古典モンテカルロ法とその応用

Classical Monte Carlo method and its applications

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Error estimation (Correction for the previous lecture)

Error due to finite number of sampling

$$\bar{A} \equiv \frac{1}{T}\sum_{t=1}^{T} \hat{A}(\Gamma(t))$$

$\langle \cdots \rangle$:average over trajectories (initial condition)

Standard error: $\epsilon^2 = \langle \bar{A}^2 \rangle - \langle \bar{A} \rangle^2$

$$\epsilon^2 = \left\langle \frac{1}{T^2}\sum_{t_1=1}^{T}\sum_{t_2=1}^{T} A_{t_1}A_{t_2} \right\rangle - \left\langle \frac{1}{T}\sum_{t=1}^{T} A_t \right\rangle$$

$$= \frac{1}{T^2}\sum_{t_1=1}^{T}\sum_{t_2=2}^{T} C_{AA}(|t_2 - t_1|)$$

$$= \frac{1}{T^2}\sum_{\Delta t=1}^{T-1} 2(T-\Delta t)C_{AA}(\Delta t) + \frac{C_{AA}(0)}{T}$$

$$\underset{T\to\infty}{\sim} \frac{1+2\tau}{T}C_{AA}(0) \quad \Rightarrow \quad \epsilon \propto \sqrt{\frac{1+2\tau}{T}}$$

$$C_{AA}(\Delta t) \sim C_{AA}(0)e^{-\Delta t/\tau}$$

$$\Delta t = |t_2 - t_1|$$

In order to reduce the error, we want to reduce τ

Outline

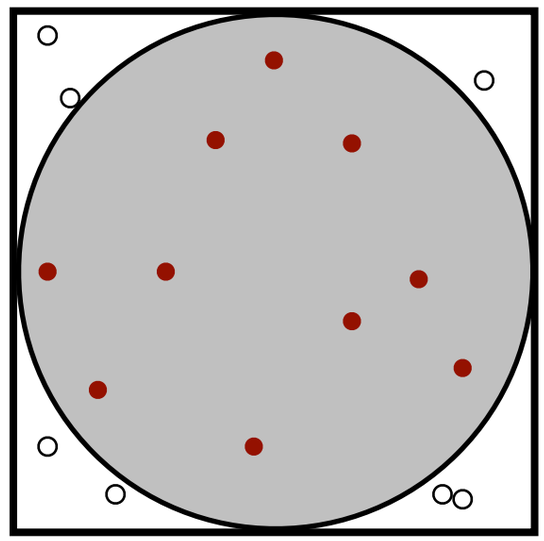
- Standard Monte Carlo method
  - Importance sampling and Markov Chain Monte Carlo
    - Metropolis-Heisting sampling
    - Heat-bath sampling (Gibbs sampling)
- Application to classical spin systems
  - Local update, Global update
- Computational Science using Monte Carlo method
  - Important tips to obtain reliable results
  - Application and analysis in the case of critical phenomena

Monte Carlo method: Randomized algorithm

Randomized algorithm: It changes its behavior depending on (psuedo) random numbers on execution.

Example :

Area of a circle: $\int_{x^2+y^2\leq 1} dxdy$



Algorithm

$N_a = 0 \quad N = 0$ initialize

loop i

$x_i \in [-1, 1]$

$y_i \in [-1, 1]$ take uniform random numbers

$N = N + 1$

if $x_i^2 + y_i^2 \leq 1$ then $N_a = N_a + 1$

end loop

$$\frac{N_a}{N} \to \pi$$

With statistical error proportional to $\frac{1}{\sqrt{N}}$

Monte Carlo Integration: General aspect

Monte Carlo Integration

$$\int d\Gamma f(\Gamma) = \int d\Gamma \frac{f(\Gamma)}{P(\Gamma)} P(\Gamma) = \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle$$

$P(\Gamma)$: probability distribution

Estimate an integral as an expectation value under $P(\Gamma)$

Previous example: $P(\Gamma)$ = uniform distribution
obtained by a rejection sampling

Merit of Monte Carlo Integration

The error is basically independent on the dimension of Γ.

$$\epsilon \propto O(N^{-1/2})$$

N : sampling number

The error of usual numerical quadrature (eg. trapezoidal formula)
exponentially increases as increase the dimension of Γ

eg. trapezoidal formula $\epsilon \propto O(N^{-2/d})$

Application to higher dimensions: The curse of dimensionality(次元の呪い)

Rejection sampling is inefficient for higher dimensions

Volume ratio between "*n*-dimensional hyper cubic" (with L=2) and "*n*-dimensional hyper sphere" (with r=1)

$$r = \frac{\pi^{n/2}/\Gamma(\frac{n}{2}+1)}{2^n} \sim \left(\frac{\pi}{en}\right)^{n/2}$$

Asymptotic form of *Γ*-function

$$\Gamma(x) \sim \left(\frac{x}{e}\right)^x$$

For larger *n*, the ratio exponentially decreases!

→ Error of the rejection sampling increases exponentially.

Even if we can directly generate uniform distribution, uniform sampling is inefficient

$\int d\Gamma f(\Gamma)$: Several sampling points, $|f(\Gamma)| \ll 1$, don't contribute the integral so much.

If $|f(\Gamma)| \ll 1$

If we could pick up relevant points $|f(\Gamma)| \gg 1$ the efficiency largely increases!

→ **Importance sampling**

Importance Sampling

Sampling the "important" points mainly

$$\int d\Gamma f(\Gamma) = \int d\Gamma \frac{f(\Gamma)}{P(\Gamma)} P(\Gamma) = \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle$$

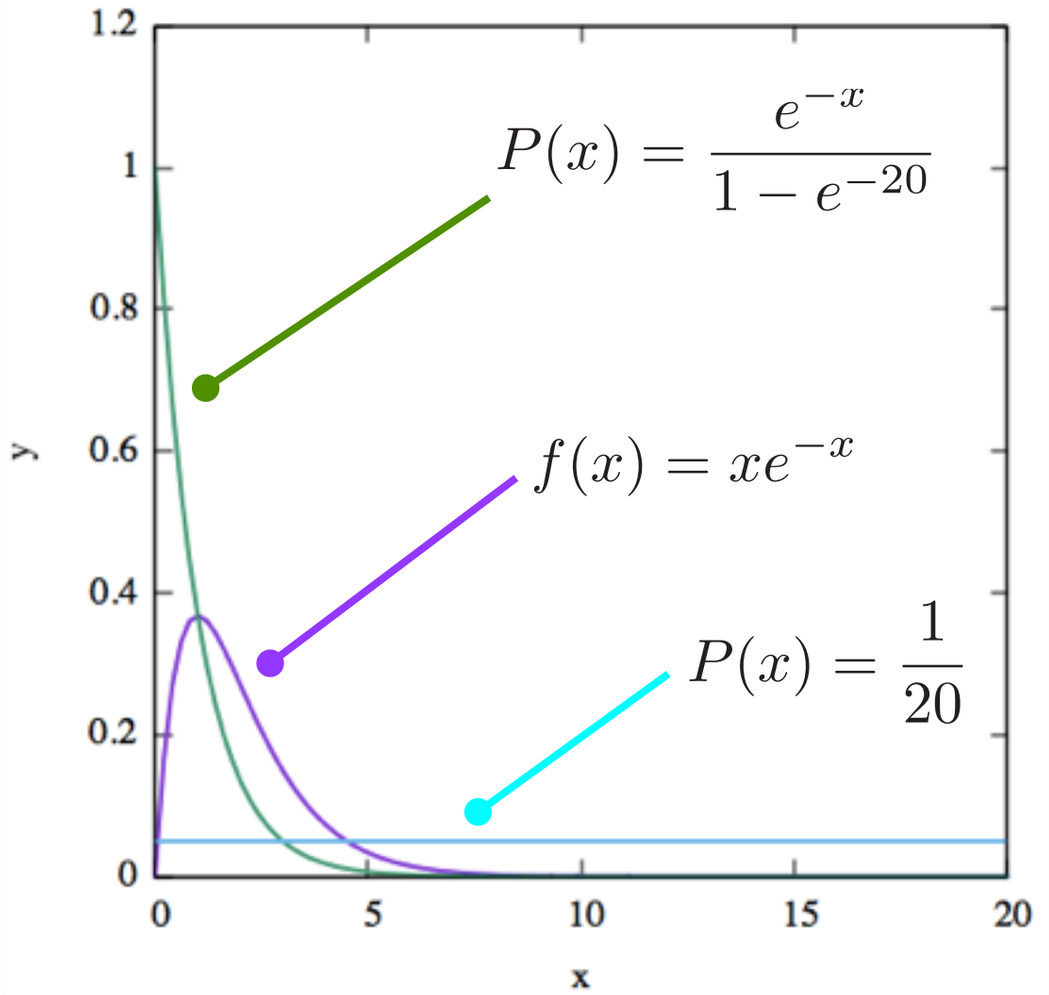
Chose $P(\Gamma)$ close to $f(\Gamma)$.

If we can choose $P(\Gamma) \propto f(\Gamma)$,
it is the best.

However, it is unrealistic!

Because, in order to normalize $f(\Gamma)$,
we have to know the value of integral,
which is the answer we want to know.

Example of importance sampling



Markov Chain Monte Carlo (MCMC)

We can generate $P(\Gamma)$ as the steady state of a stochastic process

A sampling point move in Γ "randomly".

Master equation for general Markov process

$$\rho_{t+1}(\Gamma) = \rho_t(\Gamma) + \sum_{\Gamma'} W_{\Gamma' \to \Gamma} \rho_t(\Gamma') - \sum_{\Gamma'} W_{\Gamma \to \Gamma'} \rho_t(\Gamma)$$

$W_{\Gamma \to \Gamma'}$:transition probability from Γ to Γ'

$\rho_t(\Gamma)$: probability for appearance of Γ at time t

$$\sum_{\Gamma'} W_{\Gamma \to \Gamma'} = 1$$

$$\sum_{\Gamma} \rho_t(\Gamma) = 1$$

Markov process:

A future move depends only on the present state and independent of the past states.

If a Markov process becomes a steady state in the long time limit,

$$\lim_{t \to \infty} \rho_t(\Gamma) = P(\Gamma)$$

We can sample points with distribution $P(\Gamma)$ along this stochastic process.

Markov Chain Monte Carlo: convergence condition

Conditions for transition probability for converging to $P(\Gamma)$.

1. "**Ergodicity**"
   - Any two states Γ and Γ' are connected by W with finite steps.
     - If we regard W as a matrix, this condition means

$$^{\exists}T > 0, ^{\forall}(\Gamma, \Gamma'), \quad [(W)^t]_{\Gamma,\Gamma'} > 0, (^{\forall}t \geq T)$$

2. "**Balance Condition**"
   - The "flows" of probabilities are balanced for $P(\Gamma)$.

$$^{\forall}(\Gamma, \Gamma'), \quad \sum_{\Gamma'} W_{\Gamma\to\Gamma'} P(\Gamma) = \sum_{\Gamma'} W_{\Gamma'\to\Gamma} P(\Gamma')$$

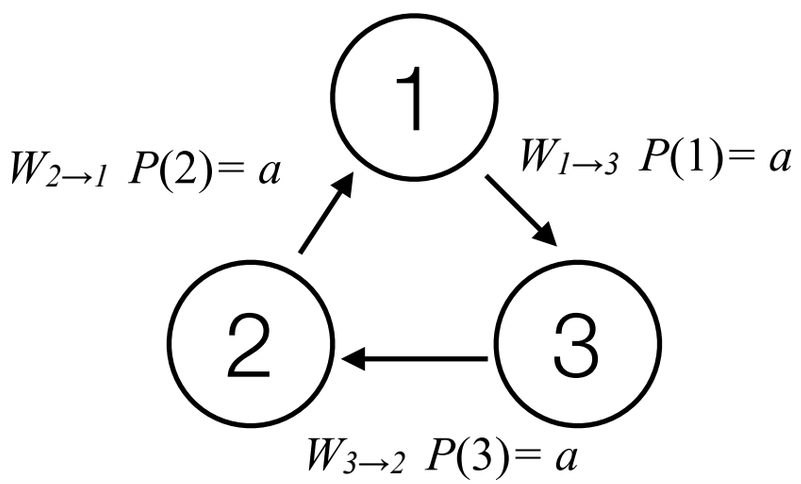
Special case:

Detailed balance condition

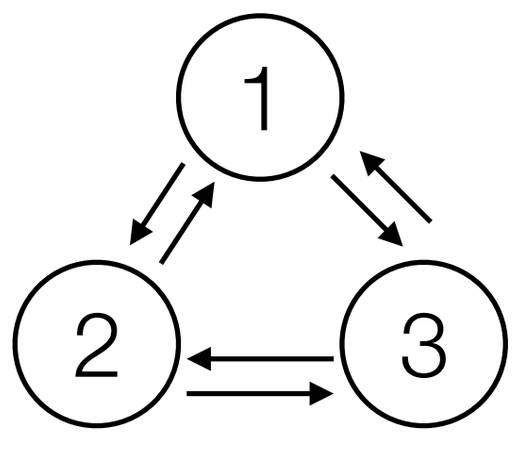
$$W_{\Gamma\to\Gamma'} P(\Gamma) = W_{\Gamma'\to\Gamma} P(\Gamma')$$

No microscopic flow
in the steady state

Balance condition with flow



Detailed balance condition



Metropolis-Heisting sampling

Step 0: Prepare an initial state $\Gamma_0 \in \{\Gamma\}$

loop t

1. Make next candidate state Γ' randomly from a proposal distribution $q(\Gamma'|\Gamma_t)$
2. Make uniform random number $r \in [0, 1]$
3. Select the next state Γ_{t+1} based on r as

$$\Gamma_{t+1} = \begin{cases} \Gamma', & r \leq a(\Gamma_t \to \Gamma') \\ \Gamma_t, & \text{otherwise} \end{cases}$$

Acceptance probability: $a(\Gamma_t \to \Gamma') = \min\left(1, \frac{P(\Gamma')q(\Gamma_t|\Gamma')}{P(\Gamma_t)q(\Gamma'|\Gamma_t)}\right)$

When $q(\Gamma_t|\Gamma') = q(\Gamma|\Gamma_t)$ → $a(\Gamma_t \to \Gamma') = \min\left(1, \frac{P(\Gamma')}{P(\Gamma_t)}\right)$ Metropolis sampling

(example) $\Gamma = x \in (-\infty, \infty)$

$x' = x_t + \epsilon \quad , \epsilon \in [-\sigma, \sigma]$ → $q(x'|x_t) = q(x_t|x')$

Metropolis-Heisting sampling: Detailed balance

Transition probability = (proposal probability) × (Acceptance probability)

$$W_{\Gamma\to\Gamma'} = q(\Gamma'|\Gamma)a(\Gamma\to\Gamma')$$

$$a(\Gamma\to\Gamma') = \min\left(1, \frac{P(\Gamma')q(\Gamma|\Gamma')}{P(\Gamma)q(\Gamma'|\Gamma)}\right)$$

* When $P(\Gamma')q(\Gamma|\Gamma') > P(\Gamma)q(\Gamma'|\Gamma)$

$$W_{\Gamma\to\Gamma'} = q(\Gamma'|\Gamma)$$

$$W_{\Gamma'\to\Gamma} = \frac{q(\Gamma'|\Gamma)P(\Gamma)}{P(\Gamma')}$$

It satisfies the detailed balance condition.

$$W_{\Gamma\to\Gamma'}P(\Gamma) = W_{\Gamma'\to\Gamma}P(\Gamma')$$

Thus, by using Metropolis-Heisting sampling,
we can calculate an ensemble average!

$$\langle O\rangle \equiv \int d\Gamma O(\Gamma)P(\Gamma)$$

$$= \lim_{T\to\infty}\frac{1}{T}\sum_{t=0}^{T-1} O(\Gamma_t)$$

Heat-bath sampling (Gibbs sampling)

Suppose we only change a part of variables in Γ

$$\Gamma = (\Gamma^1, \Gamma^2, \Gamma^3, \cdots, \Gamma^N) \quad \Rightarrow \quad \Gamma' = (\Gamma^{1\prime}, \Gamma^2, \Gamma^3, \cdots, \Gamma^N)$$

In this case, we may calculate "conditional" probability distribution of Γ^1,

$$P(\Gamma^1 | \Gamma^2, \Gamma^3, \cdots \Gamma^N) = \frac{P(\Gamma)}{\int d\Gamma^1 P(\Gamma)}$$

Then we can chose a transition probability satisfying the detailed balance condition

$$W_{\Gamma \to \Gamma'} = P(\Gamma^{1\prime} | \Gamma^2, \Gamma^3, \cdots \Gamma^N)$$

We generate the next Γ' directly from the conditional probability!

- The transition probability is independent on the present Γ^1.
- In general, it is not easy to produce the conditional probability distribution from uniform random numbers.

There is no general principle determining which of Metropolis and Heat-bath samplings is more efficient.

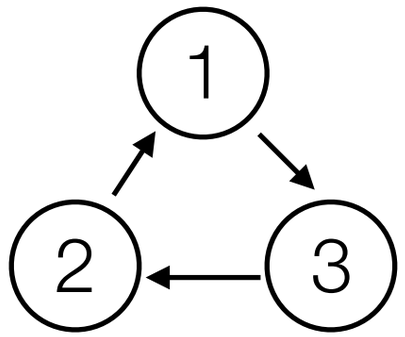
Sampling Based on balance condition

We do not necessarily use the detailed balance condition.

By using more general balance condition,
we can make "rejection free" transition probabilities

$W_{\Gamma \to \Gamma} = 0$:The state necessarily changes to another state

eg. Suwa-Todo method



H. Suwa, and S. Todo, Phys. Rev. Lett. **105**, 120603 (2010).

"詳細釣り合いを満たさないモンテカルロ法"

諏訪秀麿, 藤堂眞治, 日本物理学会誌, **66**, 370 (2011).

Application to replica exchange Monte Carlo for molecular dynamics simulation

S. G. Itoh and H. Okumura, J. Chem. Theory Comput. **9**, 570 (2013).

Application to Classical spin system

Classical spin system

Model Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i^z$$

Nearest Neighbor interaction

e.g.

Ising spin: $S_i = \pm 1$

Heisenberg spin: $S_i = (S_i^x, S_i^y, S_i^z)$

MCMC method:

Target steady state is $P(\Gamma) = \frac{1}{Z} e^{-\beta \mathcal{H}(\Gamma)}$

$$\langle \hat{O} \rangle = \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} \hat{O}(\Gamma_t)$$

Γ_t: sampling points along Markov chain

Calculate expectation values under Canonical Ensemble

$$\langle \hat{O} \rangle = \frac{1}{Z} \int d\Gamma \hat{O}(\Gamma) e^{-\beta \mathcal{H}(\Gamma)}$$

e.g.

Energy: $\hat{E}(\Gamma) = \mathcal{H}$

Squared Energy: $\hat{E}^2(\Gamma) = (\mathcal{H})^2$

Heat capacity:

$$\frac{\langle \hat{E}^2 \rangle - \langle \hat{E} \rangle^2}{k_B T^2}$$

Squared Magnetization: $\hat{M}_z^2(\Gamma) = \left(\frac{1}{N} \sum_i S_i^z \right)^2$

Local update

Local update: We try to change a part of spins (typically single spin) at transitions along Markov chain

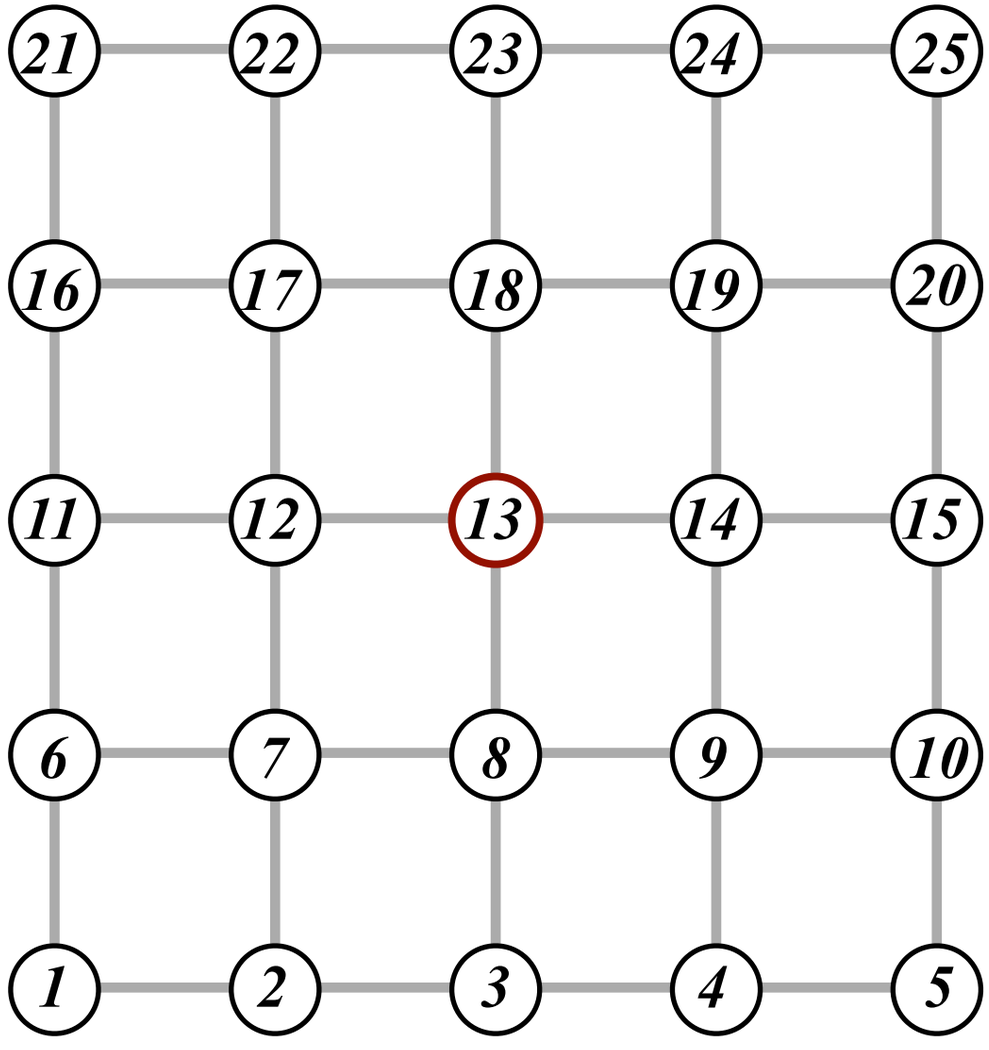
$$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$$

$$\Rightarrow \Gamma' = (S_1, S_2, \cdots, S'_{13}, \cdots, S_{25})$$

From Γ to Γ', we fix $S_1, S_2, .. S_{12}, S_{14}, S_{15}, \ldots, S_{25}$, and try to change only S_{13}.

In this local update, we can easily estimate the transition probability W because the change of Hamiltonian (Energy) is determined only locally.

* If the Hamiltonian contains long range interactions, the energy estimation becomes more costful.



Metropolis method:

*Proposal probability satisfies

$$q(\Gamma|\Gamma') = q(\Gamma'|\Gamma).$$

eg. $S_i' = -S_i$ for Ising spin.

$$a(\Gamma \to \Gamma') = \min\left(1, \frac{P(\Gamma')}{P(\Gamma)}\right)$$

$$\frac{P(\Gamma')}{P(\Gamma)} = e^{-\beta[\mathcal{H}(\Gamma')-\mathcal{H}(\Gamma)]} = e^{-\beta\Delta E}$$

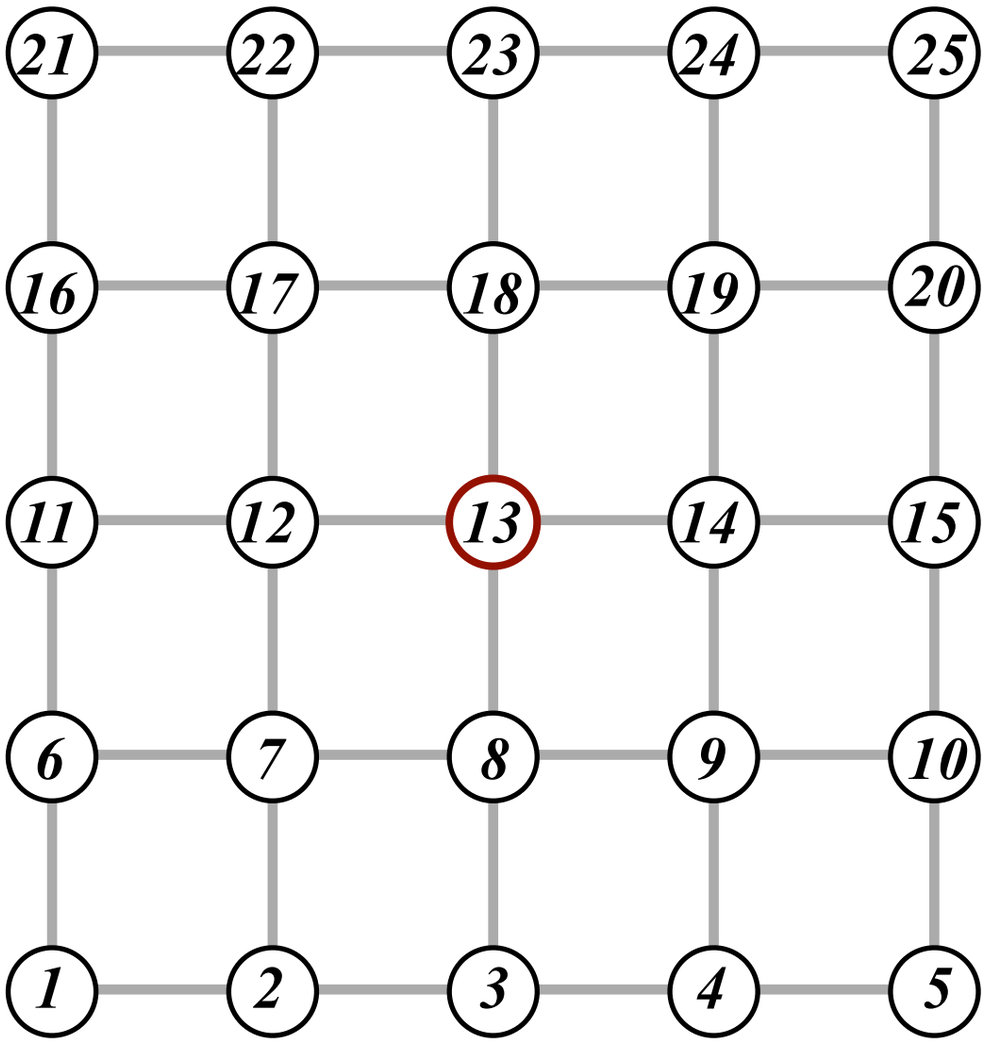
* We don't need partition function Z!

For local update on the square lattice,

$$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$$

$$\Rightarrow \quad \Gamma' = (S_1, S_2, \cdots, S'_{13}, \cdots, S_{25})$$

$$\Delta E = -J(S_8 + S_{12} + S_{14} + S_{18})(S'_{13} - S_{13}) - h[(S^z_{13})' - S^z_{13}]$$



Metropolis method with local update: summary

Step 0: Prepare an initial state $\Gamma_0 = (S_1, S_2, \cdots, S_N)$

loop t

select i-th site

1. Make next candidate state Γ' by changing S_i
   - Ising : $S_i' = -S_i$
   - XY, Heisenberg: $S_i' = S_i + \delta S$ or random unit vector
2. Calculate $\Delta E = \mathcal{H}(\Gamma') - \mathcal{H}(\Gamma)$
3. Make random number $r \in [0, 1]$
4. Select the next state Γ_{t+1} based on r as

$$\Gamma_{t+1} = \begin{cases} \Gamma' & r \leq e^{-\beta \Delta E} \\ \Gamma_t & \text{otherwise} \end{cases}$$

Calculate $O(\Gamma_t)$

Typically we choose
- random state ($T \to \infty$)
- ordered state ($T \to 0$)

If energy decreases ($\Delta E < 0$), we "accept" new state with probability 1.

It tends to sample low energy states.

Importance sampling in the canonical ensemble!

Usually, we observe quantities at least after N-spins are tried to change

Heat-bath method:

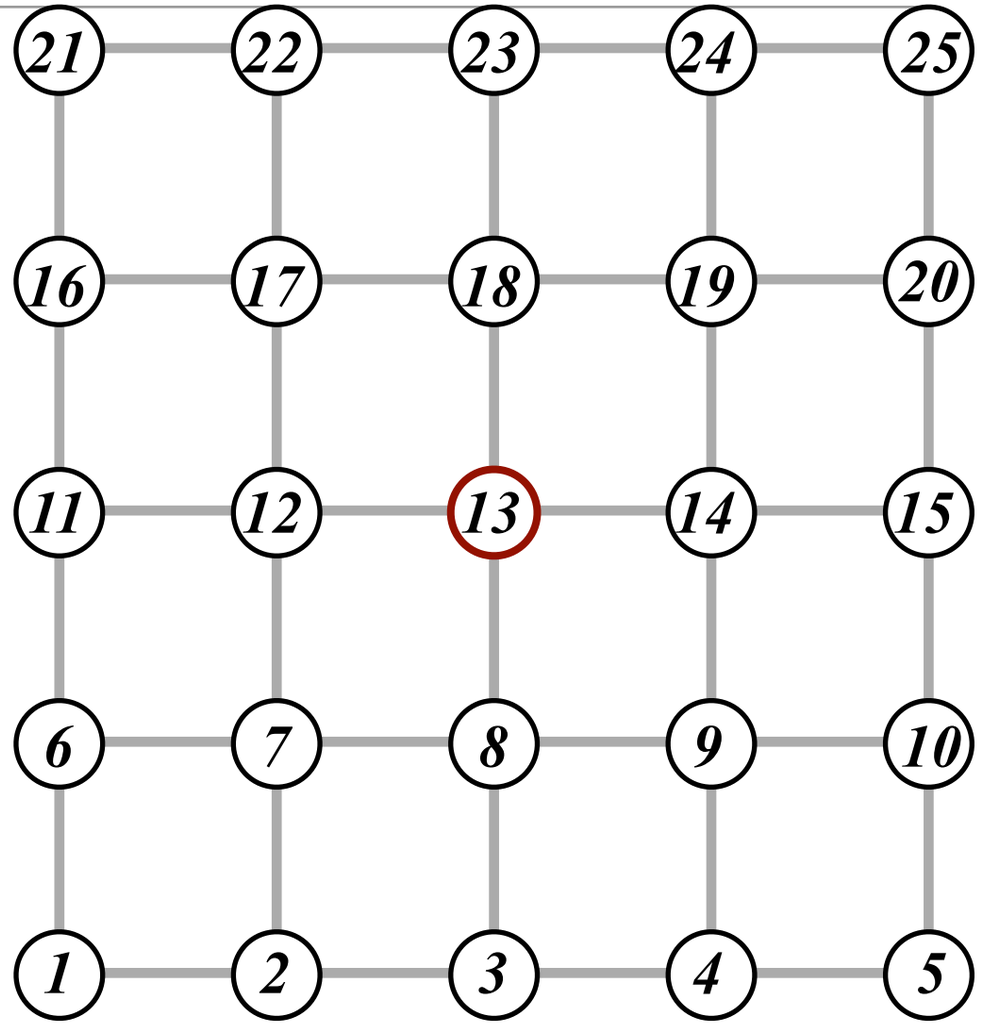
$$\Gamma = (S_1, S_2, \cdots, S_{13}, \cdots, S_{25})$$

$$\Rightarrow \quad \Gamma' = (S_1, S_2, \cdots, S'_{13}, \cdots, S_{25})$$

$$W_{\Gamma\to\Gamma'} = P(S'_{13}|S_1, S_2, \cdots S_{12}, S_{14}, \cdots, S_{25})$$

$$= \frac{P(\Gamma')}{\int dS_{13} P(\Gamma)}$$

$$= \frac{e^{\beta[J(S_8+S_{12}+S_{14}+S_{18})S'_{13}+h(S^z_{13})']}}{\int dS_{13} e^{\beta[J(S_8+S_{12}+S_{14}+S_{18})S'_{13}+h(S^z_{13})']}}$$



In the case of Ising or Heisenberg spins,
we can easily generate this probability distribution

Ising: $W_{\Gamma\to\Gamma'} = \dfrac{e^{\beta h_{\rm eff} S'_{13}}}{e^{\beta h_{\rm eff} S'_{13}} + e^{-\beta h_{\rm eff} S'_{13}}}$

Scaler value

$h_{\rm eff} \equiv J(S_8 + S_{12} + S_{14} + S_{18}) + h$

Heisenberg: $W_{\Gamma\to\Gamma'} = \dfrac{(\beta|h_{\rm eff}|)e^{\beta h_{\rm eff}\cdot S'_{13}}}{[e^{\beta|h_{\rm eff}|} - e^{-\beta|h_{\rm eff}|}]}$

Three component vector

$h_{\rm eff} \equiv J(S_8 + S_{12} + S_{14} + S_{18}) + h\hat{e}_z$

Heat-bath method with local update: summary

Step 0: Prepare an initial state $\Gamma_0 = (S_1, S_2, \cdots, S_N)$

loop t

select i-th site

1. Calculate effective field h_{eff}
2. Generate S'$_i$ based on the probability
$$P(S_i') \propto e^{\beta h_{\text{eff}} S_i'}$$
(for Ising and Heisenberg spins, it can be generated from uniform random number)
3. The next state Γ_{t+1} is Γ'

Calculate O(Γ_t)

Usually, we observe quantities at least after N-spins are tried to change

Typically we choose
- random state ($T \to \infty$)
- ordered state ($T \to 0$)

$r \in [0, 1]$:uniform random number

Ising : $$S_i' = \begin{cases} 1 & r \le P(1) \\ -1 & \text{otherwise} \end{cases}$$

Heisenberg:

(in polar co-ordinate with z // h_{eff})

$$S_x' = \sin\theta\cos\phi$$
$$S_y' = \sin\theta\sin\phi$$
$$S_z' = \cos\theta$$

$r_1, r_2 \in [0, 1]$:uniform random number

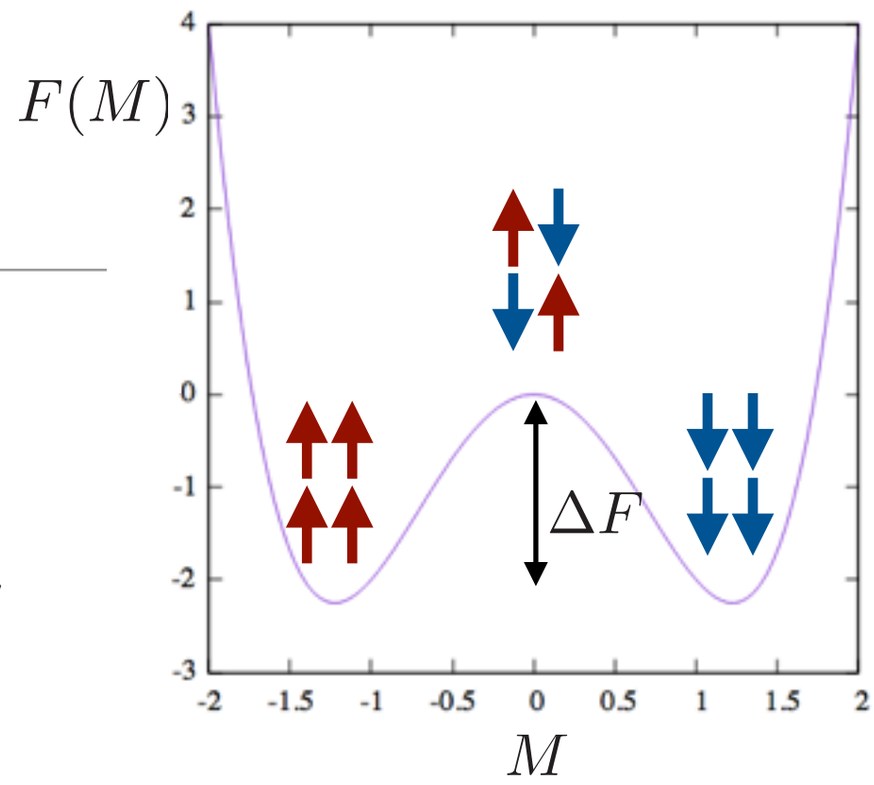
$$\phi = 2\pi r_1$$
$$\cos\theta = -1 + \frac{1}{\beta|h_{\text{eff}}|} \times \ln[r_2 + (1 - r_2)e^{2\beta|h_{\text{eff}}|}]$$

Problems in local update

Sampling efficiency largely decreases for

1. Critical phenomena
   - Divergence of relaxation time: $\tau \propto |T - T_c|^{-z\nu}$
2. 1st order phase transition (phase coexistence)
3. Low temperature phase with discrete symmetry (e.g. Ising model)
   - Exponentially small probability to move other local minima: $\tau \propto \exp\left[\frac{\Delta F}{T}\right]$

Free energy landscape



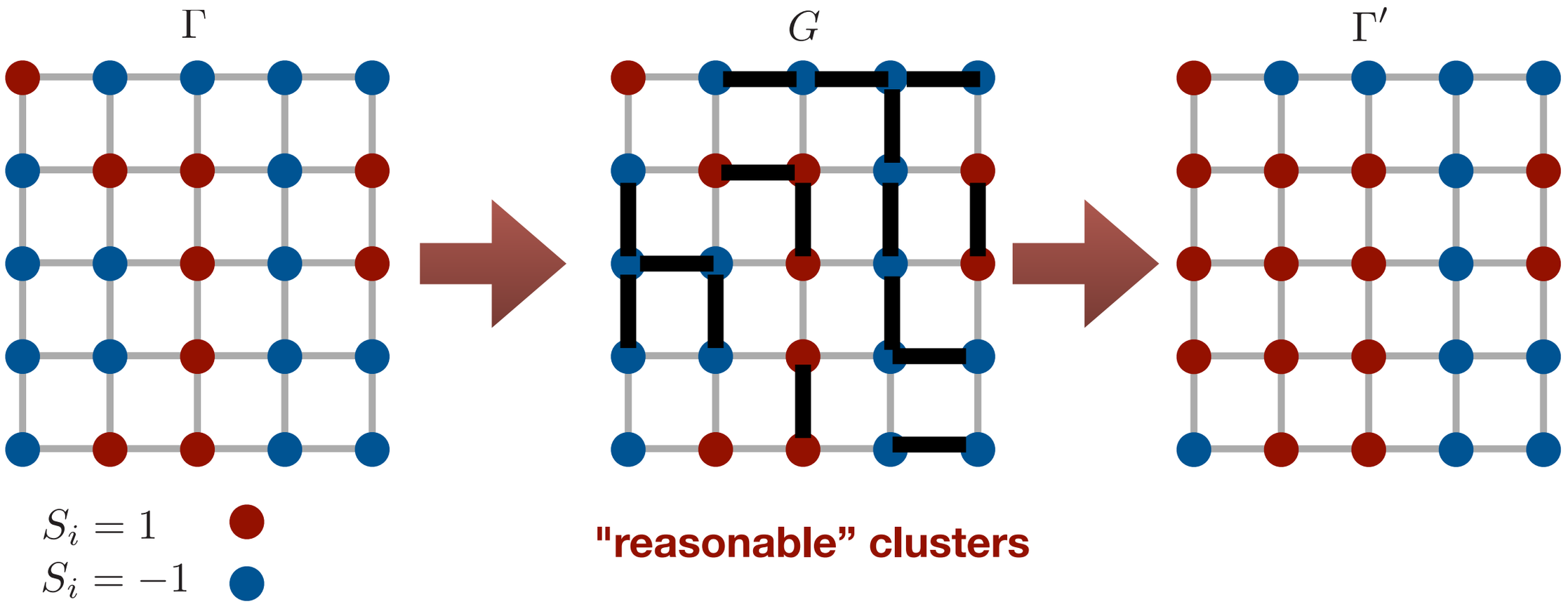
Part of these difficulties can be reduced by using "global update"

Simultaneous change of spins in "large cluster"

Cluster update method

Idea of cluster updates

- From a spin configuration Γ, we can define "reasonable" clusters G.
- When we "flip" all spins on a cluster G and make new configuration Γ', the free energy difference between Γ and Γ' is not so large.
- We can change the configuration drastically with higher probability.



How to make a cluster configuration?

Fortuin-Kasteleyn mapping (for Ising model)

Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j \ , S_i = \pm 1$$

P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Jpn, Suppl. **26**, 11 (1969)

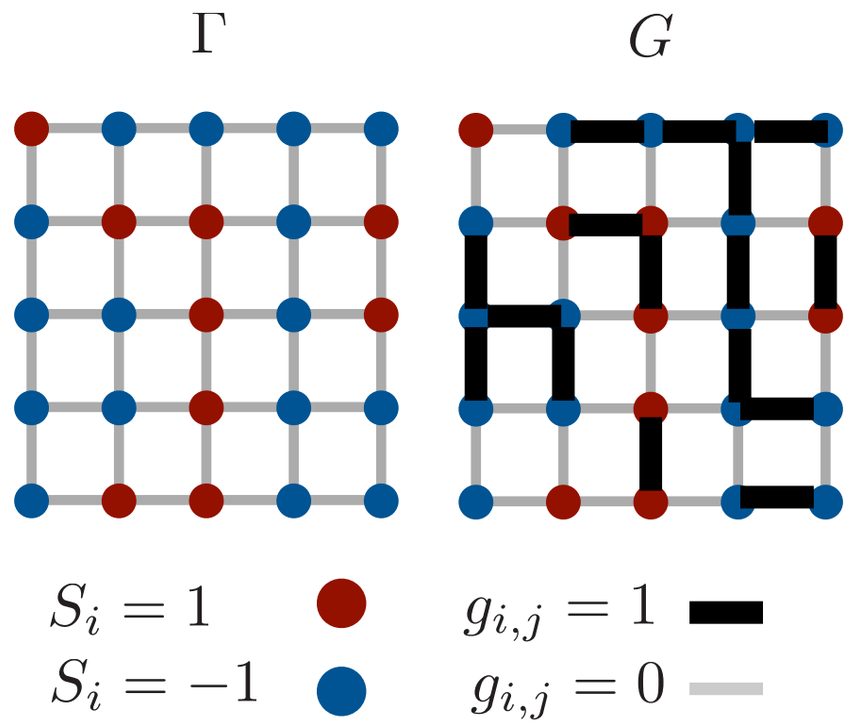
C. M. Fortuin and P. W. Kasteleyn, Physica **57**, 536 (1972)

$$e^{\beta J S_i S_j} = \underbrace{e^{-\beta J}}_{g=0} + \underbrace{\delta_{S_i,S_j}(e^{\beta J} - e^{-\beta J})}_{g=1} = \sum_{g=0,1} w(g, S_i, S_j)$$

$$Z = \sum_{\Gamma} e^{\beta J \sum_{\langle i,j \rangle} S_i S_j}$$

$$= \sum_{G} \sum_{\Gamma} \prod_{\langle i,j \rangle} w(g_{i,j}, S_i, S_j)$$

$G = \{g_{i,j}\}$ $\quad$ $\Gamma = \{S_i\}$



Markov chain in extended (G, Γ) space

$$Z = \sum_G \sum_\Gamma \prod_{\langle i,j \rangle} w(g_{i,j}, S_i, S_j) = \sum_G \sum_\Gamma W(G,\Gamma)$$

$$\cdots \to \Gamma_t \to G_t \to \Gamma_{t+1} \to G_{t+1} \to \cdots$$

Transition probabilities

$$W_{\Gamma \to G} = \frac{W(G,\Gamma)}{W(\Gamma)}, W_{G \to \Gamma} = \frac{W(G,\Gamma)}{W(G)}$$

$$= \prod_{\langle i,j \rangle} w_{(S_i,S_j)\to g_{ij}} \quad = \prod_{C_j} P(\{S_i \in C_j\})$$

cluster formed from g=1 links

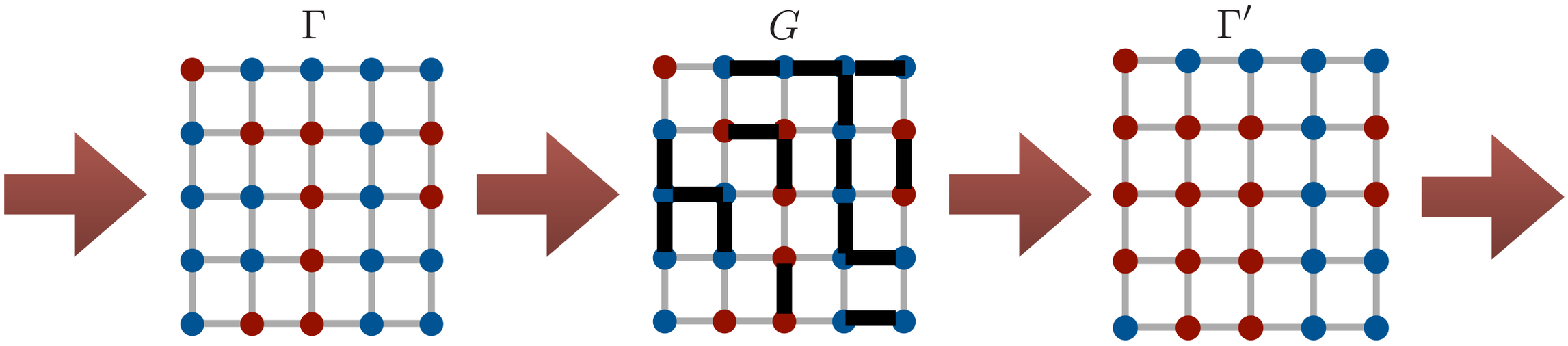
$$W(\Gamma) = \sum_G W(G,\Gamma)$$

$$W(G) = \sum_\Gamma W(G,\Gamma)$$

$$w_{(S_i,S_j)\to 0} = \begin{cases} 1 & (S_i \neq S_j) \\ e^{-2\beta J} & (S_i = S_j) \end{cases}$$

$$P(\{S_i \in C_j\}) = 1$$

(If all spin in cluster is pointing same direction)



Swendsen-Wang algorithm

Swendsen-Wang algorithm

R. H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58**, 86 (1987)

Step 0: Prepare an initial state $\Gamma_0 = (S_1, S_2, \cdots, S_N)$

loop *t*

loop <i,j>

- if $S_i = S_j$, generate a random number
  - if $r \leq 1 - e^{-2\beta J}$ connects *i* and *j* ($g_{ij}=1$)

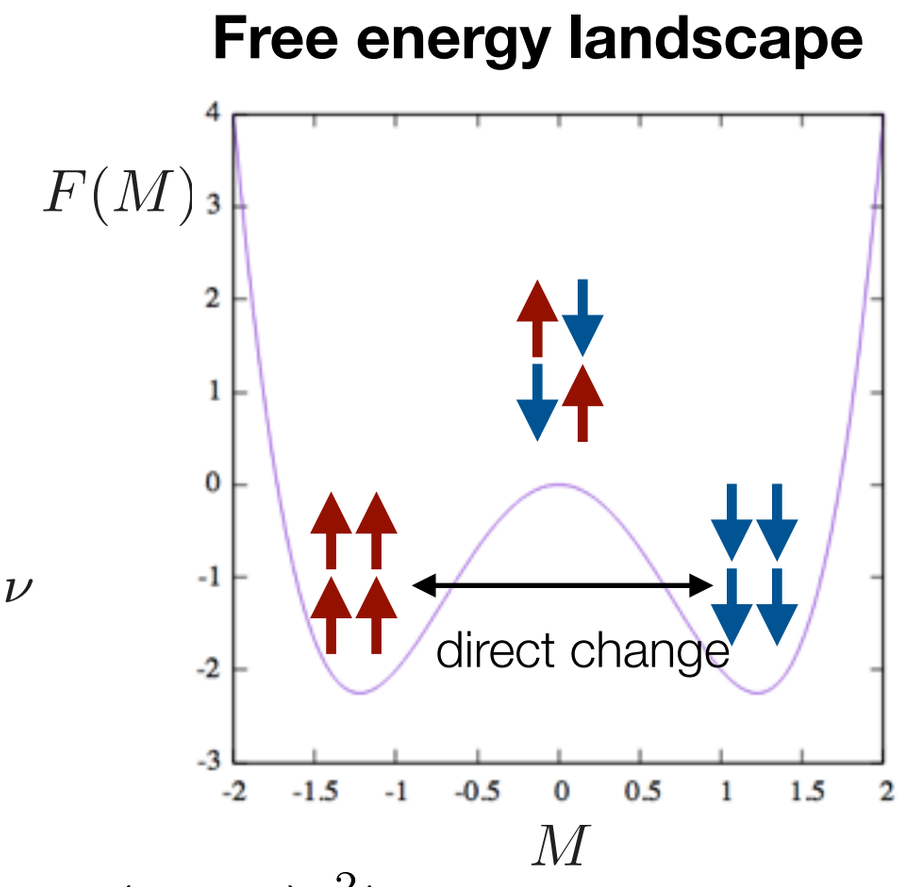
end loop <i,j>

- Make clusters using algorithms (e.g. union find)
- Change spins on the same clusters simultaneously with probability 1/2 (using random number)

Calculate $O(\Gamma_t)$

Merit of cluster update

1. For low temperature phase, the system easily transit other minima
   - Minima are related to the symmetry of the Hamiltonian
2. For critical phenomena “the dynamical critical exponent become much smaller
   - Swendsen-Wang : $z \simeq 0 \quad \tau \propto |T - T_c|^{-z\nu}$
3. Graph representation closely related to physics
   - e.g. Magnetic susceptibility in SW: $\chi = \frac{\beta}{N} \left\langle \sum_C \left(\sum_{i \in C} S_i \right)^2 \right\rangle$
   - By using observable based on graph, statistical error is largely reduced “Improved estimator”



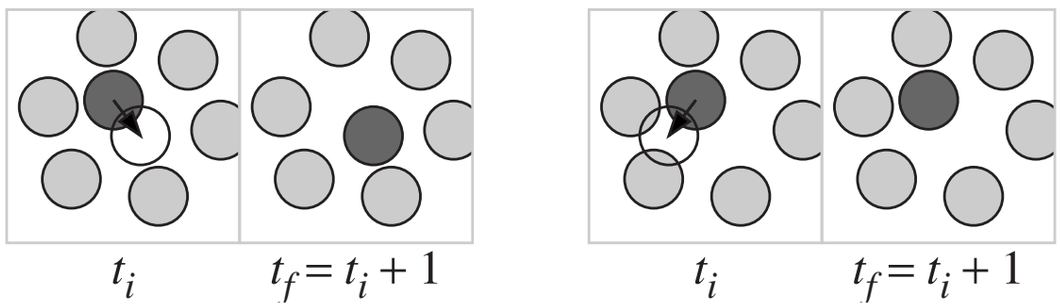
*Linear size of cluster ~ ξ

Event-chain Monte Carlo

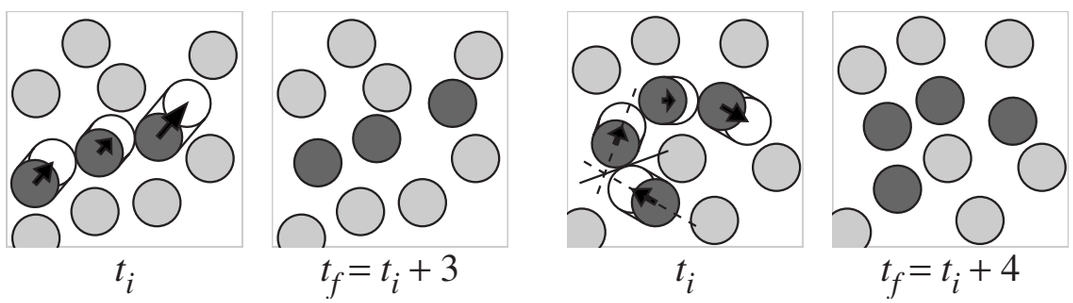
A "global" update for particle system (hard spheres)

E. P. Bernard, W. Krauth, and D. B. Wilson, Phys. Rev. E **80**, 056704 (2009)

local update

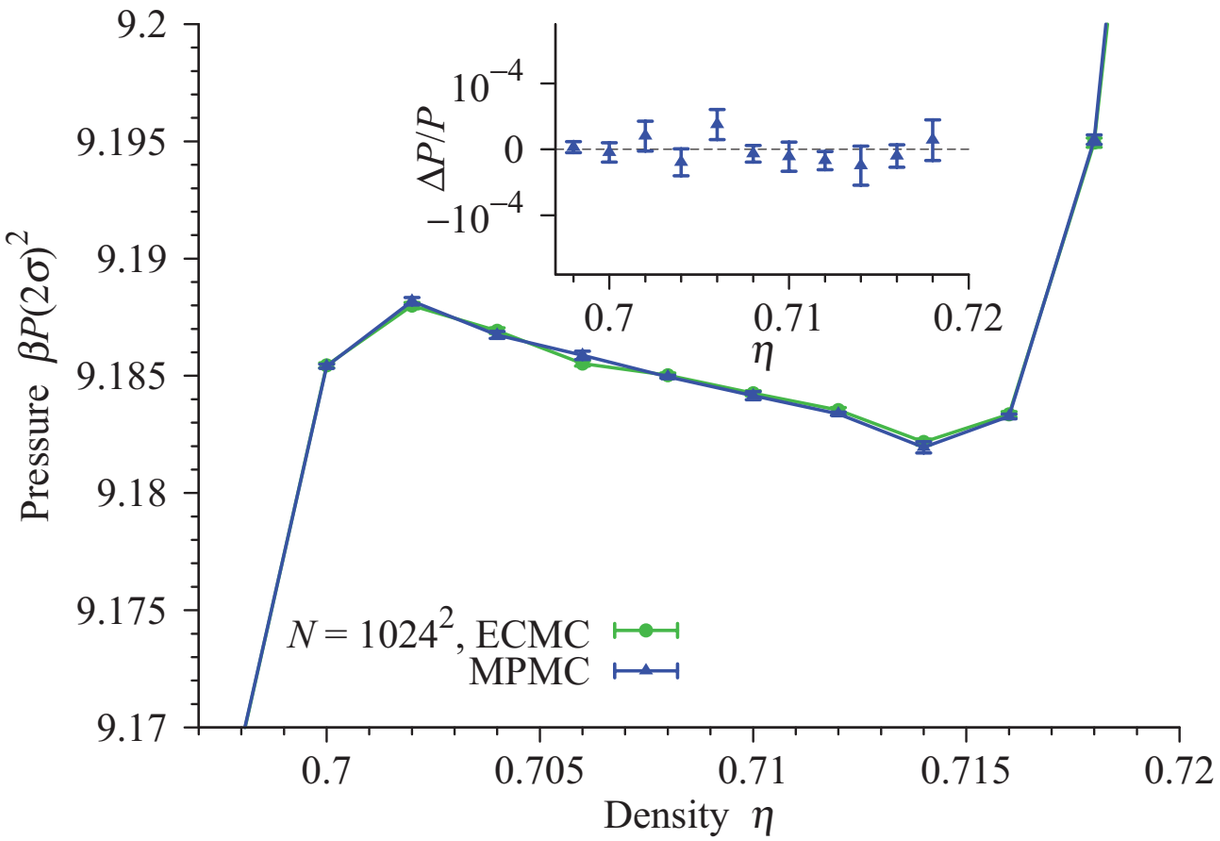


event chain update



Application to 2d melting

M. Engel *et al,* Phys. Rev. E **87**, 042134 (2013)



Computational science using MC methods

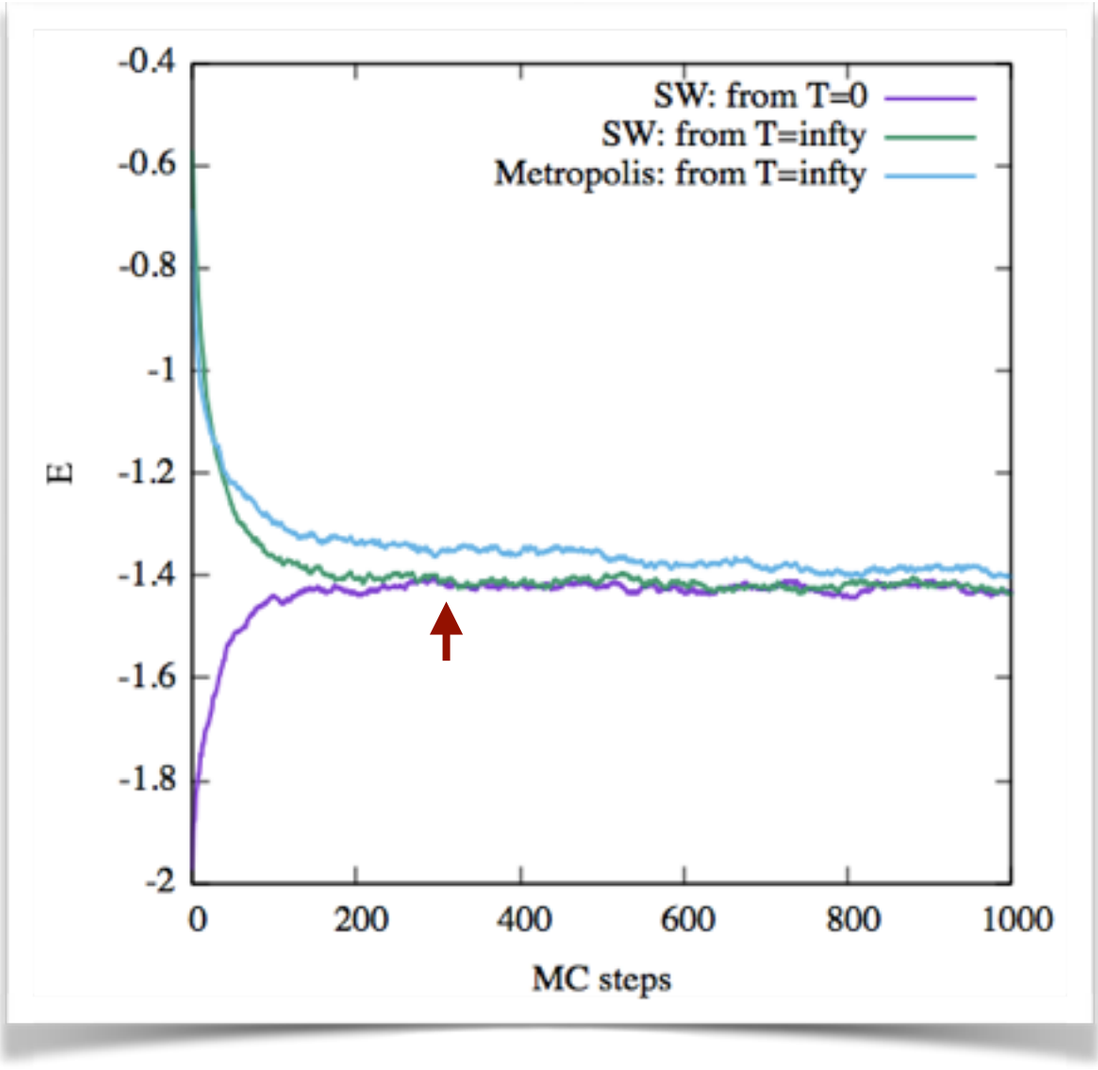
Important tips for real calculations 1

In each calculation, we have to check the convergence.

If the correlation time is very long, obtained data (expectation values) might be biased from the initial state Γ_0.

Usual procedure:

- Discard initial several MC steps
- Change MC steps and compare results
- Change Initial state
- ….



Important tips for real calculations 2

We need to estimate the statistical errors.

$$\bar{A} \equiv \frac{1}{T}\sum_{t=1}^{T} \hat{A}(\Gamma(t))$$

Standard error: $\epsilon^2 = \langle \bar{A}^2 \rangle - \langle \bar{A} \rangle^2$ $\qquad \epsilon \propto \sqrt{\dfrac{1+2\tau}{T}}$

Maximum likelihood estimation for standard error

Prepare "independent" M samples for $\bar{A}$: $\{\bar{A}_1, \bar{A}_2, \cdots, \bar{A}_M\}$

$$\sigma^2(M) = \frac{\frac{1}{M}\sum_i \bar{A}_i^2 - \left(\frac{1}{M}\sum_i \bar{A}_i\right)^2}{M-1}$$

$$\lim_{M\to\infty} \sigma^2(M) = \epsilon^2$$

Make "error bar" based on σ, and use it for data analysis.

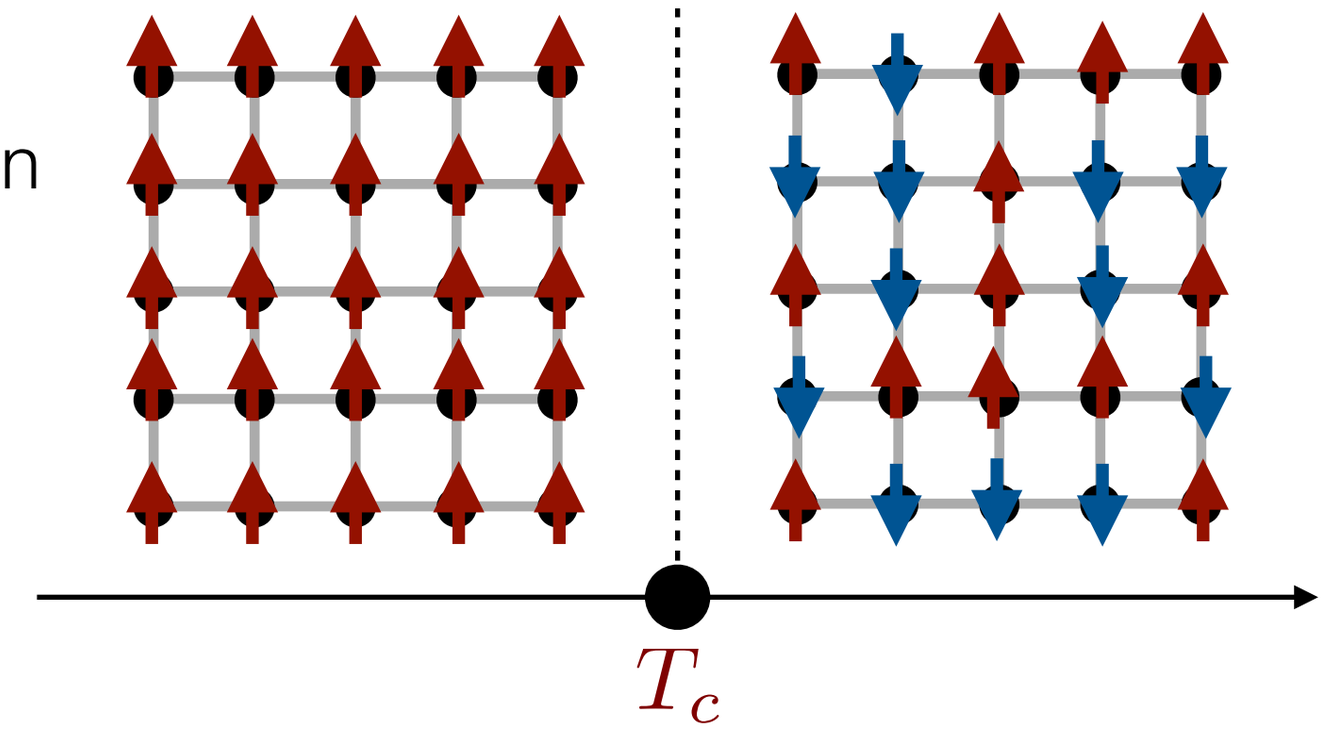
Example: Application for critical phenomena

- Square lattice Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j$$

  - Continuous phase transition at $T=T_c$

$$T_c/J = \frac{2}{\ln(1+\sqrt{2})} = 2.26918531\ldots$$



  - $T>T_c$: Paramagnetic
  - $T<T_c$: Ferromagnetic

- Monte Carlo Simulation using ALPS (spinmc)
  - spinmc: Simulator for classical spin system by MCMC

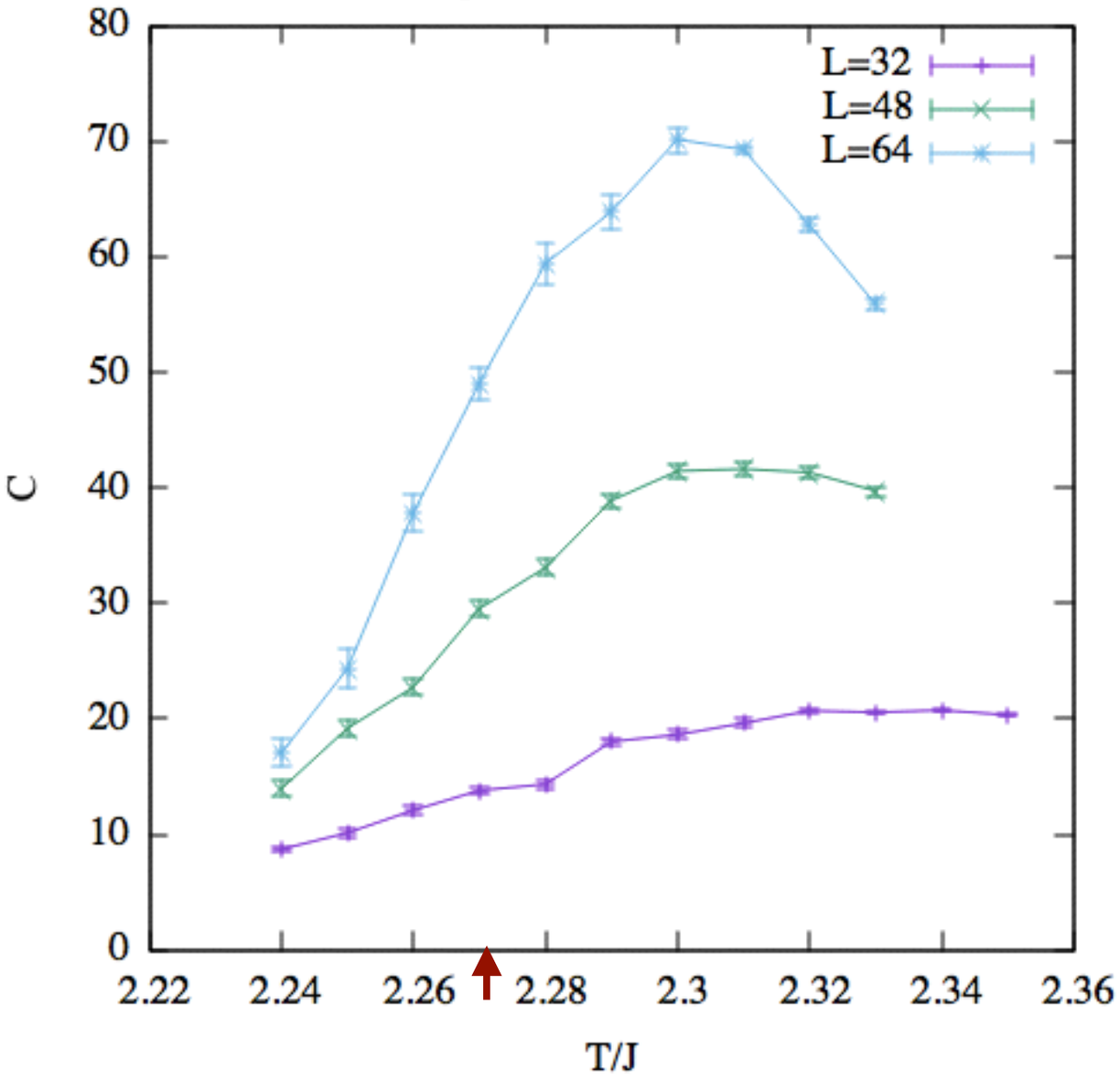
ALPS（Applications and Libraries for Physical Simulation)

- Set of libraries and applications for a variety of lattice models.
- Support for spin models, Hubbard model, Kondo lattice model, …
- A lot of solvers for models:
  - Classical/Quantum Monte Carlo, Exact Diagonalization, Density Matrix Renormalization Group (DMRG), Dynamical Mean Field Theory (DMFT), Time Evolving Block Decimation (TEBD), …
- We can select efficient solver for your problems.
- It can be applicable to the frontier research.

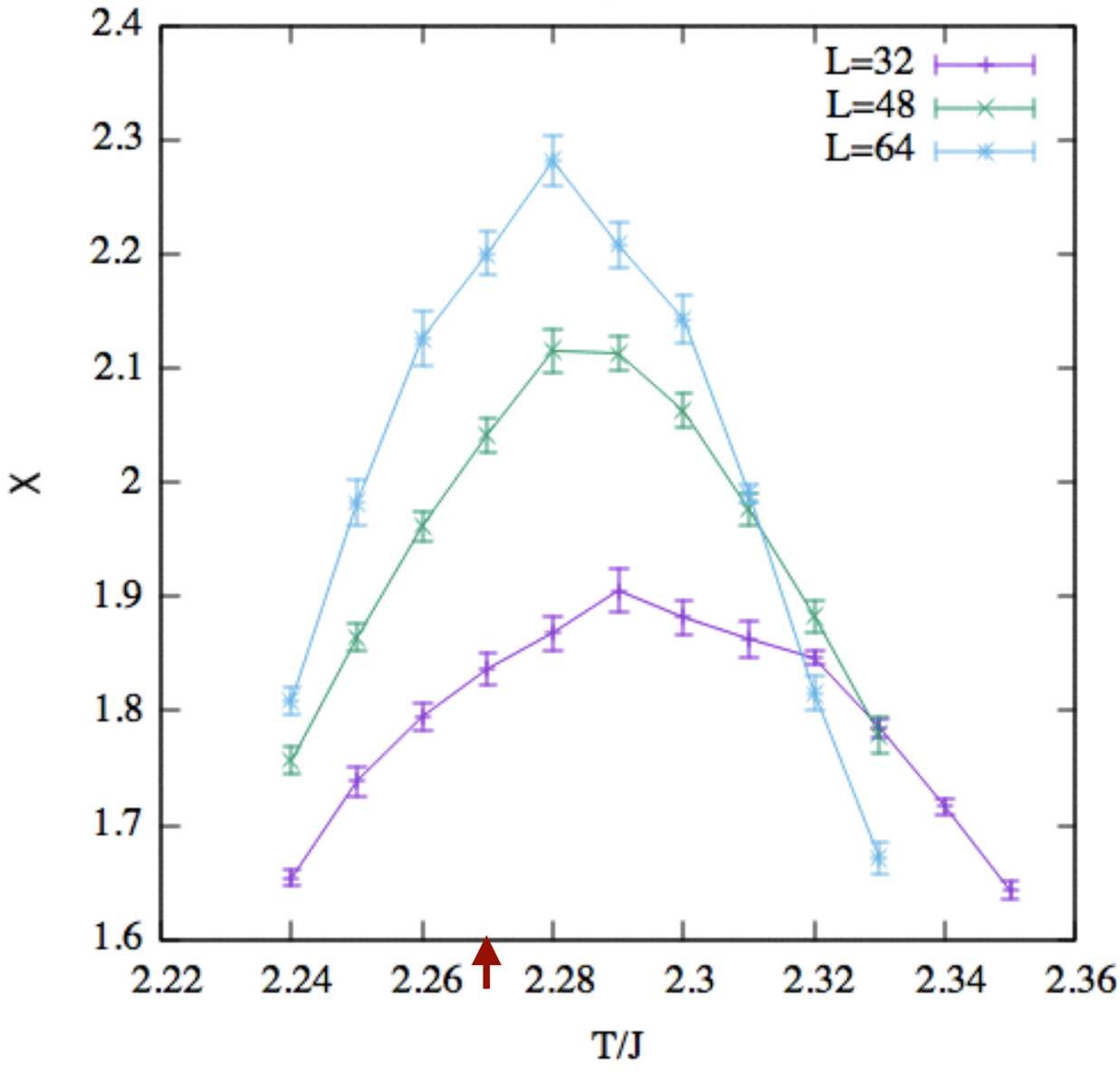
ALPS Wiki http://alps.comp-phys.org/mediawiki/index.php/Main_Page

Calculated data (ALPS tutorial 7b)

Specific heat



Susceptibility



$$T_c/J \simeq 2.269$$

Data analysis: Finite size scaling (outline)

Near the critical point (transition temperature):

The singular part of the free energy density satisfies finite size scaling

$$f_s(t, h, L) = L^{-d} f_s(tL^{y_t}, hL^{y_h})$$

$$t = T - T_c$$

y_t, y_h :scaling exponent $\Longleftrightarrow$ $y_t = 1/\nu, \quad y_h = \gamma/(2\nu)$

By taking derivatives, we see

$$M^2 = \frac{\partial^2 f}{\partial h^2} = L^{2y_h - d} g(tL^{y_t}, 0) \quad \text{(we set } h=0\text{)}$$

Physical quantity obeys common scaling function independent of L.

$\Rightarrow$ At the critical point, $M^2 \sim L^{-x_{M2}} \quad (x_{M2} \equiv d - 2y_h)$

x: scaling dimension

If x =0, it has no size dependence at the critical point!

Binder ratio

Binder ratio

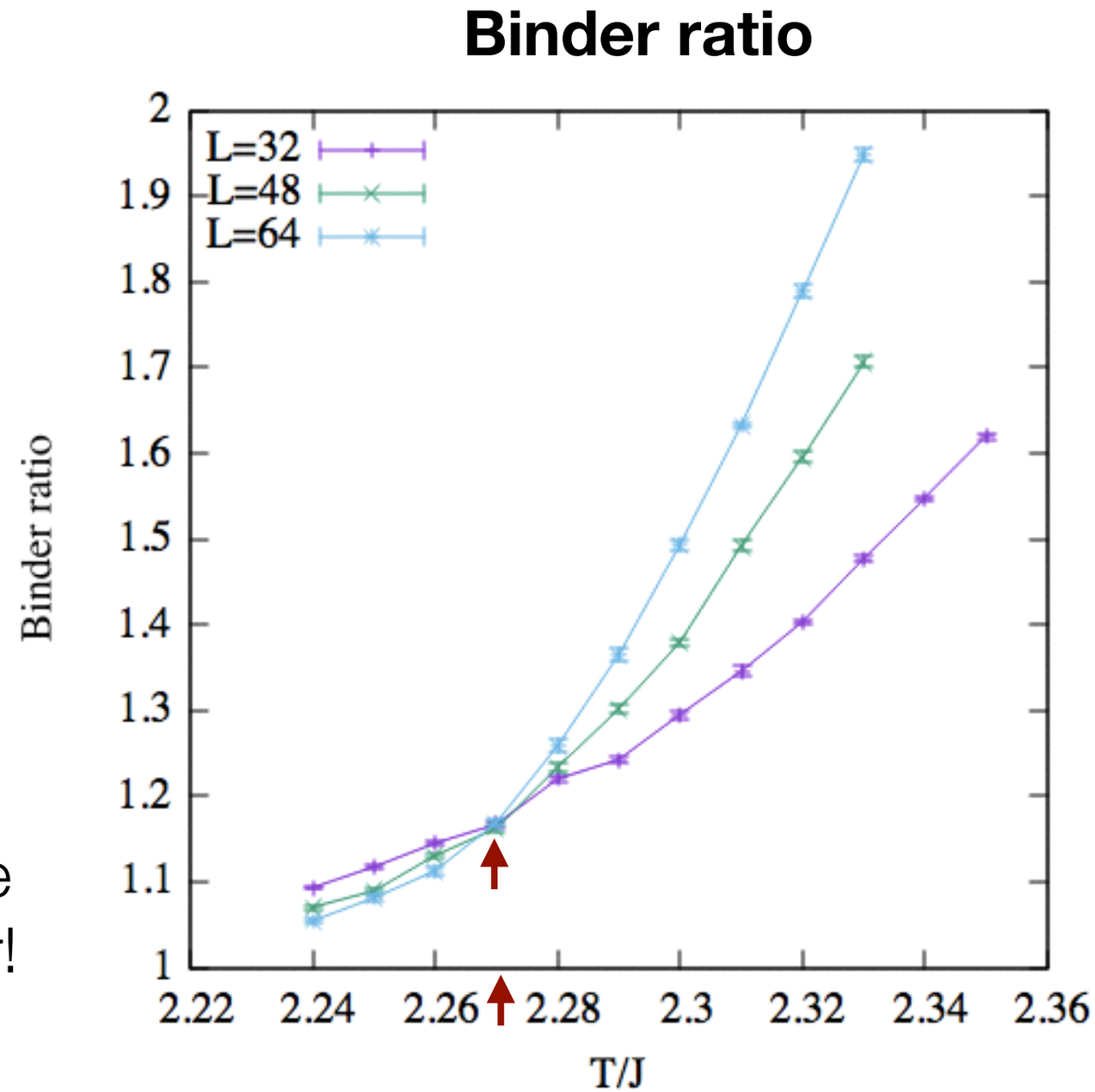
$$b = \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}$$

$$b = 3 \quad (T \to \infty)$$

$$b = 1 \quad (T \to 0)$$

The scaling dimension of b is exactly zero.

At Tc, the size dependence disappears in leading order!



$$T_c/J \simeq 2.269$$

Finite size scaling

Binder ratio

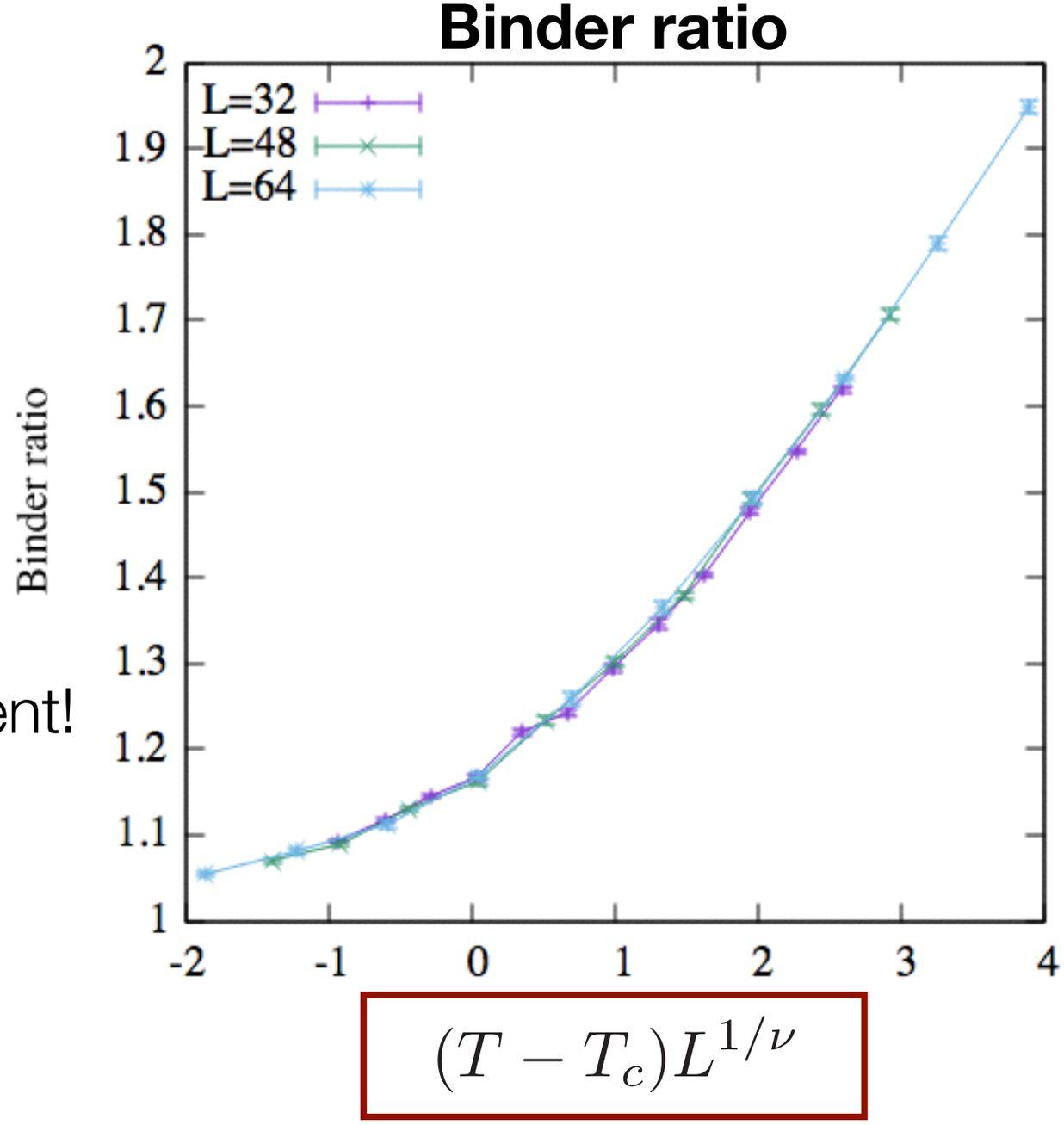
$$b = \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}$$

finite size scaling around Tc

$$b = f((T - T_c)L^{1/\nu})$$

We can determine critical exponent!

$$\nu = 1$$



Exercise: autocorrelation of MCMC (not a report)

See correlation time or autocorrelation function of
Ising model calculated by Monte Carlo simulation.

- Around Tc, how does the correlation time behave by varying the temperature?
- At Tc, how about the size (L) dependence?
- Does the correlation time depend on the algorithms?

To perform these exercise, you can use,

- Your own code
- ALPS (it is not straight forward to see the correlation time...)
- My sample codes for jupyter notebook (or python2.7).
  - In order to run the sample code you need
    - numpy, and numba
    - numba is used for speed up. In case you do not want to install numba, please use Ising_wo_jit.py .

usage: *jupyter notebook* → select Ising.ipynb

python Ising.py

Next week

Classical

第１回：　物理学における多体問題
第２回：　多体問題における困難
第３回：　古典統計力学模型と数値計算
第４回：　古典モンテカルロ法とその応用
第５回：　分子動力学法とその応用
(Molecular dynamics simulation and its applications)
第６回：　拡張アンサンブル法によるモンテカルロ計算

Quantum

第７回：　量子統計力学模型と数値計算
第８回：　量子モンテカルロ法
第９回：　量子モンテカルロ法の応用
第１０回：　量子多体問題と巨大な疎行列の線形代数
第１１回：　クリロフ部分空間法の量子多体問題への応用
第１２回：　巨大な疎行列と量子統計力学
第１３回：　多体問題の並列計算アルゴリズム