Metropolis Monte Carlo Simulation: Q & A

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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;
}
```

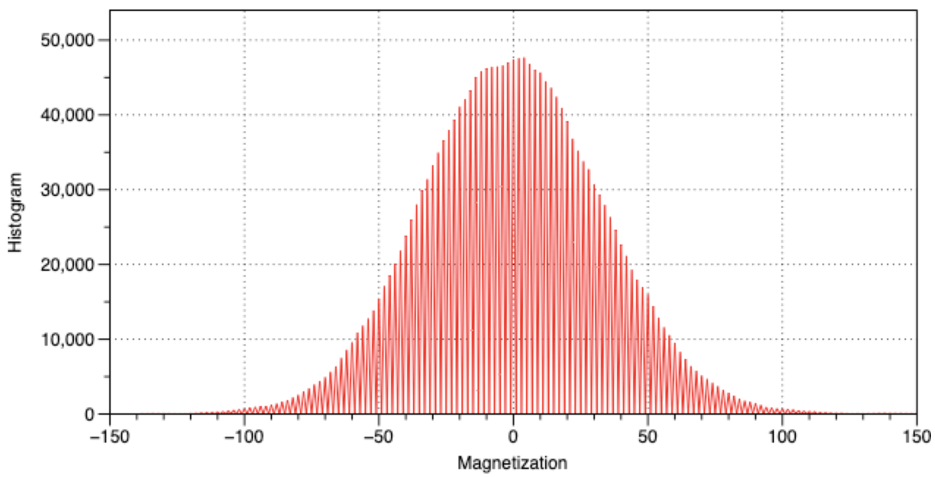
Magnetization Histogram

Q: Why so many zero entries in my histogram?

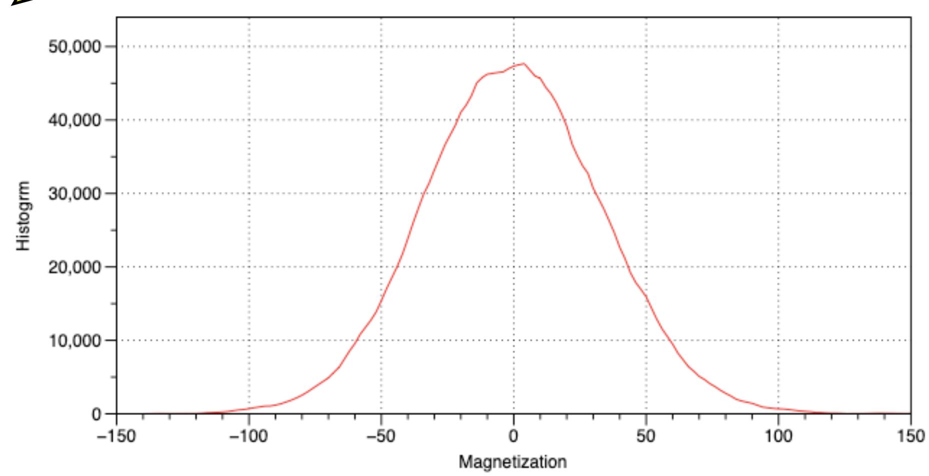
A: Spin flip conserves the parity of the total magnetization, thus no occurrence of odd magnetization.

$runM \leftarrow L^2 = 400\ (L = 20)$ // 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: $\alpha_{m,n} = \begin{cases} 1/N & Hamming\_distance(m,n) = 1 \\ 0 & \text{else} \end{cases}$

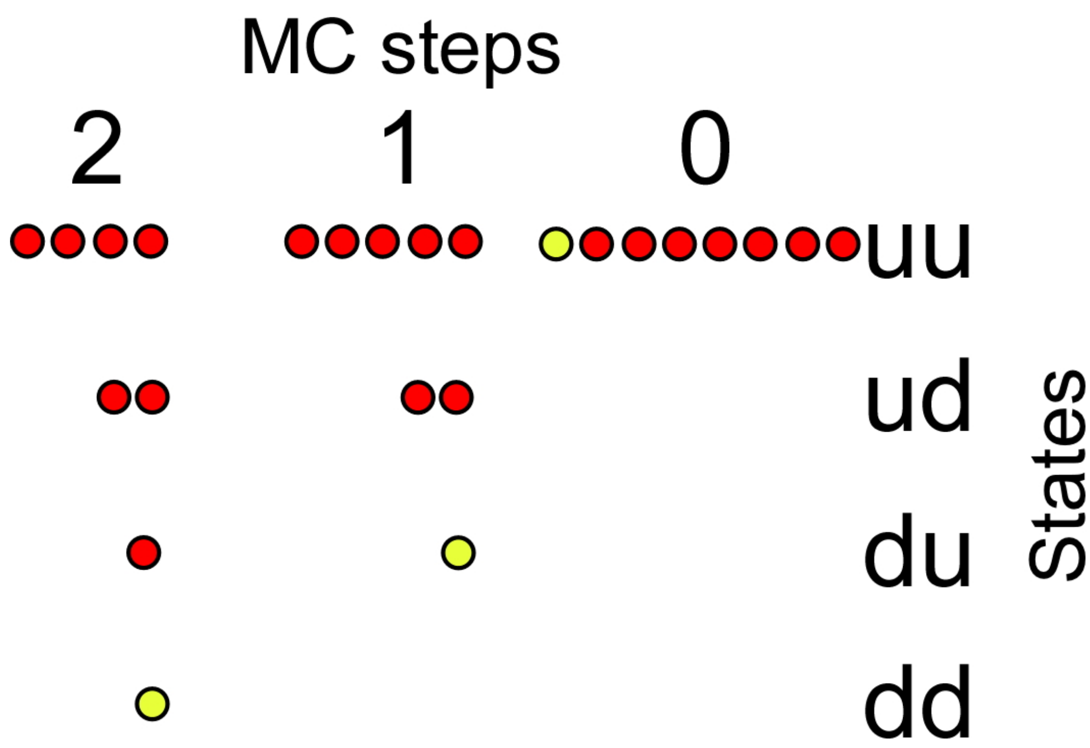
Example: $N = 3$ **($2^N = 8$ states)**

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

Q: Where Is Matrix-Vector Multiplication?

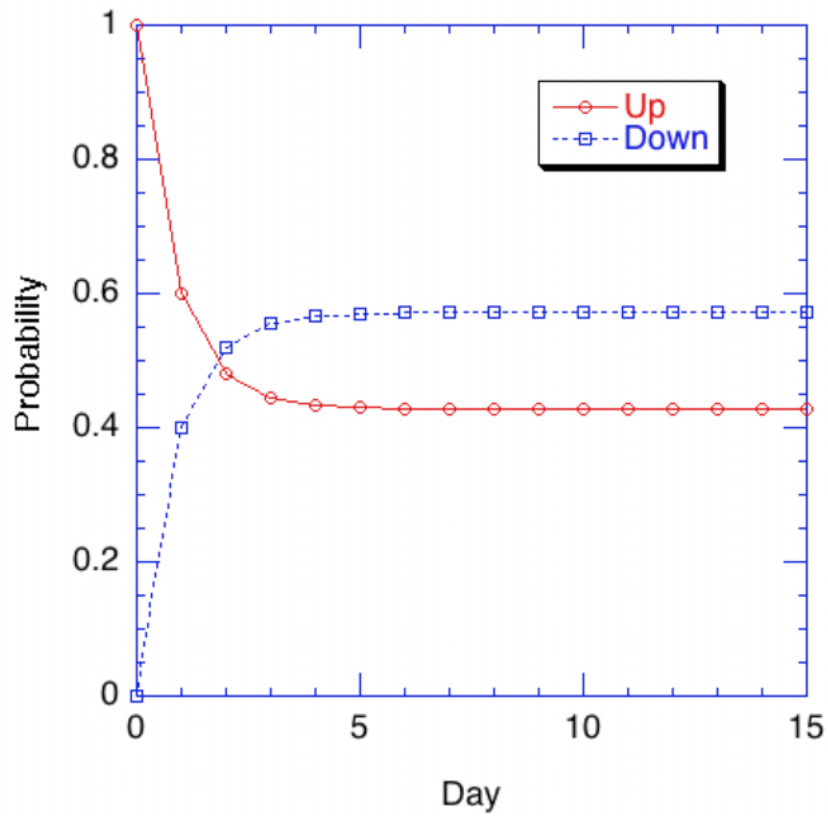
A: The probability density vector is replaced by an ensemble of individual MC sequences in Markov-chain MC; the ensemble average is then replaced by time average.

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



Example: Two-Level System

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



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

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

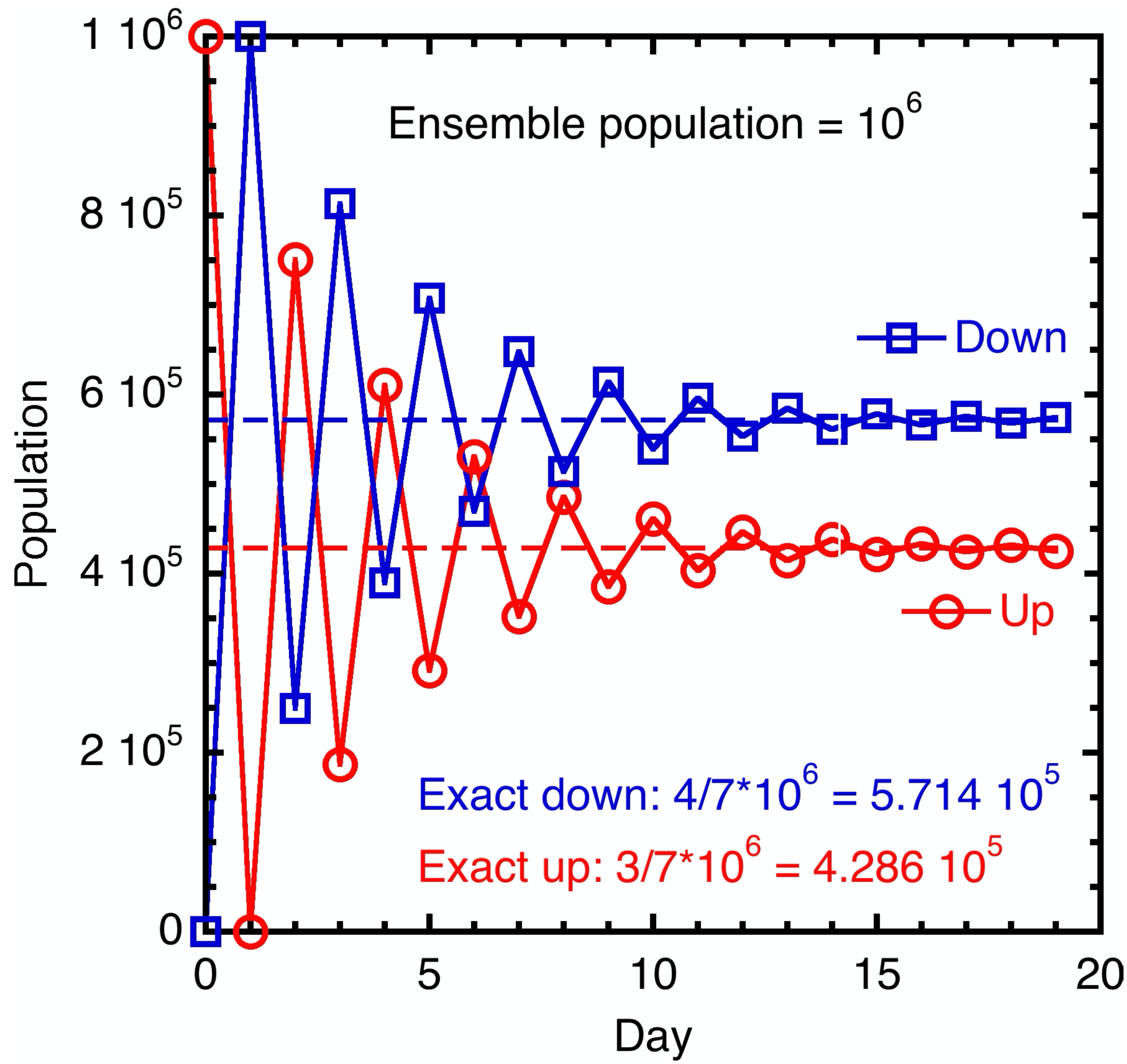
$$\boldsymbol{\Pi} = \begin{pmatrix} \pi_{\uparrow\uparrow} & \pi_{\uparrow\downarrow} \\ \pi_{\downarrow\uparrow} & \pi_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} 1-\alpha_{\downarrow\uparrow} & \alpha_{\uparrow\downarrow}(\rho_{\uparrow}/\rho_{\downarrow}) \\ \alpha_{\downarrow\uparrow}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

Q: How to represent the probability distribution?
A: An ensemble of many samples

Ensemble-Average MC

```c
#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

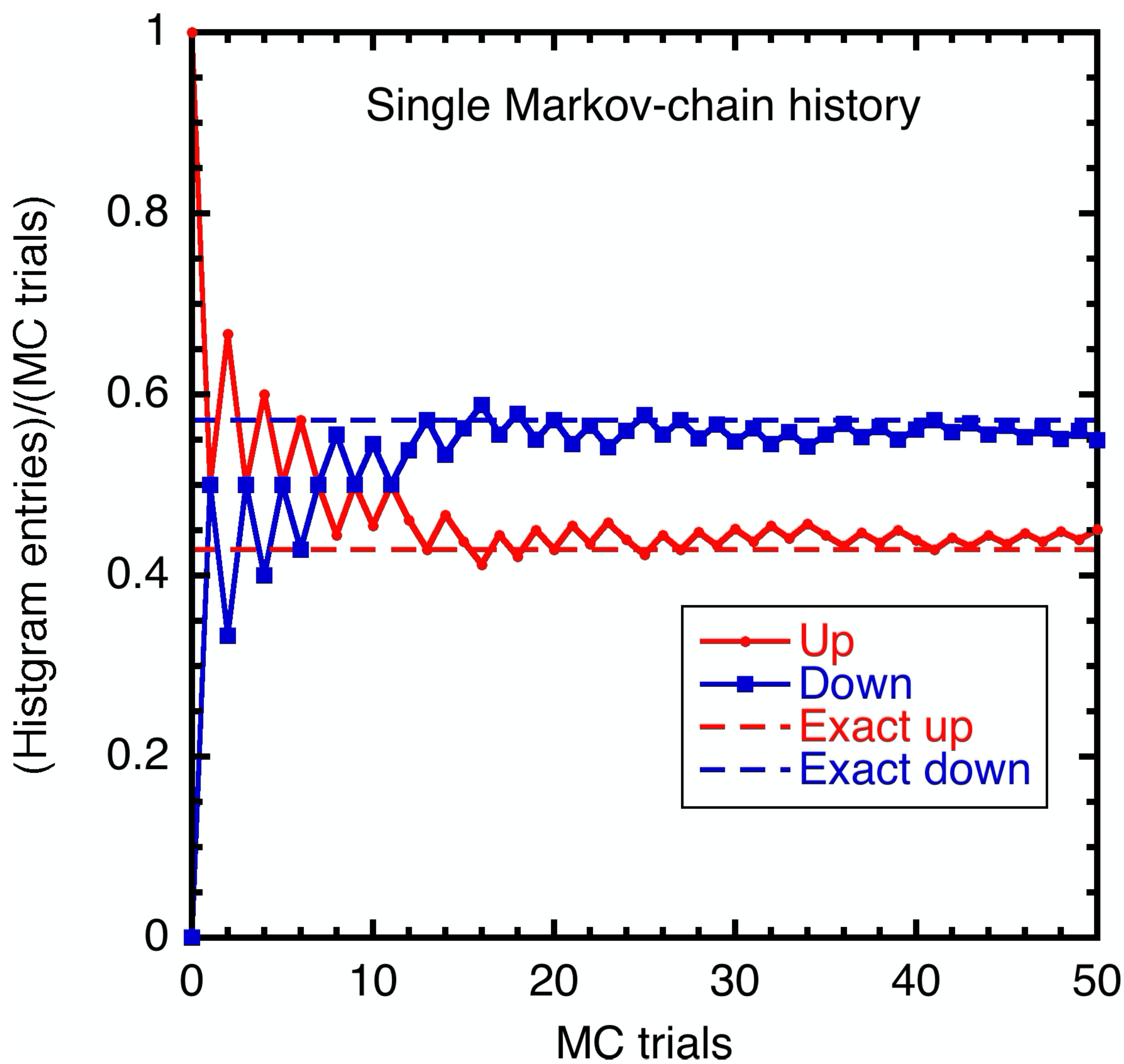
```
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#define NTRY 1000  /* ensemble size */
#define TRNS 3.0/4.0  /* up-to-down conditional probability */

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;
}
```

Ergodic hypothesis

Time-Average MC Result

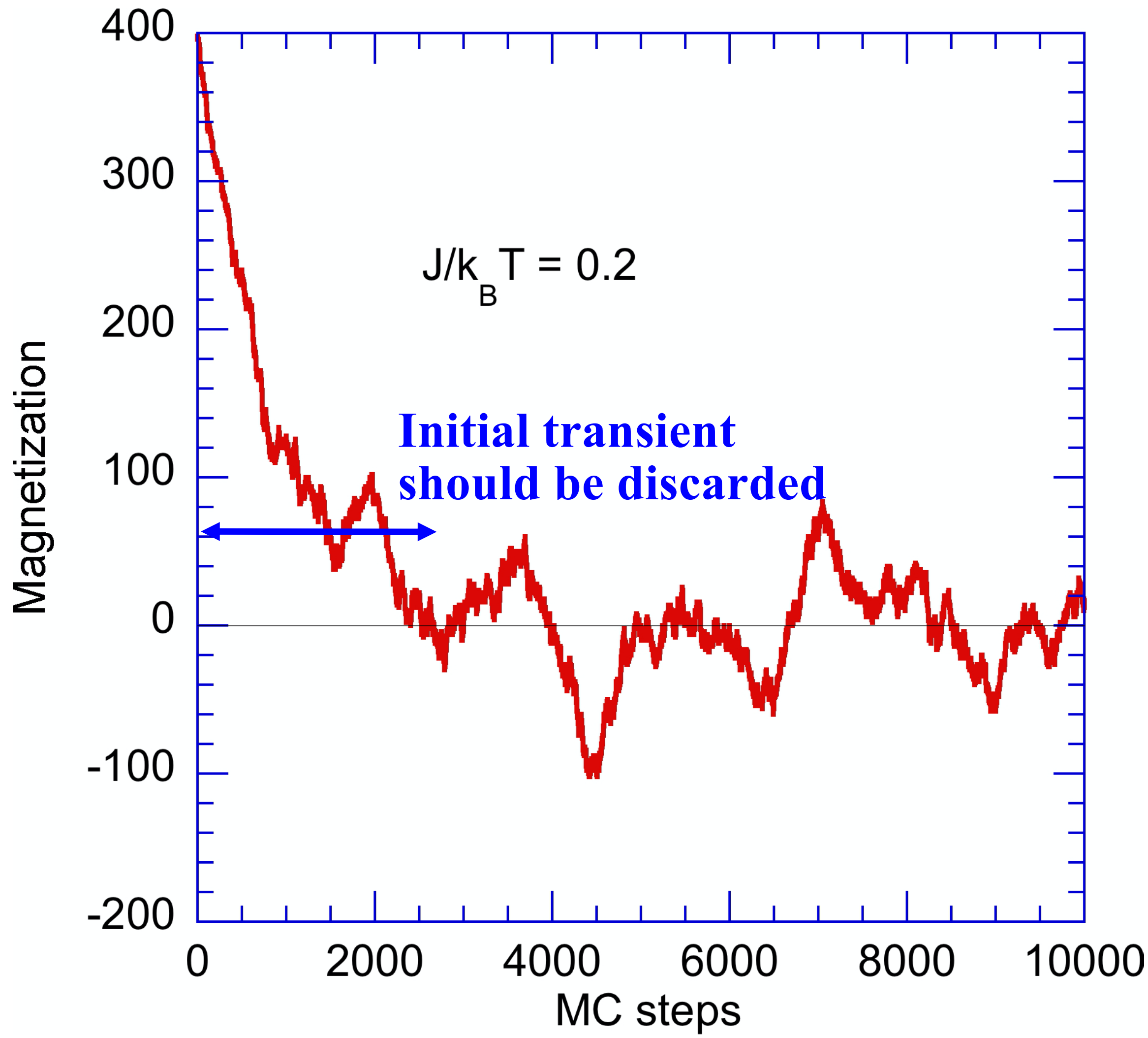
Try	Up	Down
0	1	0
1	1	1
2	2	1
3	2	2
4	3	2
5	3	3
6	4	3
7	4	4
8	4	5
9	5	5
10	5	6
11	6	6
12	6	7
13	6	8
14	7	8
15	7	9
16	7	10
17	8	10
18	8	11
19	9	11
20	9	12

Cumulative histogram



Q: Need Equilibration Steps?

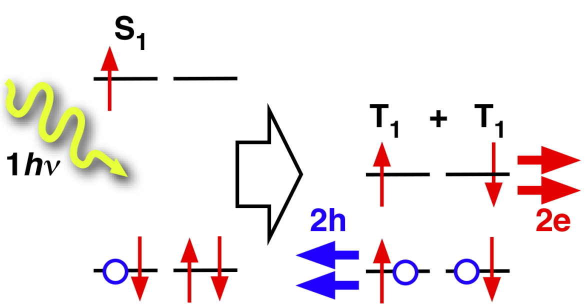
A: Yes, statistics should be taken after the memory of the initial configuration is lost

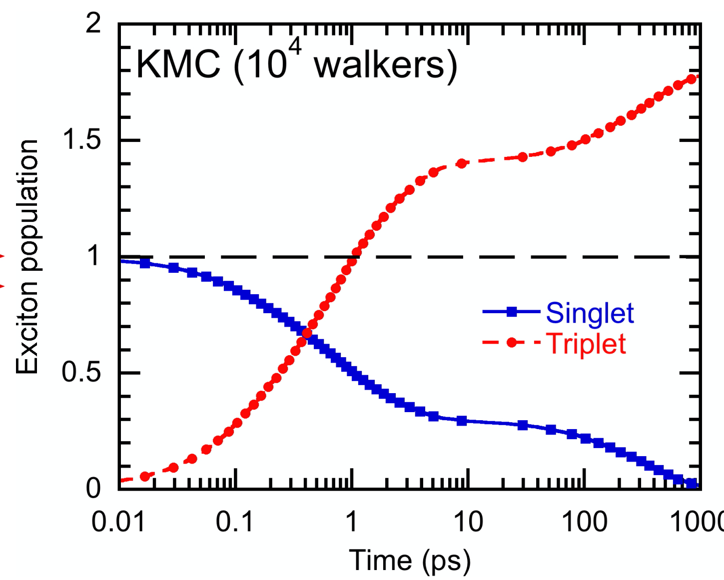


Metropolis MC *vs.* Kinetic MC

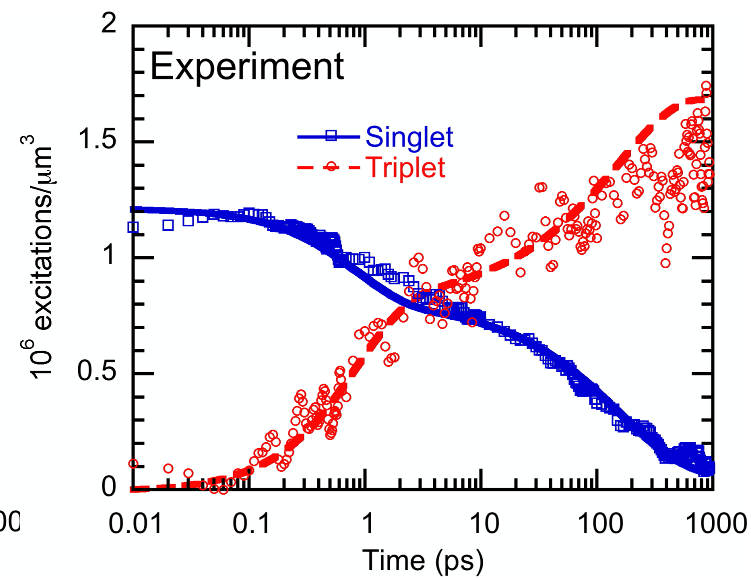
- **Metropolis MC:** Given probability density ρ_α $(\alpha = 1, \dots, N_{\text{states}})$ calculate statistical average of a physical quantity as $\langle A \rangle = \Sigma_\alpha \rho_\alpha A_\alpha$ where the transition-probability matrix $\pi_{\alpha\beta}$ is an artifact for importance sampling

- **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?

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.

Arianna W. Rosenbluth

Rosenbluth in 2013

Born Arianna Wright September 15, 1927

Contents [hide]

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 $p(x) \propto \exp(-u(x)/k_\mathrm{B}T) = \exp(-Kx^2/2k_\mathrm{B}T)$ 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)