Transition path sampling algorithm for discrete many-body systems

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Giovanni Gallavotti’s 70th birthday conference
Tanti auguri!
Outline

1 Introduction

2 The path Monte Carlo algorithm

3 Results for the 2d ferromagnetic Ising model

4 Conclusions
Consider a stochastic system moving in a potential with at least two deep energy minima $A$ and $B$:

- At low enough temperature, the system spends most of the time in state $A$ or $B$
- Rare and quick transitions between the two states, with transition rate $k_{A\rightarrow B}$
- The transition can follow one of many possible transition paths, each path having a different weight
- The transition rate is determined by the **total** weight of the paths: both **energy** and **entropy** matter

For many-body systems, the problem of calculating $k_{A\rightarrow B}$ is extremely difficult.

The aim of this talk is to present an algorithm to compute $k_{A\rightarrow B}$ in generic stochastic systems with many discrete variables.
Transition path sampling

The literature on this problem is, of course, immense. Most algorithms are designed for continuous systems.

- **Transition path sampling**: (C. Dellago, D. Chandler et al. JCP 1998)
  - Construct the probability $P[x(t)]$ that describes the weight of a given path $x(t)$ (a path integral)
  - Add the constraint that paths start in $A$ and end in $B$ to obtain $P_{AB}[x(t)]$
  - Construct a Monte Carlo sampling of paths from $P_{AB}[x(t)]$
  - Use this sampling to compute the transition probability as a function of time
    - A totally unbiased and exact method
    - Only requires the knowledge of the dynamics and the two states $A$ and $B$
    - Gives very detailed information on the transition paths
    - However, sampling might not be easy...
    - ... and a thermodynamic integration is needed to compute the transition rate

So far, this method has been implemented only for continuous systems. The aim of our work is to implement this idea for discrete systems.
Ising spin systems

The method works for general discrete stochastic systems, but let’s consider an example for concreteness:

- A system of $N$ spins $\sigma = \{\sigma_i\}$, with Hamiltonian $H(\sigma) = -\sum_{i=1}^{N} b_i \sigma_i - \sum_{i,j} J_{ij} \sigma_i \sigma_j$.
- Master equation for $p_t(\sigma)$: $\partial_t p_t(\sigma) = \sum_{\sigma'} [w_{\sigma;\sigma'} p_t(\sigma') - w_{\sigma';\sigma} p_t(\sigma)]$
- One spin flip at a time: $\sigma_{\uparrow i}$ is the configuration $\sigma$ with spin $i$ flipped.
- Energy variation: $\Delta E = H(\sigma) - H(\sigma_{\uparrow i}) = -2h_i \sigma_i$ with $h_i = b_i + \sum_{j(\neq i)} J_{ij} \sigma_j$.
- $w_{\sigma;\sigma_{\uparrow i}} = w(\Delta E) = w(-2h_i \sigma_i)$
- Simple Glauber dynamics with detailed balance: $w(\Delta E) = e^{-\beta \Delta E} w(-\Delta E)$
  Here we choose: $w(\Delta E) = w_0 e^{-\beta \Delta E/2}$ with $w_0 = 1$ (unit of time).
- Then $\partial_t p_t(\sigma) = \sum_i [e^{\beta h_i \sigma_i} p_t(\sigma_{\uparrow i}) - e^{-\beta h_i \sigma_i} p_t(\sigma)]$

The single spin flip assumption is important to simplify the method
The fact that the flip rate only depends on a few “neighbors” is also important

Instead, detailed balance is not needed for the method to work!
Any (local) choice of the single spin flip rate is allowed
Definitions: two-state model

A two-state model is described by:

$$\partial_t \left( \begin{array}{c} p_A(t) \\ p_B(t) \end{array} \right) = \left( \begin{array}{cc} -k_{A\rightarrow B} & k_{B\rightarrow A} \\ k_{A\rightarrow B} & -k_{B\rightarrow A} \end{array} \right) \cdot \left( \begin{array}{c} p_A(t) \\ p_B(t) \end{array} \right)$$

The evolution operator has:

- one zero eigenvalue, corresponding to the steady-state solution
- one non-zero eigenvalue $\Delta = k_{A\rightarrow B} + k_{B\rightarrow A}$, the “energy gap”

The probability to be in $B$ at time $t$ given that the system was in $A$ at time $t = 0$ is

$$Z_{AB}(t) = \frac{k_{A\rightarrow B}}{k_{A\rightarrow B} + k_{B\rightarrow A}} \left[ 1 - e^{-(k_{A\rightarrow B} + k_{B\rightarrow A})t} \right].$$

The probability that the system has passed at least once by $B$ after a time $t$, given that it started in $A$, is:

$$Z_{AB}^*(t) = 1 - e^{-k_{A\rightarrow B}t}.$$

The mean first passage time is:

$$\text{MFPT}_{A\rightarrow B} = \int_0^\infty dt \ t \frac{dZ_{AB}^*}{dt} = \frac{1}{k_{A\rightarrow B}}.$$

At “short” times $k_{A\rightarrow B} t \ll 1$ we have $Z_{AB}(t) \approx Z_{AB}^*(t) \approx k_{A\rightarrow B} t$.

Our aim is to be able to compute $Z_{AB}(t)$ for a complex many-body system, and extract from it the rate $k_{A\rightarrow B}$.
An example: the Curie-Weiss model

Mean field Curie-Weiss model: \( J_{ij} = 1/(2N), \forall i, j \) and \( b_i = 0 \).
\( H(\sigma) = M(\sigma)^2/(2N) \) depends only on global magnetization.

The free energy at constant \( M = mN \) is:
\[
\beta f(m) \equiv \lim_{N \to \infty} \frac{\beta}{N} F(mN) = -\frac{\beta}{2} m^2 + \frac{1+m}{2} \log \frac{1+m}{2} + \frac{1-m}{2} \log \frac{1-m}{2}
\]
and has two minima at \( \pm m^\ast \) for \( T < 1 \) separated by a barrier in \( m = 0 \).

One can write a reduced Master equation:
\[
\partial_t \rho_t(M) = w_+(M - 2) \rho_t(M - 2) + w_-(M + 2) \rho_t(M + 2) - [w_-(M) + w_+(M)] \rho_t(M)
\]
which is a simple one dimensional random walk in \( M \) space.

An explicit calculation of the mean first passage time gives for \( N \to \infty \):
\[
\text{MFPT}_{A \to B} = \frac{\pi}{\beta} \sqrt{\frac{1}{[1 - \beta(1 - (m^\ast)^2)](\beta - 1)}} e^{\beta N[f(0) - f(m^\ast)]}
\]
**An example: the Curie-Weiss model**

Mean field Curie-Weiss model: $J_{ij} = 1/(2N), \forall i, j$ and $b_i = 0$. $H(\sigma) = M(\sigma)^2/(2N)$ depends only on global magnetization.

The function $Z_{AB}(t)$ can be computed diagonalizing numerically the master equation up to $N = 400$:

- At very short times, it is very small: a minimal time is required to perform the transition!
- At intermediate times $\tau_{\text{trans}} \ll t \ll 1/k_{A \rightarrow B}$, it is linear: $Z_{AB}(t) \sim k_{A \rightarrow B} \times (t - \tau_{\text{trans}})$
- The transient scales as $\tau_{\text{trans}} \sim \log N$

![Graphs showing the behavior of $Z_{AB}(t)/Z_{AB}(T)$ and $\tau_{\text{trans}}$ as a function of $N$.](image)
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A simple argument: for large $N$, $\dot{m}(t) \sim -f'[m(t)] + \eta(t)/N$, where $\eta$ is a white noise.

Linearizing around $m = 0$, $\dot{m}(t) = |f''(0)|m(t) + \eta(t)/N$, then $\langle m(t)^2 \rangle \sim (\exp(2|f''(0)|t)/N^2$. Starting in $m = 0$ it takes a time $\sim \log N$ to leave the unstable point and go to either $A$ or $B$. 
The function $Z_{AB}(t)$

$\tau_{\text{trans}}$ is dominated by the time it takes to make the transition from the top of the barrier. We have to measure $Z_{AB}(t)$ on a time scale $\tau_{\text{trans}} \ll t \ll 1/k_{A \rightarrow B}$. 
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The path action

Assign a probability $P_A(\sigma)$ to define the initial state and an indicator function $\chi_B(\sigma) = 1$ if $\sigma \in B$ and zero otherwise.

$$dP(\sigma(t)) = P_A[\sigma(0)] \mathcal{P}[\sigma(t)] \chi_B[\sigma(T)]$$

Probability of a path $\sigma(t)$ of the system of $N$ spins, going from $\sigma(0) \in A$ to $\sigma(T) \in B$ in a time $T$.

Continuum limit for a path with $M$ jumps labeled by $(t_m, \sigma_m)$, $m = 0, \ldots, M$ and $\sigma_m = \sigma(t_m^+)$.

Use the single-spin flip form of the rates and call $i_m$ the spin that flips at time $t_m$ and $h^m_i$ the local field on spin $i$ in configuration $\sigma_m$:

$$dP(\sigma(t)) = P_A(\sigma(0)) \left\{ \prod_{m=1}^{M} \exp \left[ - \left( t_m - t_{m-1} \right) \sum_i w(2h^m_i \sigma^m_i) \right] \prod_{m=1}^{M-1} w(2h^m_{i_m} \sigma^m_{i_m}) dt_m \right\} \chi_B(\sigma(T))$$
Heat bath sampling

Update one spin path at each step, according to the conditional probability $d\mathbb{P}(\sigma_i(t)|\sigma_{\backslash i}(t))$

A Delete one spin path $i$ chosen at random

B The conditional probability for $i$ depends on $h_i(t)$, the field of all other spins $j$. It also depends on the fields $\bar{h}_j$ that each of these spins feel in the absence of $i$. Divide the trajectory into $K$ time intervals, denoted by $k$, on which these fields are constant.

C Draw a value of the spins at the boundaries of the $K$ intervals.

D Draw the trajectory inside each of the intervals, with fixed boundaries.

F. Krzakala, A. Rosso, G. Semerjian, FZ, PRB 2008
The conditional probability

\[ h_i(t) = t_1 \text{ for } k = 1, t_2 \text{ for } k = 2, t_3 \text{ for } k = 3 \]

Define the operator \( \mathcal{L}^k_i \), a \( 2 \times 2 \) matrix:

\[ \langle \sigma' | \mathcal{L}^k_i | \sigma \rangle = \begin{cases} -w(2h_i^k \sigma) - \sum_{j \neq i} w(2\sigma^k_j (\bar{h}^k_j + J_{ji} \sigma)) & \text{for } \sigma' = \sigma \\ w(2h_i^k \sigma) & \text{for } \sigma' = -\sigma \end{cases} \]

then

\[ \mathbb{P}(\{\sigma_i^k\}|\sigma_i(t)) \propto e^{h_i^A \sigma_i^A} \prod_{k=1}^{K} \langle \sigma_i^k | e^{(t_k - t_{k-1}) \mathcal{L}^k_i} | \sigma_i^{k-1} \rangle \left\{ \prod_{k=1}^{K-1} w(2\sigma_{j_k}^k (\bar{h}^k_{j_k} + J_{j_k,i} \sigma_i^k)) \right\} e^{h_i^B \sigma_i^B} \]

From this one dimensional chain representation we can draw easily the boundary values \( \sigma_i^k \).
Generate the trajectory inside each interval

Recursions between paths:

\[ \sigma_{-} = \int \mathrm{d}u \]

\[ \sigma_{+} = \int \mathrm{d}u \]

To generate a path of length \( \lambda \), with \( \sigma(0) = \sigma, \sigma(\lambda) = \sigma \):

- With probability \( \frac{e^{\lambda} \langle \sigma| \mathcal{L} | \sigma \rangle}{\langle \sigma | e^{\lambda \mathcal{L}} | \sigma \rangle} \), set \( \sigma(t) = \sigma \) for \( t \in [0, \lambda] \)
- Otherwise
  - Draw \( u \in [0, \lambda] \) with probability density proportional to \( e^{u} \langle \sigma| \mathcal{L} | \sigma \rangle \langle -\sigma | e^{(\lambda - u) \mathcal{L}} | \sigma \rangle \)
  - Set \( \sigma(t) = \sigma \) for \( t \in [0, u] \)
  - Generate a path of length \( \lambda - u \) with \( \sigma(u) = -\sigma, \sigma(\lambda) = \sigma \)

To generate a path of length \( \lambda \), with \( \sigma(0) = \sigma, \sigma(\lambda) = -\sigma \):

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- Set \( \sigma(t) = \sigma \) for \( t \in [0, u] \)
- Generate a path of length \( \lambda - u \) with \( \sigma(u) = -\sigma, \sigma(\lambda) = -\sigma \)
The path Monte Carlo algorithm

The calculation of the transition rate

Using this path Monte Carlo algorithm, we can compute averages over the measure
\[d\mathbb{P}(\sigma(t)) = P_A[\sigma(0)] \mathcal{P}[\sigma(t)] \chi_B[\sigma(T)]\]
of all paths that go from \(A\) to \(B\) in time \(T\).

How do we extract the rate from this?

The function \(Z_{AB}(T)\) is the partition function associated with this measure:

\[Z_{AB}(T) = \int d\mathbb{P}[\sigma(t)] = \sum_{\sigma(t)} P_A[\sigma(0)] \mathcal{P}[\sigma(t)] \chi_B[\sigma(T)]\]

so we must use thermodynamic integration:

\[Z_{AB}(T, \mu(1)) = Z_{AB}(T, \mu(0)) e^{\int_0^1 ds U_{AB}(T, \mu(s)) \frac{d\mu}{ds}}\]

\[U_{AB}(T, \mu) = \frac{\partial \log Z_{AB}(T, \mu)}{\partial \mu}\]

where \(\mu(s)\) is an interpolation path between \(Z_{AB}(T, \mu(0))\), that is assumed to be easily calculable, and \(Z_{AB}(T, \mu(1)) = Z_{AB}(T)\).

The choice of the optimal interpolation path depends on the system under investigation.
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The 2d ferromagnetic Ising model

We consider the 2d Ising model on a square lattice with \( J_{ij} = 1 \) for nearest neighbors and zero otherwise, and \( b_i = 0 \).

We work at \( \beta = 1 > \beta_c = 0.4407 \) where \( m_{eq} = 0.999275 \ldots \)

We choose

\[
P_A(\sigma_A) = \frac{\exp(h_A M_A)}{(2 \cosh h_A)^N} = \prod_{i=1}^{N} \frac{e^{h_A \sigma_i^A}}{2 \cosh h_A}
\]

\[
\chi_B(\sigma_B) = \exp[-h_B (M^* - M_B) \Theta (M^* - M_B)]
\]

with \( h_A = -3 \) and \( h_B = 1 \), \( M^* = [0.56N] \) so the system goes from the down (A) to the up (B) state.
Thermodynamic integration

We perform the integration starting from $\beta = 0$ and changing $\beta$ up to $\beta = 1$.
At $\beta = 0$ spins are independent, then:

$$p_{up}(t) = \frac{1}{2} \left[ 1 + (2p_{up}(0) - 1)e^{-2t} \right] \text{ with } p_{up}(0) = e^{h_A}/(2 \cosh(h_A)).$$

Probability that the system has magnetization $M$ at time $t$:

$$P_t(M) = \left( \frac{N}{N+M} \right) p_{up}(t)^{(N+M)/2}(1 - p_{up}(t))^{(N-M)/2}$$

The partition function at $\beta = 0$ is:

$$Z_{AB}(T, \beta = 0) = \sum_M P_T(M) e^{-h_B(M^* - M)\theta(M^* - M)}$$
Results for the 2d ferromagnetic Ising model

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Probability that the system has magnetization $M$ at time $t$:

$$P_t(M) = \left( \frac{N}{N + M} \right) p_{up}(t)^{(N+M)/2} (1 - p_{up}(t))^{(N-M)/2}$$

The partition function at $\beta = 0$ is:

$$Z_{AB}(\mathcal{T}, \beta = 0) = \sum_M P_T(M) e^{-h_B(M^* - M)\theta(M^* - M)}$$

We have:

$$U_{AB}(\mathcal{T}, \beta) = \frac{\partial \log Z_{AB}(\mathcal{T}, \beta)}{\partial \beta} = \left\langle \sum_{k=1}^{L} (t_k - t_{k-1}) \sum_i w(2h^k_i \sigma^k_i) h^k_i \sigma^k_i - \sum_{k=1}^{L-1} h^k_{ik} \sigma^k_{ik} \right\rangle_{AB, \mathcal{T}, \beta}$$

$$Z_{AB}(\mathcal{T}, \beta) = Z_{AB}(\mathcal{T}, \beta = 0) e^{\int_0^\beta d\beta' U_{AB}(\mathcal{T}, \beta')}$$
Thermodynamic integration

\[ Z_{AB}(T, \beta) = Z_{AB}(T, \beta = 0) \ e^{\int_0^\beta d\beta' \ U_{AB}(T, \beta')} \]

A single point for \( N = 81 \) and \( T = 150 \) needed a CPU time \( \sim 500 \) hours (one month). We need 12 points for \( Z_{AB}(T) \): 1 year of CPU time.

The limit \( T \to \infty \) can be calculated via a standard Monte Carlo: very useful for small \( \beta \).
The function $Z_{AB}(t)$

Black dots: thermodynamic integration
Red and blue lines: results from Dellago et al. trick
Green points are obtained via standard Monte Carlo to check the accuracy of the method
For large $t$: $Z_{AB}(t) = k_{A\rightarrow B} \times (t - \tau_{\text{trans}})$
Results for the 2d ferromagnetic Ising model

Transition rate and transient time

- Transition rate $k_{A \rightarrow B} \sim \exp(-2\Sigma L)$
- Transient time $\tau_{\text{trans}} \propto N^2$
- A change in prefactors around $L = 8$
A typical transition path

- The transition state is a stripe of + spins in the − background
- Explains the exponential factor $\exp(-2\Sigma L)$ (F. Martinelli, JSP 1994)
- Once the stripe is formed, its growth is an unbiased random walk:
  - One move of the interface requires diffusion of a kink on a length $L$: takes a time $\sim N$
  - Moving the interface by $L$ requires $N$ such steps: $N \times N = N^2$
A simple model for the interface

Assume that the height of the interface is a single valued function \( h_i \)

\[ H_I = 2L + 2 \sum_{i=1}^{L+1} |h_i - h_{i-1}| \quad \text{with} \quad h_0 = h_{L+1} = 0. \]

\[ Z_I = e^{-2\beta L} \sum_{h_1 \ldots h_L} e^{-2\beta \sum_{i=1}^{L+1} |h_i - h_{i-1}|} = e^{-2\beta L} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left( \frac{e^{4\beta} - 1}{e^{4\beta} + 1 - 2e^{2\beta} \cos(k)} \right)^{L+1} \equiv e^{-L\Sigma} \]

Asymptotic results:

- For small \( L \) and large \( \beta \), \( h_i = 0 \) dominates: \( \Sigma = 2\beta \)
- For \( L \rightarrow \infty \), via a saddle point at \( k = 0 \): \( \Sigma = 2\beta + \log(\tanh(\beta)) \)
  (this is the correct result obtained by Onsager!)
- The crossover length increases with \( \beta \) and diverges for \( \beta \rightarrow \infty \)
- At \( \beta = 1 \), the crossover is roughly around \( L \sim 10 \), consistent with our data
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Conclusions

- A new algorithm to perform constrained path sampling of discrete many-body systems
- Based on the Transition Path Sampling strategy of Dellago, Chandler et al. and on the Quantum Monte Carlo heat bath algorithm of Krzakala et al.
- Works for generic stochastic processes with local interactions; detailed balance is not necessary
- Combined with thermodynamic integration, can be used to compute transition rates
- Gives detailed information on:
  ◦ the typical transition paths
  ◦ the time-dependent transition probability $Z_{AB}(t)$
  ◦ the transition rate $k_{A \rightarrow B}$
  ◦ the transient time $\tau_{\text{trans}}$, related to the barrier crossing time
- An application to the 2d Ising ferromagnetic model gives consistent results