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From Quarks and Gluons to Nuclear Forces and Structure

Lecture 6: Intro to Hybrid Monte Carlo II

July 23, 2019 | Thomas Luu, IAS-4

Goal of today’s lecture

Apply HMC to more sophisticated problems:

- 1-site Hubbard Model
- 2-D Ising model vI
- 2-D Ising model vII
- Alternative to least-squares fitting

You choose which one to implement!

- Pitfalls of HMC
  - 1-D anHarmonic Oscillator

Recap of HMC

- Given action S, make an *artificial* Hamiltonian:

$$\mathcal{H}[p,\phi] = \frac{1}{2}\sum_i p_i^2 + S[\phi]$$

- For each degree of freedom ϕ_i there is a "*conjugate momentum*" p_i, which one samples from a normal distribution
- Now calculate EoMs:

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

- Integrate EoMs for some trajectory length using leapfrog integration
- Accept/Reject

Let's do this for our Hubbard example

Recall the partition function:

$$\mathcal{Z} = \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t - 1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}} e^{-\frac{1}{2\tilde{U}}\phi_t^2} \right] \det\left(M[\phi] M[-\phi] \right) = \int \mathcal{D}[\phi] e^{-\frac{1}{2\tilde{U}} \sum_t \phi_t^2 + \log\det(M[\phi]M-\phi])}$$

where $M[\phi]_{t',t} = \delta_{t't} - \mathcal{B}_{t'} e^{-\phi_t} \delta_{t',t+1}$ and

$$\mathcal{B}_t = \begin{cases} +1 & (0 \leq t < N_t) \\ -1 & (t = N_t) \end{cases}$$

So the artificial Hamiltonian is

$$\mathcal{H}[p, \phi] = \frac{1}{2} \sum_t p_t^2 + \frac{1}{2\tilde{U}} \sum_t \phi_t^2 - \log\det\left(M[\phi] M - \phi] \right)$$

Equations of motions with matrices

$$\mathcal{H}[p,\phi] = \frac{1}{2}\sum_t p_t^2 + \frac{1}{2\tilde{U}}\sum_t \phi_t^2 - \log\det\left(M[\phi]M - \phi]\right)$$

Equations of motion:

$$\dot{\phi}_j = \frac{\partial \mathcal{H}}{\partial p_j} = p_j \qquad \text{(easy)}$$

$$\dot{p}_j = -\frac{\partial \mathcal{H}}{\partial \phi_j} = -\frac{\phi_j}{\tilde{U}} + \frac{1}{2}\left(\frac{1}{\det\left(M[\phi]M[-\phi]\right)}\frac{\partial}{\partial \phi_j}\det\left(M[\phi]M[-\phi]\right)\right)$$

Derivatives of determinants

Assume Q is some square matrix and invertible. Then we have Jacobi's formula[1]

$$\frac{\partial}{\partial \phi_j} \det Q[\phi] = \det Q[\phi] \,\mathrm{tr}\left(Q[\phi]^{-1} \frac{\partial}{\partial \phi_j} Q[\phi] \right)$$

Setting $Q[\phi] = M[\phi]M[-\phi]$, and using the chain rule and cyclic properties of the trace, one gets

$$\begin{aligned} \dot{p}_j &= -\frac{\phi_j}{\tilde{U}} + \frac{1}{2}\,\mathrm{tr}\left((M[\phi]M[-\phi])^{-1} \frac{\partial}{\partial \phi_j} (M[\phi]M[-\phi]) \right) \\ &= -\frac{\phi_j}{\tilde{U}} + \frac{1}{2}\,\mathrm{tr}\left(M[\phi]^{-1} \frac{\partial}{\partial \phi_j} M[\phi] + M[-\phi]^{-1} \frac{\partial}{\partial \phi_j} M[-\phi] \right) \end{aligned}$$

where

$$\frac{\partial}{\partial \phi_j} M[\phi]_{t',t} = \delta_{j,t} \mathcal{B}_{t'} e^{-\phi_t} \delta_{t',t+1}$$

[1] `https://en.wikipedia.org/wiki/Jacobi%27s_formula`

The trace simplifies greatly in this case. . .

Artificial Hamiltonian:

$$\mathcal{H}[p,\phi] = \frac{1}{2}\sum_t p_t^2 + \frac{1}{2\tilde{U}}\sum_t \phi_t^2 - \log\det\left(M[\phi]M - \phi]\right)$$

Equations of motion:

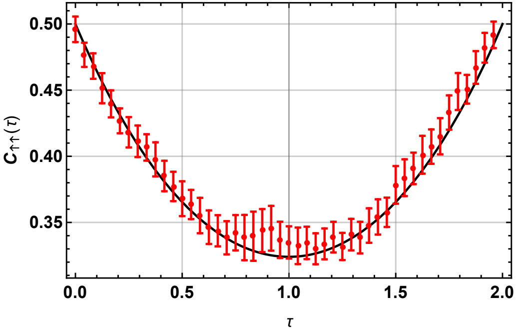
$$\begin{aligned}\dot{\phi}_j &= p_j \\ \dot{p}_j &= -\frac{\phi_j}{\tilde{U}} + \mathcal{B}_{j+1}\left(e^{-\phi_j}M^{-1}[\phi]_{j+1,j} - e^{\phi_j}M^{-1}[-\phi]_{j,j+1}\right)\end{aligned}$$

Note that the "force equation" for the conjugate momenta requires matrix *inversion*. This can be very expensive for large systems!

HMC Integration of the Hubbard model (1 site)

- Use HMC to generate an ensemble $\{\phi\}$ of size N_{cfg}
- Estimate correlator via (compare to what was done in lecture 4!)

$$C_{\uparrow\uparrow}(\tau) \approx \frac{1}{N_{cfg}} \sum_{\vec{\phi}\in\{\phi\}} M^{-1}_{\tau,0}[\phi]$$



$\beta = 2$, $U = 2$, $N_{md} = 4$, MD trajectory length=1, $N_t = 48$, $N_{cfg} = 2000$

Now let's look at the *normal* Ising model

Here's the Hamiltonian again:

$$H(s,h) = -J\sum_{\langle i,j\rangle} s_i s_j - h\sum_i s_i \ ,$$

Here $\langle i,j\rangle$ denotes nearest neighbor interactions.
Let's rewrite this as

$$H = -\frac{J}{2}\sum_{ij} s_i K_{ij} s_j - h\sum_i s_i$$

Here K_{ij} is a *connectivity* matrix and the sum over i,j is unrestricted.

The connectivity matrix K_{ij}

Examples of connectivity matrix (with periodic boundary conditions):

2×2 lattice

$$K = \begin{pmatrix} 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \\ 2 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 \end{pmatrix},$$

has eigenvalues -4, 4, 0, 0

3×3 lattice:

$$K = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix},$$

with eigenvalues 4, -2, -2, -2, -2, 1, 1, 1, 1

4×4 lattice:

$$K = \begin{pmatrix}
0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0
\end{pmatrix},$$

and has eigenvalues -4, 4, -2, -2, -2, -2, 2, 2, 2, 2, 0, 0, 0, 0, 0, 0

Can we just apply the HS transformation?

Formally yes, but numerically *NO*!

- Recall the form of the HS transformation:

$$e^{\frac{1}{2}\sum_{ij} s_i U_{ij} s_j} = \int_{-\infty}^{\infty} \frac{1}{\sqrt{\det U}} \left[\prod_i \frac{d\phi_i}{\sqrt{2\pi}}\right] e^{-\frac{1}{2}\sum_{ij}\phi_i U_{ij}^{-1}\phi_j + \sum_i \phi_i s_i} ,$$

- For this equation to be numerically stable, all eigenvalues of U must be positive!
- This is NOT the case for our connectivity matrix K!

But the eigenvalues of K are bounded!

- The eigenvalues λ of K satisfiy $|\lambda| \leq 4$.
- We use this fact to make a stable HS transformation
- To do this, we add 0 to the Hamiltonian (add and subtract a constant)

Watch!

$$
\begin{aligned}
H &= -\frac{J}{2}\sum_{ij} s_i K_{ij} s_j - h\sum_i s_i \\
&= -\frac{J}{2}\sum_{ij} s_i \left(K_{ij} + \mathcal{C}\delta_{ij}\right) s_j + \frac{\mathcal{C}J}{2}\sum_i s_i^2 - h\sum_i s_i \\
&= -\frac{J}{2}\sum_{ij} s_i \left(K_{ij} + \mathcal{C}\delta_{ij}\right) s_j + \frac{\mathcal{C}JN}{2} - h\sum_i s_i \\
&= -\frac{J}{2}\sum_{ij} s_i \tilde{K}_{ij} s_j + \frac{\mathcal{C}JN}{2} - h\sum_i s_i \ ,
\end{aligned}
$$

where $\tilde{K}_{ij} \equiv K_{ij} + \mathcal{C}\delta_{ij}$.

Now apply HS transformation

- The eigenvalues of $\tilde{K}$ are all greater than 4 as long as $\mathcal{C} > 4$.
- This shift of the eigenvalues is compensated by the term $\mathcal{C}J\sum_i s_i^2 = \mathcal{C}JN$, which is just an overall constant to the Hamiltonian.
- In principle, we don't care about overall shifts in the energy, but we keep track of it since we will need it when we (you) derive the form of the operators for the internal energy, specific heat, etc. . .

Here we go! :

$$
\begin{aligned}
\mathcal{Z} &= \sum_{\{s_i\}=+1} e^{\frac{\beta J}{2}\sum_{ij} s_i K_{ij} s_j + \beta h \sum_i s_i} \\
&= \sum_{\{s_i\}=+1} e^{\frac{\beta J}{2}\sum_{ij} s_i \tilde{K}_{ij} s_j + \beta h \sum_i s_i - \mathcal{C}\beta J\Lambda/2} \\
&= \sum_{\{s_i\}=+1} \int_{-\infty}^{\infty} \frac{1}{\sqrt{\det \tilde{K}}} \left[\prod_i \frac{d\phi_i}{\sqrt{2\pi\beta J}}\right] e^{-\frac{1}{2\beta J}\sum_{ij}\phi_i \tilde{K}_{ij}^{-1}\phi_j + \sum_i s_i(\beta h + \phi_i) - \frac{\mathcal{C}\beta J\Lambda}{2}} .
\end{aligned}
$$

You know how to do the rest!

In particular, since the argument is "linear" in the spins, we can integrate out the spins (just like in the long-distance Ising model)

$$\begin{aligned}
\mathcal{Z} &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{\det \tilde{K}}} \left[\prod_i \frac{d\phi_i}{\sqrt{2\pi\beta J}}\right] \sum_{\{s_i\}=+1} e^{-\frac{1}{2\beta J}\sum_{ij}\phi_i \tilde{K}^{-1}_{ij}\phi_j + \sum_i s_i(\beta h+\phi_i) - \mathcal{C}\beta J\Lambda/2} \\
&= \int_{-\infty}^{\infty} \frac{1}{\sqrt{\det \tilde{K}}} \left[\prod_i \frac{d\phi_i}{\sqrt{2\pi\beta J}}\right] e^{-\frac{1}{2\beta J}\sum_{ij}\phi_i \tilde{K}^{-1}_{ij}\phi_j - \frac{\mathcal{C}\beta J\Lambda}{2}} \times \left[\prod_i 2\cosh(\beta h+\phi_i)\right] \\
&= \frac{e^{-\frac{\mathcal{C}\beta J\Lambda}{2}}}{\sqrt{\det \tilde{K}}} \int_{-\infty}^{\infty} \left[\prod_i \frac{d\phi_i}{\sqrt{2\pi\beta J}}\right] e^{-\frac{1}{2\beta J}\sum_{ij}\phi_i \tilde{K}^{-1}_{ij}\phi_j + \sum_i \log(2\cosh(\beta h+\phi_i))} .
\end{aligned}$$

One last thing. We change variables to simplify some expressions: $\tilde{\phi}_i \equiv \frac{\phi_i}{\sqrt{\beta J}}$. This gives:

$$\boxed{\mathcal{Z} = \frac{e^{-\frac{\mathcal{C}\beta J\Lambda}{2}}}{\sqrt{\det \tilde{K}}} \int_{-\infty}^{\infty} \left[\prod_i \frac{d\tilde{\phi}_i}{\sqrt{2\pi}}\right] e^{-\frac{1}{2}\sum_{ij}\tilde{\phi}_i \tilde{K}^{-1}_{ij}\tilde{\phi}_j + \sum_i \log(2\cosh(\beta h+\sqrt{\beta J}\tilde{\phi}_i))}} .$$

The artificial Hamiltonian and EoMs

Here is the artificial Hamiltonian:

$$\begin{aligned}\mathcal{H}(\mathbf{p},\tilde{\phi}) &= \frac{\mathbf{p}^2}{2} + \mathcal{S}[\tilde{\phi}] \\ &= \frac{\mathbf{p}^2}{2} + \frac{\tilde{\phi}\cdot\tilde{K}^{-1}\cdot\tilde{\phi}}{2} - \sum_i \log(2\cosh(\beta h + \sqrt{\beta J}\tilde{\phi}_i))\ ,\end{aligned}$$

and the corresponding EoMs:

$$\begin{aligned}\dot{\tilde{\phi}}_i &= \frac{\partial}{\partial p_i}\mathcal{H} = p_i \\ \dot{p}_i &= -\frac{\partial}{\partial\tilde{\phi}_i}\mathcal{H} = -\frac{\partial}{\partial\tilde{\phi}_i}\mathcal{S} = -\tilde{K}_{ij}^{-1}\tilde{\phi}_j + \sqrt{\beta J}\tanh(\beta h + \sqrt{\beta J}\tilde{\phi}_i)\end{aligned}$$

In this case, the force equations also involve an inverse of a matrix, $\tilde{K}^{-1}$, but this only has to be solved once and stored for future use (as opposed to $M^{-1}[\phi]$ in the Hubbard example).

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Operators in this basis

Here I just give you the expressions for some operators. You should derive them yourself[2] to confirm that I didn't make any mistakes!

$$\langle m\rangle = \frac{1}{N\beta}\frac{\partial}{\partial h}\log(\mathcal{Z}) \implies O[\tilde\phi] = \frac{1}{N}\sum_i \tanh(\beta h + \sqrt{\beta J}\tilde\phi_i)$$

$$\langle \beta\epsilon\rangle = -\frac{\beta}{N}\frac{\partial}{\partial \beta}\log(\mathcal{Z}) \implies O[\tilde\phi] = \frac{\mathcal{C}\beta J}{2} - \frac{1}{N}\sum_i \left(\beta h + \sqrt{\beta J}\frac{\tilde\phi_i}{2}\right)\tanh(\beta h + \sqrt{\beta J}\tilde\phi_i)$$

$$\langle s_i s_j\rangle = \frac{1}{\mathcal{Z}}\frac{1}{\beta^2}\partial_{h_i}\partial_{h_j}\mathcal{Z} \implies O[\tilde\phi] = \tanh(\beta h_i + \sqrt{\beta J}\tilde\phi_i)\tanh(\beta h_j + \sqrt{\beta J}\tilde\phi_j)$$

[2] And you should derive other expressions that I did not give, e.g. specific heat, susceptibility.

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An alternative discretization of the Ising model. . .

Let's do a change of variables. We define the field ψ via

$$\tilde{\phi}_i = \tilde{K}_{ij}\psi_j - \frac{\beta h_i}{\sqrt{\beta J}} \ .$$

A little bit of algebra shows that

$$S[\tilde{\phi}] \to \frac{1}{2}\psi_i \tilde{K}_{ij}\psi_j - \frac{1}{\sqrt{\beta J}}\beta h_i \psi_i - \sum_i \log\left(2\cosh(\sqrt{\beta J}\tilde{K}_{ij}\psi_j)\right) + \frac{1}{2\beta J}\beta h_i \tilde{K}^{-1}_{ij}\beta h_j$$

$$\equiv S[\psi] + \frac{1}{2\beta J}\beta h_i \tilde{K}^{-1}_{ij}\beta h_j \ .$$

And the metric becomes

$$\mathcal{D}[\tilde{\phi}] \equiv \frac{e^{-\frac{\mathcal{C}\beta J\Lambda}{2}}}{\sqrt{\det \tilde{K}}}\left[\prod_i \frac{d\tilde{\phi}_i}{\sqrt{2\pi}}\right] \to e^{-\frac{\mathcal{C}\beta J\Lambda}{2}}\sqrt{\det \tilde{K}}\left[\prod_i \frac{d\psi_i}{\sqrt{2\pi}}\right] \ .$$

Do we have fermions???

The artificial Hamiltonian and EoMs in this version...

Here is the artificial Hamiltonian:

$$\begin{aligned}\mathcal{H}(\mathbf{p},\psi) &= \frac{\mathbf{p}^2}{2} + \mathcal{S}[\psi] \\ &= \frac{\mathbf{p}^2}{2} + \frac{1}{2}\psi_i\tilde{K}_{ij}\psi_j - \frac{1}{\sqrt{\beta J}}\beta h_i\psi_i - \sum_i \log\left(2\cosh(\sqrt{\beta J}\tilde{K}_{ij}\psi_j)\right) .\end{aligned}$$

The equations of motion are again simple to derive (repeated indices are summed),

$$\begin{aligned}\dot{\psi}_i &= \frac{\partial}{\partial p_i}\mathcal{H} = p_i \\ \dot{p}_i &= -\frac{\partial}{\partial \psi_i}\mathcal{H} = -\frac{\partial}{\partial \psi_i}\mathcal{S} = -\tilde{K}_{ij}\psi_j + \frac{\beta h}{\sqrt{\beta J}} + \sqrt{\beta J}\tilde{K}_{ij}\tanh(\sqrt{\beta J}\tilde{K}_{jl}\psi_l) .\end{aligned}$$

Note that there are NO matrix inversions in the force equations, just matrix multiplication (of a sparse matrix).

Some operators in this basis (version II)

Here I just give you the expressions for some operators (again check that I didn't make any mistakes!). First define

$$\frac{1}{N}\sum_{ij}\tilde{K}^{-1}_{ij} \equiv \mathcal{K}$$

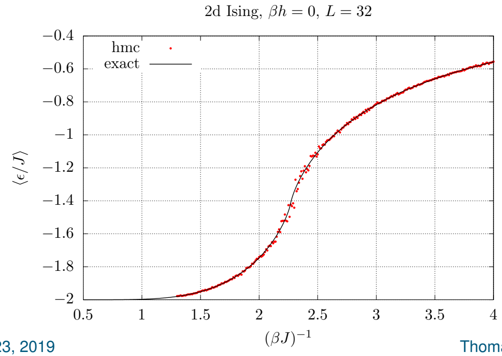
$$\langle m\rangle = \frac{1}{N\beta}\frac{\partial}{\partial h}\log(\mathcal{Z}) \implies O[\tilde{\phi}] = \frac{1}{\sqrt{\beta J}}\frac{1}{N}\sum_i \psi_i - \frac{h}{J}\mathcal{K}$$

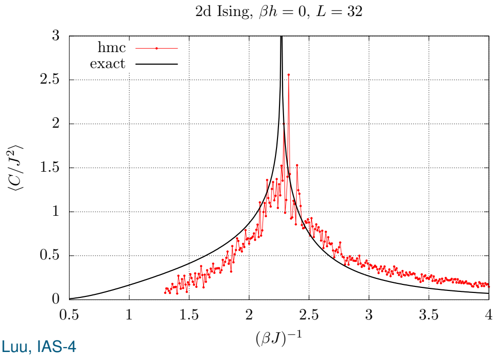
$$\langle \beta\epsilon\rangle = -\frac{\beta}{N}\frac{\partial}{\partial\beta}\log(\mathcal{Z})$$

$$\implies O[\tilde{\phi}] = \frac{\mathcal{C}\beta J}{2} + \frac{(\beta h)^2\mathcal{K}}{2\beta J} - \frac{\beta h}{2N\sqrt{\beta J}}\sum_i \psi_i - \frac{\sqrt{\beta J}}{2N}\sum_i \tilde{K}_{i\alpha}\psi_\alpha \tanh\left(\sqrt{\beta J}\tilde{K}_{i\beta}\psi_\beta\right)$$

The code

- I provide you with `C++` code to do both versions
- Can run in any dimensions D
- Unfortunately, it is not well documented
- But it runs faster than my python scripts!





Sampling fit parameters with HMC

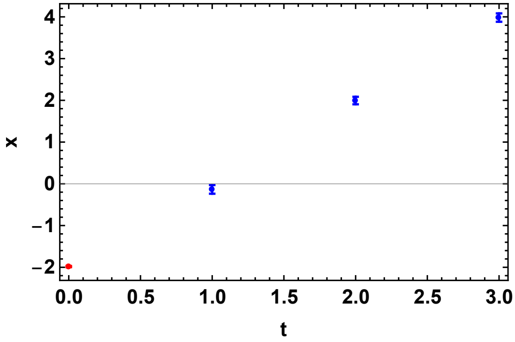
- Let's say you have some data

	t	x	err
$V1$	1	-0.133250	0.1037669
$V2$	2	1.995190	0.0900265
$V3$	3	3.983042	0.1004825

- And now you want to fit a line to the data

$$F(t) = a\,t + b$$

- Also assume you have some *prior* knowledge of b: $\bar{b} = -1.983(12)$.



Standard way of doing things. . .

Maximum-likelihood method equates to maximizing the probability

$$f(x|a,b)f(a)f(b) \propto \exp\left(-\sum_i \frac{(x_i - F(t_i))^2}{2\Delta x_i^2}\right) \exp\left(\frac{-(\overline{b}-b)^2}{2\cdot\Delta\overline{b}^2}\right)$$

$$\propto \exp\left(-\frac{1}{2}\left[\sum_i \frac{(x_i - F(t_i))^2}{\Delta x_i^2} + \frac{(\overline{b}-b)^2}{\Delta\overline{b}^2}\right]\right)$$

which is equivalent to minimizing the argument of the exponential, i.e. least-squares minimization.

But I want HMC to take over the world!!!

We define an artificial Hamiltonian!

$$\mathcal{H}\left(p_a, p_b, a, b\right) = \frac{p_a^2}{2} + \frac{p_b^2}{2} - \log[f(x|a,b)f(a)f(b)]$$
$$= \frac{p_a^2}{2} + \frac{p_b^2}{2} + \frac{1}{2}\left[\sum_i \frac{(x_i - F(t_i))^2}{\Delta x_i^2} + \frac{(\overline{b} - b)^2}{\Delta\overline{b}^2}\right]$$

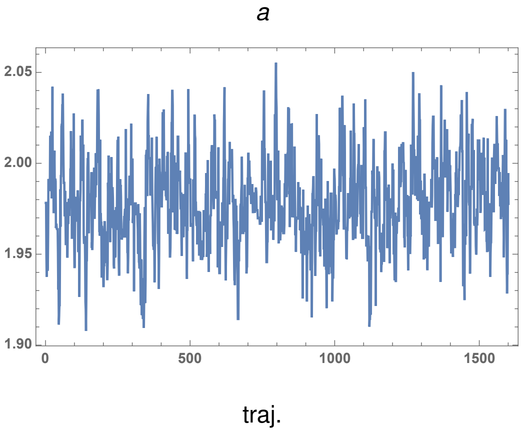
with corresponding EoMs:

$$\begin{aligned} \dot{a} &= p_a, & \dot{p}_a &= -\tfrac{\partial\mathcal{H}}{\partial a} \\ \dot{b} &= p_b, & \dot{p}_b &= -\tfrac{\partial\mathcal{H}}{\partial b} \end{aligned}$$

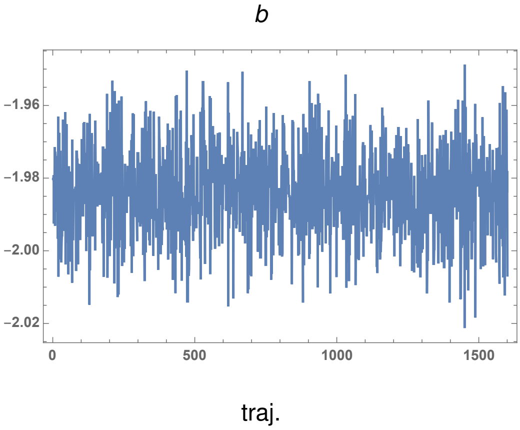
You can even include correlations (if you know them)! This is a general expression:

$$H\left(p_a, p_b, a, b\right) = \frac{p_a^2}{2} + \frac{p_b^2}{2} + \frac{1}{2}\sum_{r,r'}\left(\overline{w}(r) - f_{a,b}(r)\right)\overline{C}^{-1}\left(r, r'\right)\left(\overline{w}\left(r'\right) - f_{a,b}\left(r'\right)\right)$$
$$= \frac{p_a^2}{2} + \frac{p_b^2}{2} + \frac{1}{2}\chi^2(a,b)$$

And the rest is old news!



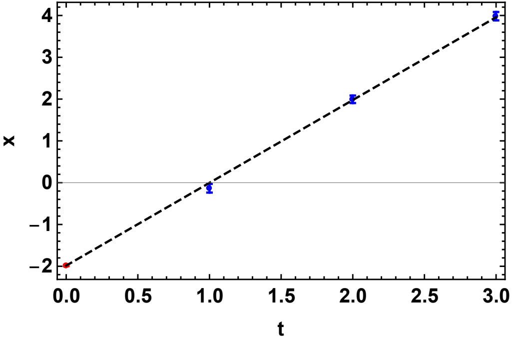
$$a = 1.98241 \pm 0.0285312$$



$$b = -1.98727 \pm 0.0239101$$

Error analysis in this case

- You'll still need to perform an autocorrelation analysis and perform binning to reduce autocorrelations (if needed)
- However, the fluctuations of the variables are dictated by Δx_i.
- This means that the standard deviation of these fluctuations are the true error (NOT the bootstrap standard deviations)
- In other words, don't do bootstrap in this case

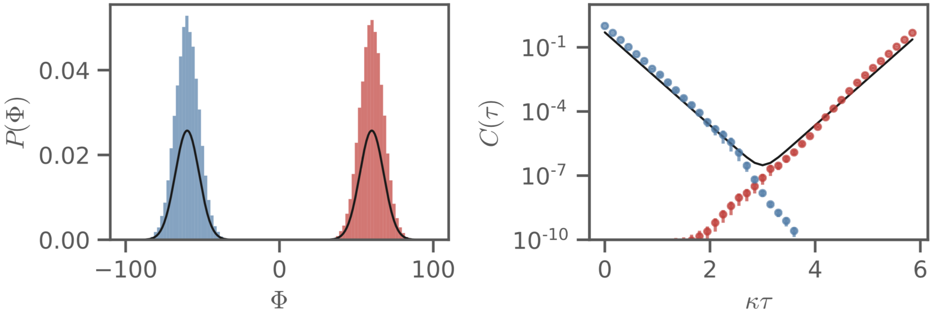


Try this on Prof. Shindler's exercise related to fitting the effective mass!

Some pitfalls

- Though some problems may not have a *formal* ergodic problem they have a *practical* ergodic problem

$N_x = 1,\ N_t = 40, \quad U/\kappa = 10,\ \kappa\beta = 6$



This is the 1-site Hubbard model!

Calculation of $\det M$ and M^{-1}

- The calculation of $\det M$ is *time consuming*
- For large systems, must make use of "stochastic (noisy) estimates" of $\det M$ (e.g. pseudo-fermions)
- One never actually solves for the entire M^{-1}, but instead solves $M.x = b$ for select "source" vectors b
- Use iterative *Krylov* solvers (and its many flavors) to do such solves

But the biggest pitfall of all. . .

- Remember the 1-D anHarmonic problem?
- I could here also apply the HS transformation to reduce the x^4 term to x^2:

$$\int \mathcal{D}[x]e^{-S_\omega[x]-\lambda\omega x^4} \to \int \mathcal{D}[\phi]\mathcal{D}[x]e^{-\frac{\phi^2}{4\omega\lambda}}e^{-S_\omega[x]-i\phi x^2}$$
$$= \int \mathcal{D}[\phi]e^{-\frac{\phi^2}{4\omega\lambda}-\frac{1}{2}\log\det M[\phi]}$$

- Looking good so far, right? Now I just introduce conjugate momenta for each ϕ_i, determine EoMs, and apply HMC

What could be so hard???

The sign problem!

- The issue is with $\log \det M[\phi]$, which can be *complex* in this case
- We don't know how to interpret probabilities with complex terms!
- This is known colloquially as the *sign problem*
- There are some limiting cases where "solutions", or better "work-arounds" exist that can deal with this problem (e.g. re-weighting, expansion around real part, etc. . .)
- And as you might imagine, most of the interesting physics occurs in regimes where the sign problem is severe
  - Finite baryon density QCD
  - Doped condensed matter systems

But if you want the Fields Medal, solve the sign problem!

Guys, it's been an honor! So let's end with a challenge problem!

Come back to the Ising model.

- Up till now, you've (hopefully) calculated the spin-spin correlator in position space

$$g(r) = \frac{1}{N}\sum_i \langle s_i s_{i+r}\rangle = \frac{1}{NN_t^2}\sum_{i,t,\tau}\langle s_{i,\tau} s_{i+r,\tau+t}\rangle$$

- Calculate the (symmetric) spin-spin correlator in time!

$$g(t) = \frac{1}{N^2 N_t}\sum_{i,r,\tau}\langle s_{i,\tau} s_{i+r,\tau+t}\rangle$$

- This requires some manipulation of the codes I gave you, but believe it or not, you have all the tools to do this!
- If you do do this, email me your results!