MATH327: StatMech and Thermo

Thursday, 7 May 2026

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Something to consider

Suppose we want to *approximately* compute expectation values

$$\langle \mathcal{O} \rangle = \sum_{i=1}^{M} \mathcal{O}_i \, p_i = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{O}_i \, e^{-\beta E_i} = \frac{\sum_{i=1}^{M} \mathcal{O}_i \, e^{-\beta E_i}}{\sum_{i=1}^{M} e^{-\beta E_i}}.$$

How many of the system's micro-states do we really need to analyse?

Recap

Mean-field approx. of Ising model

Transition, critical exponent, reliability

Plan

Numerical methods (broadly applicable)

Module review / exam prep

How to do numerical calcs in less than age of universe?

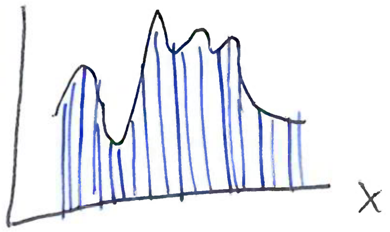
Crucial for interacting statistical systems (including 3d Ising)

Sample small subset of micro-states to approximate $\langle \mathcal{O} \rangle$

pseudo-random → "Monte Carlo" methods

纺

Illustrate: Estimate integral by evaluating integrand at random points



$$\int_{-1}^{1} dx \int_{-1}^{1} dy \; H(1-\{x^2+y^2\}) = \text{area of disk with radius } 1 = \pi$$

$$H(r) = \begin{cases} 1 & \text{for } r \geq 0 \\ 0 & \text{for } r < 0 \end{cases}$$

Monte Carlo integration most useful for high-dim'l integrals like $\langle O \rangle$ for $N \gg 1$ interacting statistical systems!

$$\frac{\text{length of calc.}}{\text{age of universe}} \ll 1$$

$\therefore$ very small fraction of micro-state

How can this give reliable approx.?

High-T Ising model: All p_i roughly equal

$\langle O \rangle$ determined by degeneracies

Large degeneracy $\rightarrow$ more likely to sample... could be ok

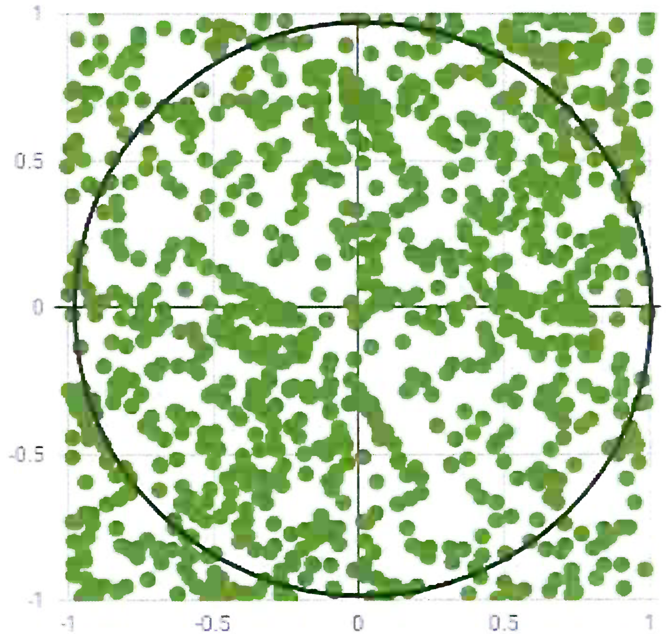
Low-T: $\langle O \rangle$ dominated by ground state(s)

other contributions suppressed $\sim e^{-E/T}$

Solution: Sample w_i with prob. $p_i \propto e^{-\beta E_i}$

without knowing p_i distribution

Importance sampling algorithms use pseudo-randomness to find large p_i without bias



fraction: $\frac{\pi}{4}$

Example: MRRTT algorithm (1953)

Start from any micro-state

Pseudo-random change $\to \Delta E$

$P_{accept} = \min\{1, \exp(-\beta \Delta E)\}$ otherwise reject

$\to$ New micro-state (possibly unchanged)

Repeat!

Sequence of micro-state ~~is~~ is Markov chain $\xrightarrow{w_1} \xrightarrow{w_2} \xrightarrow{w_3} \ldots$

Each w_i based on previous one, no memory

$$\frac{P(A\to B)}{P(B\to A)} = \frac{\min\{\cancel{1}, e^{-\beta(E_B - E_A)}\}}{\min\{1, \cancel{e^{-\beta(E_A - E_B)}}\}} = e^{-\beta(E_B - E_A)} = \frac{e^{-\beta E_B}}{e^{-\beta E_A}} = \frac{p_B}{p_A} \checkmark$$

To avoid bias, must (in principle) be able to reach any w_i from any other w_j

Ergodicity of random update (customized for system)

May take many updates to produce statistically independent w_i

$\to$ auto-correlation increase costs and uncertainties $\propto 1/\sqrt{S}$

independent samples

For spin systems, huge benefits from ~~updating~~ flipping "cluster" of spins, not just one

Reduce "critical slowing down" near 2nd-order phase trans. with fluctuations on all length scale