Monte Carlo for classical and quantum mechanics.

These lectures will be covering strategies complementing standard treatment in stat physics.

Standard setting: Given H, perform probabilistic sampling of classical d-dim or quantum $d+1$ configurations and calculate $\langle O \rangle$.

Data driven setting: Given set of data $D = \{\mathbf{x}_1, \mathbf{x}_2\}$, construct underlying probability distribution.

0.1 Important underying concepts

- Non-deterministic sampling of 'configurations', like spin. According to their weight $P(\mathbf{x}) = \frac{W(\mathbf{x})}{Z}$
- In Quantum integrate over space and imaginary time (temperature), starting and ending in the same configuration.
- Restricted Boltzmann machine: layers of ising spins (hidden and visible)
- Markov chains: Configuration of chains: configuration at time ℓ depends on $\mathbf{x}_\ell$ only. This leads to correlations between $\mathbf{x}_\ell$ and $\mathbf{x}_{\ell+1}$.
- Expectation values

$$\langle O \rangle = \frac{1}{Z} \operatorname{Tr}\{O \mathrm{e}^{-\beta H}\} = \frac{\sum_{\mathbf{x}} O(\mathbf{x}) W_{\mathbf{x}}}{\sum_{\mathbf{x}} W_{\mathbf{x}}}$$

Markov chain gives a sequence of configurations which we can use to approximate the true probability distribution from a frequency point of view. In particular we get a data set from the stationary distribution. Then can estimate

$$P(\mathbf{x}) \simeq P_{\text{data}}(\mathbf{x}) = \frac{1}{\|D\|} \sum_{\mathbf{x}_i \in D} \delta_{\mathbf{x}, \mathbf{x}_i}$$

Now if you have bad update rule, becomes important ot think about whether monte carlo chain samples correlated with neighbours

$$A_O(t) = \frac{\langle O(i+t) O(i) \rangle - \langle O \rangle^2}{\langle O^2 \rangle - \langle O \rangle^2}$$

Generally $A_O(t) \sim e^{-t/\tau_0}$, has characteristic decay time. Affects warm up time (no correlation to initial state), and variance, but not averages.

0.2 Designing monte carlo updates

Want to find most efficient way to update, relatively uncorrelated, and must reach equilibrium distsribution.

Example (Metropolis)**.** Based on *detailed balance* and *ergodicity* Consider to configurations $\mathbf{x}_\mu$ and $\mathbf{x}_\nu$, what is transition probability $T(\mu \to \nu)$ or alternatively writte $T(\nu, t+1 | \mu, t) = T(\nu | \mu)$. Detailed balance is

$$T(\nu|\mu) P_{\text{eq}}(\mathbf{x}_\mu) = T(\mu|\nu) P_{\text{eq}}(\mathbf{x}_\nu)$$

Usefull way of splitting up probability distribution

$$T(\mu \to \nu) = g(\mu \to \nu)A(\mu \to \nu) = \text{(selection probability)(acceptance ratio)}$$

In generalised metropolis is given by

$$A(\mu \to \nu) = \min\left\{1, \frac{p(x_\nu)}{p(x_\mu)}\frac{g(\nu \to \mu)}{g(\mu \to \nu)}\right\}$$

For example ising model with random spin flip have

$$A(\mu \to \nu) = \min\left\{1, \mathrm{e}^{\beta(E_\nu - E_\mu)}\right\}$$

Another example is a restricted boltzmann machine with hidden and visible states $\mathbf{h}$ and $\mathbf{v}$ with hamiltonian

$$H = -\sum_{ij} W_{ij} v_i h_j - \sum_i b_i v_i - \sum_j c_j h_j$$

Selection probability goes (Block Gibbs sampling) $\mathbf{v} \to \mathbf{h} \to \mathbf{v}$, has selection probability $p(\mathbf{v}|\mathbf{h}) = \prod_i p(v_i|\mathbf{h})$ where $p(v_i|\mathbf{h}) = \sigma(\sum_j W_{ij}h_j + b_i)$, then the acceptance ratio can be written

$$A(\mathbf{v}, \mathbf{h} \to \mathbf{v}', \mathbf{h}) = \min\left\{1, \frac{p(\mathbf{v}', \mathbf{h})}{p(\mathbf{v}, \mathbf{h})}\frac{p(v|h)}{p(v'|h)}\right\} = 1$$

A good place to get into machine learning as a physicist. been replaced with convolution neural network

0.3 Ergodicity

Starting from any $\mathbf{x}_\mu$ the MC algorithm can get to any $\mathbf{x}_\mu$ in a finite number of steps. This can affect many important What is a $\mathbb{Z}_2$ gauge theory? A classical part of toric code has a double redundancy in the fact that can flip all spins in plaquette.

Exercise. Design a MC update that are ergodic in the low-energy state of classical toric code

1. Single spin flip Creates two spin flips $E_\nu - E_\mu = 4J$, is exponentially unlikely to get accepted.
2. Gauge flips all spins in a star has no change in energy, can always be accepted. Is this ergodic? No! Non-ergodic in topological sector!
3. Non-local loop moves!

1 Quantum Monte Carlo

Involves the sampling of a $d + 1$ dimensional classical configuration. The extra dimension is imaginary time, and we need to be able sample world lines with positive measure. A variety of methods exists (World-line, SSE, aux.field,PIMC for the continuum, VMC) Most of these are affected by sign problem of the configurations. (Not VariationalMonteCarlo).

QMC: What are the configurations $\mathbf{x}_i$, weights $W_{\mathbf{x}_i}$, transition probabilities etc. Will talk about SSE

1.1 Stochastic Series Expansion

Taylor expansion of the partition function

$$Z = \mathrm{Tr}\left\{e^{-\beta H}\right\} = \sum_{\alpha}\sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle\alpha|H^n|\alpha\rangle$$

Now insert $n-1$ resolutions of the identity between the hamiltonians

$$Z = \sum_{\{\alpha_i\}}\sum_{n} \frac{\beta^n}{n!} \langle\alpha_0| - H\,|\alpha_1\rangle\langle\alpha_1| - H\,|\alpha_2\rangle \ldots \langle\alpha_{n-1}|H|\alpha_n\rangle$$

where $\alpha_n = \alpha_0$. Strategy is importance sample from sum/traces. let $Z = \sum_{\mathbf{x}} W_{\mathbf{x}}$ can be used in MCMC. If any $W_{\mathbf{x}} < 0$ there is a sign problem; cannot intepret these directly as probabilities.

Example. Spin 1/2 heisenberg $H = J\sum_{\langle ij\rangle} \mathbf{S}_i{\cdot}\mathbf{S}_j = J\sum_b \left[S^z_{b_i}S^z_{b_j} + \frac{1}{2}\left(S^+_{b_i}S^-_{b_j} + \text{h.c.}\right)\right]$ Go into z spin basis, and insert the diagonal and off-diagonal elements. Need all terms to be give positive contributions.

- Diagonal sign problem can be fixed by adding a big constant to hamiltonian
- Off-diagonal is less trivial, as the operators may be positive or negative. In 1-D is solved by the periodic boundary condition, so will always have even number terms.
- In 2D biparte eg square, negative signs also always occur in even numbers, so no sign problem. On non-bipartite lattice can have odd number of negative values.
- In arbitrary dimernsion If any path can be found that takes an odd number of hops to return to original configuration a sign problem will occur.

The way of *solving the sign problem* is finding a local basis rotation that that makes the off-diagonal matrix elements all positive. A good example is applying a unitary rotation on a sublattice A.

A *Stoquastic hamiltonians* is one which all Ground state wavefunction is strictly real-positive.

- AFM heisenberg XY on bipartite
- Bosons with unfrustrated hopping
- Transverse field ising model/Rydberg atoms

1.2 Ergodicity in QMC

How does one sample off diagonal states? Remember to think about topological sectors.