Metropolis Monte Carlo Simulation: Q & A

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Metropolis Inequalities

Q: Why my ising.c doesn't compile on USC Discovery cluster* (discovery.usc.edu)?

A: Please load the standard software module and use Gnu C compiler (gcc) instead of cc.

```
[anakano@discovery1]$ module purge
[anakano@discovery1]$ module load usc
[anakano@discovery1]$ gcc -o ising ising.c -lm
[anakano@discovery1]$ ./ising
Input JdivT HdivT Sta_step
0.2 0.0 2000000
avgM & sigM = -6.847660e-01 3.389275e+01
```

Remember to plot the absolute value of magnetization

*We are not providing a class account on Discovery for this course, but you are welcome to use it if you already have an account.

Metropolis Inequalities

Q: How to handle *exp_val* = $\exp(-\delta V / k_B T) = 1$?

A: Either accept it unconditionally or conditionally with probability 1; let us (arbitrarily) pick: `if (exp_val > 1.0) {}`

Q: How to accept an attempt with probability *exp_val*?

A: Let us use

```
else if ((rand()/(double)RAND_MAX) <= exp_val) {}
```

Always *true* for *exp_val*=1.0, and correct probability if *exp_val* is rational with denominator *RAND_MAX* and *rand*() ∈ [1,*RAND_MAX*].*

```
// Our pick for assignment 3
if (exp_val > 1.0) {
  s[i][j] = s_new;
  runM += 2.0*s_new;
}
else if (rand()/(double)RAND_MAX <= exp_val) {
  s[i][j] = s_new;
  runM += 2.0*s_new;
}
```

*Linear-congruential random-number generator would return an integer in the range [1,*RANDMAX-1*], while certain library returns [0,*RANDMAX*], introducing 10^{-9} discretization error (which we have in general *exp_val* values anyways).

Metropolis Inequalities (2)

Q: Could we get over with just one if statement (no else)?

A: Yes we can, though with slightly more computation.

```
// Not our pick for assignment 3
if (exp_val > 1.0) {
  s[i][j] = s_new;
  runM += 2.0*s_new;
}
else if (rand()/(double)RAND_MAX <= exp_val) {
  s[i][j] = s_new;
  runM += 2.0*s_new;
}
```

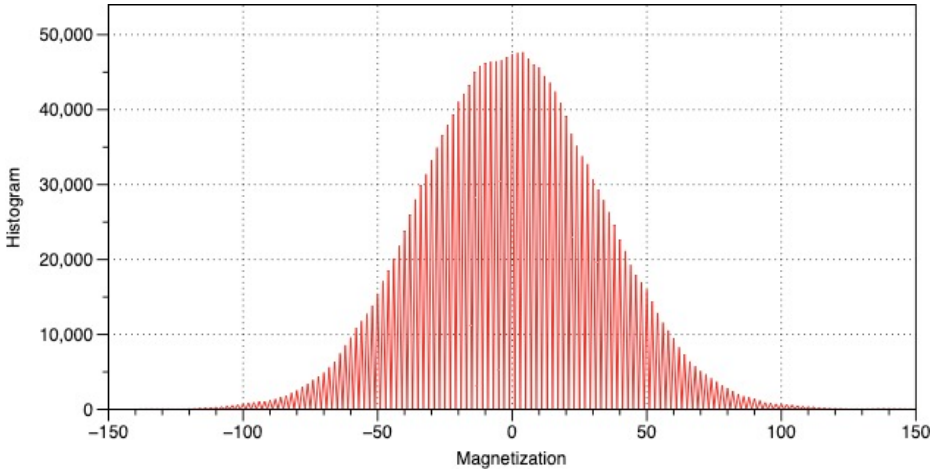
Magnetization Histogram

Q: Why so many zero entries in my histogram?

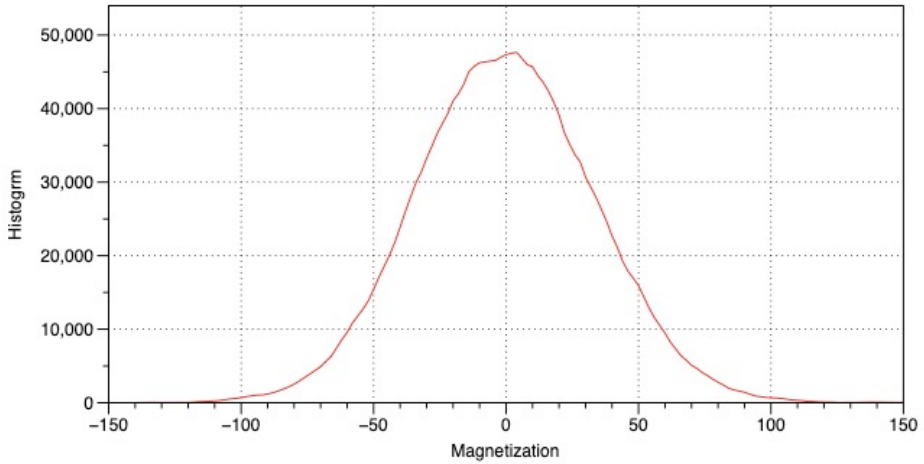
A: Spin flip conserves the parity of the total magnetization, thus no occurrence of odd magnetization.

$runM \leftarrow L^2 = 400\ (L = 20)$ // Initialization (cold start)

$runM \mathrel{+}= 2 \times s\_new$ // At each spin flip



This is perfectly fine



Or eliminate all zero entries

Proving Metropolis Algorithm

Q: How much detailed is required?

A: Just show that Metropolis transition-probability matrix: (1) satisfies the detailed-balanced condition; and consequently (2) fixed-point property, *i.e.*, the desired probability is its eigenvector with eigenvalue 1.

Metropolis Transition-probability matrix

$$\pi_{m,n} = \overbrace{\min\left(\frac{\rho_m}{\rho_n}, 1\right)}^{\text{accept/reject}} \overbrace{\alpha_{m,n}}^{\text{symmetric attempt}}$$

Detailed-balance condition

$$\pi_{mn}\rho_n = \pi_{nm}\rho_m$$

Equal population flux

Fixed-point

$$\boldsymbol{\Pi\rho} = 1 \bullet \boldsymbol{\rho}$$
$$\sum_n \pi_{mn}\rho_n = \rho_m$$

Once you get there, stuck forever

(Filtering) Since all other eigenvalues are less than 1 in absolute value, we get there no matter what is the initial probability

Q: What Is α_{mn} in Ising MC?

States: $m, n \in \left\{ s^N = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_N \end{pmatrix} \middle| \, s_i = \uparrow, \downarrow; i = 1, \ldots, N \right\}$

$$\pi_{m,n} = \overbrace{\min\left(\frac{\rho_m}{\rho_n}, 1\right)}^{\text{accept/reject}} \overbrace{\alpha_{m,n}}^{\text{attempt}}$$

Attempt matrix: $\alpha_{m,n} = \begin{cases} 1/N & Hamming\_distance(m,n) = 1 \\ 0 & \text{else} \end{cases}$

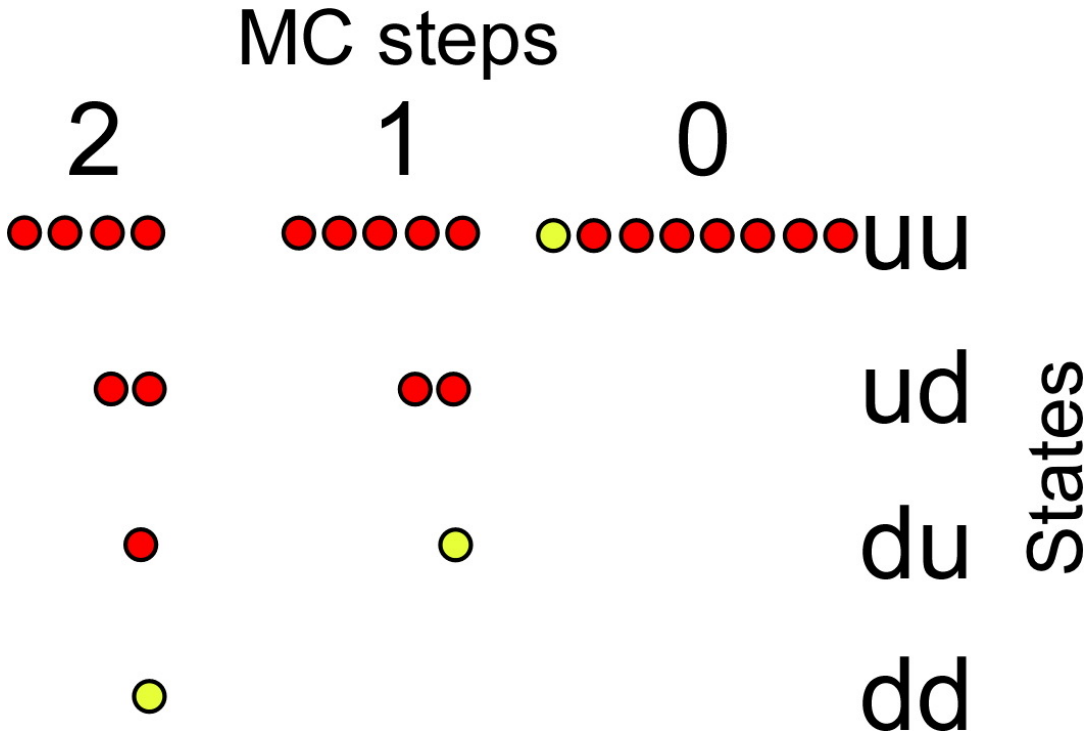
Example: $N = 3$ ($2^N = 8$ states)

$$\begin{pmatrix} \uparrow\uparrow\uparrow \\ \uparrow\uparrow\downarrow \\ \uparrow\downarrow\uparrow \\ \uparrow\downarrow\downarrow \\ \downarrow\uparrow\uparrow \\ \downarrow\uparrow\downarrow \\ \downarrow\downarrow\uparrow \\ \downarrow\downarrow\downarrow \end{pmatrix} = \begin{pmatrix} & 1/3 & 1/3 & & 1/3 & & & \\ 1/3 & & & 1/3 & & 1/3 & & \\ 1/3 & & & 1/3 & & & 1/3 & \\ & 1/3 & 1/3 & & & & & 1/3 \\ 1/3 & & & & & 1/3 & 1/3 & \\ & 1/3 & & & 1/3 & & & 1/3 \\ & & 1/3 & & 1/3 & & & 1/3 \\ & & & 1/3 & & 1/3 & 1/3 & \end{pmatrix} \begin{pmatrix} \uparrow\uparrow\uparrow \\ \uparrow\uparrow\downarrow \\ \uparrow\downarrow\uparrow \\ \uparrow\downarrow\downarrow \\ \downarrow\uparrow\uparrow \\ \downarrow\uparrow\downarrow \\ \downarrow\downarrow\uparrow \\ \downarrow\downarrow\downarrow \end{pmatrix}$$

Q: Where Is Matrix-Vector Multiplication?

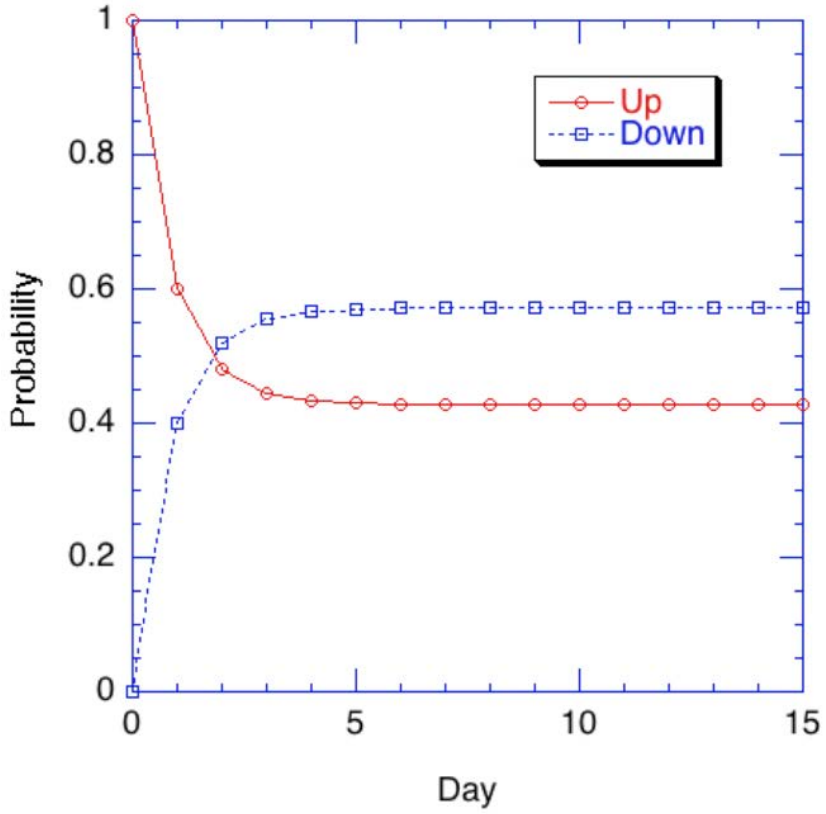
A: The probability density vector is replaced by an ensemble of individual MC sequences in Markov-chain MC; the ensemble average is then replaced by time average.

$$\boldsymbol{\rho}^{(t+1)} = \boldsymbol{\Pi}\boldsymbol{\rho}^{(t)}$$



Example: Two-Level System

$$\Pi = \begin{array}{c} \\ \uparrow \\ \downarrow \end{array} \begin{array}{c} \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{pmatrix} a & 1-b \\ 1-a & b \end{pmatrix} \end{array} = \begin{pmatrix} 0.6 & 0.3 \\ 0.4 & 0.7 \end{pmatrix} \quad (a = 0.6, b = 0.7)$$



$$\begin{pmatrix} p_{\uparrow}^{(t)} \\ p_{\downarrow}^{(t)} \end{pmatrix} = \begin{pmatrix} 0.6 & 0.3 \\ 0.4 & 0.7 \end{pmatrix}^{t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \xrightarrow{t \to \infty} \begin{pmatrix} 0.4286 \\ 0.5714 \end{pmatrix} \begin{matrix} 3/7 \\ 4/7 \end{matrix}$$

Equilibrium probability

A Metropolis Monte Carlo

Your only knowledge = equilibrium probability distribution

$$\boldsymbol{\rho} = \begin{pmatrix} 3/7 \\ 4/7 \end{pmatrix}$$

A choice of attempt matrix

$$\alpha_{\uparrow\downarrow} = \alpha_{\downarrow\uparrow} = 1$$

Detailed-balanced transition-probability matrix

$$\boldsymbol{\Pi} = \begin{pmatrix} \pi_{\uparrow\uparrow} & \pi_{\uparrow\downarrow} \\ \pi_{\downarrow\uparrow} & \pi_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} 1-\alpha_{\downarrow\uparrow} & \alpha_{\uparrow\downarrow}(\rho_\uparrow/\rho_\downarrow) \\ \alpha_{\downarrow\uparrow} & 1-\alpha_{\uparrow\downarrow}(\rho_\uparrow/\rho_\downarrow) \end{pmatrix}$$
$$= \begin{pmatrix} 1-1 & 1 \bullet 3/4 \\ 1 & 1-1 \bullet 3/4 \end{pmatrix} = \begin{pmatrix} 0 & 3/4 \\ 1 & 1/4 \end{pmatrix}$$

Q: How to represent the probability distribution?

A: An ensemble of many samples

Ensemble-Average MC

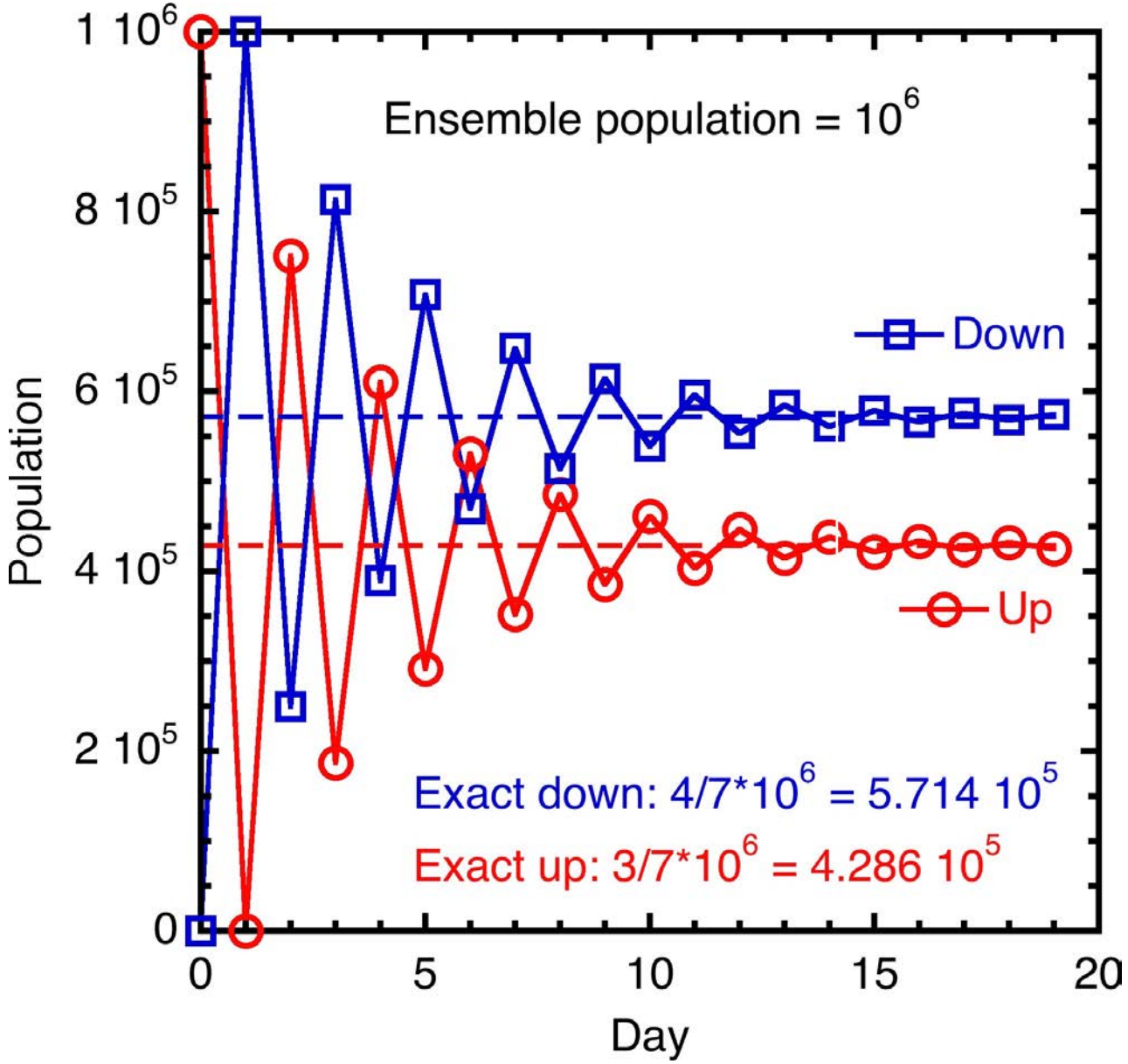
```
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#define NTRY 20  /* # of MC trials */
#define NENS 1000000  /* ensemble size */
#define TRNS 3.0/4.0  /* up-to-down conditional probability */

int main() {
  int s;  /* spin state: 0 = up; 1 = down */
  int hist[NTRY][2];  /* histgram */
  int try,walker;

  srand((unsigned)time((long *)0));
  for (try=0; try<NTRY; try++) for (s=0; s<2; s++) hist[try][s] = 0;

  for (walker=0; walker<NENS; walker++) {
    s = 0;  /* up on day 0 */
    ++(hist[0][s]);
    for (try=1; try<NTRY; try++) {
      if (s == 0) s = 1;  /* unconditional down move */
      else if (rand()/(double)RAND_MAX < TRNS) s = 0;  /* conditional up move */
      ++(hist[try][s]);  /* accumulate the average */
    }
  }
  for (try=0; try<NTRY; try++) printf("%d %d %d\n",try,hist[try][0],hist[try][1]);
  return 0;
}
```

Ensemble-Average MC Result



Time-Average MC

```
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#define NTRY 1000  /* ensemble size */
#define TRNS 3.0/4.0  /* up-to-down conditional probability */

int main() {
  int s;  /* spin state: 0 = up; 1 = down */
  int hist[NTRY][2];  /* histgram */
  int try,i;

  srand((unsigned)time((long *)0));
  for (try=0; try<NTRY; try++) for (s=0; s<2; s++) hist[try][s] = 0;

  s = 0;  /* up on day 0 */
  ++(hist[0][s]);
  for (try=1; try<NTRY; try++) {
    if (s == 0) s = 1;  /* unconditional down move */
    else if (rand()/(double)RAND_MAX < TRNS) s = 0;  /* conditional up move */
    for (i=0; i<2; i++) hist[try][i] = hist[try-1][i];
    ++(hist[try][s]);  /* accumulate the average */
  }

  for (try=0; try<NTRY; try++)
    printf("%d %d %d\n",try,hist[try][0],hist[try][1]);

  return 0;
}
```

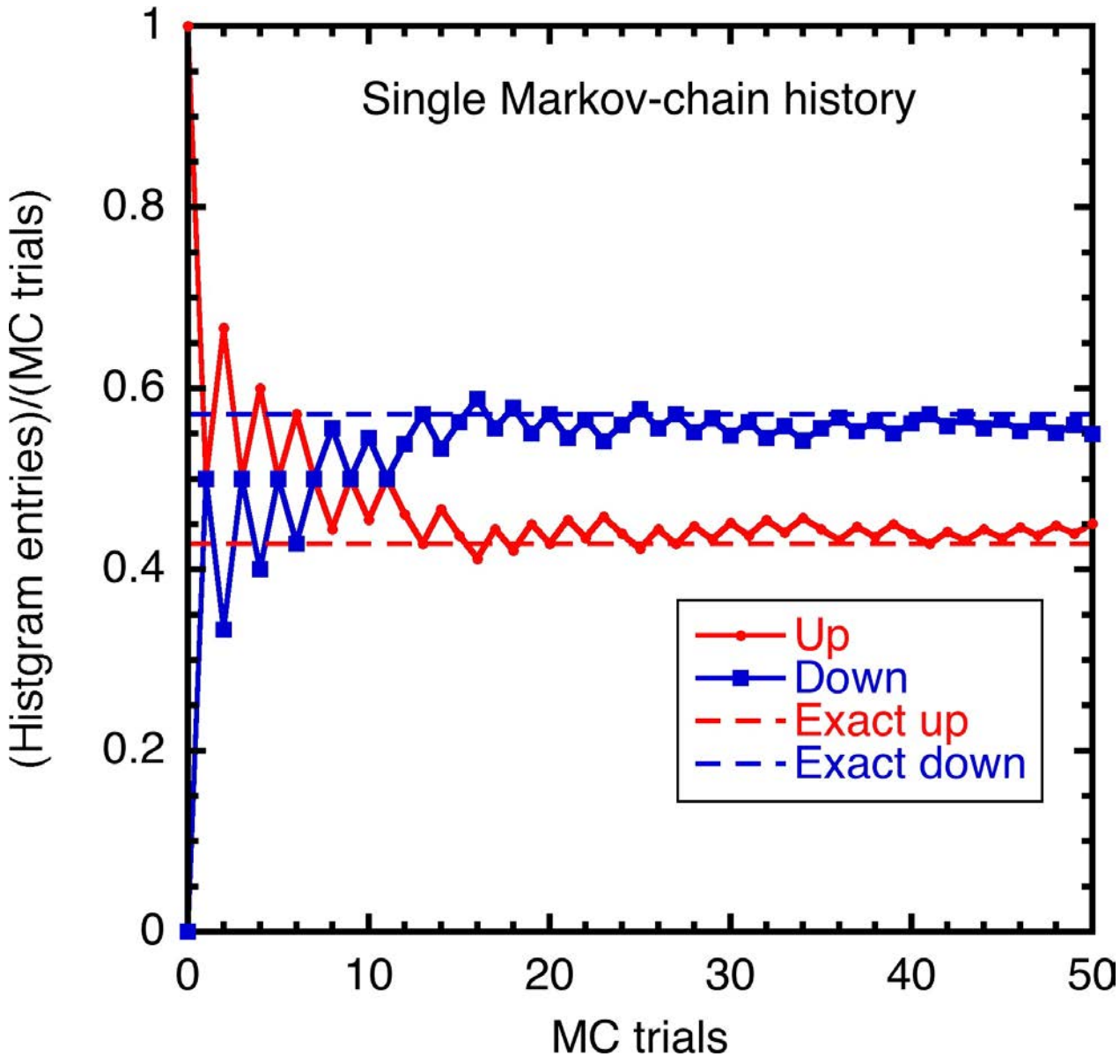
Replace ensemble average by time average of one walker

Ergodic hypothesis

Time-Average MC Result

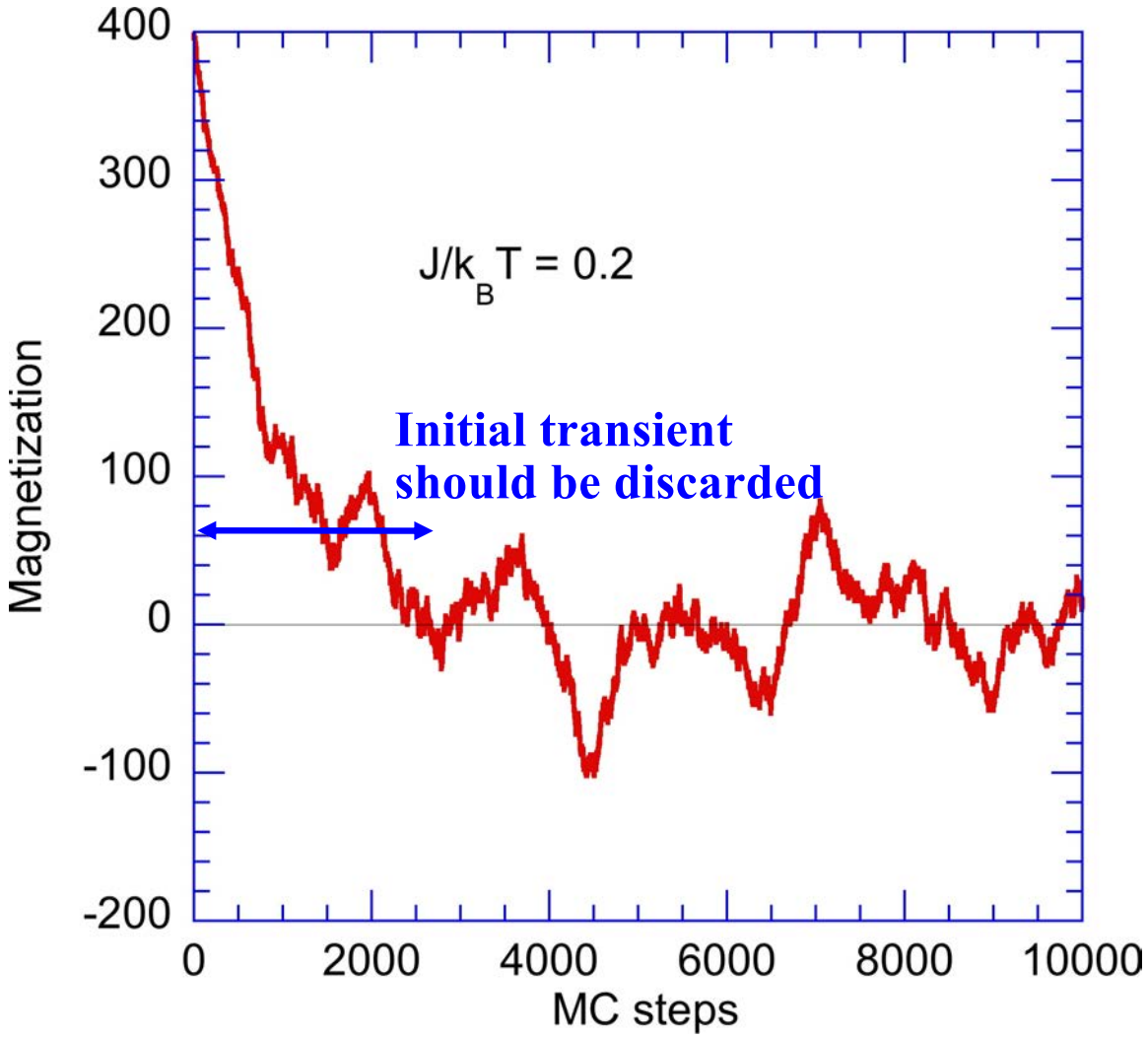
Try	Up	Down
0	1	0
1	1	1
2	2	1
3	2	2
4	3	2
5	3	3
6	4	3
7	4	4
8	4	5
9	5	5
10	5	6
11	6	6
12	6	7
13	6	8
14	7	8
15	7	9
16	7	10
17	8	10
18	8	11
19	9	11
20	9	12

Cumulative histogram



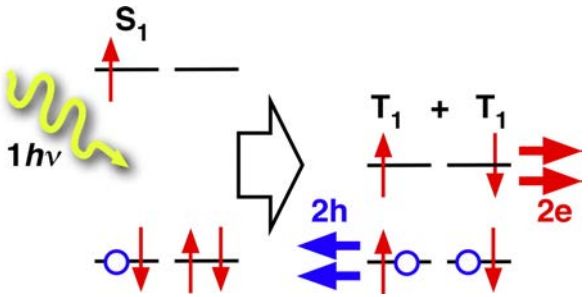
Q: Need Equilibration Steps?

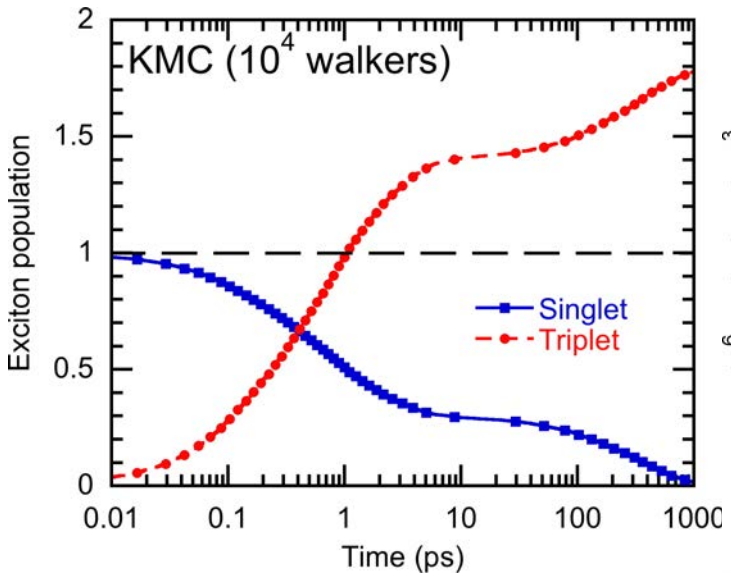
A: Yes, statistics should be taken after the memory of the initial configuration is lost



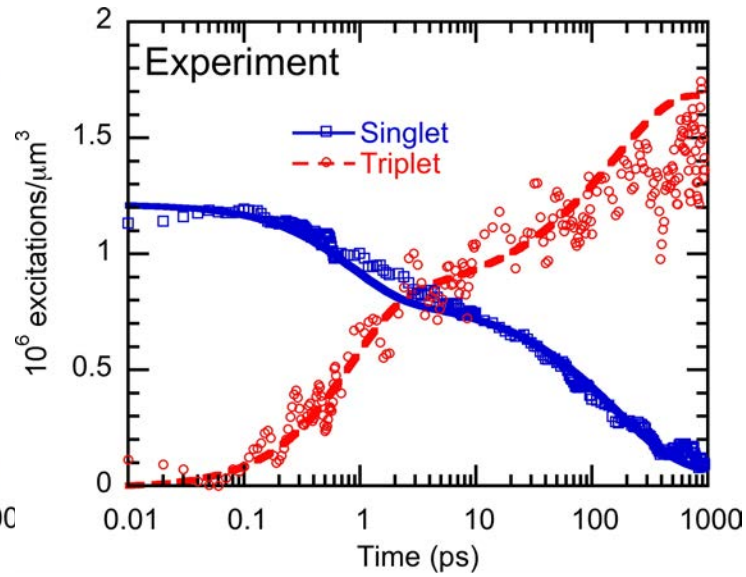
Metropolis MC *vs.* Kinetic MC

- **Metropolis MC:** Given probability density ρ_α $(\alpha = 1, \ldots, N_{\text{states}})$ calculate statistical average of a physical quantity as $\langle A \rangle = \Sigma_\alpha \rho_\alpha A_\alpha$ where the transition-probability matrix $\pi_{\alpha\beta}$ is an artifact for importance sampling
- **Kinetic MC:** Given transition-rate matrix $\pi_{\alpha\beta}$ (calculated, *e.g.*, based on the transition state theory) & initial distribution $\rho_\alpha(t = 0)$, obtain the time variation of $\rho_\alpha(t)$ by solving the master equation represented by an ensemble of state samples, $d\rho_\alpha/dt = -\Sigma_\beta \pi_{\beta\alpha}\rho_\alpha + \Sigma_\beta \pi_{\alpha\beta}\rho_\beta$





W. Mou *et al.*
APL **102,** 173301 ('13)



S. T. Roberts *et al.*
JACS **134**, 6388 ('12)

Metropolis Algorithm?

Equation of State by Fast Computing Machines

Journal of Chemical Physics 21 (6), 1087-1093 (1953)
Received March 6, 1953; Published June 1953

NICHOLAS METROPOLIS
ARIANNA W. ROSENBLUTH
MARSHALL N. ROSENBLUTH
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EDWARD TELLER
Department of Physics, University of Chicago

Who invented the algorithm ..?

ARIANNA & MARSHALL ROSENBLUTH

not

Nicholas Metropolis

https://www.youtube.com/watch?v=MaSGXhsMk1U

A slide taken from a recent presentation by Michael Klein, giving proper credit to the creators of the "Metropolis algorithm" (M. Klein)

https://aiichironakano.github.io/phys516/Battimelli-ComputerMeetsPhysics-Springer20.pdf, p. 29

RIP Arianna

Arianna W. Rosenbluth

From Wikipedia, the free encyclopedia

Arianna Rosenbluth (September 15, 1927 – December 28, 2020) was an American physicist who contributed to the development of the Metropolis–Hastings algorithm. She wrote the first full implementation of the Markov chain Monte Carlo method.

Contents [hide]

Arianna W. Rosenbluth

Rosenbluth in 2013

Born	Arianna Wright September 15, 1927

Early life and education [edit]

Arianna Rosenbluth (née Wright) was born on September 15, 1927, in Houston, Texas.

Death [edit]

Arianna died on December 28, 2020 in the greater Los Angeles, California area.

https://en.wikipedia.org/wiki/Arianna_W._Rosenbluth

Coordinate Transformation?

- **Box-Muller algorithm:** For a harmonic oscillator, $u(x) = Kx^2/2$, Boltzmann probability density (which is Gaussian $p(x) \propto \exp(-u(x)/k_B T) = \exp(-Kx^2/2k_B T)$ can be generated by coordinate transformation
- **Boltzmann generator:** Machine learning of coordinate transformation such that the probability density is Gaussian in the transformed coordinate system, $z(x)$, for complex, multidimensional $u(x)$

F. Noe *et al*.
Science **365,** 1001 ('19)