact integrator)}$$

Integration over $\mathcal{D}[p']$ above (no integration over $\mathcal{D}[p]$ since it is constrained by Hamilton's equations) gives the same detailed balance result, namely,

$$e^{-S[\phi]} P(\phi'|\phi) = e^{-S[\phi']} P(\phi|\phi')$$

The Accept/Reject method corrects numerical errors of the MD integrator! (when averaged over the ensemble)

First application of *HMC*: The long-distance Ising model

- Here we set $J_{ij} = \frac{J}{N}$ and $h_i = h \quad \forall\, i, j$:

$$\begin{aligned} H(s,h) &= -\frac{1}{2}\frac{J}{N}\sum_{i,j} s_i s_j - h\sum_i s_i \\ &= -\frac{1}{2}\hat{J}\sum_{i,j} s_i s_j - h\sum_i s_i \end{aligned}$$

- Our partition function:

$$\mathcal{Z} = \sum_{\{s_i\}=\pm 1} e^{-\beta H(s,h)} = \sum_{\{s_i\}=\pm 1} e^{\beta J\left(\frac{1}{2N}\sum_{i,j} s_i s_j + \frac{h}{J}\sum_i s_i\right)}$$

- But the total spin $s = \sum_i s_i$. So we can simplify the sum over spins

$$\sum_{i,j} s_i s_j = \left(\sum_i s_i\right)^2 = s^2 \implies \mathcal{Z} = \sum_{\{s_i\}=\pm 1} e^{\beta J\left(\frac{1}{2N}s^2 + \frac{h}{J}s\right)}$$

Now apply HS transformation

Recall:

$$e^{-\frac{1}{2}|U|s^2} = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi|U|}} e^{-\frac{\phi^2}{2|U|} \pm i\phi s}$$

$$e^{\frac{1}{2}|U|s^2} = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi|U|}} e^{-\frac{\phi^2}{2|U|} \pm \phi s}$$

In our case, $U = \beta J/N = \beta\hat{J}$. Assume $J > 0$ (ferromagnetic case):

$$\mathcal{Z} = \sum_{\{s_i\}=\pm 1} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}} + (\beta h \pm \phi)s}$$

Now sum over all spins!

$$\mathcal{Z}[J>0] = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} \sum_{\{s_i\}=\pm 1} e^{(\beta h \pm \phi)s}$$

$$= \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} \prod_{i=1}^{N} \sum_{s_i=\pm 1} e^{(\beta h \pm \phi)s_j}$$

$$= \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} \prod_{i=1}^{N} 2\cosh(\beta h \pm \phi)$$

$$= \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} [2\cosh(\beta h \pm \phi)]^N = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}} + N\log[2\cosh(\beta h \pm \phi)]}$$

Expectation values of operators O

As usual, the expectation value of some operator O is simply

$$\langle O \rangle = \frac{1}{\mathcal{Z}} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} O[\phi] e^{-\frac{\phi^2}{2\beta\hat{J}} + N \log[2\cosh(\beta h + \phi)]}$$

$$= \int_{-\infty}^{\infty} d\phi \; O[\phi] \; \mathbb{P}[\phi]$$

where

$$\mathbb{P}[\phi] = \frac{1}{\mathcal{Z}} \frac{e^{-\frac{\phi^2}{2\beta\hat{J}} + N \log[2\cosh(\beta h + \phi)]}}{\sqrt{2\pi\beta\hat{J}}} \, .$$

Goal: Generate ensemble of ϕ using HMC

Multiply top and bottom by 1

$$1 = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} e^{-p^2/2}$$

Have

$$\langle O \rangle = \frac{1}{\tilde{\mathcal{Z}}} \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} O[\phi] e^{-\frac{p^2}{2} - \frac{\phi^2}{2\beta\hat{J}} + N \log(2\cosh(\beta h + \phi))}$$

where

$$\begin{aligned} \tilde{\mathcal{Z}} &= \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{p^2}{2} - \frac{\phi^2}{2\beta\hat{J}} + N \log(2\cosh(\beta h + \phi))} \\ &= \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\mathcal{H}[p,\phi]} \end{aligned}$$

Derive equations of motion from $\mathcal{H}[p, \phi]$

Problem: Derive the following expressions

$$\dot{\phi} = \frac{\partial}{\partial p}\mathcal{H} = p$$

$$\dot{p} = -\frac{\partial}{\partial \phi}\mathcal{H} = -\frac{\phi}{\beta \hat{J}} + N \tanh(\beta h + \phi)$$

Problem: code up the leapfrog integrator

- Draw $p_0 \in \mathcal{N}_{0,1}$
- Set $(\Pi, \Phi) = (p_0, \phi_0)$
- First (half) step of leapfrog:

$$\Phi = \Phi + \frac{\epsilon}{2}\Pi$$

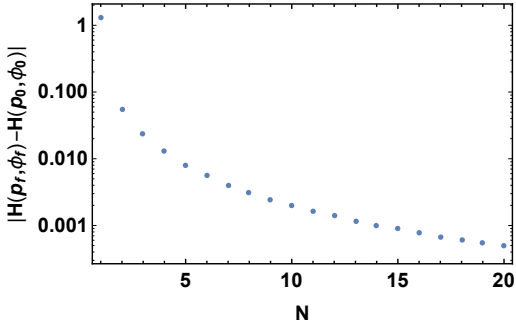
- $N_{md} - 1$ steps (repeat $N_{md} - 1$ times):

$$\Pi = \Pi - \epsilon\left(\frac{\Phi}{\beta\hat{J}} - N\tanh(\beta h + \Phi)\right)$$
$$\Phi = \Phi + \epsilon\Pi$$

- Last step of leapfrog:

$$\Pi = \Pi - \epsilon\left(\frac{\Phi}{\beta\hat{J}} - N\tanh(\beta h + \Phi)\right)$$
$$\Phi = \Phi + \frac{\epsilon}{2}\Pi$$

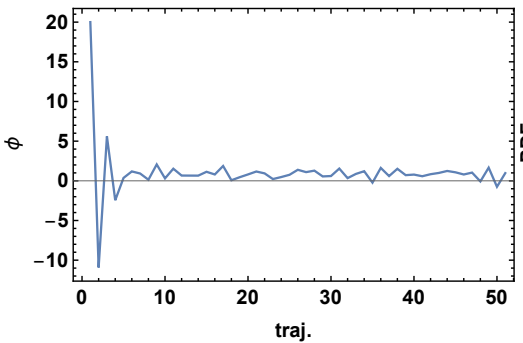
- Set $(p_f, \phi_f) = (\Pi, \Phi)$

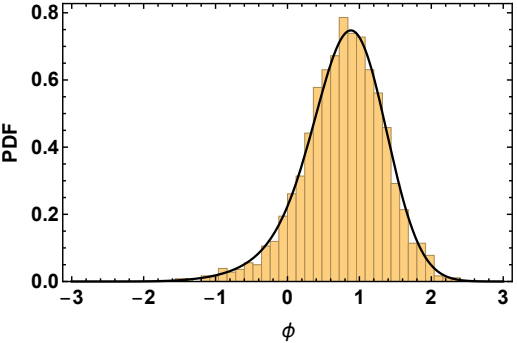


Since this is a numerical integrator, we do not have exact constants of motions but should find that $\mathcal{H}(p_f, \phi_f) = \mathcal{H}(p_0, \phi_0) + \mathcal{O}(\epsilon^2)$, which can be improved by increasing N_{md} while keeping the overall trajectory length constant.

Combine with Metropolis-Hastings to generate ensemble!

Et voilà! You now have implemented HMC!





Now you can calculate observables!

Let's define some observables

The average magnetization per site and energy persite are given by

$$\begin{aligned}
\langle m \rangle = \frac{1}{N}\left\langle \sum_i s_i \right\rangle = \frac{1}{N}\langle s \rangle &= \frac{1}{\mathcal{Z}}\frac{1}{N}\sum_{\{s_i\}=\pm 1} s e^{\beta J\left(\frac{1}{2N}s^2+\frac{h}{J}s\right)} \\
&= \frac{1}{Z}\sum_{\{s_i\}=\pm 1}\frac{1}{N\beta}\frac{\partial}{\partial h}e^{\beta J\left(\frac{1}{2N}s^2+\frac{h}{J}s\right)} \\
&= \frac{1}{N\beta}\frac{\partial}{\partial h}\log(\mathcal{Z}) \\
\langle \epsilon \rangle = \frac{1}{N}\langle H \rangle &= -\frac{1}{N}\frac{\partial}{\partial \beta}\log(\mathcal{Z})
\end{aligned}$$

Problem:

Show that the corresponding operators in this case is

$$O[\phi] = \begin{cases} \tanh(\beta h + \phi) & \text{(magnetization)} \\ \frac{1}{2\beta N} - \frac{\phi^2}{2\beta^2 J} - h\tanh(\beta h + \phi) & \text{(energy)} \end{cases}$$

Code up HMC and calculate some observables!

Calculate, for example, the magnetization and energy as a function βJ and βh.

- This problem is meant only as a warmup to HMC.
  - There is only one degree of freedom on the long-range Ising model: ϕ
  - $\frac{k}{d} > \frac{1}{2}$!
- Thus this problem does not show the power of HMC, which is the ability to do *global* updates.

This comes tomorrow!