

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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Outline

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

Standard Monte Carlo method

Monte Carlo method: Randomized algorithm

Randomized algorithm:

It changes its behavior depending on (pseudo) random numbers on execution.

Example :

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

Algorithm (rejection sampling)

$N_a \leftarrow 0, N_s \leftarrow 0$ initialize

loop i

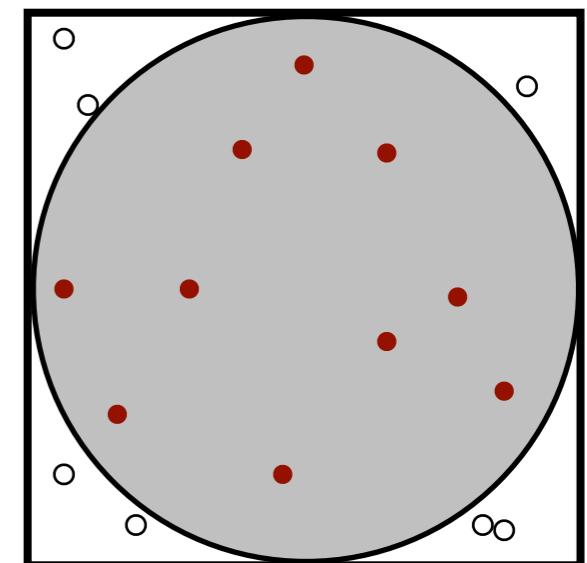
$$x_i \in [-1, 1]$$

take uniform
random numbers

$$y_i \in [-1, 1]$$

$$N_s \leftarrow N_s + 1$$

if $x_i^2 + y_i^2 \leq 1$ then $N_a \leftarrow N_a + 1$
end loop



$$\lim_{N_s \rightarrow \infty} \frac{N_a}{N_s} = \frac{\pi}{4}$$

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

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

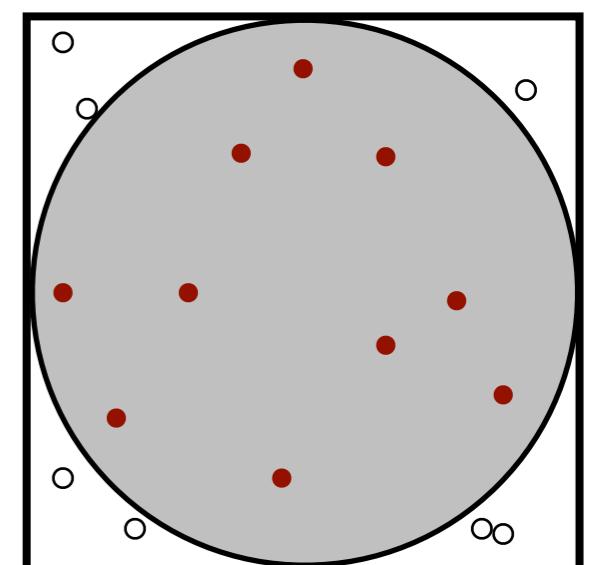
Estimate an integral as **an expectation value under $P(\Gamma)$**

Previous example:

$$\Gamma = \{(x, y); -1 \leq x \leq 1, -1 \leq y \leq 1\}$$

$$f(\Gamma) = \begin{cases} 1 & \sqrt{x^2 + y^2} \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

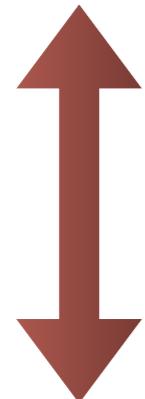
$P(\Gamma) = \text{const.}$ (Uniform distribution)



Monte Carlo Integration: General aspect

Merit of Monte Carlo Integration

The error is (usually) independent on the dimension of Γ .



$$\epsilon \sim \sqrt{\frac{\sigma_f^2}{N_s}} \propto O(N_s^{-1/2})$$

N_s : sampling number

σ_f^2 : Variance

$$\sigma_f^2 = \left\langle \left[\frac{f(\Gamma)}{P(\Gamma)} \right]^2 \right\rangle - \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle^2$$

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

eg. trapezoidal formula

$$\epsilon \propto O(N_s^{-2/d})$$

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

Rejection sampling is inefficient for higher dimensions

Volume ratio between “ d -dimensional hyper cubic” (with $L=2$) and
“ d -dimensional hyper sphere” (with $r=1$)

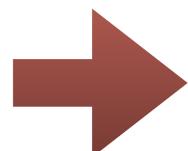
$$r = \frac{V_{\circ}}{V_{\square}} = \frac{\pi^{d/2}/\Gamma(\frac{d}{2} + 1)}{2^d} \sim \left(\frac{e\pi}{2d}\right)^{d/2}$$

Asymptotic form of Γ -function

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

For larger d , the ratio exponentially decreases!

$$\text{And, } \sigma_f^2 = \left\langle \left[\frac{f(\Gamma)}{P(\Gamma)} \right]^2 \right\rangle - \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle^2 = V_{\circ}^2 \left(\frac{1}{r} - 1 \right) \sim O(r^{-1})$$



(Relative) Error of the rejection sampling increases exponentially.

$$\epsilon \sim O((rN_s)^{-1/2}) = O\left(\left(\frac{2d}{e\pi}\right)^{d/4} N_s^{-1/2}\right)$$

More efficient way?

Sample points where $|f(\Gamma)|$ takes large value!
(eg. points within the sphere)



Importance sampling

Importance sampling and Markov Chain Monte Carlo

Sampling with uniform distribution

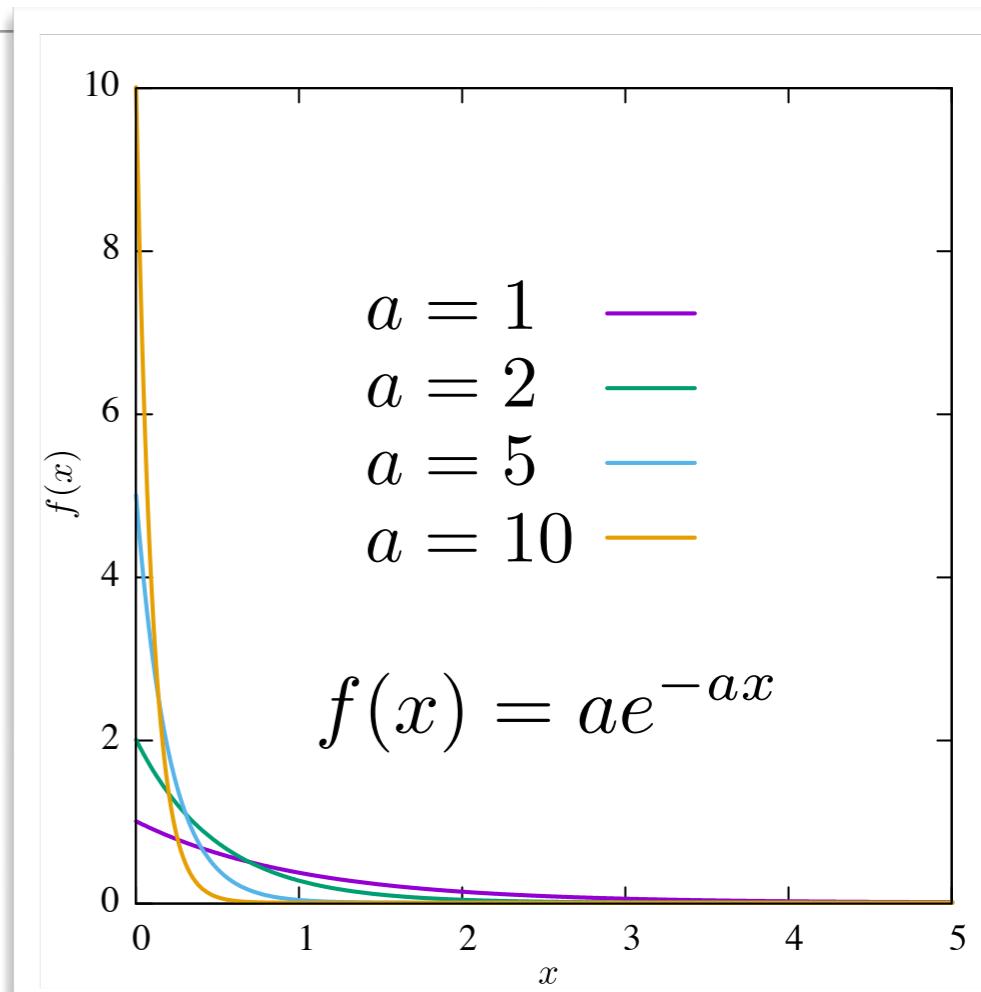
$$\int d\Gamma f(\Gamma) = \int d\Gamma \frac{f(\Gamma)}{P(\Gamma)} P(\Gamma) \quad \text{with } P(\Gamma) = \text{const.}$$

When $f(\Gamma)$ is "narrow", the sampling becomes inefficient, as like the rejection sampling.

For example, $f(x) = ae^{-ax}$, $x \in [0, l]$

$$\rightarrow \sigma_f^2 \sim \frac{la}{2} \sim O(la) \rightarrow \epsilon \sim O\left(\sqrt{la/N_s}\right)$$

The error increases as the parameter a increases.



This situation typically occurs in a sampling for statistical mechanics.

$$\langle \hat{O} \rangle \equiv \int d\Gamma \hat{O}(\Gamma) \underline{P_{\text{eq}}(\Gamma)}$$

It corresponds to $f(\Gamma) = \hat{O}(\Gamma) P_{\text{eq}}(\Gamma)$

Equilibrium distribution, e.g.,
 $P_{\text{eq}}(\Gamma) \propto e^{-\beta \mathcal{H}(\Gamma)}$

$$\mathcal{H}(\Gamma) = \textcolor{red}{O}(N)$$

N : number of particles or spins

Importance Sampling

Importance sampling

Chose $P(\Gamma)$ close to $f(\Gamma)$. (e.g. $P(\Gamma) \propto f(\Gamma)$)

$$\rightarrow \sigma_f^2 = \left\langle \left[\frac{f(\Gamma)}{P(\Gamma)} \right]^2 \right\rangle - \left\langle \frac{f(\Gamma)}{P(\Gamma)} \right\rangle^2 \text{ Becomes small!}$$

However it is **not so easy**, in practice!

In order to perform Monte Carlo sampling,
 $P(\Gamma)$ must be **easily generated** from pseudo random numbers.

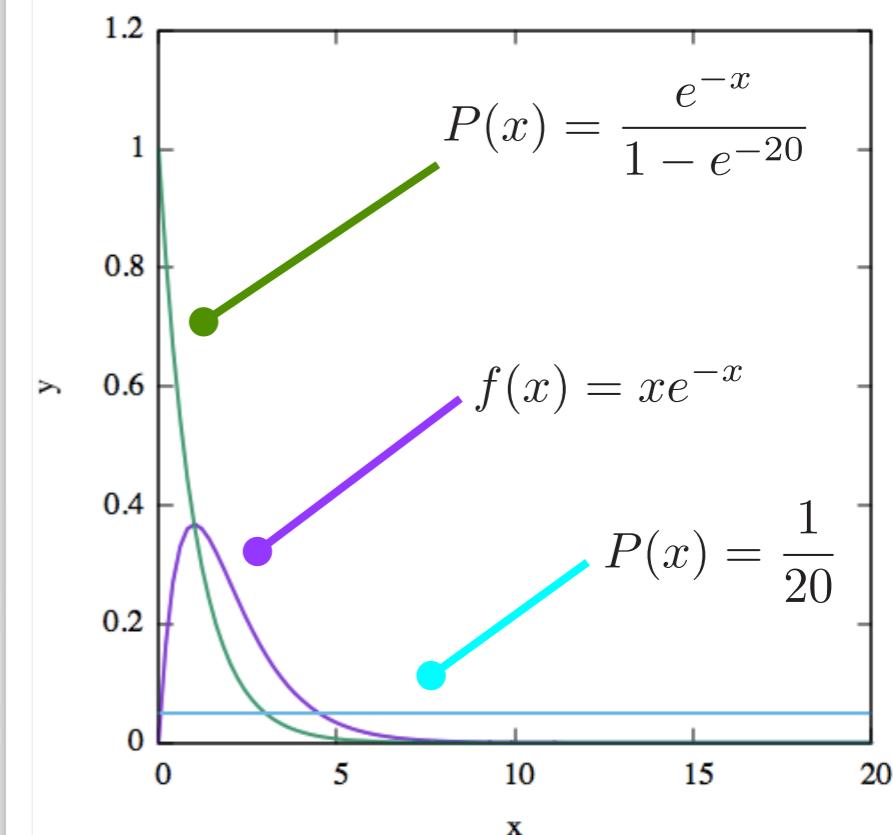


$$P_{\text{eq}}(\Gamma) \propto e^{-\beta \mathcal{H}(\Gamma)}$$

- We do not know the normalization constant
- It is too complex

How can we perform the importance sampling?

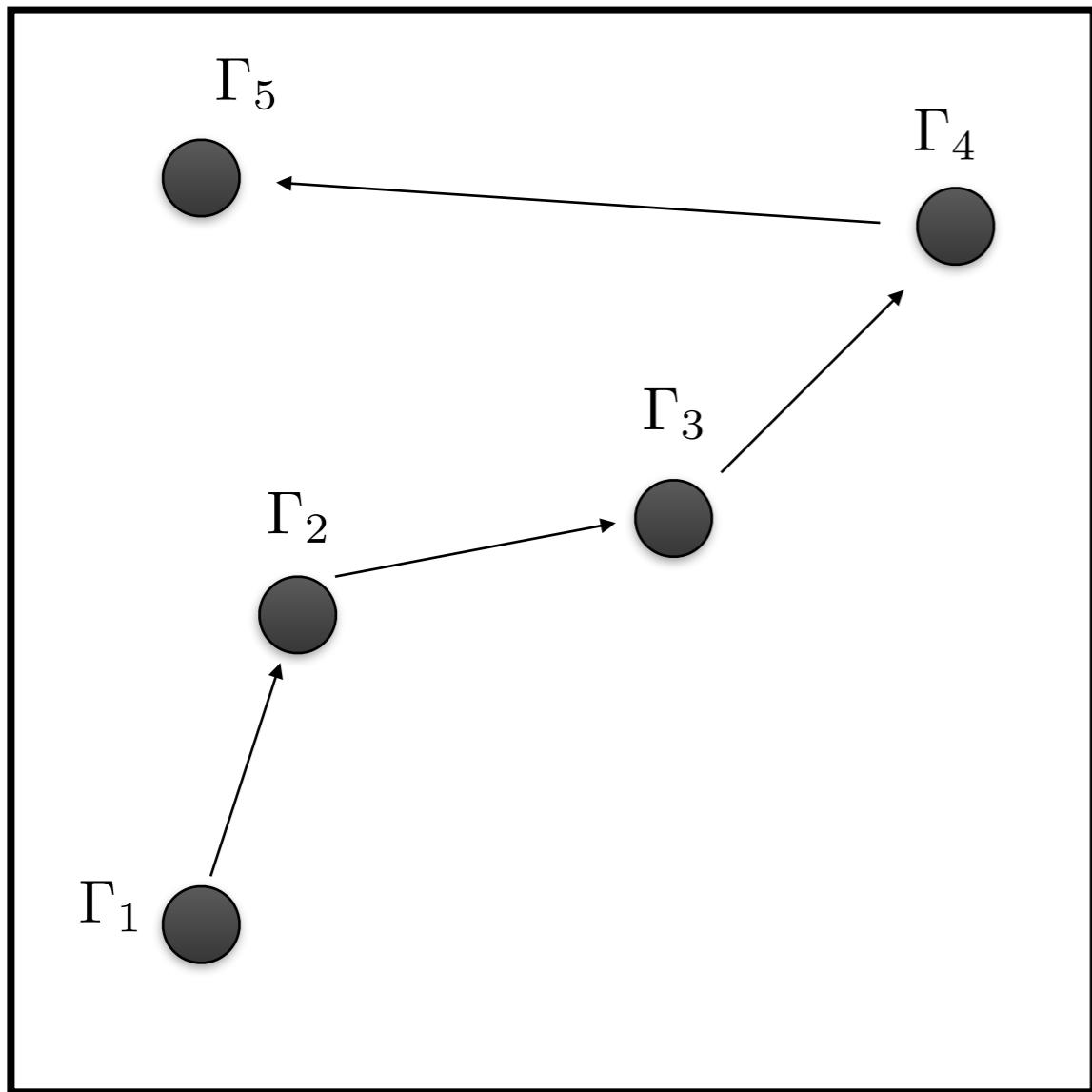
Example of importance sampling



Markov Chain Monte Carlo (MCMC)

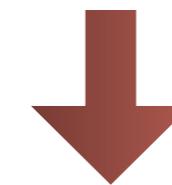
We might generate a $P(\Gamma)$ as the steady state of a stochastic process.

A sampling point move in Γ “randomly”.



Markov process:

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



The **transition probability** to Γ_{t+1} depends on Γ_t .

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

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

Markov Chain Monte Carlo (MCMC)

Master equation for general Markov process

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

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

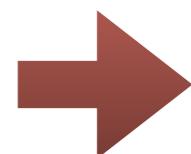
$$\sum_{\Gamma'} W_{\Gamma \rightarrow \Gamma'} = 1$$

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

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

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

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



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

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

2. “Balance Condition”

- The “flows” of probabilities are balanced for $P(\Gamma)$.

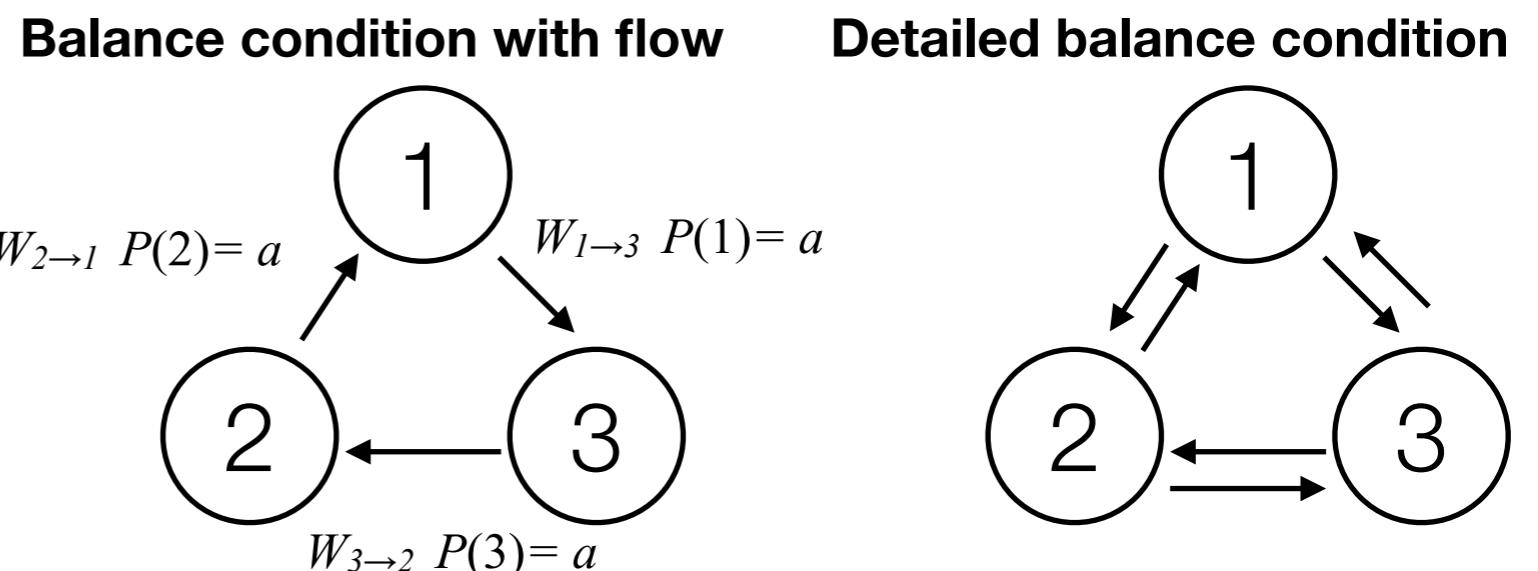
$$\forall \Gamma, \sum_{\Gamma'} W_{\Gamma \rightarrow \Gamma'} P(\Gamma) = \sum_{\Gamma'} W_{\Gamma' \rightarrow \Gamma} P(\Gamma')$$

Special case:

Detailed balance condition

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

No microscopic flow
in the steady state



Examples of MCMC

Example: 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

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

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

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

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

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

Metropolis-Hastings sampling: Detailed balance

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

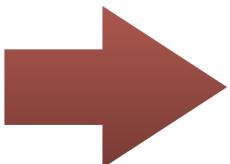
$$W_{\Gamma \rightarrow \Gamma'} = q(\Gamma' | \Gamma) a(\Gamma \rightarrow \Gamma')$$

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

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

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

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



It satisfies the **detailed balance condition**.

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

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

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

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

Note:

We do not need to know
the normalization constant.

Example: Heat-bath sampling (Gibbs sampling)

Suppose we only change a part of variables in Γ

$$\Gamma = (\Gamma^1, \Gamma^2, \Gamma^3, \dots, \Gamma^N) \rightarrow \Gamma' = (\Gamma^{1'}, \Gamma^2, \Gamma^3, \dots, \Gamma^N)$$

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

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

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

$$W_{\Gamma \rightarrow \Gamma'} = P(\Gamma^{1'} | \Gamma^2, \Gamma^3, \dots, \Gamma^N)$$

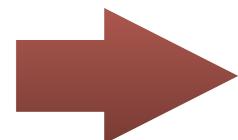
We generate the next Γ' directly from the conditional probability!

- 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.

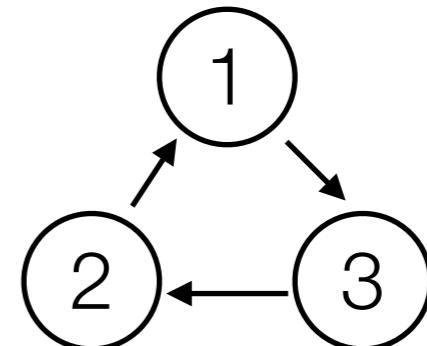
Sampling based on the balance condition

We do not necessarily use the detailed balance condition.



By using more general balance condition,
we can make “rejection free” transition probabilities.

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



e.g. 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”

諏訪秀磨, 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

Local update

Classical spin system

Model Hamiltonian

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

e.g.

Ising spin: $S_i = \pm 1$

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

Nearest Neighbor
interaction

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:

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

**Squared
Magnetization:**

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

MCMC method:

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

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

Γ_t : sampling points along Markov chain

Local update

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

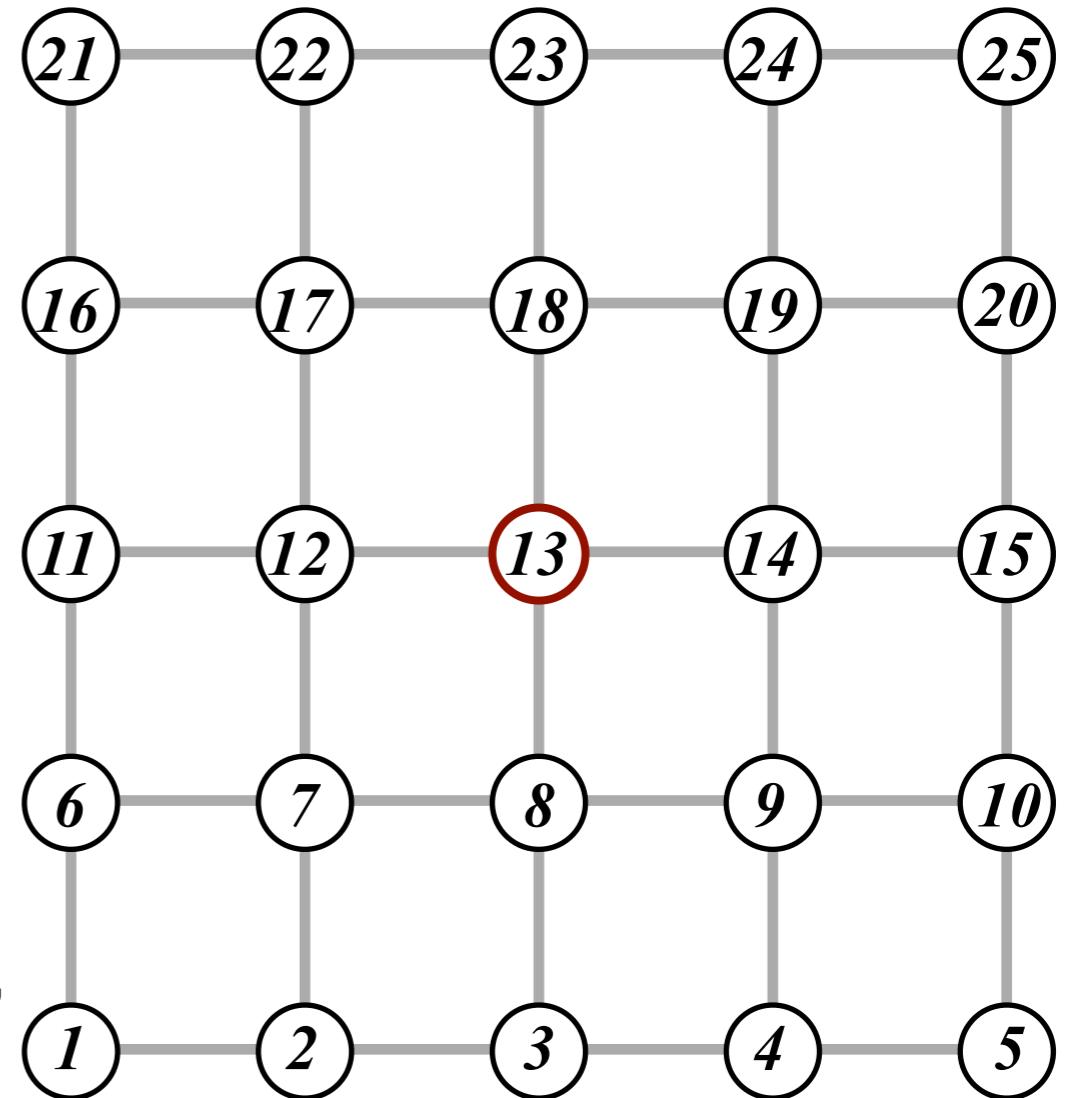
$$\Gamma = (S_1, S_2, \dots, S_{13}, \dots, S_{25})$$

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

From Γ to Γ' , we fix $S_1, S_2, \dots, S_{12}, S_{14}, S_{15}, \dots, S_{25}$, 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:

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

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

* We don't need partition function Z !

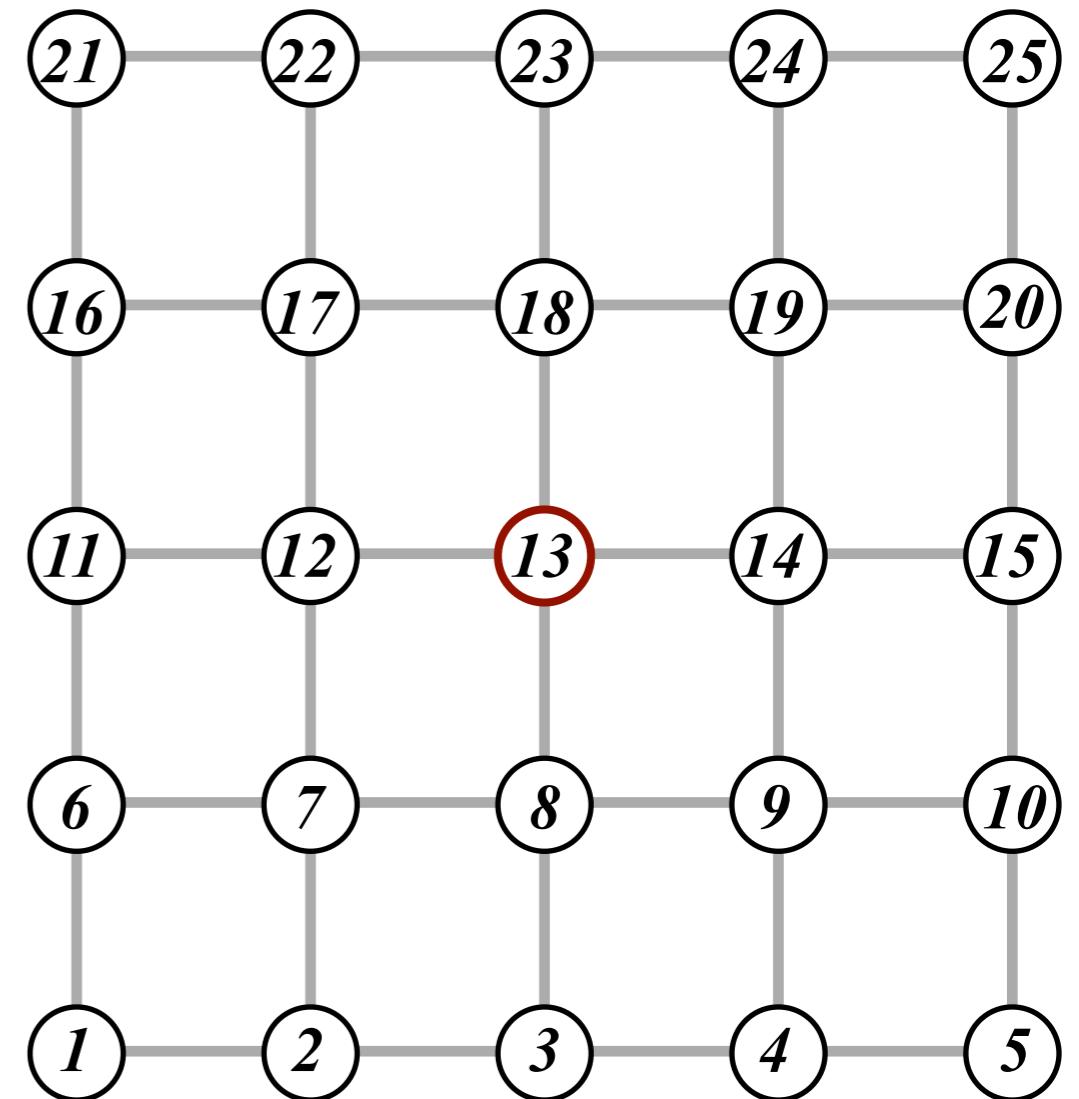
For local update on the square lattice,

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

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

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

*Proposal probability satisfies
 $q(\Gamma|\Gamma') = q(\Gamma'|\Gamma)$.
eg. $S'_i = -S_i$ for Ising spin.



Metropolis method with local update: summary

Step 0: Prepare an initial state $\Gamma_0 = (S_1, S_2, \dots, S_N)$
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 ($T \rightarrow \infty$)
- ordered state ($T \rightarrow 0$)

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:

(Will be skipped)

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

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

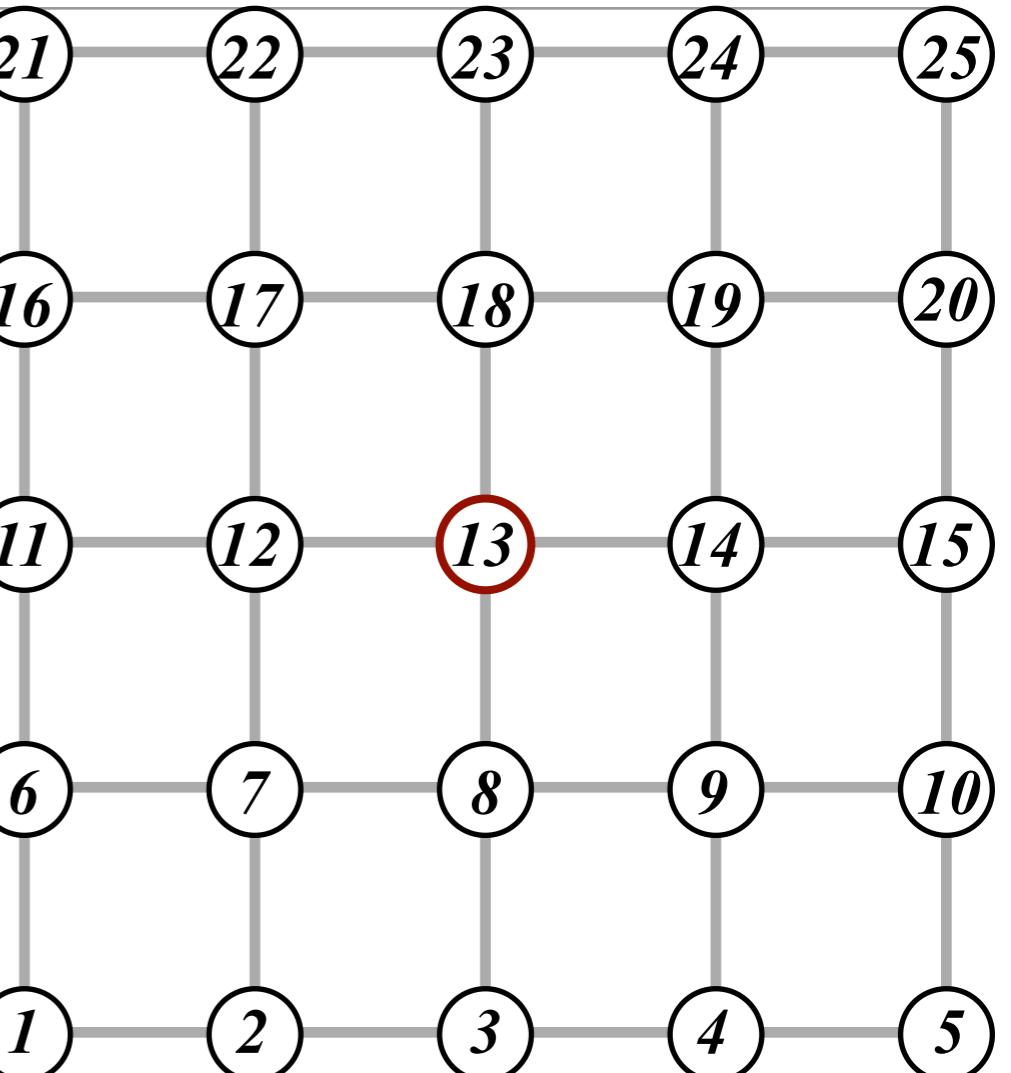
$$W_{\Gamma \rightarrow \Gamma'} = P(S'_{13} | S_1, S_2, \dots, S_{12}, S_{14}, \dots, S_{25})$$

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

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

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

Ising: $W_{\Gamma \rightarrow \Gamma'} = \frac{e^{\beta h_{\text{eff}} S'_{13}}}{e^{\beta h_{\text{eff}} S'_{13}} + e^{-\beta h_{\text{eff}} S'_{13}}}$



Scalar value

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

Three component vector

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

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

Heat-bath method with local update: summary

(Will be skipped)

Step 0: Prepare an initial state $\Gamma_0 = (S_1, S_2, \dots, S_N)$
loop t
select i -th site

Typically we choose
• random state ($T \rightarrow \infty$)
• ordered state ($T \rightarrow 0$)

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'

$r \in [0, 1]$:uniform random number
Ising : $S'_i = \begin{cases} 1 & r \leq P(1) \\ -1 & \text{otherwise} \end{cases}$

Heisenberg:
(in polar co-ordinate with $z // h_{\text{eff}}$)

$$\begin{aligned} S'_x &= \sin \theta \cos \phi \\ S'_y &= \sin \theta \sin \phi \\ S'_z &= \cos \theta \end{aligned}$$

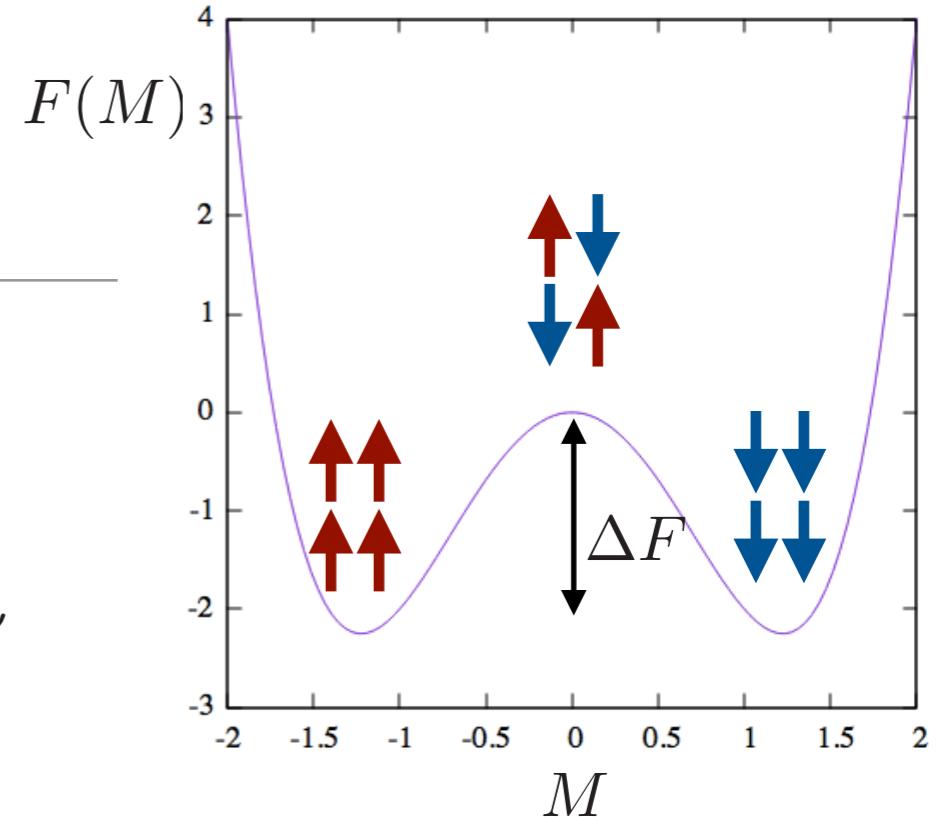
$r_1, r_2 \in [0, 1]$:uniform random number

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

Calculate $O(\Gamma_t)$

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

Free energy landscape



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:

$$\tau \propto \exp \left[\frac{\Delta F}{T} \right]$$

Part of these difficulties can be reduced by using “global update”.

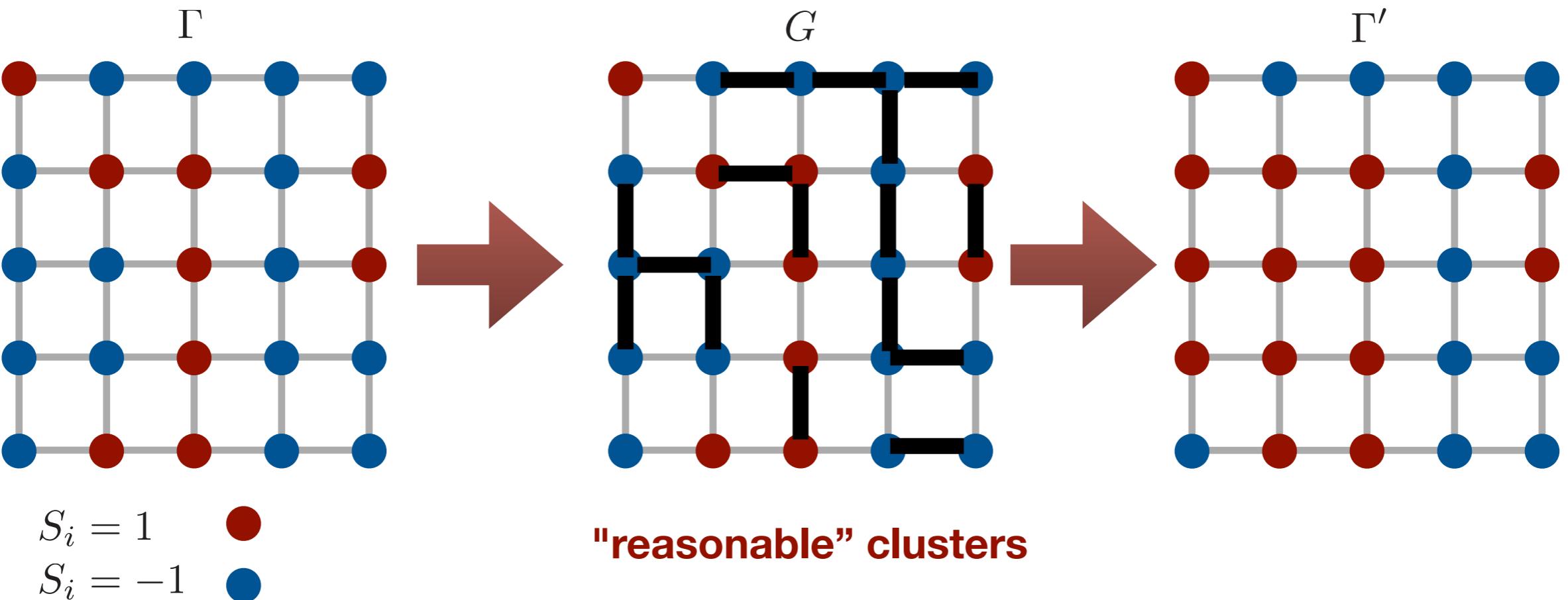
Simultaneous change of spins in “large cluster”

Cluster update

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).

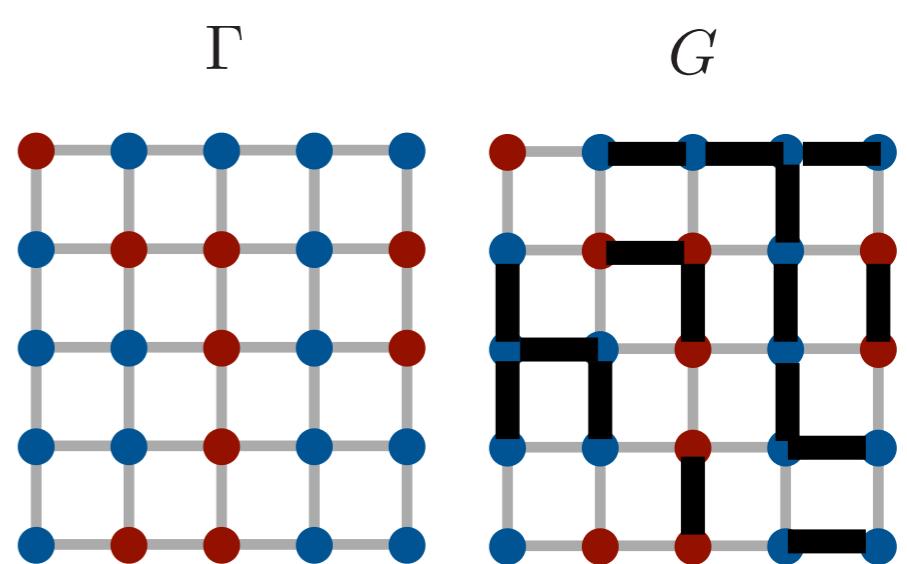
$$e^{\beta J S_i S_j} = \sum_{g=0} e^{-\beta J} + \sum_{g=1} \delta_{S_i, S_j} (e^{\beta J} - e^{-\beta J}) = \sum_{g=0,1} w(g, S_i, S_j)$$

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

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

$$G = \{g_{i,j}\}$$

$$\Gamma = \{S_i\}$$



$$S_i = 1 \quad \bullet$$

$$S_i = -1 \quad \circ$$

$$g_{i,j} = 1 \quad \blacksquare$$

$$g_{i,j} = 0 \quad \square$$

Markov chain in extended (G, Γ) space

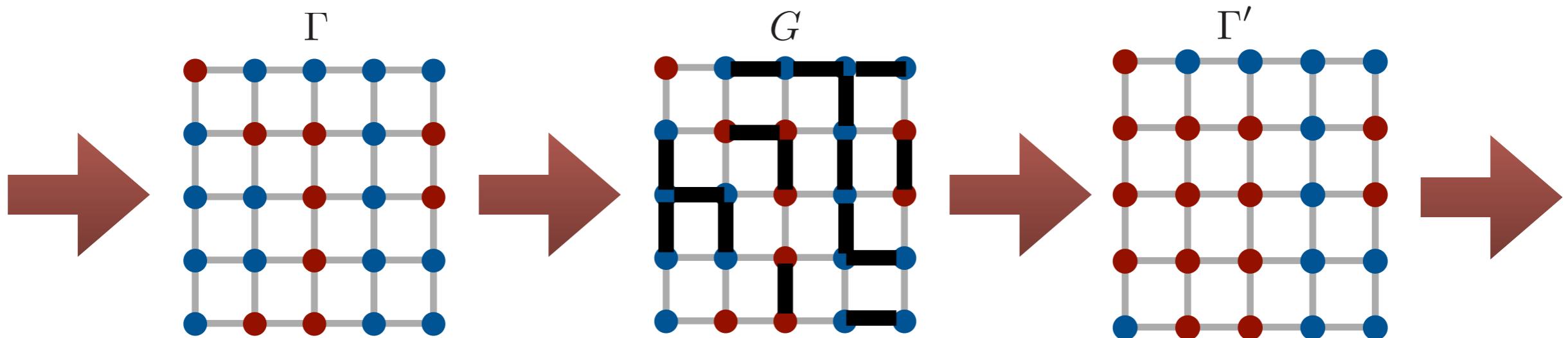
$$Z = \sum_G \sum_{\Gamma} \prod_{\langle i,j \rangle} w(g_{i,j}, S_i, S_j) = \sum_G \sum_{\Gamma} W(G, \Gamma)$$

We consider to update Γ and G alternatively:

$$\cdots \rightarrow (G_{t-1}, \Gamma_t) \rightarrow (\textcolor{red}{G}_t, \Gamma_t) \rightarrow (G_t, \Gamma_{t+1}) \rightarrow (\textcolor{red}{G}_{t+1}, \Gamma_{t+1}) \rightarrow \cdots$$

This update can be symbolically written as

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



Markov chain in extended (G, Γ) space

We assign the transition probabilities as follows:

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

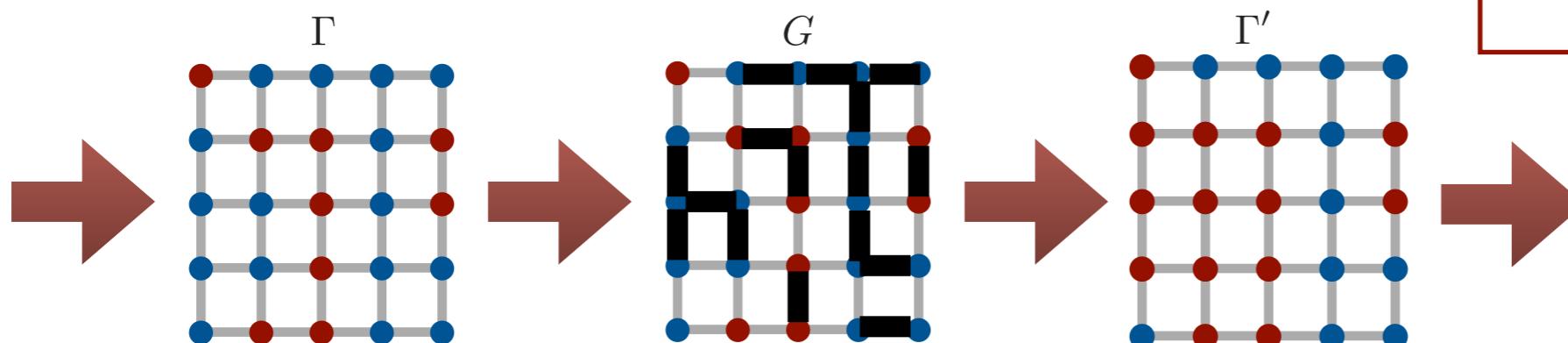
Transition probabilities (as like the heat bath)

$$\Gamma \rightarrow G' : W_{(G, \Gamma) \rightarrow (G', \Gamma)} = \frac{W(G', \Gamma)}{\sum_{G''} W(G'', \Gamma)} = \prod_{\langle i, j \rangle} w_{(S_i, S_j) \rightarrow g_{ij}}$$

$$G \rightarrow \Gamma' : W_{(G, \Gamma) \rightarrow (G, \Gamma')} = \frac{W(G, \Gamma')}{\sum_{\Gamma''} W(G, \Gamma'')} = \prod_{C_j} P(\{S_i \in C_j\})$$

cluster formed
from $g=1$ links

$P(\{S_i \in C_j\}) = 1$
(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 $\underline{\Gamma_0 = (S_1, S_2, \dots, S_N)}$

loop t

 loop $\langle i, j \rangle$

- 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 $\langle i, j \rangle$

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

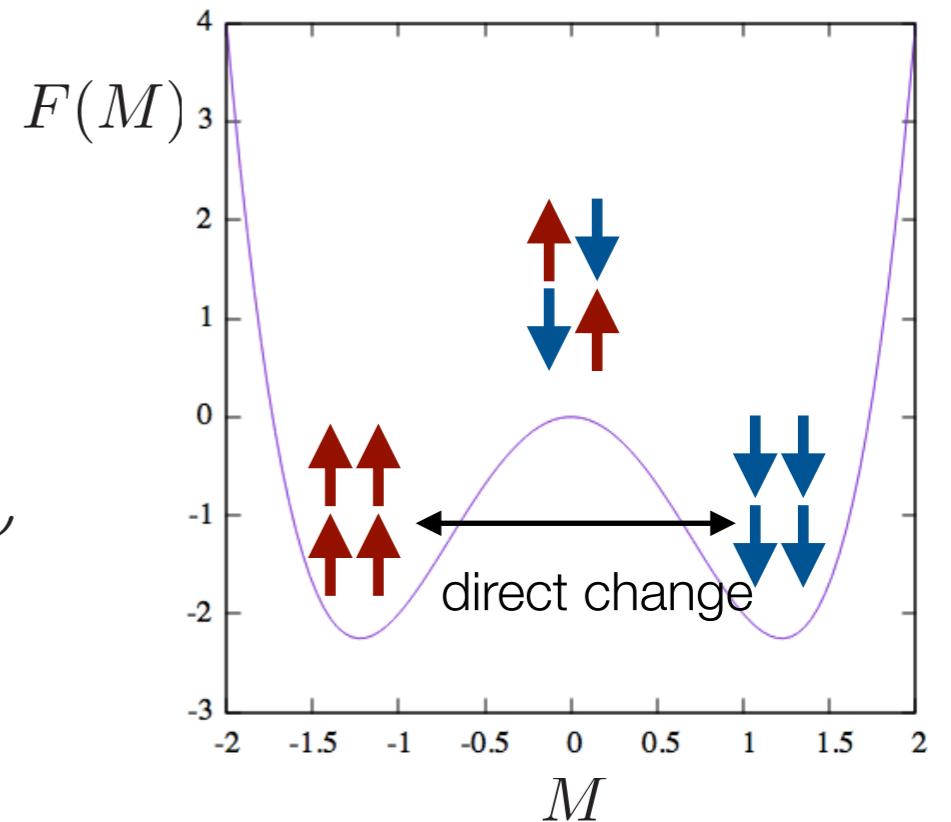
(Under a finite magnetic field, we need to modify the probability.)

Calculate $O(\Gamma_t)$

Merits of cluster update

1. For low temperature phase, the system easily moves to other minima.
 - Minima are related to the symmetry of the Hamiltonian.
2. For critical phenomena the dynamical critical exponent becomes much smaller.
 - Swendsen-Wang : $z \simeq 0 \quad \tau \propto |T - T_c|^{-z\nu}$
3. Graph representation is 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”

Free energy landscape

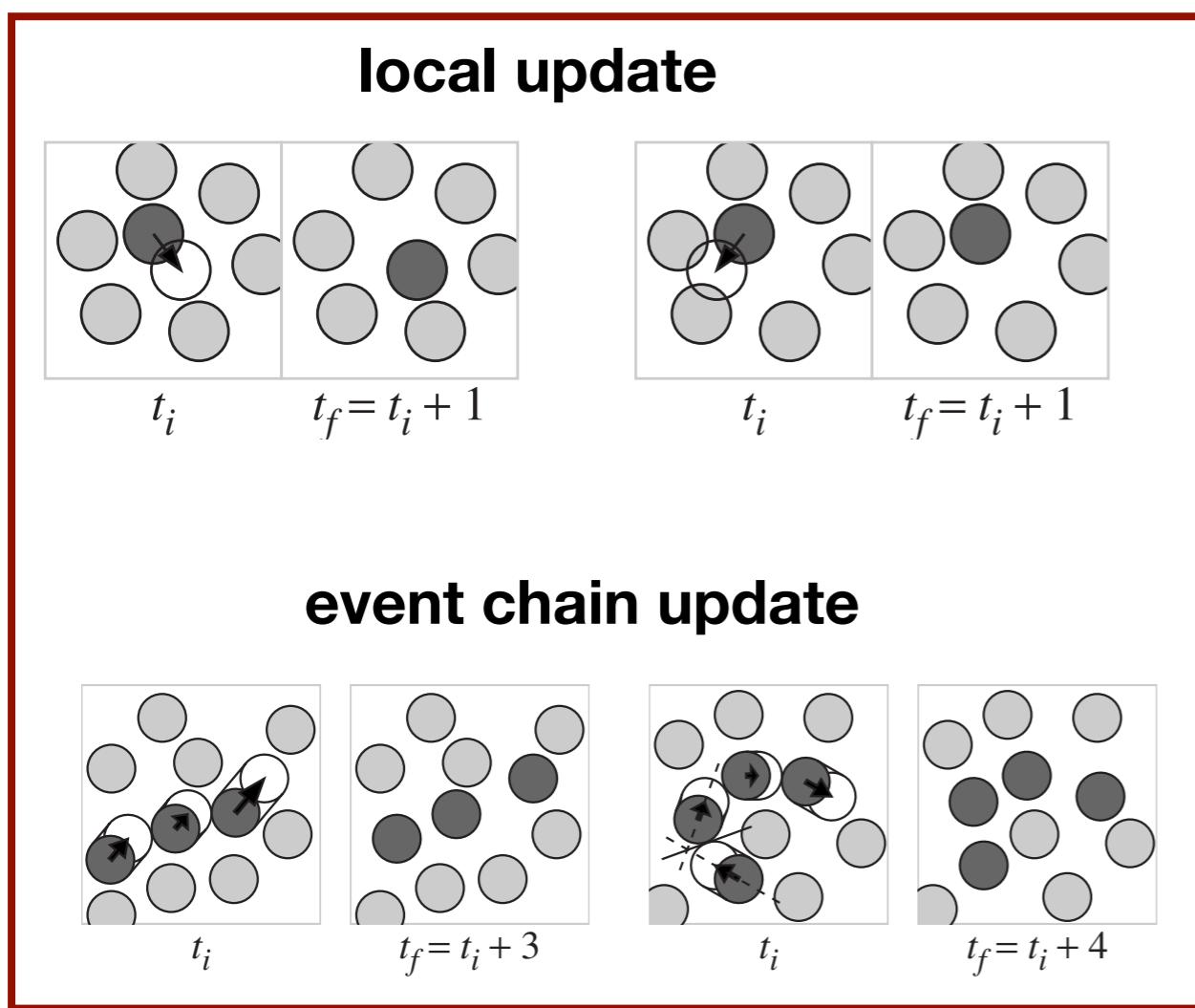


*Linear size of cluster $\sim \xi$

Event-chain Monte Carlo

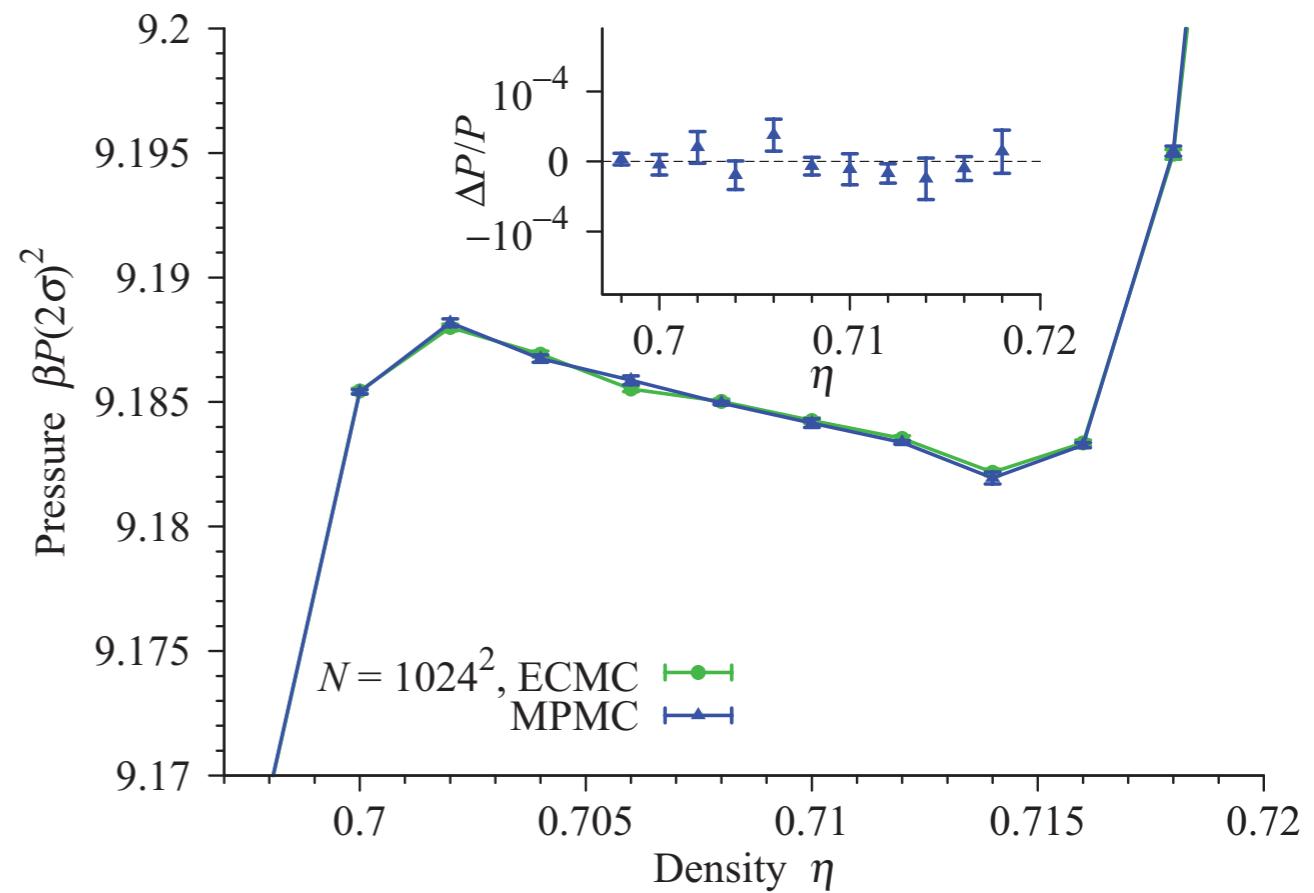
A "global" update for particle system (hard spheres)

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



Application to 2d melting

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



*Application of the event-chain MC to classical spin systems:

M. Michel, J. Mayer, and W. Krauth, Euro Phys. Lett. **112**, 20003 (2015).

Y. Nishikawa, M. Michel, W. Krauth, and K. Hukushima, Phys. Rev. E **92**, 063306 (2015).

Computational science using MCMC methods

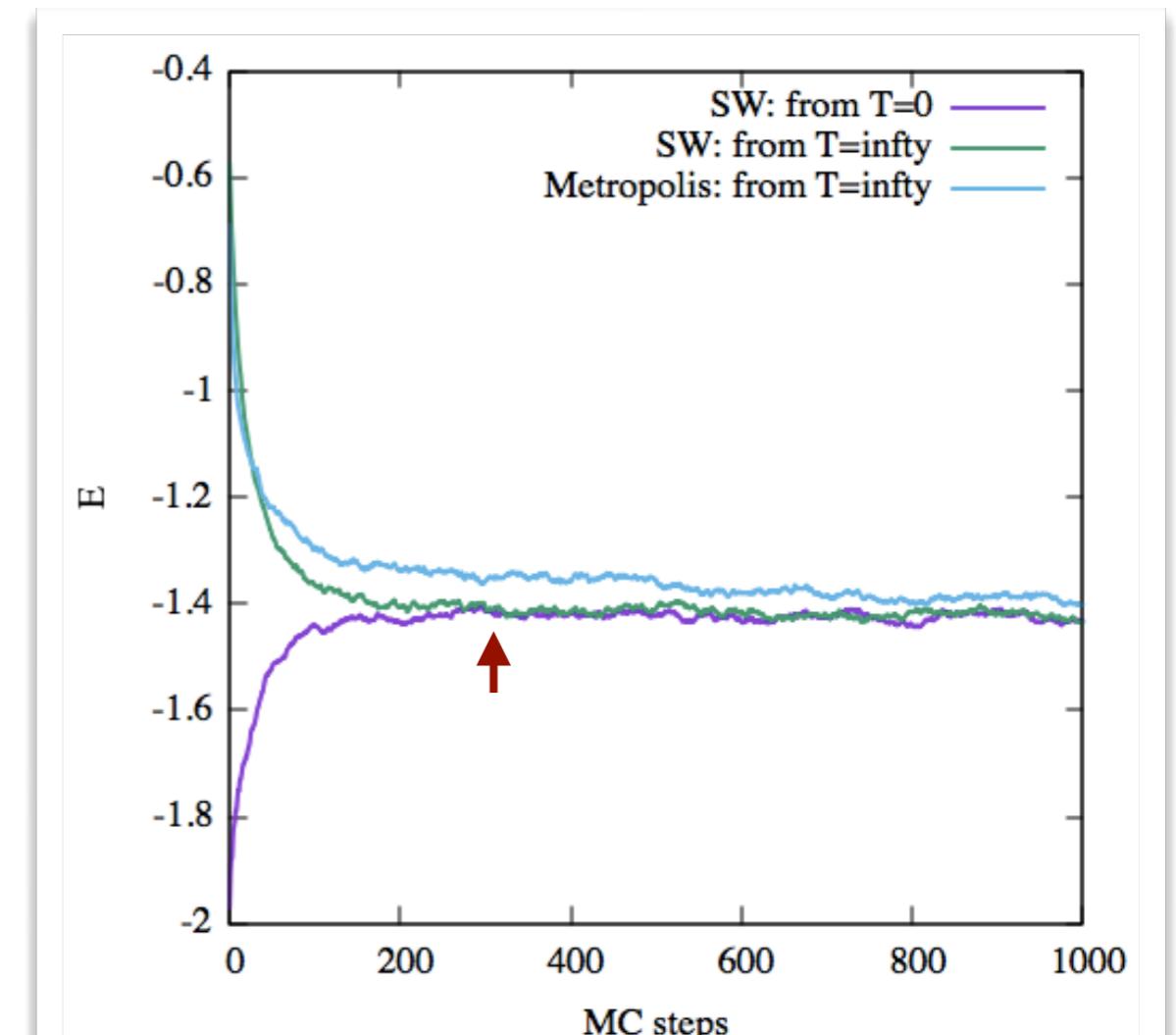
Important tips for real calculations 1

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**.

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

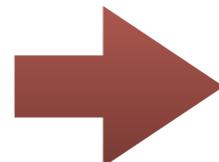
→ Standard error: $\epsilon^2 = \langle \bar{A}^2 \rangle - \langle \bar{A} \rangle^2$ $\epsilon \propto \sqrt{\frac{1 + 2\tau}{T}}$

Maximum likelihood estimation for standard error

Prepare “independent” M samples for \bar{A} : $\{\bar{A}_1, \bar{A}_2, \dots, \bar{A}_M\}$

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

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



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

Example: Application to critical phenomena

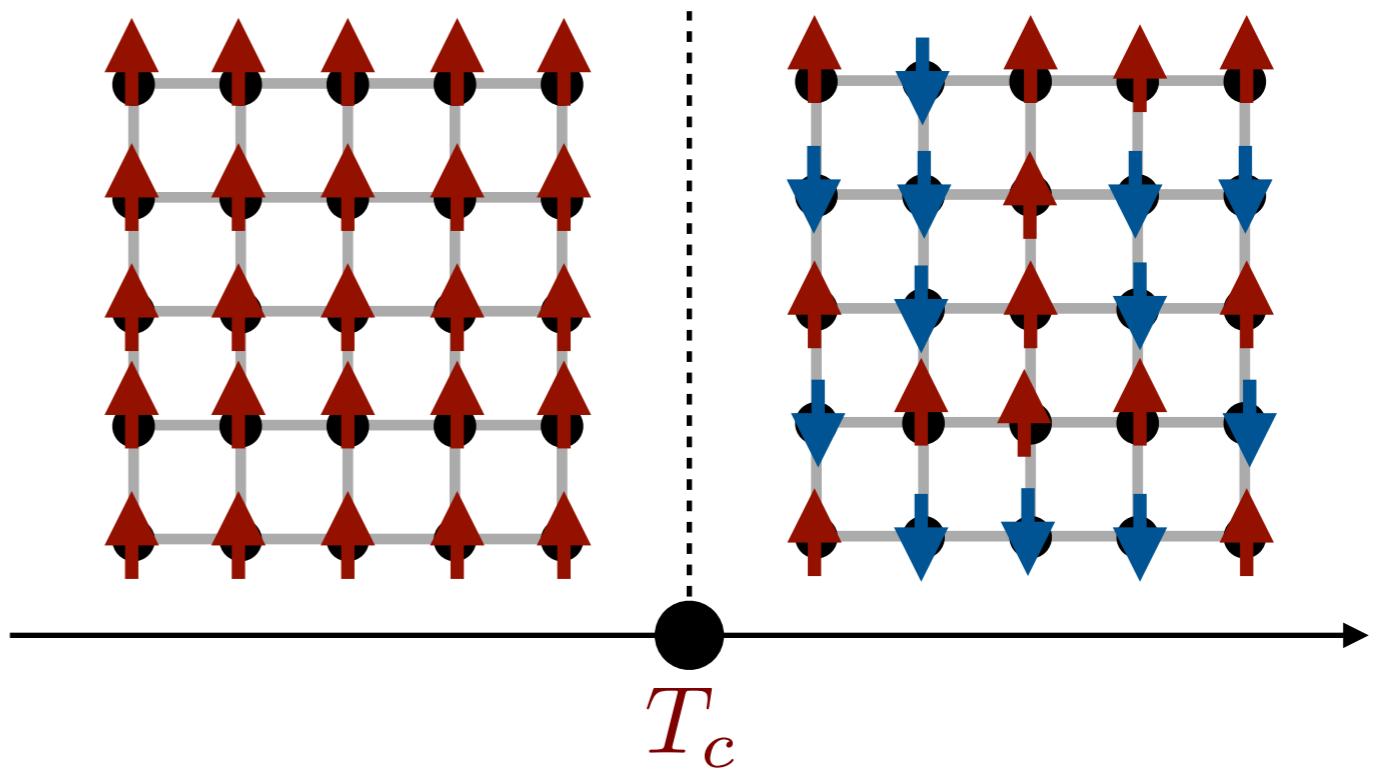
- Square lattice Ising model

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

- Continuous phase transition at $T=T_c$

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

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

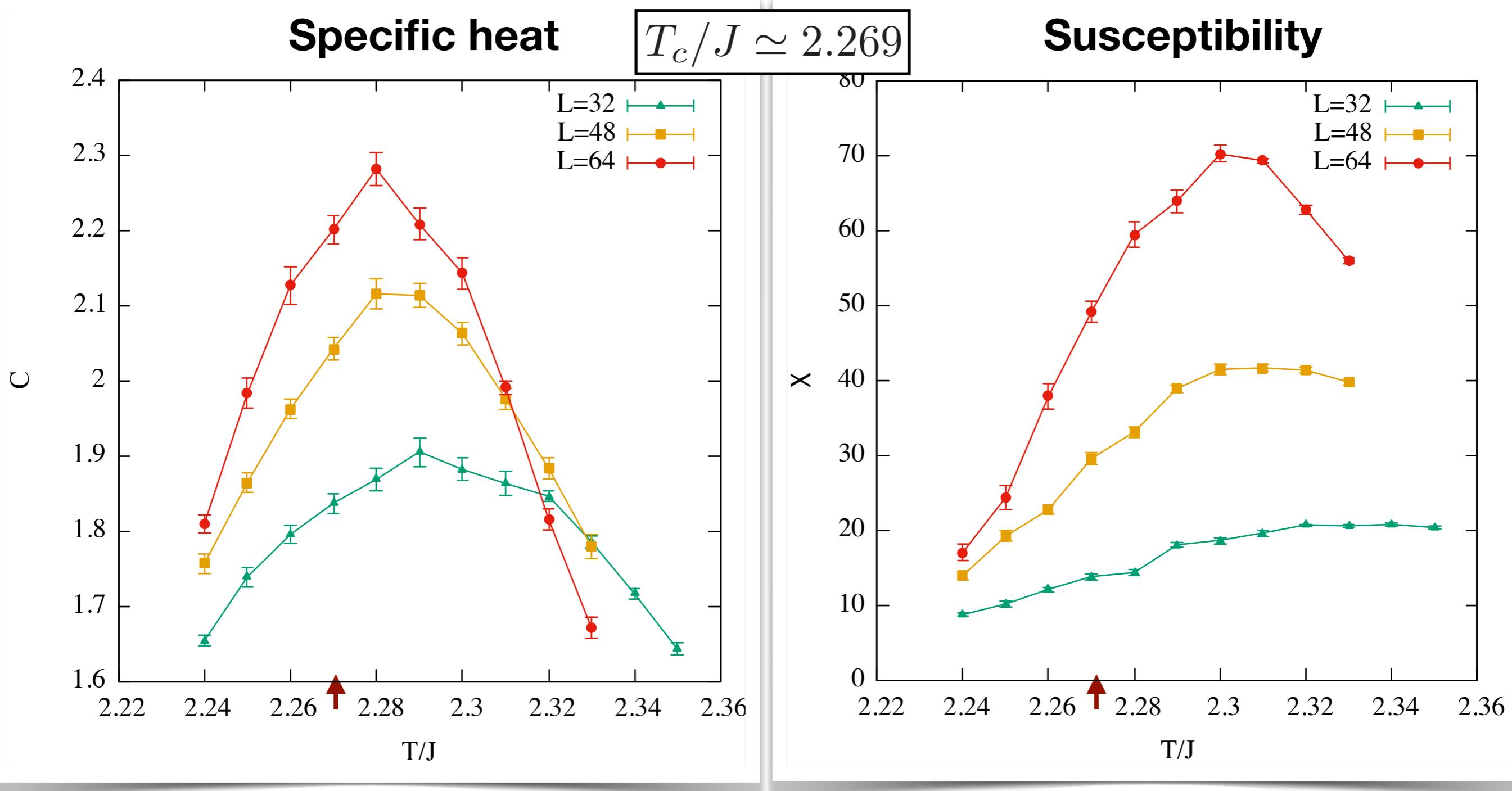


- Monte Carlo Simulations
 - Using spinmc in **ALPS**: Simulator for classical spin system by MCMC
 - My sample code

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**.

Calculated data (ALPS tutorial 7b)



$$C = N \frac{\langle E^2 \rangle - \langle E \rangle^2}{T^2}$$

$$\chi = N \frac{\langle M^2 \rangle - \langle |M| \rangle^2}{T}$$

Data analysis: Finite size scaling (outline)

Near the critical point (transition temperature):

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

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

$$t = T - T_c$$

$$y_t, y_h : \text{scaling exponent} \longleftrightarrow y_t = 1/\nu, \quad y_h = \gamma/(2\nu)$$

By taking derivatives, we see

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

Physical quantity obeys common scaling function independent of L .

→ At the critical point, $M^2 \sim L^{-x_{M^2}}$ $x_{M^2} \equiv d - 2y_h (= \eta)$

x : scaling dimension

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

Data analysis: Finite size scaling (outline)

Similarly, the energy and the specific heat obey:

$$E = \frac{\partial f}{\partial T} = L^{y_t-d} g_E(tL^{y_t}) = L^{1/\nu-d} g_E(tL^{1/\nu})$$

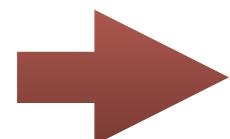
$$C = \frac{\partial^2 f}{\partial T^2} = L^{2y_t-d} g_C(tL^{y_t}) = L^{2/\nu-d} g_C(tL^{1/\nu}) = (L^{\alpha/\nu} g_C(tL^{1/\nu}))$$

Note: scaling relations $\nu d = 2 - \alpha, 2 - \eta = \frac{\gamma}{\nu}, \dots$

Scaling form of general quantities are

$$O = L^{-x_o} g_o(tL^{1/\nu})$$

When we plot O as $(x = tL^{1/\nu}, y = OL^{x_o})$



All data are on a single curve corresponding to $y = g_o(x)$.

By using this property, we can estimate critical exponents and critical temperature.

Examples: Magnetization

(Squared) Magnetization: $\langle M^2 \rangle$

$$M = \frac{1}{N} \sum_i S_i$$

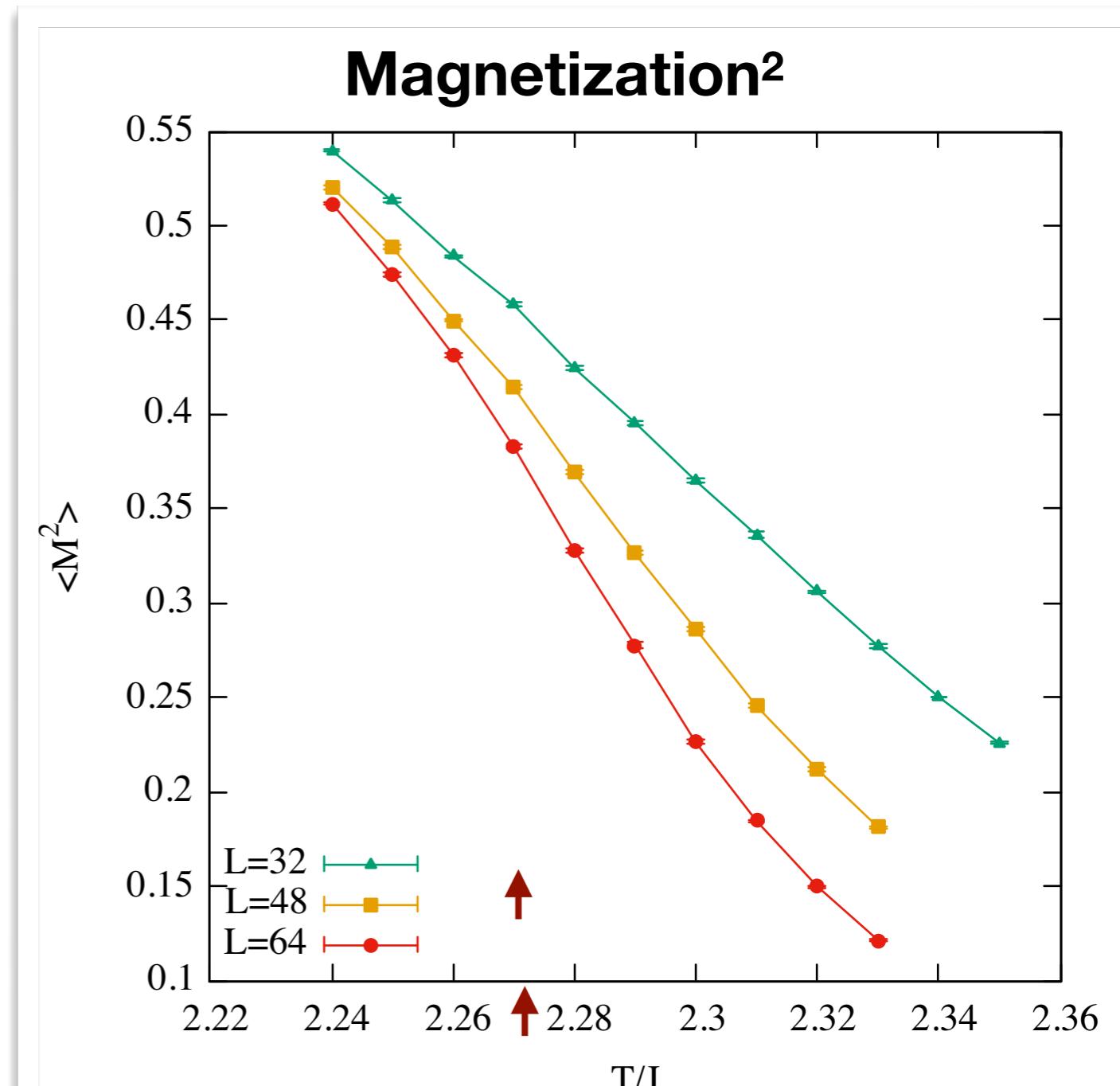
(Q. We cannot use $\langle M \rangle$. Why?)

→ In the thermodynamic limit

$$\langle M^2 \rangle \begin{cases} = 0 & (T \geq T_c) \\ \neq 0 & (T < T_c) \end{cases}$$

So, in principle, we can estimate T_c by extrapolating the data.

Can we estimate T_c more easily?



$$T_c/J \simeq 2.269$$

Examples: Binder ratio

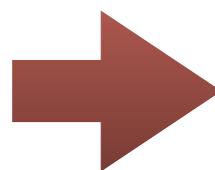
Binder ratio

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

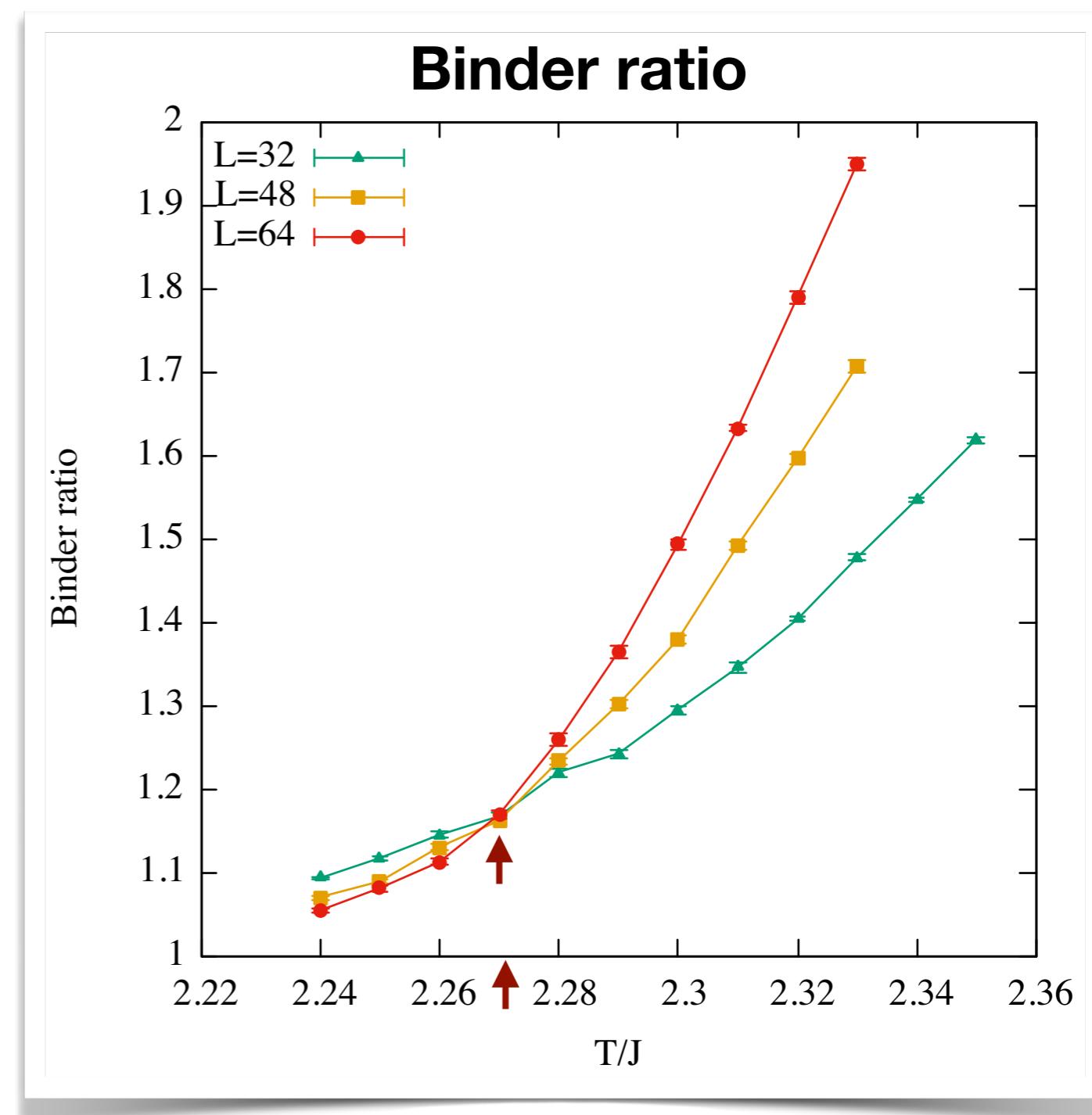
$$b = 3 \quad (T \rightarrow \infty)$$

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

The scaling dimension of b is exactly zero.



At T_c , the size dependence disappears in leading order!



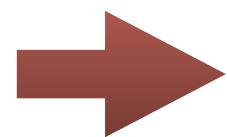
Finite size scaling: Binder ratio

Binder ratio

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

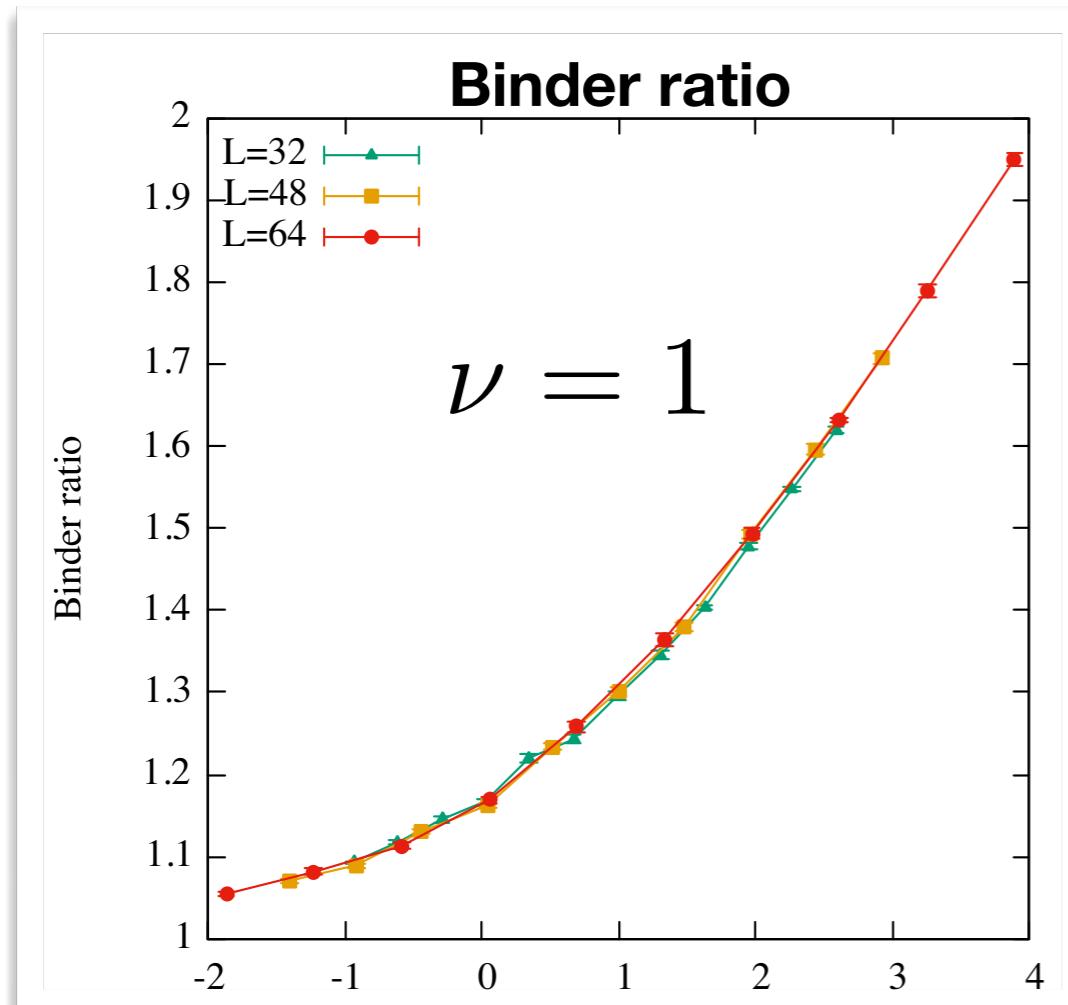
Finite size scaling around T_c

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

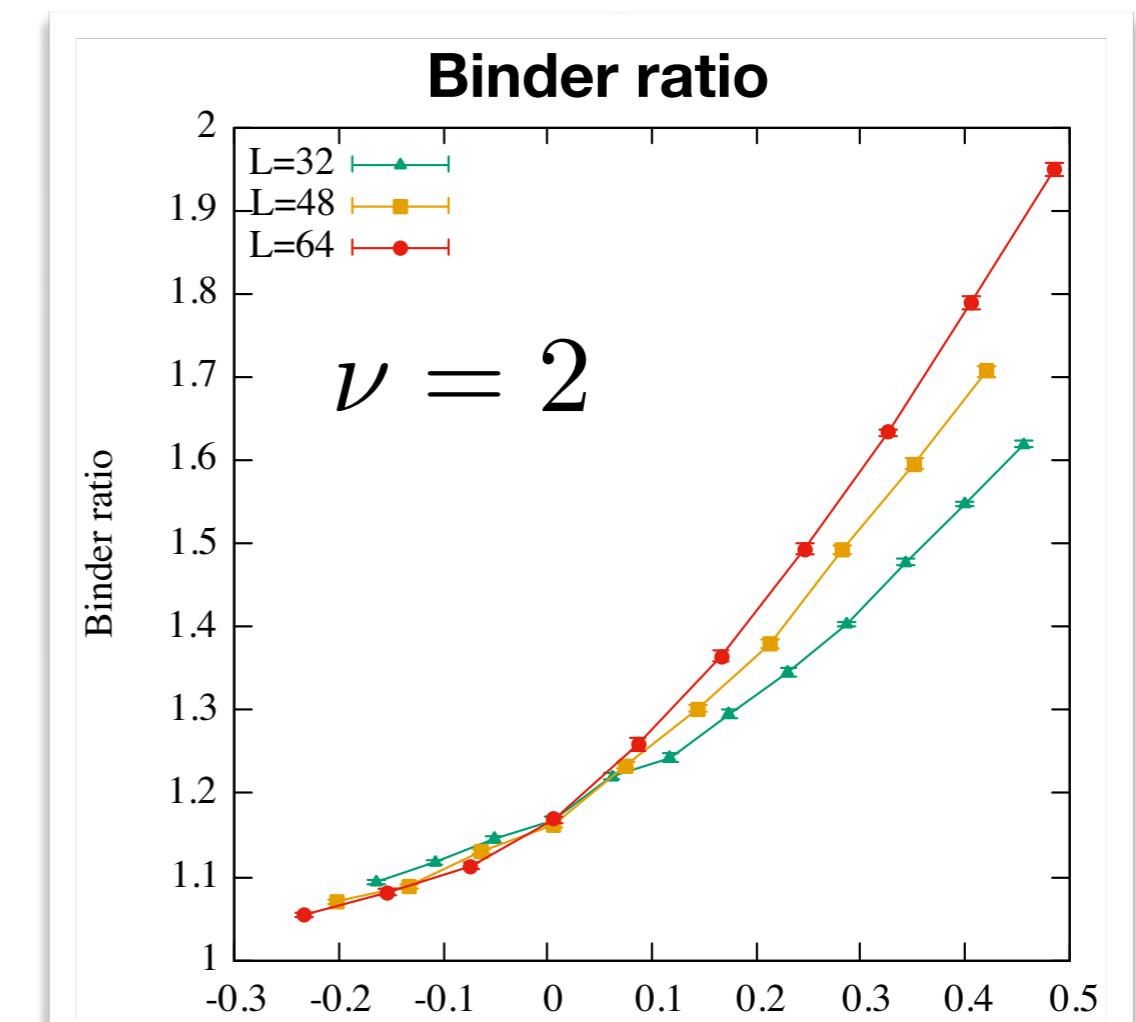


We can determine critical exponent!

$$\nu = 1$$



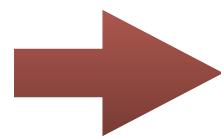
$$(T - T_c)L^{1/\nu}$$



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

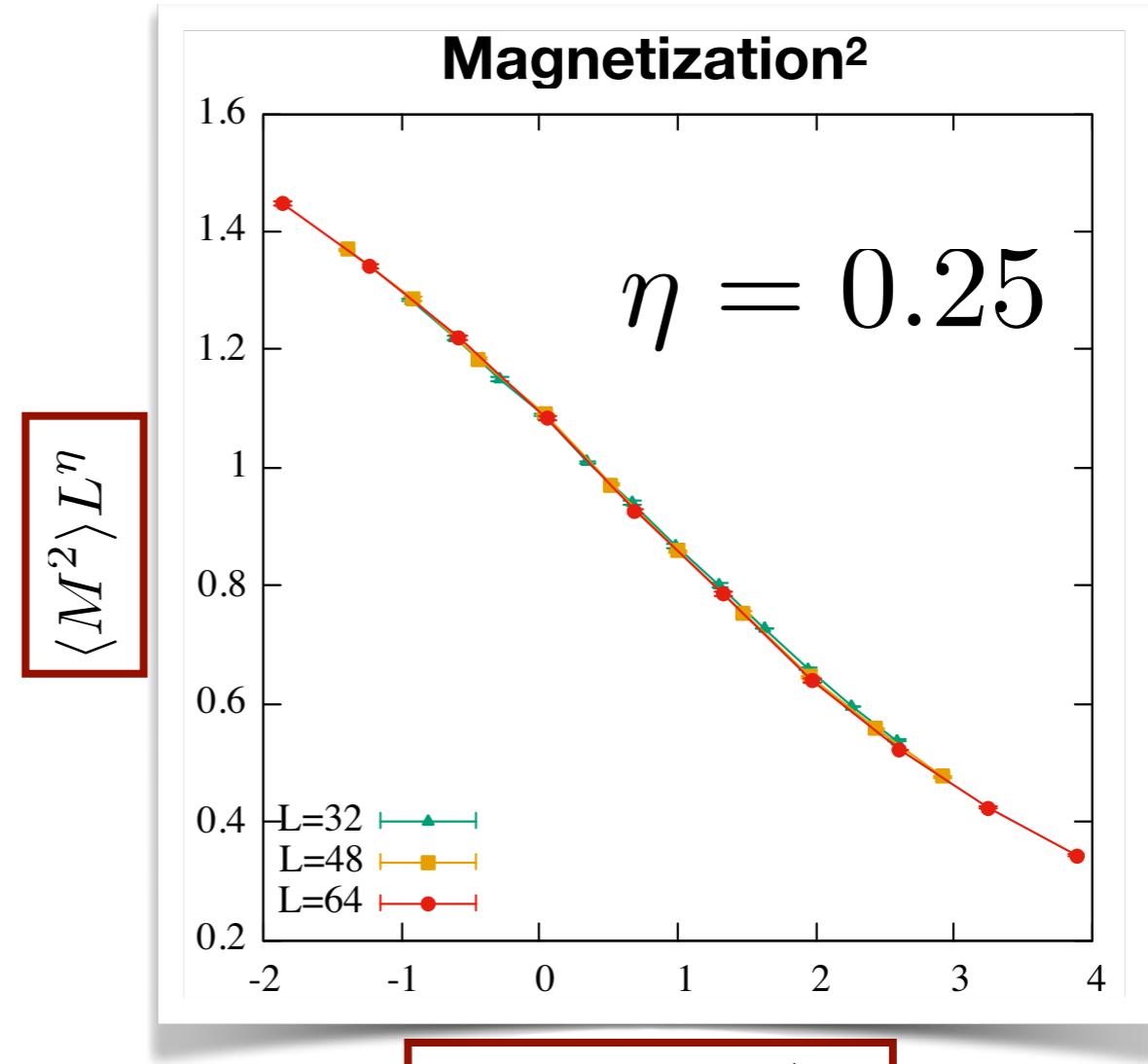
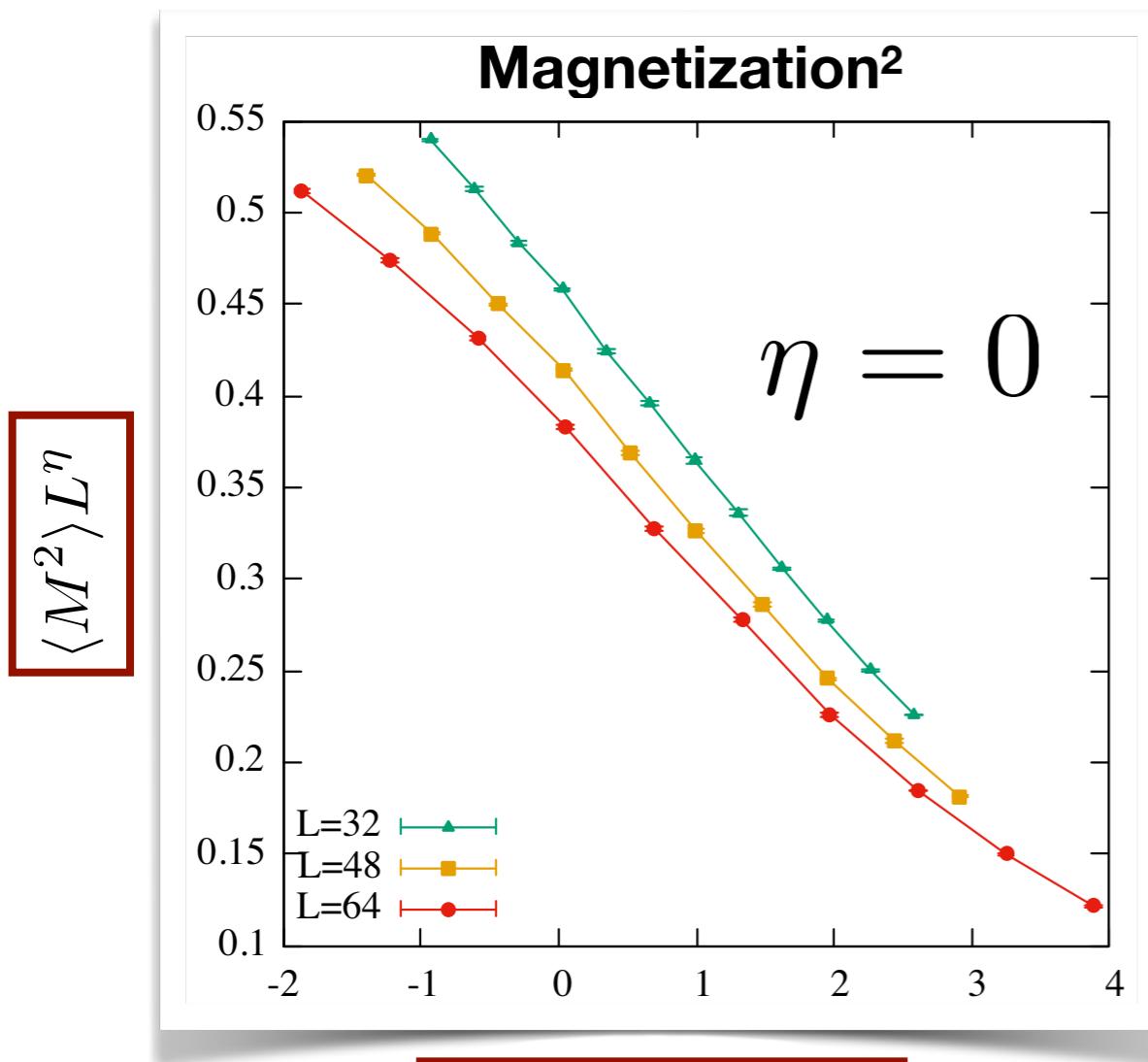
Finite size scaling: Magnetization

(Squared) Magnetization: $\langle M^2 \rangle$



By fixing $\nu = 1$ and varying η ,
we can also determine another critical exponent.

Finite size scaling around T_c
 $\langle M^2 \rangle = L^{-\eta} g((T - T_c)L^{1/\nu})$



Exercises and sample codes

Exercises (not a report)

Exercise1: autocorrelation of MCMC

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

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

Exercise2: finite size scaling

Try the finite size scaling of, eg. binder ratio, in the case of Ising model.

- Calculate physical quantities for various system size (L).
- Plot them without scaling, and see they are actually different.
- Try finite size scaling by assuming values of critical exponents.
 - Even if you know the exact value, it is worth trying several different values.

How to perform the exercises

To perform these exercises, you may use

- Your own code
- ALPS (it is not straight forward to see the correlation time...)
- My sample codes for [jupyter notebook \(python3\)](#).
 - In order to run the sample codes you need
 - *numpy*, and *numba* modules (*numba* is used for speed up).
 - In case you do not want to install numba,
please use "wo_jit" versions ([It is very slow...](#)).

How to use my codes

Usage of my codes:

For jupyter notebook (Highly recommended):

jupyter notebook → select Ising-Ex1.ipynb or Ising-Ex2.ipynb

For python:

python3 Ising-Ex1.py or *python3 Ising-Ex2.py*

(In this case, you need to close figure windows to forward the analysis after you check them.)

You can see help message by "-h" option.

python3 Ising-Ex1.py -h

* --L_list of Ex2 is used, e.g.

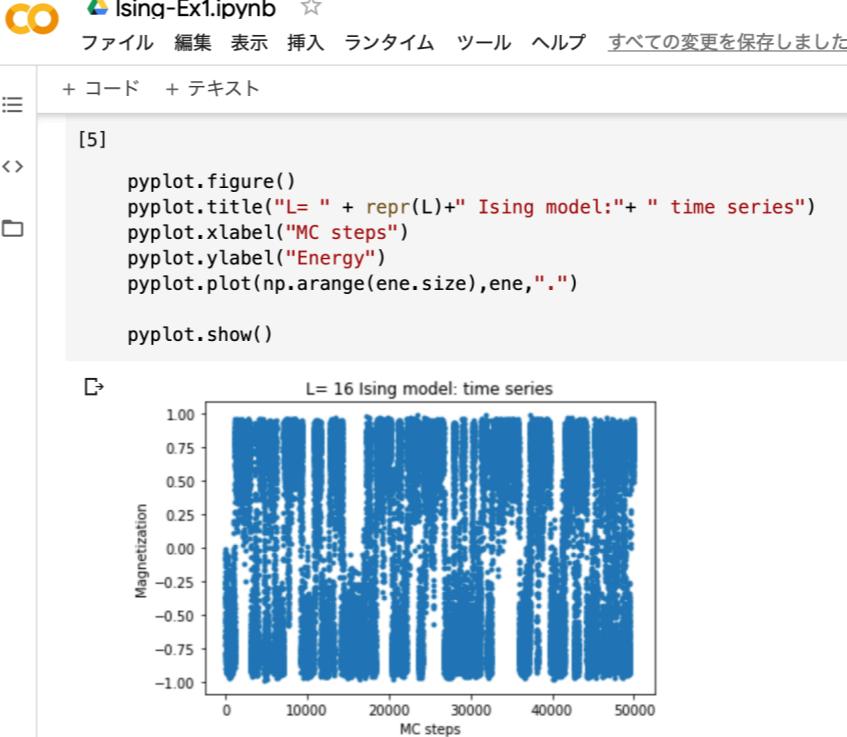
python3 Ising-Ex2.py --L_list 4 8 16 32

Do not include "[]" and ",".

Google Colab

Google Colab <https://colab.research.google.com/>

- It is a **web browser based python environment**.
 - You do not need to prepare python environment on your PC.
- You can **easily run the exercise codes** (*.ipynb) by uploading it to the google colab.
 - Before run them, you need to upload *Ising_lib.py* in addition to *.ipynb.

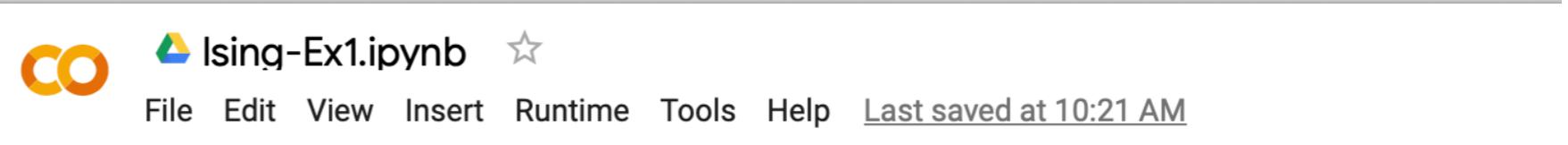


The screenshot shows the Google Colab interface. At the top, there's a toolbar with icons for file operations, a search bar, and a save button. Below the toolbar, the title "Ising-Ex1.ipynb" is visible. The main area has two code cells. The first cell, labeled [5], contains Python code for plotting a time series of magnetization. The second cell shows a plot titled "L= 16 Ising model: time series". The x-axis is labeled "MC steps" and ranges from 0 to 50,000. The y-axis is labeled "Magnetization" and ranges from -1.00 to 1.00. The plot displays a highly fluctuating blue line, indicating the time series of magnetization for a 16x16 Ising model over 50,000 Monte Carlo steps.

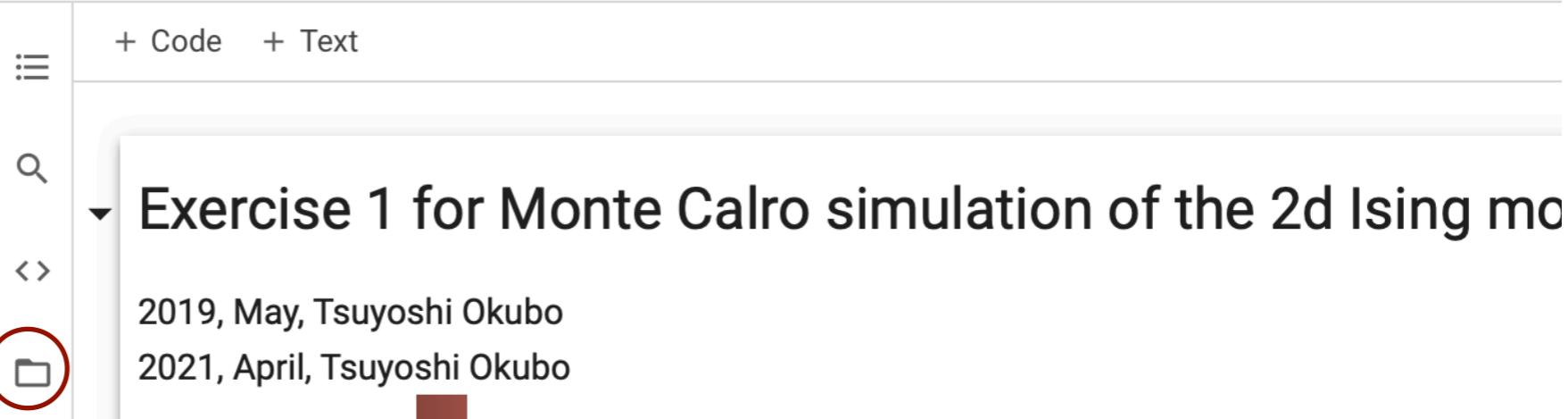
```
pyplot.figure()
pyplot.title("L= " + repr(L)+" Ising model:"+ " time series")
pyplot.xlabel("MC steps")
pyplot.ylabel("Energy")
pyplot.plot(np.arange(ene.size),ene,".")
pyplot.show()
```

How to use Google Colab

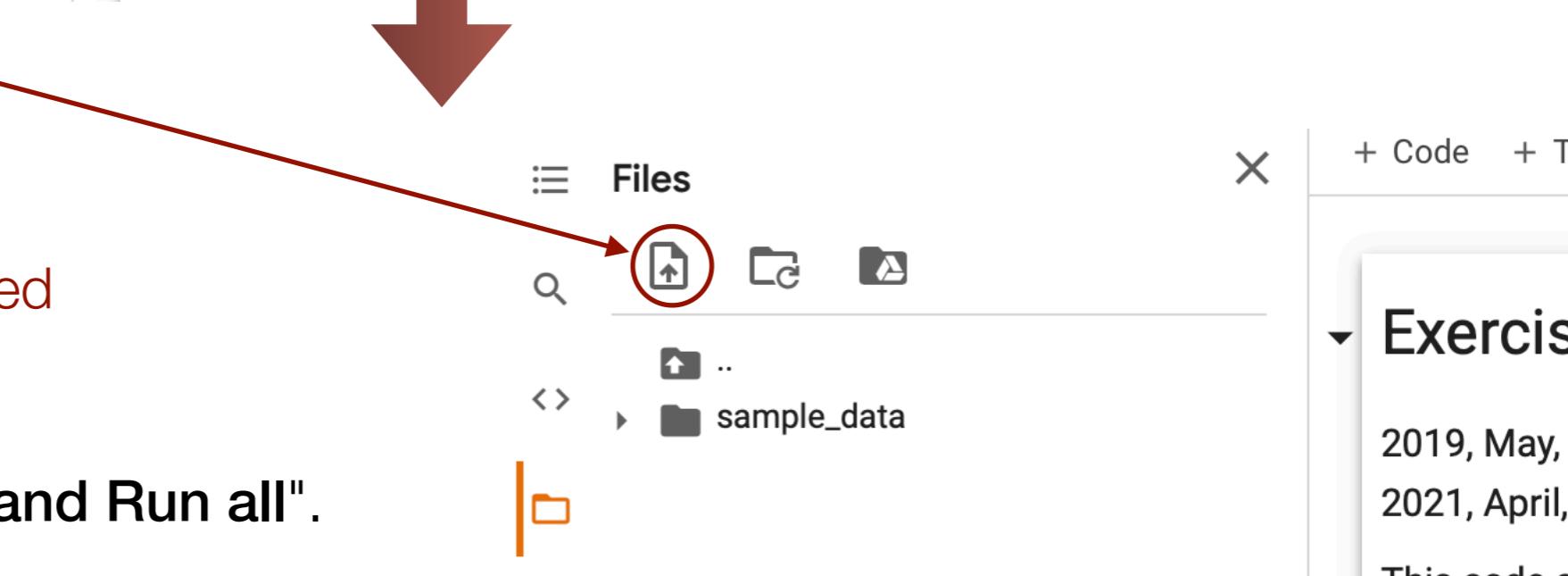
1. Open, e.g., *Ising-Ex1.ipynb*, in Google colab
 - Select "File/upload notebook" ("ファイル/ノートブックをアップロード") and upload *Ising-Ex1.ipynb*



2. Click [here](#)
(Wait a moment
for the connection)



3. Click [here](#) and upload
Ising_lib.py
(Uploaded file will be deleted
after the session finishes.)



4. Select "Runtime/Restart and Run all".



MateriApps Live:

MateriApps Live <https://cmsi.github.io/MateriAppsLive/>

- It is a collection of **softwares** for a variety of material simulations, together with **a virtual linux environment**.
- By using MA live, we can **easily install and construct environment** for computer simulation.
- Its **virtual box version** is easy to install to Win, Mac.

Examples of installed softwares:

- ALPS
- HPhi
- LAMMPS
- mVMC
- Quantum ESPRESSO
- ...

References: textbook for MCMC in the physics

- "A guide to Monte Carlo simulation in statistical physics"
D. P. Landau and K. Binder,
Cambridge university press, (2014) (4th edition).
- "Computational Physics", J. Thijssen, Cambridge University Press.
(「計算物理学」J.M.ティッセン著、松田和典他訳、シュプリンガー・フェアラーク東京.)
- "統計科学のフロンティア12 計算統計II
マルコフ連鎖モンテカルロ 法とその周辺"
伊庭幸人ほか、岩波書店.
(Unfortunately, I have not read it yet.)
-

Next (5/11)

Classical

Quantum

- 1st: Many-body problems in physics
- 2nd: Why many-body problem is hard to solve
- 3rd: Classical statistical models and numerical simulation**
- 4th: Classical Monte Carlo method and its applications**
- 5th: Molecular dynamics simulation and its applications**
- 6th: Extended ensemble method for Monte Carlo methods**
- 7th: Quantum lattice models and numerical simulation
- 8th: Quantum Monte Carlo methods
- 9th: Applications of quantum Monte Carlo methods
- 10th: Linear algebra of large and sparse matrices for quantum many-body problems
- 11th: Krylov subspace methods and their applications to quantum many-body problems
- 12th: Large sparse matrices, and quantum statistical mechanics
- 13th: Parallelization for many-body problems