Quantum Monte Carlo

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1. Monte Carlo Integration

Integrating a function

- Convert the integral to a discrete sum

$$\int_a^b f(x)dx = \frac{b-a}{N}\sum_{i=1}^{N} f\left(a + i\frac{b-a}{N}\right) + O(1/N)$$

- Higher order integrators:
  - Trapezoidal rule:

$$\int_a^b f(x)dx = \frac{b-a}{N}\left(\frac{1}{2}f(a) + \sum_{i=1}^{N-1} f\left(a + i\frac{b-a}{N}\right) + \frac{1}{2}f(b)\right) + O(1/N^2)$$

  - Simpson rule:

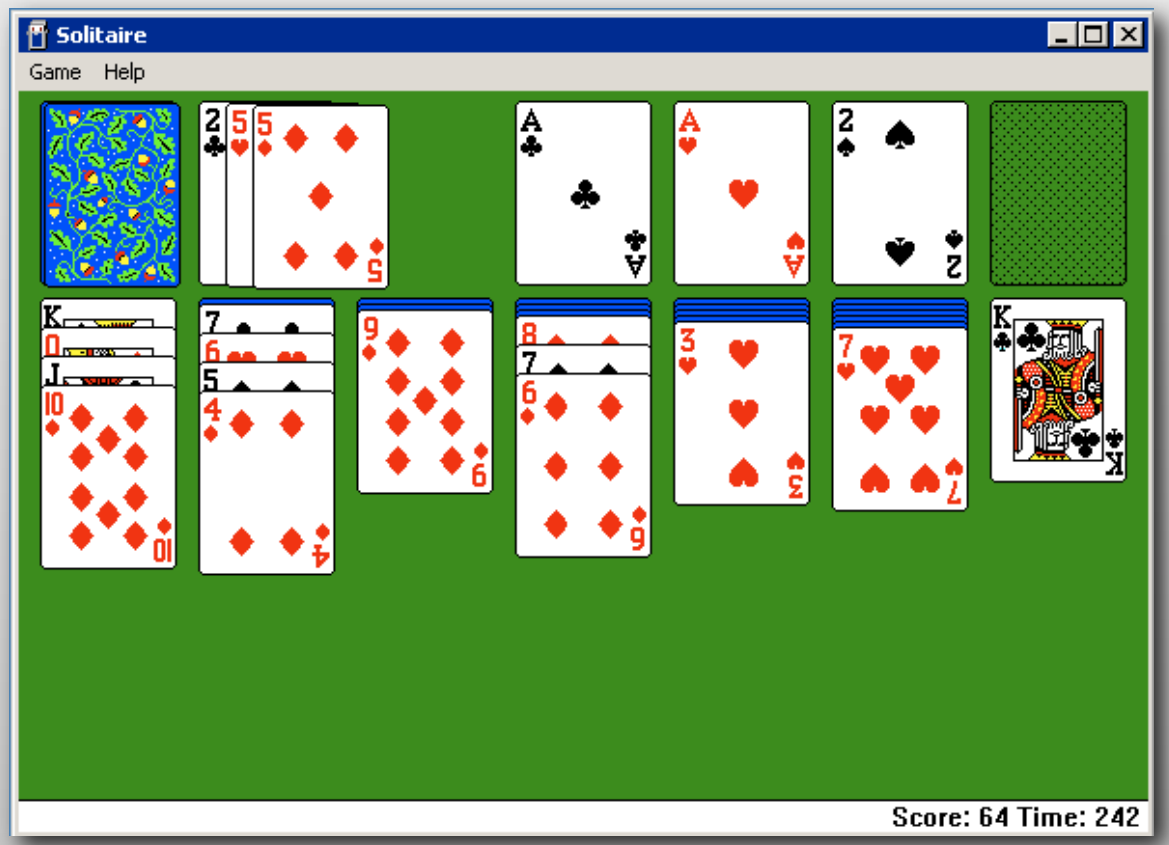
$$\int_a^b f(x)dx = \frac{b-a}{3N}\left(f(a) + \sum_{i=1}^{N-1}(3-(-1)^i) f\left(a + i\frac{b-a}{N}\right) + f(b)\right) + O(1/N^4)$$

High dimensional integrals

- Simpson rule with M points per dimension
  - one dimension the error is $O(M^{-4})$
  - d dimensions we need $N = M^d$ points
    the error is order $O(M^{-4}) = O(N^{-4/d})$
- An order - n scheme in 1 dimension
  is order - n/d d in d dimensions!
- In a statistical mechanics model with N particles we have $6N$-dimensional integrals ($3N$ positions and $3N$ momenta).
- Integration becomes extremely inefficient!

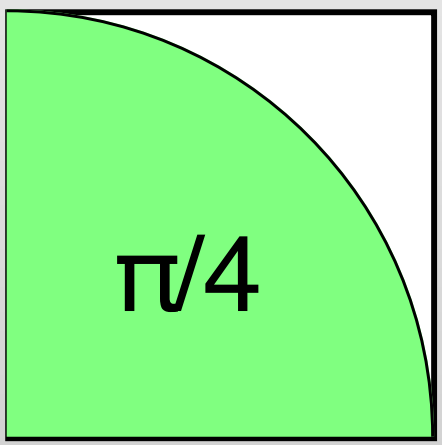
Ulam: the Monte Carlo Method

- What is the probability to win in Solitaire?
  - Ulam's answer: play it 100 times, count the number of wins and you have a pretty good estimate



Throwing stones into a pond

- How can we calculate π by throwing stones?
- Take a square surrounding the area we want to measure:

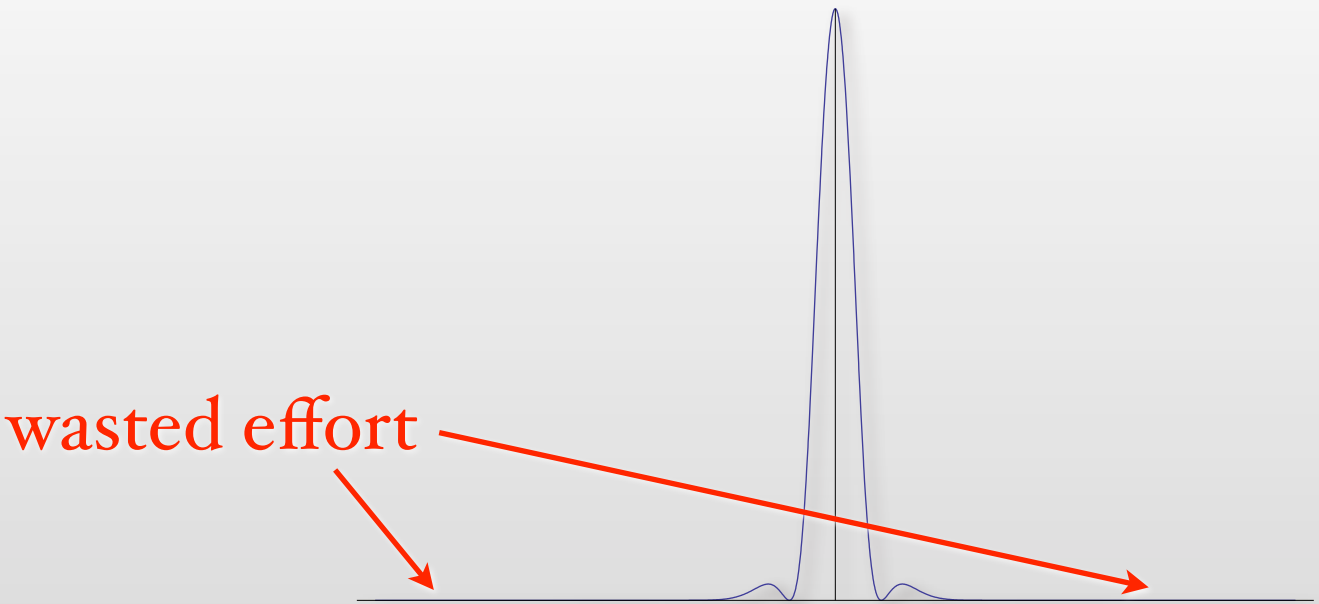


- Choose M pairs of random numbers (x, y) and count how many points (x, y) lie in the interesting area

Monte Carlo integration

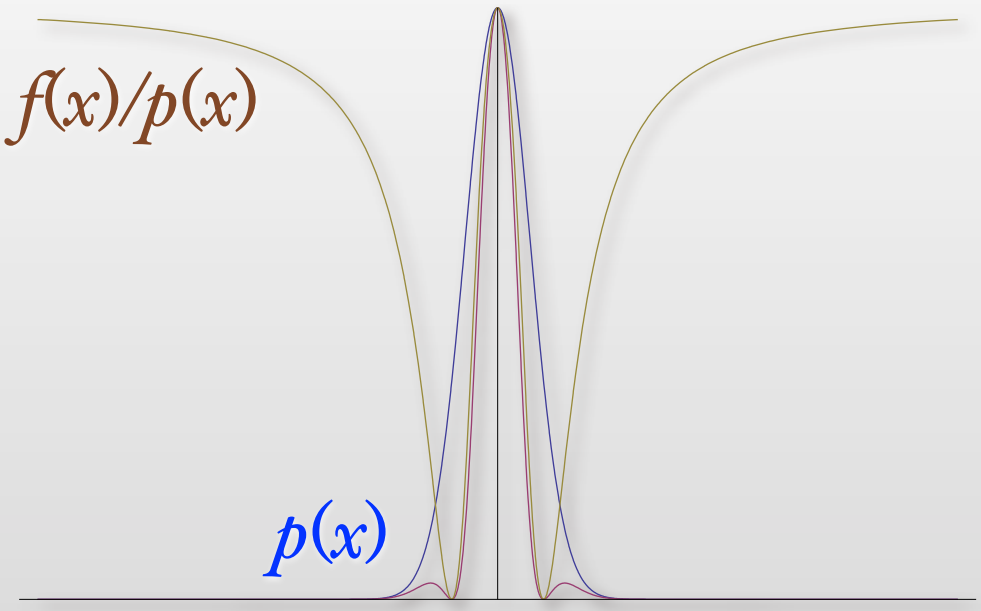
- Consider an integral $$\langle f \rangle = \int_\Omega f(\vec{x}) d\vec{x} \Big/ \int_\Omega d\vec{x}$$
- Instead of evaluating it at equally spaced points evaluate it at M points x_i chosen randomly in Ω:
$$\langle f \rangle \approx \frac{1}{M} \sum_{i=1}^{M} f(\vec{x}_i)$$
- The error is statistical:
$$\Delta = \sqrt{\frac{\mathrm{Var}\, f}{M}} \propto M^{-1/2}$$
$$\mathrm{Var}\, f = \langle f^2 \rangle - \langle f \rangle^2$$
- In d>8 dimensions Monte Carlo is better than Simpson!

Sharply peaked functions



- In many cases a function is large only in a tiny region
- Lots of time wasted in regions where the function is small
- The sampling error is large since the variance is large

Importance sampling



- Choose points not uniformly but with probability $p(x)$:

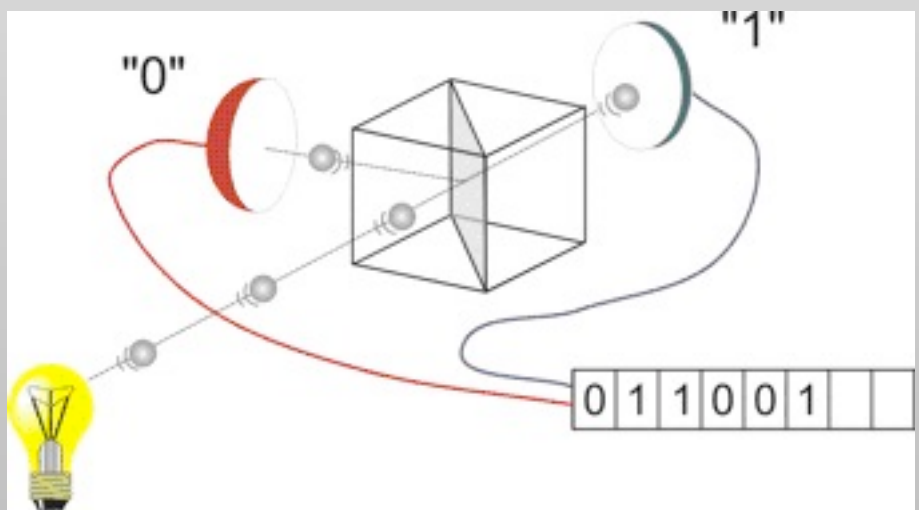
$$\langle f \rangle = \left\langle \frac{f}{p} \right\rangle_p := \int_\Omega \frac{f(\vec{x})}{p(\vec{x})} p(\vec{x}) d\vec{x} \Big/ \int_\Omega d\vec{x}$$

- The error is now determined by Var f/p
- Find p similar to f and such that p-distributed random numbers are easily available

2. Generating Random Numbers

Random numbers

- Real random numbers are hard to obtain
  - classical chaos (atmospheric noise)
  - quantum mechanics
- Commercial products: quantum random number generators
  - based on photons and semi-transparent mirror
  - 4 Mbit/s from a USB device, too slow for most MC simulations



http://www.idquantique.com/

Pseudo Random numbers

- Are generated by an algorithm
- Not random at all, but completely deterministic
- Look nearly random however when algorithm is not known and may be good enough for our purposes
- Never trust pseudo random numbers however!

Linear congruential generators

- are of the simple form $x_{n+1}=f(x_n)$
- A reasonably good choice is the GGL generator

$$x_{n+1} = (ax_n + c) \bmod m$$

with a = 16807, c = 0, m = $2^{31}-1$

- quality depends sensitively on a,c,m

- Periodicity is a problem with such 32-bit generators
  - The sequence repeats identically after $2^{31}-1$ iterations
  - With 500 million numbers per second that is just 4 seconds!
  - Should not be used anymore!

Lagged Fibonacci generators

$$x_n = x_{n-p} \otimes x_{n-q} \bmod m$$

- Good choices are
  - (2281,1252,+)
  - (9689,5502,+)
  - (44497,23463,+)

- Seed blocks usually generated by linear congruential
- Has very long periods since large block of seeds
- A very fast generator: vectorizes and pipelines very well

More advanced generators

- As well-established generators fail new tests, better and better generators get developed
  - Mersenne twister (Matsumoto & Nishimura, 1997)
  - Well generator (Panneton and L'Ecuyer , 2004)

- Number theory enters the generator design: predicting the next number is equivalent to solving a very hard mathematical problem

Are these numbers really random?

- No!
- Are they random enough?
  - Maybe?
- Statistical tests for distribution and correlations
- Are these tests enough?
  - No! Your calculation could depend in a subtle way on hidden correlations!
- What is the ultimate test?
  - Run your simulation with various random number generators and compare the results

Marsaglia's diehard tests

- **Birthday spacings:** Choose random points on a large interval. The spacings between the points should be asymptotically Poisson distributed. The name is based on the birthday paradox.
- **Overlapping permutations:** Analyze sequences of five consecutive random numbers. The 120 possible orderings should occur with statistically equal probability.
- **Ranks of matrices:** Select some number of bits from some number of random numbers to form a matrix over {0,1}, then determine the rank of the matrix. Count the ranks.
- **Monkey tests:** Treat sequences of some number of bits as "words". Count the overlapping words in a stream. The number of "words" that don't appear should follow a known distribution. The name is based on the infinite monkey theorem.
- **Count the 1s:** Count the 1 bits in each of either successive or chosen bytes. Convert the counts to "letters", and count the occurrences of five-letter "words".
- **Parking lot test:** Randomly place unit circles in a 100 x 100 square. If the circle overlaps an existing one, try again. After 12,000 tries, the number of successfully "parked" circles should follow a certain normal distribution.

Marsaglia's diehard tests (cont.)

- **Minimum distance test:** Randomly place 8,000 points in a 10,000 x 10,000 square, then find the minimum distance between the pairs. The square of this distance should be exponentially distributed with a certain mean.
- **Random spheres test:** Randomly choose 4,000 points in a cube of edge 1,000. Center a sphere on each point, whose radius is the minimum distance to another point. The smallest sphere's volume should be exponentially distributed with a certain mean.
- **The squeeze test:** Multiply 231 by random floats on [0,1) until you reach 1. Repeat this 100,000 times. The number of floats needed to reach 1 should follow a certain distribution.
- **Overlapping sums test:** Generate a long sequence of random floats on [0,1). Add sequences of 100 consecutive floats. The sums should be normally distributed with characteristic mean and sigma.
- **Runs test:** Generate a long sequence of random floats on [0,1). Count ascending and descending runs. The counts should follow a certain distribution.
- **The craps test:** Play 200,000 games of craps, counting the wins and the number of throws per game. Each count should follow a certain distribution.

Non-uniform random numbers

- we found ways to generate pseudo random numbers u in the interval [0,1[
- How do we get other uniform distributions?
  - uniform x in [a,b[: $x = a+(b-a)\,u$
- Other distributions:
  - Inversion of integrated distribution
  - Rejection method

Non-uniform distributions

- How can we get a random number x distributed with $f(x)$ in the interval $[a,b[$ from a uniform random number u?
- Look at probabilities:

$$P[x < y] = \int_a^y f(t)\,dt =: F(y) \equiv P[u < F(y)]$$

$$\Rightarrow x = F^{-1}(u)$$

- This method is feasible if the integral can be inverted easily
  - exponential distribution $f(x)=\lambda \exp(-\lambda x)$
  - can be obtained from uniform by $x=-1/\lambda \ln(1-u)$

Normally distributed numbers

- The normal distribution

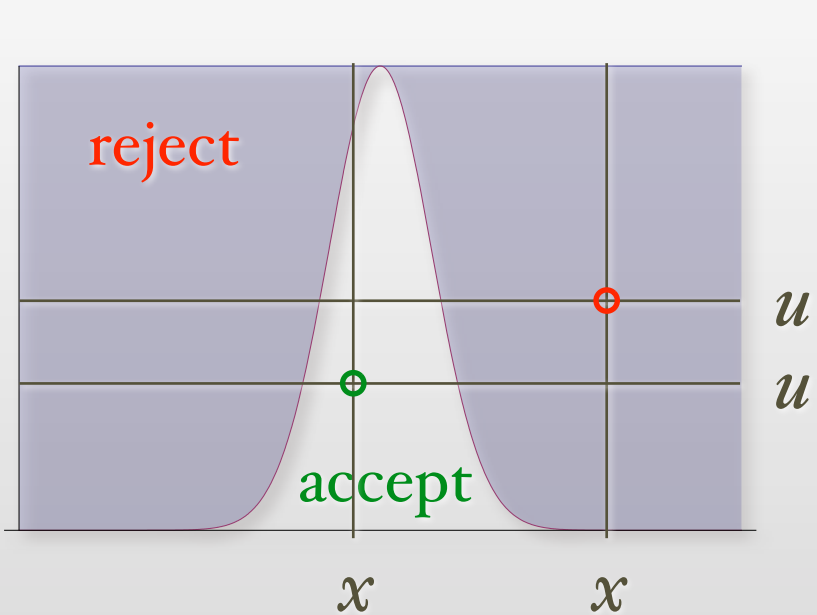
$$f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-x^2\right)$$

- cannot easily be integrated in one dimension but can be easily integrated in 2 dimensions!
- We can obtain two normally distributed numbers from two uniform ones (Box-Muller method)

$$n_1 = \sqrt{-2\ln(1-u_1)}\sin u_2$$

$$n_2 = \sqrt{-2\ln(1-u_1)}\cos u_2$$

Rejection method (von Neumann)



- Look for a simple distribution h that bounds f: $f(x) < \lambda h(x)$
  - Choose an h-distributed number x
  - Choose a uniform random number number $0 \le u < 1$
  - Accept x if $u < f(x)/\lambda h(x)$,
    otherwise reject x and get a new pair (x,u)

- Needs a good guess h to be efficient, numerical inversion of integral might be faster if no suitable h can be found

3. The Metropolis Algorithm

Monte Carlo for classical systems

- Evaluate phase space integral by importance sampling

$$\langle A \rangle = \frac{\int_{\Omega} A(c)p(c)dc}{\int_{\Omega} p(c)dc} \longrightarrow \langle A \rangle \approx \overline{A} = \frac{1}{M}\sum_{i=1}^{M} A_{c_i}$$

- Pick configurations with the correct Boltzmann weight

$$P[c] = \frac{p(c)}{Z} = \frac{\exp(-\beta E(c))}{Z}$$

- But how do we create configurations with that distribution? The key problem in statistical mechanics!

GUEST EDITORS' INTRODUCTION

the Top 10 Algorithms

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

computing in SCIENCE & ENGINEERING

The Metropolis Algorithm (1953)

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† con-

Markov chain Monte Carlo

- Instead of drawing independent samples c_i we build a Markov chain

$$c_1 \to c_2 \to \ldots \to c_i \to c_{i+1} \to \ldots$$

- Transition probabilities $W_{x,y}$ for transition $x \to y$ need to satisfy:
  - **Normalization:** $\sum_y W_{x,y} = 1$
  - **Ergodicity:** any configuration reachable from any other

$$\forall x, y \; \exists n \; : \; \left(W^n\right)_{x,y} \neq 0$$

  - **Balance:** the distribution should be stationary

$$0 = \frac{d}{dt} p(x) = \sum_y p(y) W_{y,x} - \sum_y p(x) W_{x,y} \Rightarrow p(x) = \sum_y p(y) W_{y,x}$$

  - Detailed balance is sufficient but not necessary for balance

$$\frac{W_{x,y}}{W_{y,x}} = \frac{p(y)}{p(x)}$$

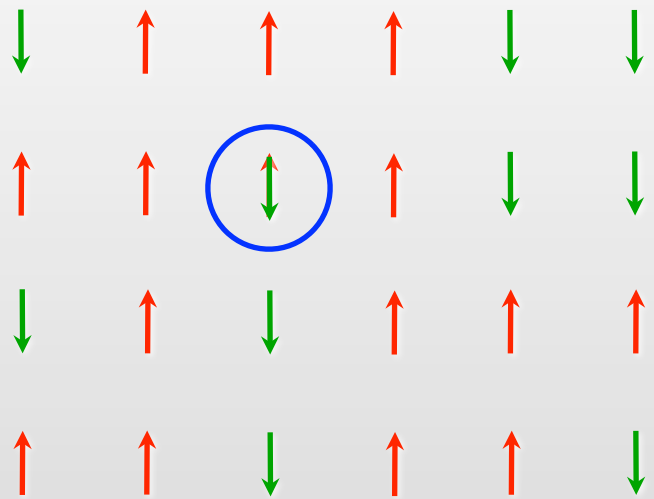
The Metropolis algorithm

- Teller's proposal was to use rejection sampling:
  - Propose a change with an a-priori proposal rate $A_{x,y}$
  - Accept the proposal with a probability $P_{x,y}$
  - The total transition rate is $W_{x,y} = A_{x,y} P_{x,y}$
- The choice

$$P_{x,y} = \min\left[1, \frac{A_{y,x} p(y)}{A_{x,y} p(x)}\right]$$

satisfies detailed balance and was first proposed by Metropolis *et al*

Metropolis algorithm for the Ising model



1. Pick a random spin and propose to flip it

2. Accept the flip with probability $P = \min\left[1, e^{-(E_{new} - E_{old})/T}\right]$

3. Perform a measurement independent of whether the proposed flip was accepted or rejected!

Equilibration

- Starting from a random initial configuration it takes a while to reach the equilibrium distribution
- The desired equilibrium distribution is a left eigenvector with eigenvalue 1 (this is just the balance condition)

$$p(x) = \sum_y p(y) W_{y,x}$$

- Convergence is controlled by the second largest eigenvalue

$$p(x,t) = p(x) + O(\exp(-\lambda_2 t))$$

- We need to run the simulation for a while to equilibrate and only then start measuring

4. Monte Carlo Error Analysis

Monte Carlo error analysis

- The simple formula $\Delta A = \sqrt{\frac{\mathrm{Var}\, A}{M}}$

  is valid only for independent samples

- The Metropolis algorithm gives us correlated samples! The number of independent samples is reduced

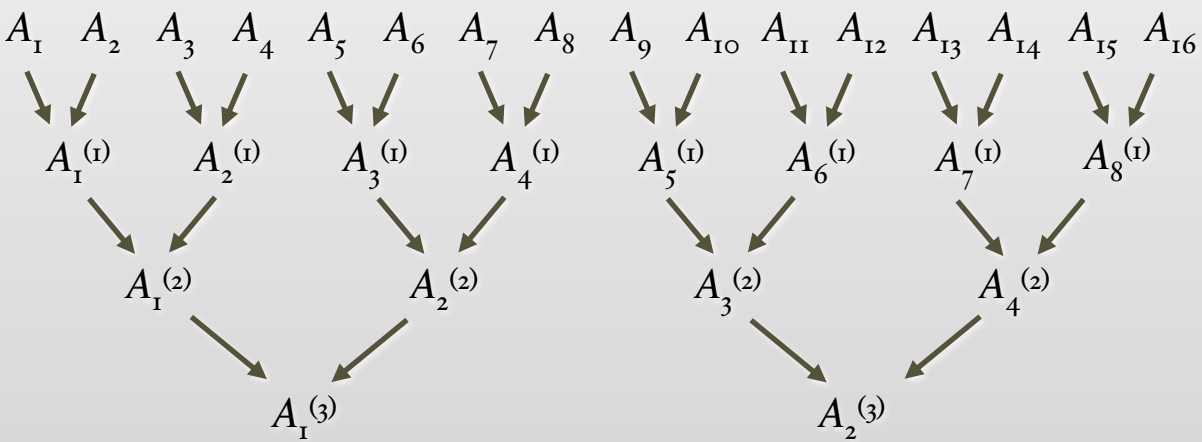
$$\Delta A = \sqrt{\frac{\mathrm{Var}\, A}{M}\left(1 + 2\tau_A\right)}$$

- The autocorrelation time is defined by

$$\tau_A = \frac{\sum_{t=1}^{\infty}\left(\langle A_{i+t} A_i \rangle - \langle A \rangle^2\right)}{\mathrm{Var}\, A}$$

Binning analysis

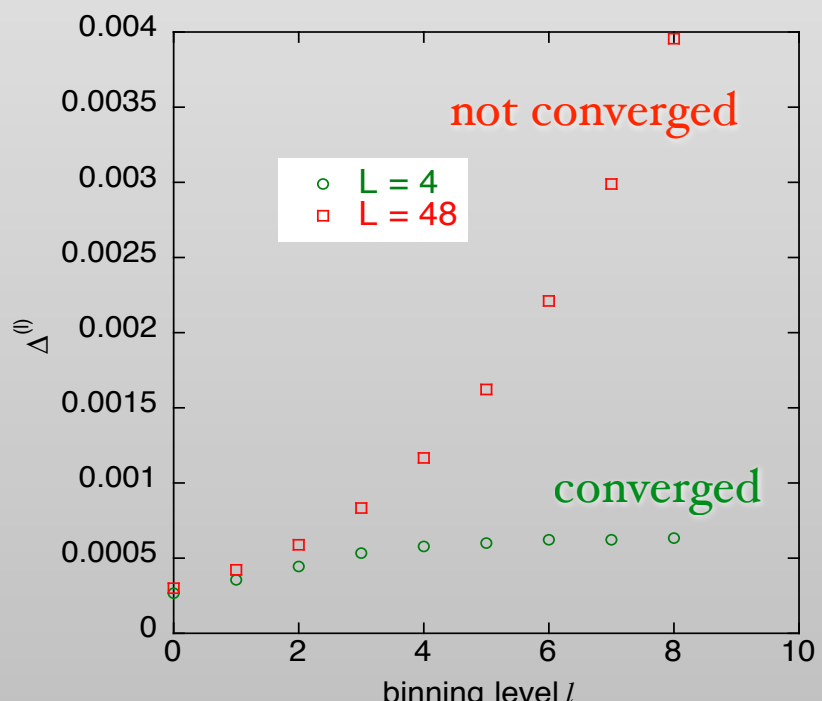
- Take averages of consecutive measurements: averages become less correlated and naive error estimates converge to real error



$$A_i^{(l)} = \frac{1}{2}\left(A_{2i-1}^{(l-1)} + A_{2i}^{l}\right)$$

$$\Delta^{(l)} = \sqrt{\operatorname{Var} A^{(l)} / M^{(l)}} \xrightarrow{l\to\infty} \Delta = \sqrt{(1+2\tau_A)\operatorname{Var} A / M}$$

$$\tau_A = \lim_{l\to\infty} \frac{1}{2}\left(\frac{2^l \operatorname{Var} A^{(l)}}{\operatorname{Var} A^{(0)}} - 1\right)$$



a smart implementation needs only O(log (*N*)) memory for *N* measurements

Seeing convergence in ALPS

- Look at the ALPS output in the first hands-on session
- 48 x 48 Ising model at the critical point
  - local updates:

Name	Count	Mean	Error	Tau	Method
Susceptibility	52529	401.08	11.3 not converged	99.1	binning

  - cluster updates:

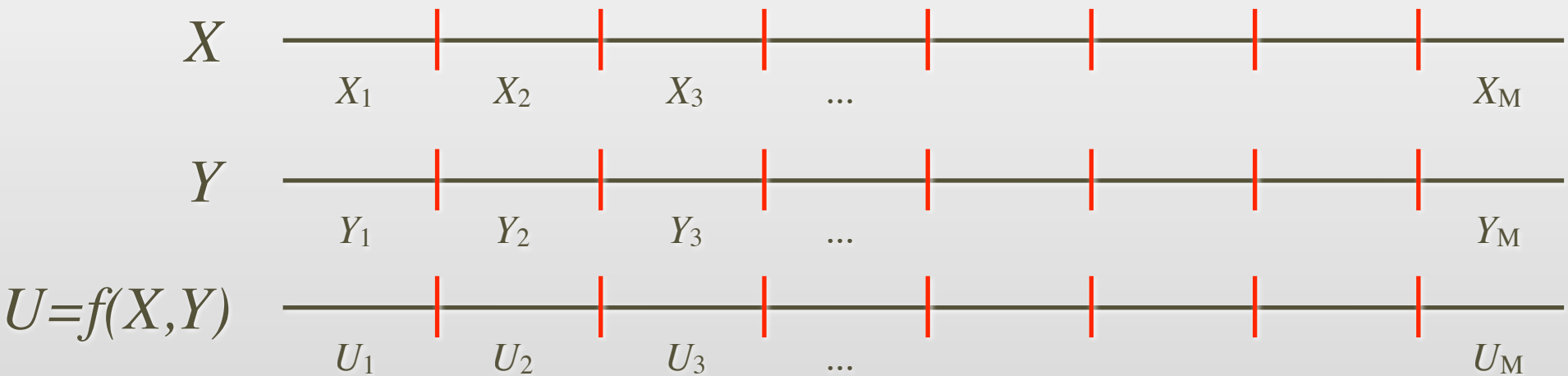
Name	Count	Mean	Error	Tau	Method
Susceptibility	113433	421.642	1.57	0.821	binning

Correlated quantities

- How do we calculate the errors of functions of correlated measurements?
  - specific heat $$c_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{T^2}$$
  - Binder cumulant ratio $$U = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$$
- The naïve way of assuming uncorrelated errors is wrong!
- It is not even enough to calculate all crosscorrelations due to nonlinearities except if the errors are tiny!

Splitting the time series

Simplest idea: split the time series and evaluate for each segment



$$\langle U \rangle \approx \overline{U} = \frac{1}{M}\sum_{i=1}^{M} U_i$$

$$\Delta U \approx \sqrt{\frac{1}{M(M-1)}\sum_{i-1}^{M}\left(U_i - \overline{U}\right)^2}$$

Problem: can be unstable and noisy for nonlinear functions such as X/Y

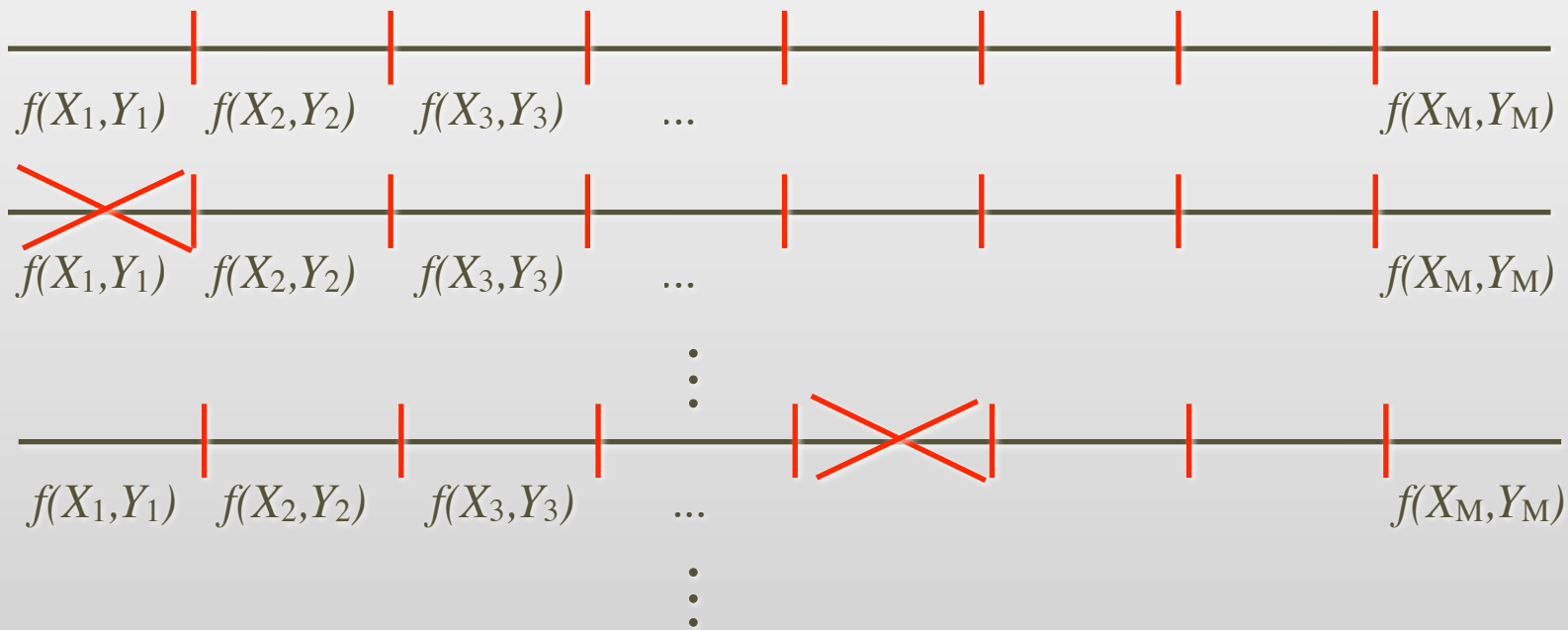
Jackknife-analysis

Evaluate the function on all and all but one segment

$$U_0 = \frac{1}{M}\sum_{i=1}^{M} f(X_i,Y_i)$$

$$U_1 = \frac{1}{M-1}\sum_{i=2}^{M} f(X_i,Y_i)$$

$$U_j = \frac{1}{M-1}\sum_{\substack{i=1 \\ i\neq j}}^{M} f(X_i,Y_i)$$



$$\langle U \rangle \approx U_0 - (M-1)(\overline{U} - U_0)$$

$$\overline{U} = \frac{1}{M}\sum_{i=1}^{M} U_i$$

$$\Delta U \approx \sqrt{\frac{M-1}{M}\sum_{i-1}^{M}\left(U_i - \overline{U}\right)^2}$$

ALPS Alea library in C++

- The ALPS class library implements reliable error analysis
  - Adding a measurement:

```
alps::RealObservable mag;
…
mag << new_value;
```

  - Evaluating measurements

```
std::cout << mag.mean() << " +/- " << mag.error();
std::cout "Autocorrelation time: " << mag.tau();
```

- Correlated quantities?
  - Such as in Binder cumulant ratios $\langle m^4 \rangle / \langle m^2 \rangle^2$
  - ALPS library uses jackknife analysis to get correct errors

```
alps::RealObsEvaluator binder = mag4/(mag2*mag2);
std::cout << binder.mean() << " +/- " << binder.error();
```

ALPS Alea library in Python

- The ALPS class library implements reliable error analysis
  - Adding a measurement:

```
mag = pyalps.pyalea.RealObservable('Magnetization');
…
mag << new_value;
```

  - Evaluating measurements

```
print mag.mean, " +/- ", mag.error;
print "Autocorrelation time: ", mag.tau;
```

- Correlated quantities?
  - Such as in Binder cumulant ratios $\langle m^4 \rangle / \langle m^2 \rangle^2$
  - ALPS library uses jackknife analysis to get correct errors

```
print mag4/(mag2*mag2)
```

5. Cluster updates: The Swendsen-Wang algorithm The loop algorithm

Autocorrelation effects

- The Metropolis algorithm creates a Markov chain

$$c_1 \to c_2 \to \ldots \to c_i \to c_{i+1} \to \ldots$$

- successive configurations are correlated, leading to an increased statistical error

$$\Delta A = \sqrt{\left\langle \left(\overline{A} - \langle A \rangle \right)^2 \right\rangle} = \sqrt{\frac{\mathrm{Var}\, A}{M} (1 + 2\tau_A)}$$

- *Critical slowing down* at second order phase transition

$$\tau \propto L^2$$

- *Exponential tunneling problem* at first order phase transition

$$\tau \propto \exp(L^{d-1})$$

Problems with local updates

- Local updates cannot change global topological properties
  - number of world lines (particles, magnetization) conserved
  - winding conserved
  - braiding conserved
  - cannot sample grand-canonical ensemble
- Critical slowing down at second order phase transitions
  - solved by cluster updates (today)
- Tunneling problem at first order phase transitions
  - solved by extended sampling techniques (Thursday)

From local to cluster updates

- Energy of configurations in Ising model
  - $-J$ if parallel: ↑ ↑ ↓ ↓
  - $+J$ if anti-parallel: ↓ ↑ ↓ ↑
- Probability for flip
  - Anti-parallel: flipping lowers energy, always accepted

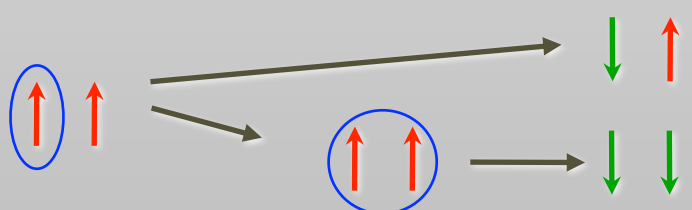
$$\Delta E = -2J \Rightarrow P = \min\left(1, e^{-2\Delta E/T}\right) = 1$$

  - Parallel:

$$\Delta E = +2J \Rightarrow P = \min\left(1, e^{-2\Delta E/T}\right) = \exp(-2\beta J)$$

no change with probability $1-\exp(-2\beta J)$!!!

Alternative: flip both!

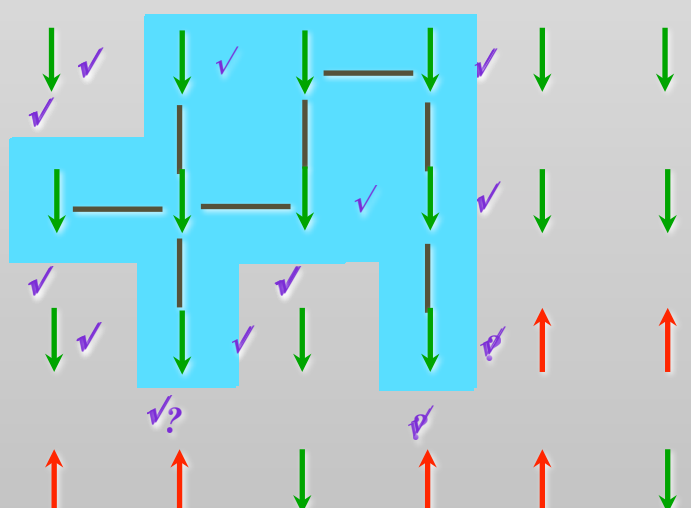


$$P = \exp(-2J/T)$$

$$P = 1-\exp(-2J/T)$$

Swendsen-Wang Cluster-Updates

- No critical slowing down (Swendsen and Wang, 1987) !!!
- Ask for each spin: "do we want to flip it against its neighbor?"
  - antiparallel: yes
  - parallel: costs energy
    - Accept with $P = \exp(-2\beta J)$
    - Otherwise: also flip neighbor! $P = 1 - \exp(-2\beta J)$
    - Repeat for all flipped spins => cluster updates



Shall we flip neighbor?

Done building cluster
Flip all spins in cluster

The secret of Monte Carlo

- Small ideas are enough to make big progress
- However one needs the right idea - most unfortunately fail