Simulated tempering and magnetizing simulations of a Potts model

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Background

• Monte Carlo (MC) and molecular dynamics (MD) simulations are extensively used in computational physics.

• To enhance the sampling efficiency, the generalized-ensemble (aka extended-ensemble) algorithms are developed and applied, such as the multicanonical algorithm (MUCA) [*], simulated tempering (ST) [**], and replica-exchange method [***] (REM) (aka parallel tempering).

Motivation

• Whether the dimensional generalization of ST helps perform simulations better.

\[ P(E, T) \propto e^{-\beta E + a(T)} \]

\[ P(E, T, h) \propto e^{-\beta (E + hM) + a(T, h)} \]

We addressed this question by applying the two-dimensional ST method to the two-dimensional Potts model (and Ising model).

“Simulated Tempering and Magnetizing” (STM)

\[
P(E, T) \propto e^{-\beta E + a(T)}
\]

\[
P(E, T, h) \propto e^{-\beta (E + hM) + a(T, h)}
\]
Reconstruction of canonical ensembles

One can reconstruct the canonical ensemble via the conditional probability.

\[ P(\{\sigma_l\}, T, h) \propto e^{-\frac{(E-hM)}{T} + a(T,h)}, \]

\[ P(\{\sigma_l\}|T_i, h_j) \propto e^{\frac{(E-h_jM)}{T_i}} \]

(Applyingly, the conditional expectation gives the canonical average.)
Reweighting techniques

They give free energy values (necessary as STM parameters $a(T, h)$) with preliminary simulations.

**WHAM**

$$n(E, M) = \frac{\sum_{T_i, h_j} n_{T_i, h_j}(E, M)}{\sum_{T_i, h_j} N_{T_i, h_j} \exp(f(T_i, h_j) - (E - h_j M)/T_i)}$$

$$f(T_i, h_j) = -\log \sum_{E, M} n(E, M) \exp(-(E - h_j M)/T_i)$$

**MBAR**

$$f(T_i, h_j) = -\log \sum_{n=1}^{N} \frac{\exp(-(E_n - h_j M_n)/T_i)}{\sum_{T_i, h_j} \sum_{k=1}^{N_T} \sum_{l=1}^{N_h} N_{T_k, h_l} \exp(f(T_k, h_l) - (E_n - h_l M_n)/T_k)}$$


Reweighting techniques

Thermal quantity

\[
\langle A \rangle_{T,h} = \sum_{n=1}^{N} W_{na} A(x_n),
\]

\[
W_{na} = \frac{1}{\langle c_a \rangle} \frac{\exp\left(-\frac{(E_n - hM_n)}{T}\right)}{\sum_{k=1}^{N_T} \sum_{l=1}^{N_h} N_{T_k,h_l} \exp\left(f(T_k, h_l) - \frac{(E_n - h_lM_n)}{T_k}\right)},
\]

\[
\langle c_a \rangle = \sum_{n=1}^{N} \frac{\exp\left(-\frac{(E_n - hM_n)}{T}\right)}{\sum_{k=1}^{N_T} \sum_{l=1}^{N_h} N_{T_k,h_l} \exp\left(f(T_k, h_l) - \frac{(E_n - h_lM_n)}{T_k}\right)}.
\]

Review of application to Ising model

Hamiltonian: \( H = E - hM, \)

where \( E = \sum_{<i,j>} \sigma_i \sigma_j, \quad M = \sum_i \sigma_i. \)

Weight: \( P(\{\sigma_i\}, T, h) \propto e^{-(E-hM)/T+a(T,h)}, \)

Two-dimensional Ising model (4X4)

At every flame, 5000 MC sweeps.
Change by 1000 MC sweeps.

ST-Freq: 50
TvsH=0.5
L=20

Binder Cumulant

Those lines can be obtained by a single run for each.

Potts Model

Hamiltonian: $H = E - hM,$
where $E = \sum_{<i,j>} \delta_{\sigma_i,\sigma_j}, \ M = \sum_i \delta_{0,\sigma_i}.$

$h > 0$
State 0 is favored.
No phase transitions.

$h = 0$
All the three states are equivalent.

$h < 0$
State 0 is disfavored.
Behave like an Ising model.
Results

- Random walks realized in $T, h, E, M, M_{\text{max}}$

$$M_{\text{max}} = \max_{j=0,1,2} \left\{ \sum_{i} \delta_{j,\sigma_i} \left( \frac{L^2}{3} \right) - \frac{L^2}{3} \right\} \times \frac{3}{2}$$

$L=80$
Dimensionless free energy

\[ \frac{f}{L^2} \]

L = 80
Density of states

Wider areas of DOS were gained by STM than by ST.
Area really enlarged?

How the area sampled is exactly different?

THERE ARE AREAS IN BLUE AREN’T THERE?

red: by STM only
green: by both
blue: by ST only

$L=40$
Area really enlarged?

How the area sampled is exactly different?

THERE ARE AREAS IN BLUE AREN'T THERE?

red: by STM only
green: by both
blue: by ST only
L=40

THERE ARE AREAS IN BLUE AREN'T THERE?
The difference zoomed up

Yes, but the red and green segments are among blue regions!

red: by STM
green: both blue: by ST
It’s not relevant

Reweighting results for $h = 0$ are shown. The reweighting techniques work properly!! Thus, those representative are sampled well with STM. The ST method draws more samples from the narrower area.
Reweighting around wide area

- Reweighting in a wide area is possible.
- Specific heat and susceptibility. \( (L=80) \)
Reweighting around wide area 2

Specific heat $C$ converges at smaller $L$ as $h$ increases.

$L=5, 10, 20, 40, \text{ and } 80$

(a) $h=0$
(b) $h=0.005$
(c) $h=0.01$
(d) $h=0.02$
As an animation
Crossover with respect to $h$ and $t$

\[ t = \frac{|T - T_c|}{T_c} \]

\[ L^{2/15} m = \psi(tL^{6/5}, hL^{28/15}) \]

\[ t^{-14/9} h \ll 1: m \sim t^{1/9} \]

\[ t^{-14/9} h \gg 1: m \sim h^{1/14} \]
How $O_{\text{max}}$ changes is different between Ising and Potts. With negative $h$ and large $L$, the system behave as two-dimensional Ising model.

$$\sim L^{(1-\beta)/\nu}$$  \hspace{1cm}  $$\sim L^{1/\nu}$$
How $O_{\text{max}}$ changes is different between Ising and Potts. With negative $h$ and large $L$, the system behave as two-dimensional Ising model.

$\sim L^{1/\nu}$
Conclusions

We applied STM method to the two-dimensional Potts model (up to $L=160$).

The tradeoff between sample density and sampling area was not relevant, and we succeeded in reweighting at various conditions.

We also depicted the crossover behaviors.