Title: Computer Simulations of Guage Theories: Monte-Carlo Method

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Abstract:

Computer Simulations of Gauge Theories

Monte-Carlo method

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August 29, 2011

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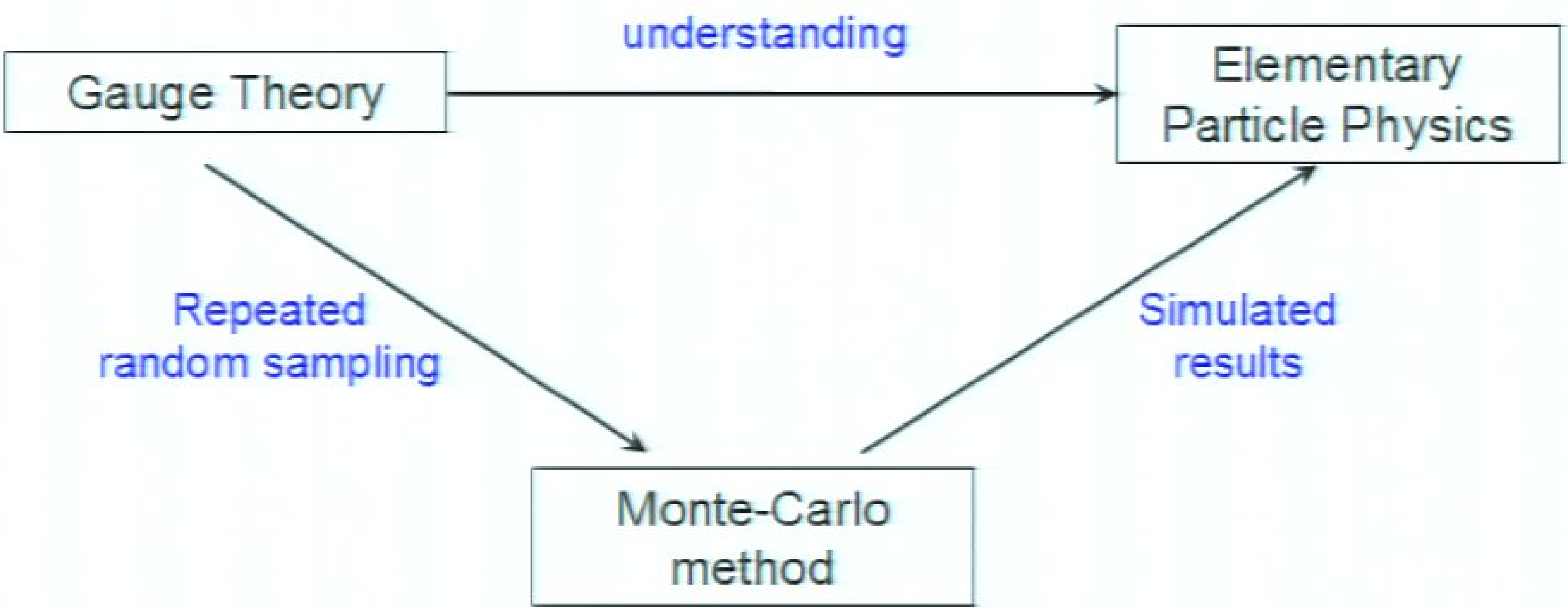
Motivation


understanding
Gauge Theory
Elementary
Particle Physics
Repeated
random sampling
Simulated
results
Monte-Carlo
method

Contents

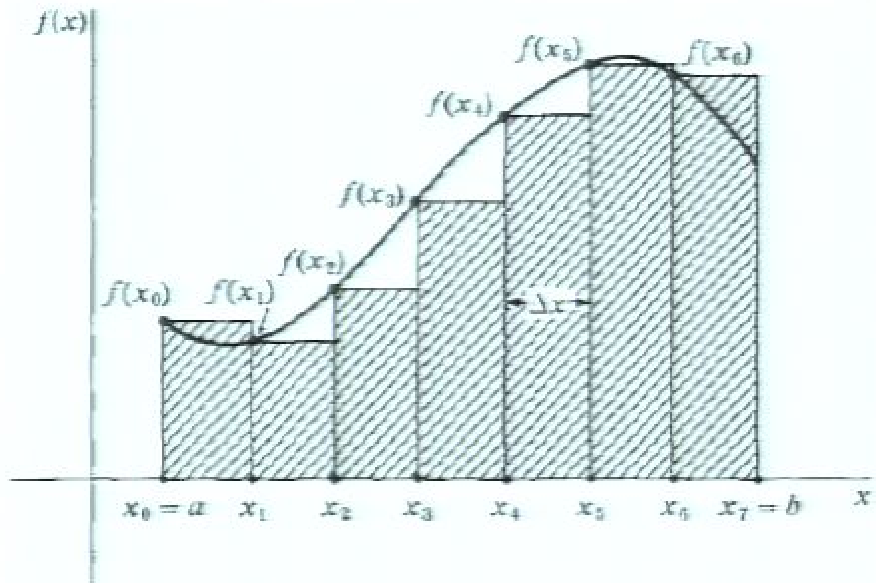
A simple example of Monte-Carlo Method

Little History

- Can be seen in Buffon's needle experiment
- Monte-Carlo integrals
  - poorly-behaved functions
  - high-dimensional spaces

A simple example of Monte-Carlo Method

Area of a region bounded by a graph using Riemann Integral



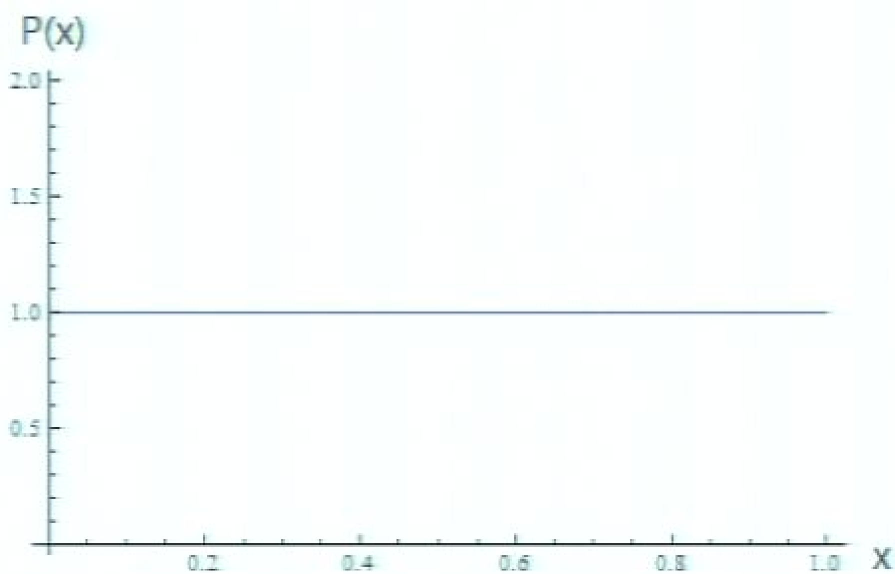
Define $I = \int_0^1 f(x)\,\mathrm{d}x$, which is the area of the region bounded by the axis and the curve $f(x)$.
Then, according to the definition of Riemann Integral,

$$I = \lim_{N \to \infty} \sum_{i=1}^{N} \Delta x f(x_i)$$

A simple example of Monte-Carlo Method

Area of a region bounded by a graph using Monte-Carlo

Introduce a random uniform distribution,



then by arranging the integral $I = \int_0^1 f(x)P(x)\,\mathrm{d}x = \langle f \rangle$.

A simple example of Monte-Carlo Method

Area of a region bounded by a graph using Monte-Carlo

So the idea is we can simply take some sample points from the range, then

Important Relation

$$I = \langle f \rangle \approx \frac{1}{N} \sum_{i=1}^{N} f(x_i) = f_N \quad \text{(estimator)}$$

Basically, the difference between these two methods is just one getting samples regularly while the other getting samples randomly.

A simple example of Monte-Carlo Method

Error

In d-dimension space, if we both get $M = N^d$ samples of f, we can prove that the error of the first method is proportional to $\frac{1}{\sqrt[d]{M}}$ whereas the error of Monte Carlo Method dies as $\frac{1}{\sqrt{M}}$.

Conclusion

when $d > 2$, Monte Carlo Methods provide us more precise results with less effort! Thus, especially in higher dimensional problems, Monte Carlo Methods are extremely useful tricks.

A simple example of Monte-Carlo Method

Importance Sampling

Furthermore, we still can rearrange the integral this way:

$$I = \int_0^1 f(x)\,\mathrm{d}x = \int_0^1 \frac{f(x)}{P(x)} P(x)\,\mathrm{d}x = \left\langle \frac{f(x)}{P(x)} \right\rangle$$

where x is random variable with arbitrary probability distribution $P(x)$ with

$$\int_0^1 P(x)\,\mathrm{d}x = 1$$

A simple example of Monte-Carlo Method

Importance Sampling

Again, define

$$I_N = \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{P(x_i)}$$

Since

$$\langle I_N \rangle = \left\langle \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{P(x_i)} \right\rangle = \frac{1}{N}N\left\langle \frac{f(x)}{P(x)} \right\rangle = \left\langle \frac{f(x)}{P(x)} \right\rangle = I$$

so I_N is a good estimator.

A simple example of Monte-Carlo Method
Importance Sampling

And

$$\Delta I_N = \frac{1}{\sqrt{N}} \sqrt{\left\langle \frac{f^2(x)}{P^2(x)} \right\rangle - \left\langle \frac{f(x)}{P(x)} \right\rangle^2}$$

Question

What distribution $P(x)$ minimizes ΔI_N ?

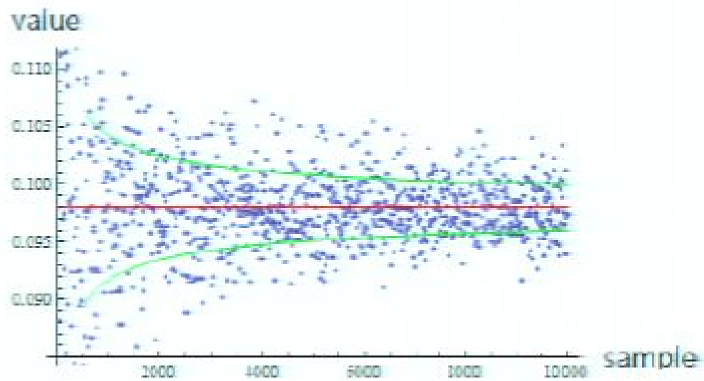
Answer: If $\frac{f(x)}{P(x)} = \text{constant} \Longrightarrow \Delta I_N = 0.$

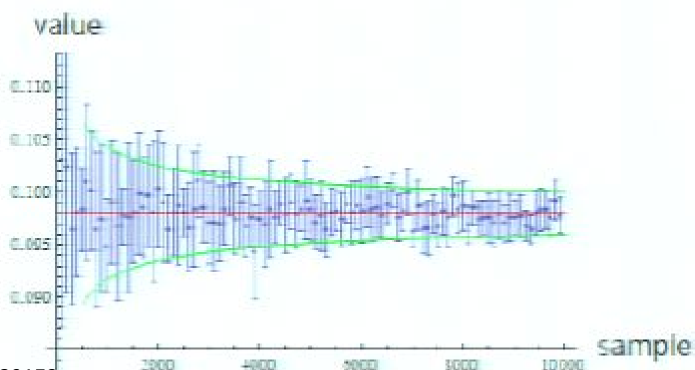
A simple example of Monte-Carlo Method

Importance Sampling

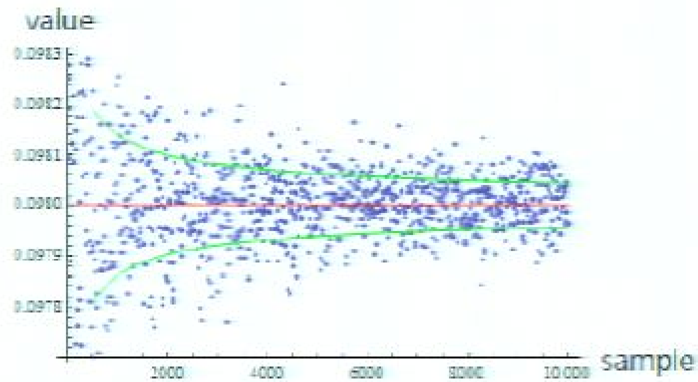
To calculate $I = \int_0^1 e^{-ax}(1 - x^2)\,\mathrm{d}x$:

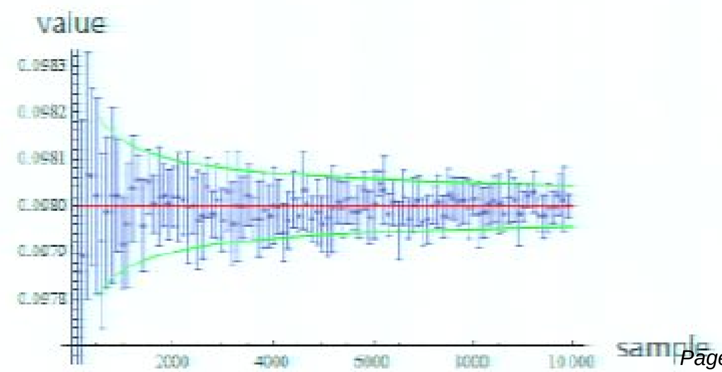
For the uniform distribution:





For the $P(x) \propto e^{-ax} (a = 10)$:

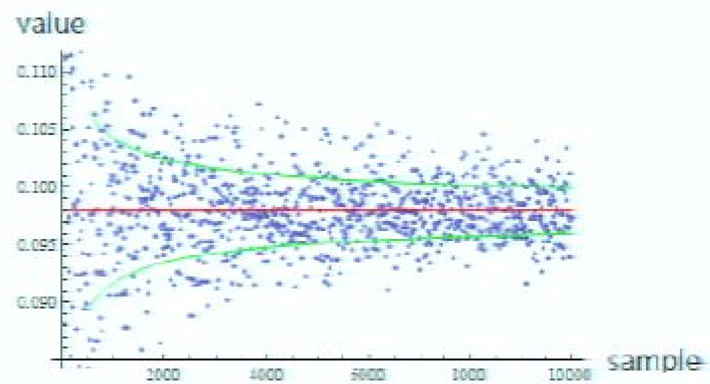


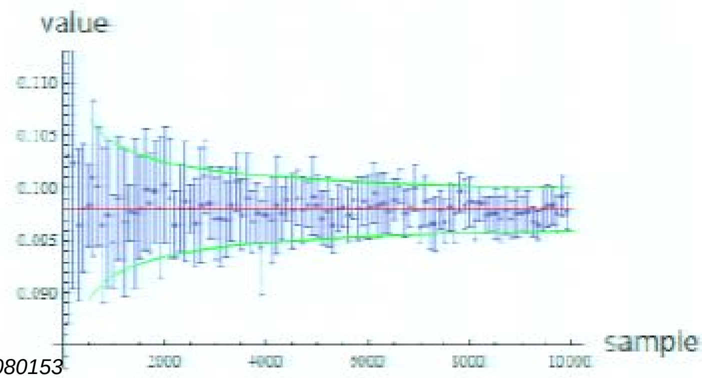


A simple example of Monte-Carlo Method
Importance Sampling

If we change these two plots to the same plot range:

For the uniform distribution:





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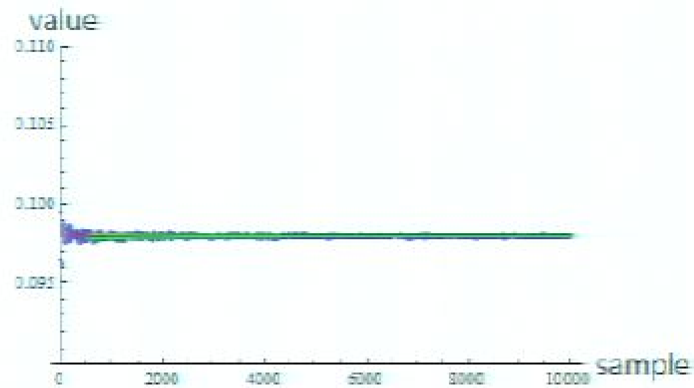

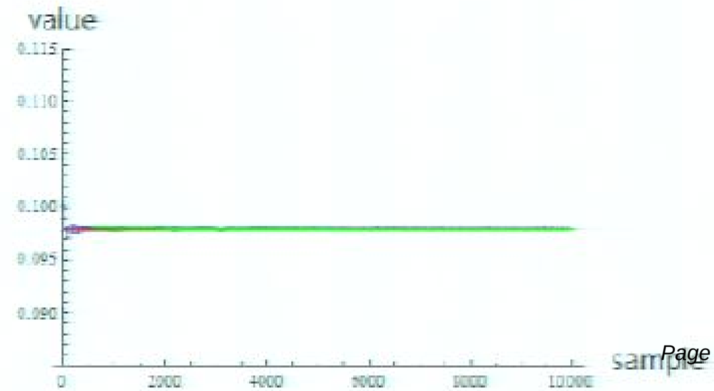

A simple example of Monte-Carlo Method

Importance Sampling

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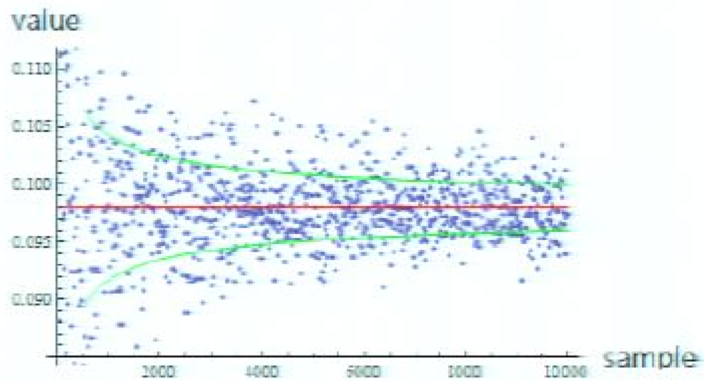

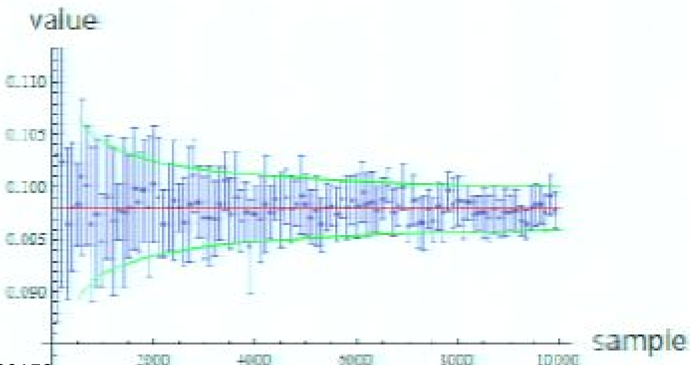

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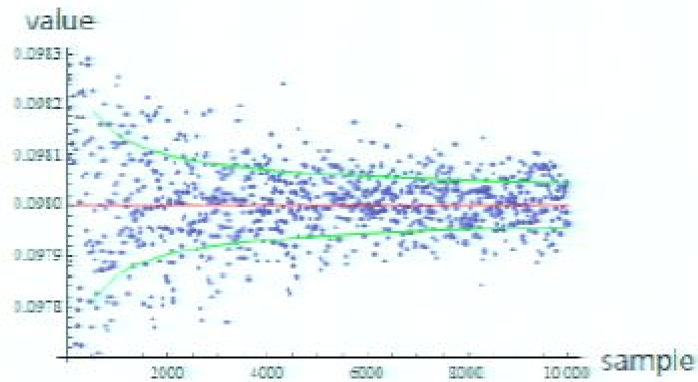

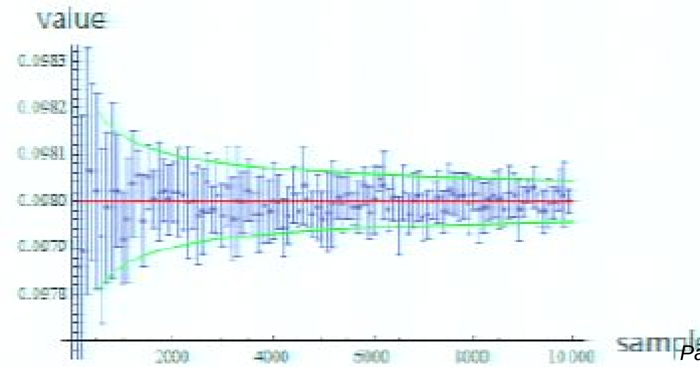

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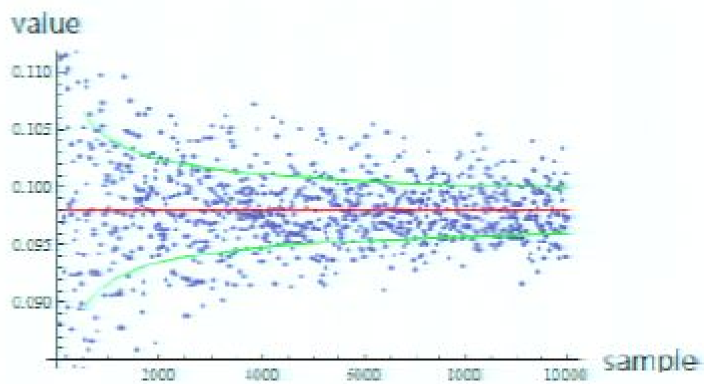

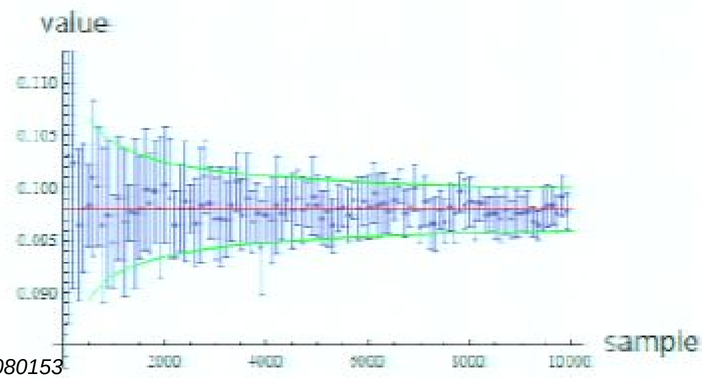

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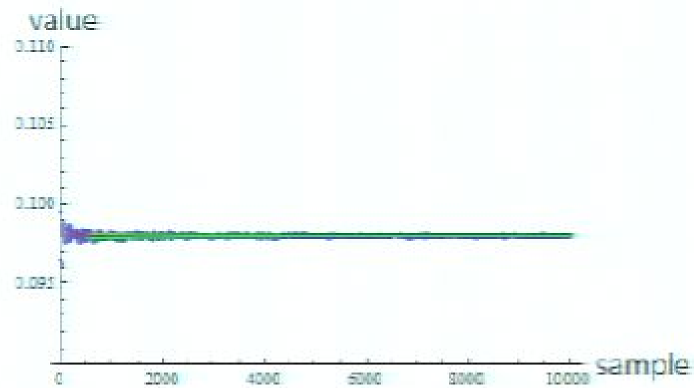
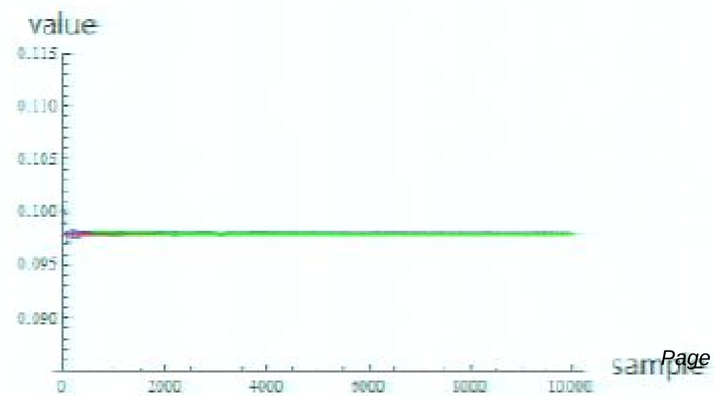




Contents

General procedure of Monte-Carlo Method

The basic idea

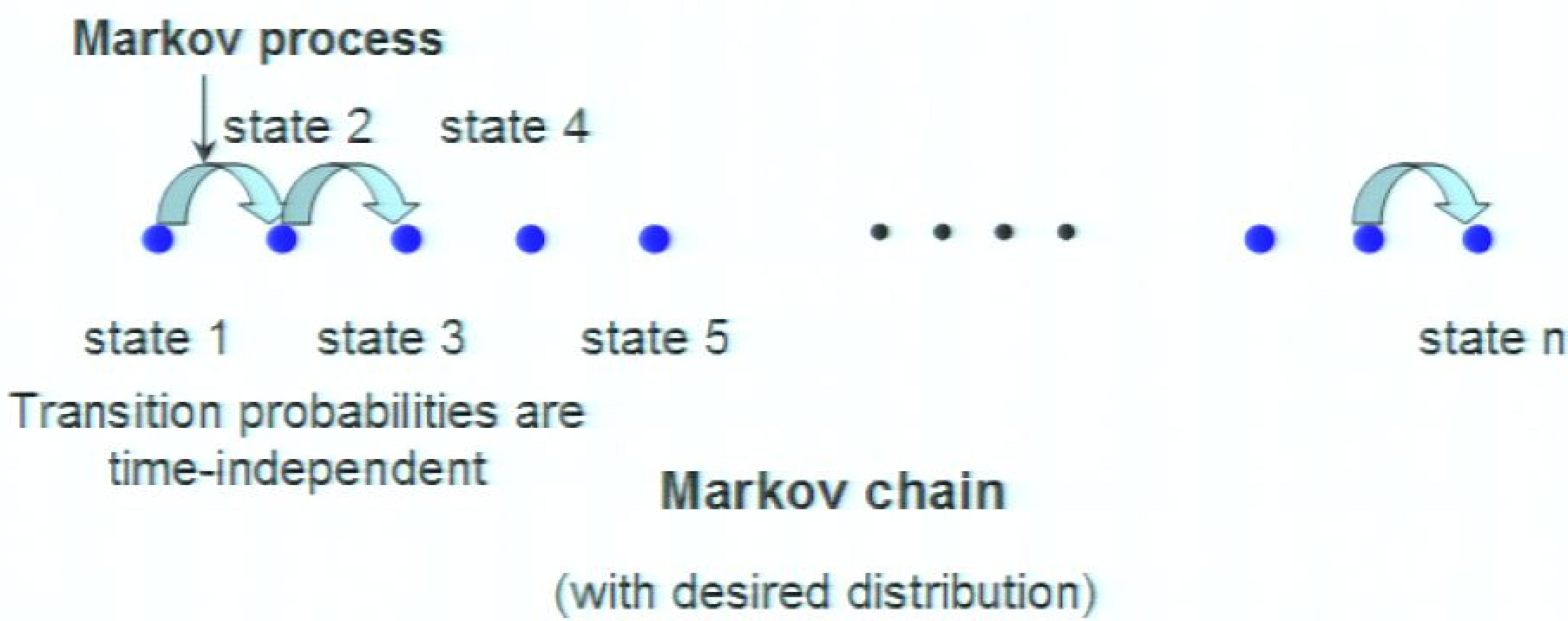
- simulate the random thermal fluctuation of the system
- expectation value $\longrightarrow$ averaging over the states passing through

General procedure of Monte-Carlo Method

- Markov processes
- Dynamics
- Detailed Balance
- The Metropolis algorithm

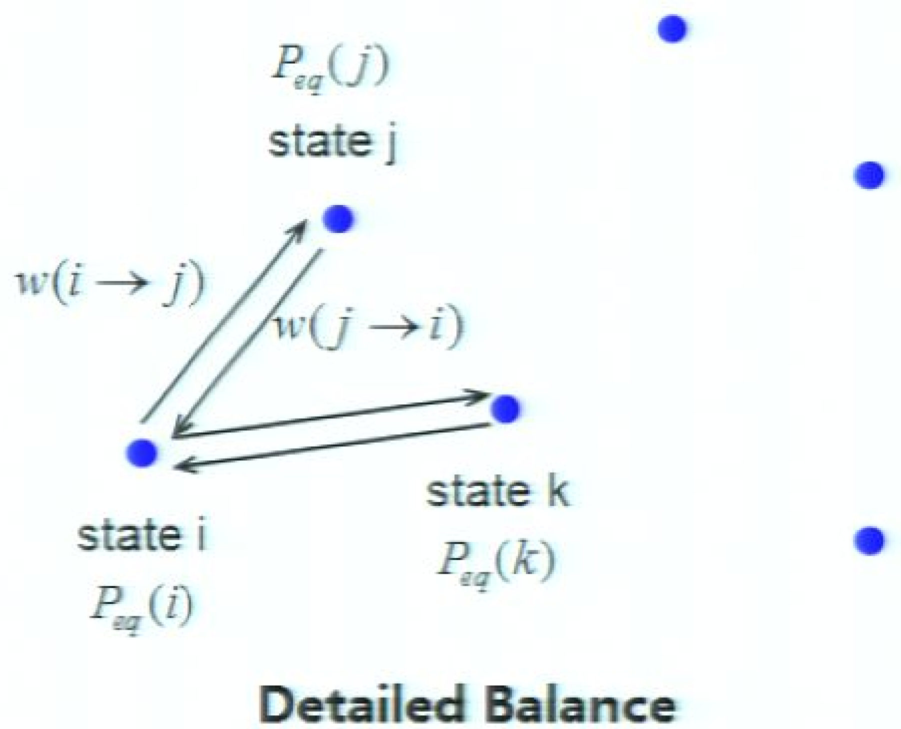
General procedure of Monte-Carlo Method

Markov processes



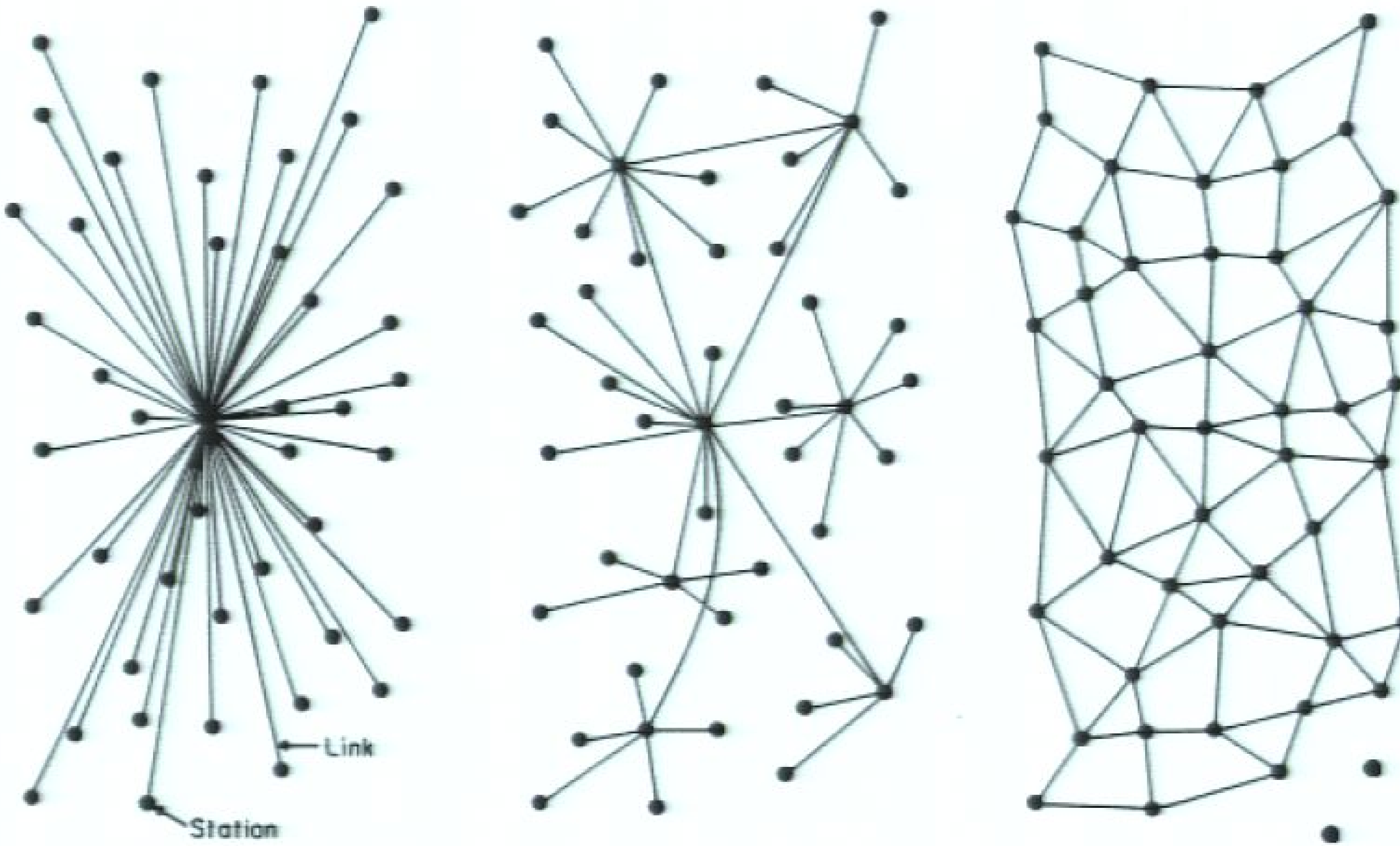
General procedure of Monte-Carlo Method
Detailed Balance

- ensures it is the correct distribution



$$P_{eq}(i)w(i \to j) = P_{eq}(j)w(j \to i)$$

General procedure of Monte-Carlo Method
Dynamics

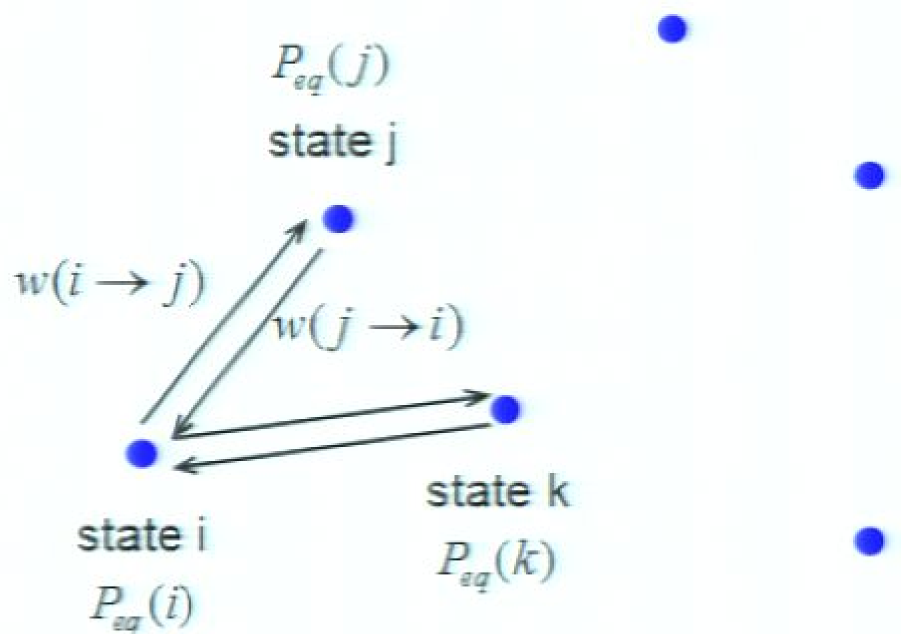


Ergodicity

General procedure of Monte-Carlo Method

Detailed Balance

- ensures it is the correct distribution



Detailed Balance

$$P_{eq}(i)w(i \to j) = P_{eq}(j)w(j \to i)$$

General procedure of Monte-Carlo Method

The Metropolis algorithm

- If we want Boltzmann distribution: $P_{eq}(i) \propto e^{-s(i)}$.
- The Metropolis algorithm requires

$$w(i \to j) = \frac{1}{q} \min \left\{ 1, \frac{P_{eq}(j)}{P_{eq}(i)} \right\}$$

where q is the number of "nearest neighbors" to which particles can jump directly from state i.

- That is, we let

$$w(i \to j) = \begin{cases} \frac{1}{q} e^{-\Delta s} & \text{if } \Delta s = s(j) - s(i) > 0 \\ \frac{1}{q} & \text{otherwise} \end{cases}$$

Contents

The Ising Model

The Ising Model

- Hamiltonian

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

  - $S_i = \pm 1$ is the state of the atom at site i
  - $\sum_{\langle i,j \rangle}$ denotes a sum over nearest-neighbor sites i and j
  - J is interpreted as the exchange constant in magnetism

- Task: compute the desired average properties from H, e.g.

$$E = \frac{\langle H \rangle_T}{N}, \quad \mathbf{M} = \frac{\langle \sum_i \vec{S}_i \rangle_T}{N}$$

The Ising Model

The Ising Model

Generally, the thermal average of any observable $A(x)$ is defined in the canonical ensemble by

$$\langle A(x)\rangle_T = \frac{1}{Z}\int e^{\frac{-H(\vec{x})}{k_B T}} A(\vec{x})\,\mathrm{d}\vec{x}$$

$$Z = \int e^{\frac{-H(\vec{x})}{k_B T}}\,\mathrm{d}\vec{x}$$

The normalized Boltzmann factor $p(\vec{x}) = \frac{1}{Z} e^{\frac{-H(\vec{x})}{k_B T}}$ plays the role of a probability density describing the statistical weight with which the configuration $\vec{x}$ occurs in thermal equilibrium.

The Ising Model

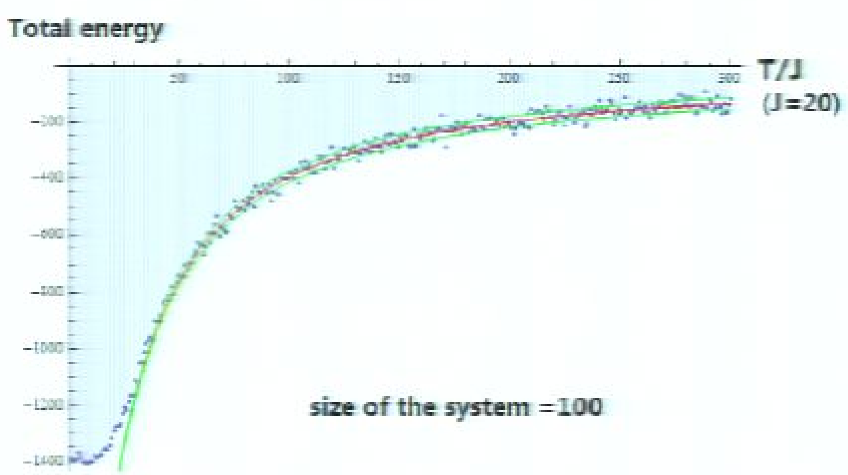
The Ising Model

Monte Carlo Scheme

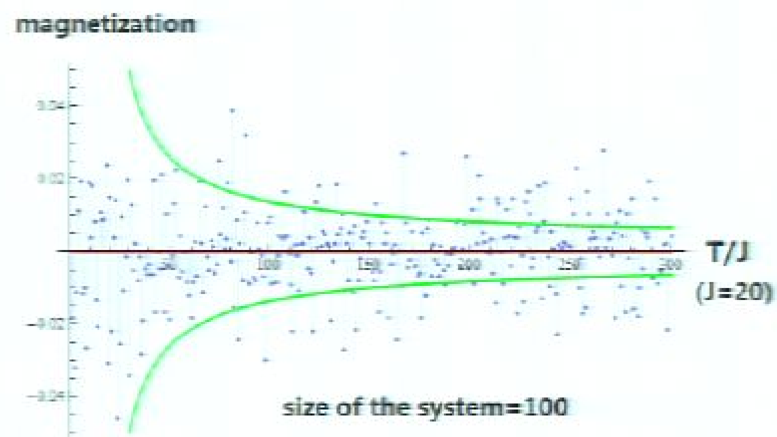
(1)	Choose an initial state.
(2)	Choose a site i randomly.
(3)	Calculate the energy change ΔH which results if the spin at site i is overturned.
(4)	Generate a random number z such that $0 < z < 1$.
(5)	If $z < e^{-\frac{\Delta H}{k_B T}}$, flip the spin.
(6)	Analyze the resulting configuration as desired, store its properties to calculate the necessary averages.
(7)	Go to (2).

The Ising Model
The Ising Model

Internal Energy



Magnetization

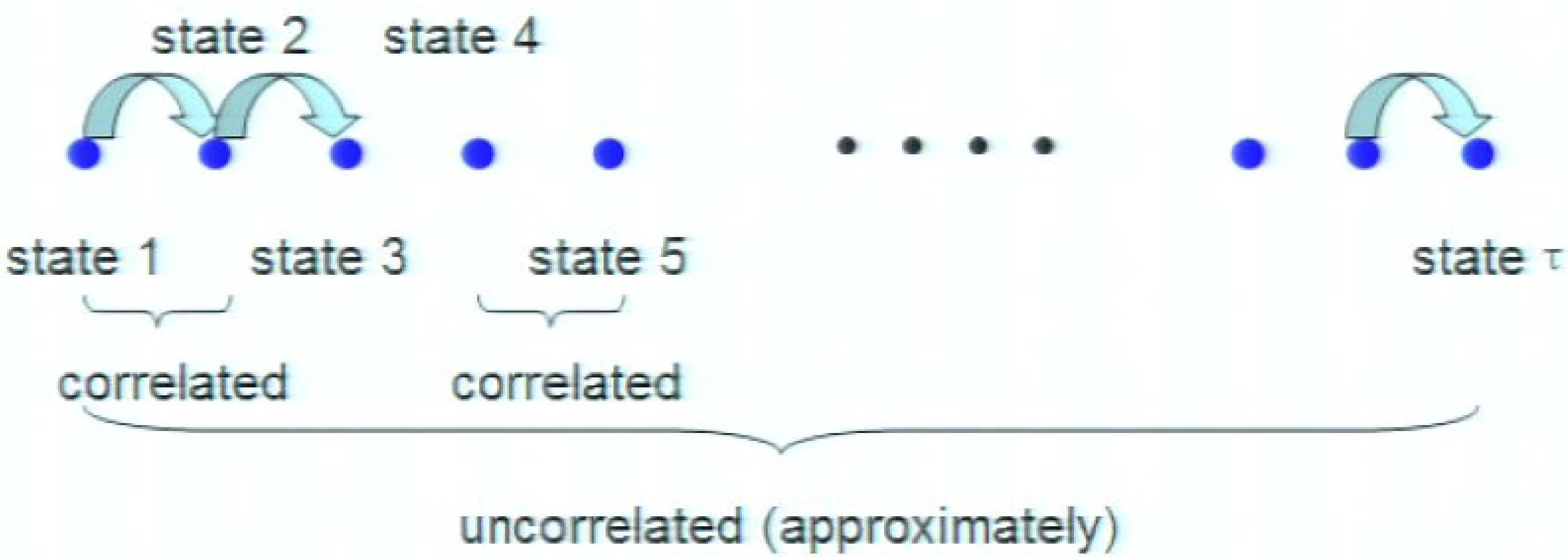


Contents

The Ising Model
Considerations

- Auto-correlation time
- Acceptance ratio

The Ising Model
Considerations
Auto-correlation time



The Ising Model
Considerations
Auto-correlation time

Let us take the example if the energy E of our Ising model.

- **time-displaced autocorrelation** $\chi(\mathbf{t})$

$$\chi(t) = \int \left[E(t') - \langle E\rangle\right]\left[E(t'+t) - \langle E\rangle\right]\, \mathrm{d}t'$$
$$= \int \left[E(t')E(t'+t) - \langle E\rangle^2\right]\, \mathrm{d}t'$$

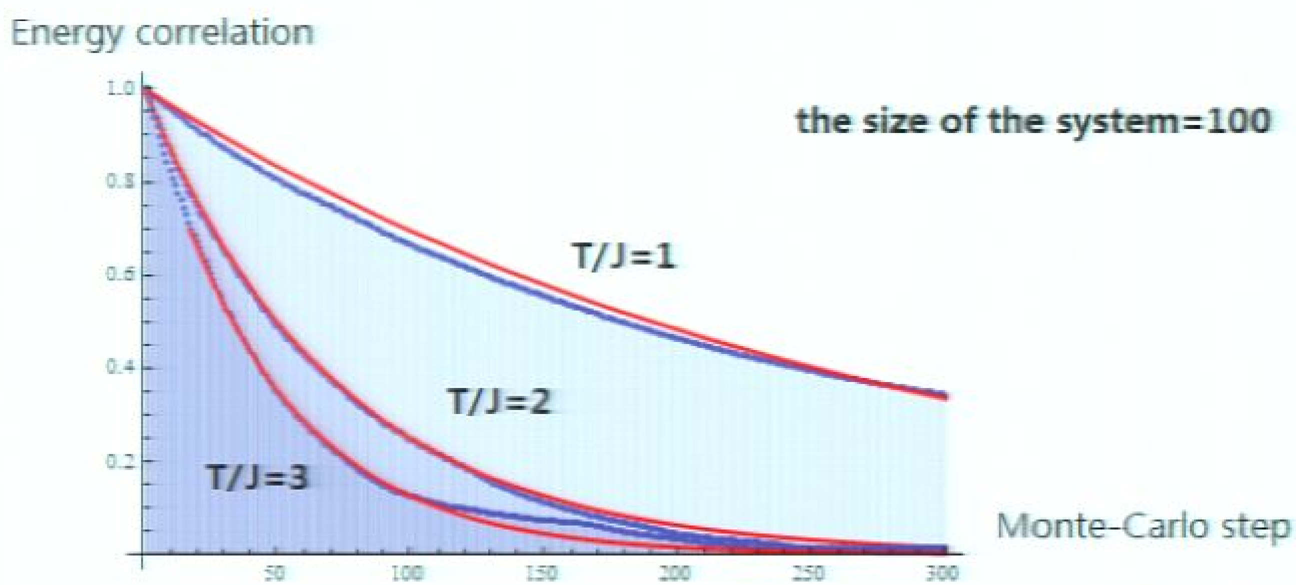
where $E(t)$ is the instantaneous value if the energy at time t and $\langle E\rangle$ is the average value.

The Ising Model
Considerations
Auto-correlation time

The typical time-scale on which it falls off is a measure of the correlation time τ of the simulation.

$$\chi(t) \sim e^{-\frac{t}{\tau}}$$

For our Metropolis simulation of the Ising model



The Ising Model

Considerations

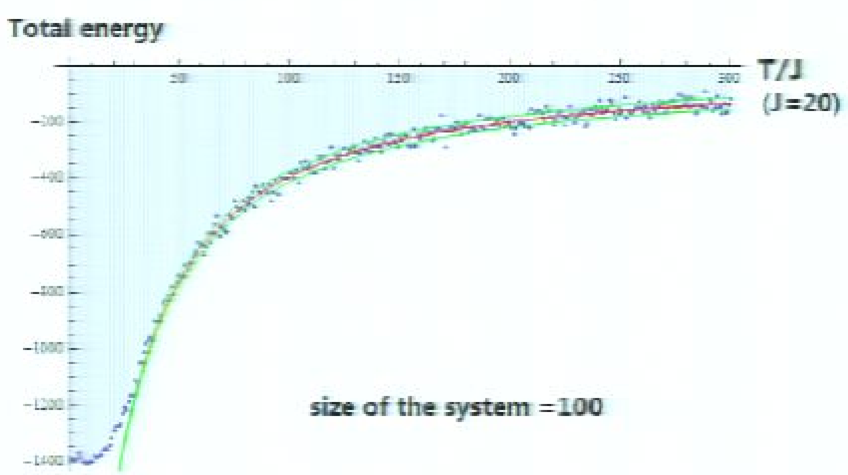
Acceptance ratio

Generally, the **acceptance ratio** is defined by

$$\text{Acceptance ratio} = \frac{\text{current state is changed to a new state}}{\text{current state remains the same state}}$$

The Ising Model
The Ising Model

Internal Energy



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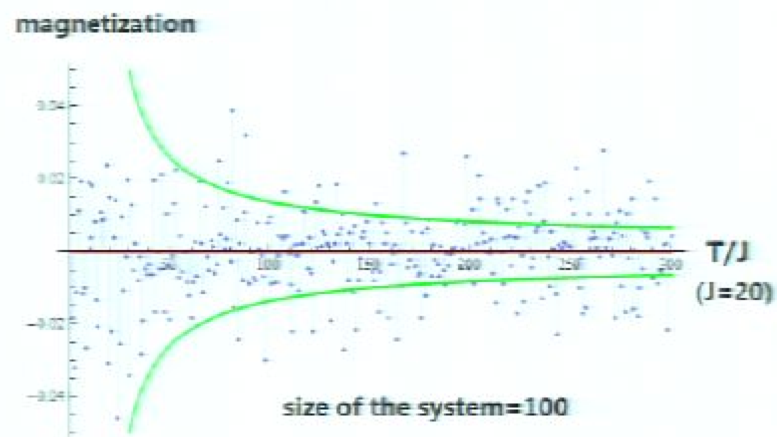

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Acceptance ratio

Generally, the **acceptance ratio** is defined by

$$\text{Acceptance ratio} = \frac{\text{current state is changed to a new state}}{\text{current state remains the same state}}$$

The Ising Model

Considerations

Acceptance ratio

At low temperature,

$\Rightarrow$ $\frac{J}{T}$ is very large.

$\Rightarrow$ Δs tends to be very large.

$\Rightarrow$ $e^{-\Delta s}$ is extremely small

$\Rightarrow$ Acceptance ratio tends to be very small.

$\Rightarrow$ the state does not move.

$\Rightarrow$ Auto-correlation time is large.

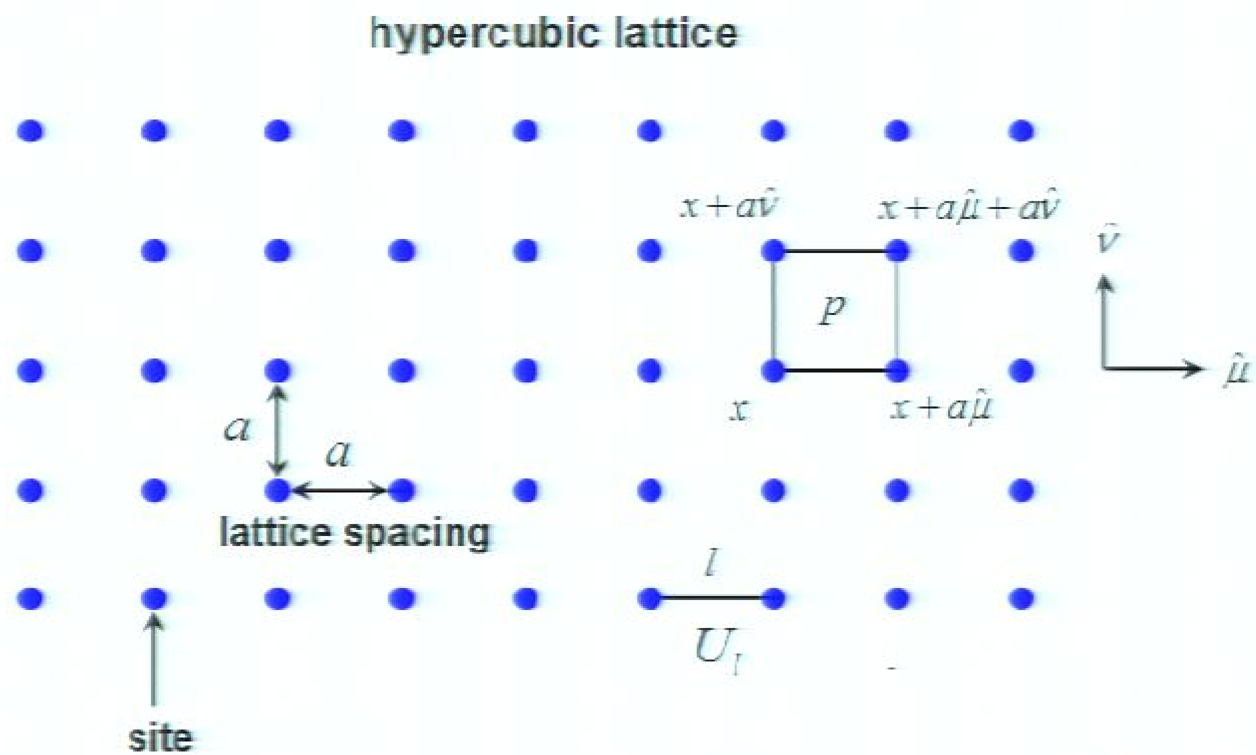
$\Rightarrow$ The statistical result is not reliable.

Contents

Application in Lattice Gauge Theories

In computer simulations for a lattice gauge theory,

- the link is represented by unitary matrices U_l
- the state of a lattice is represented by the values of the link variables U_l



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Application in Lattice Gauge Theories
One matrix in SU(N)

Example(One-matrix model)

Suppose there is a partition function:

$$Z = \int \mathrm{d}U e^{\frac{N}{\lambda}\mathrm{Re}(\mathrm{Tr}U)}$$

where $U \in SU(N)$. Note that λ is the 't Hooft coupling. It is the analogue of temperature in Ising model. Define an observable to compute:

$$W_k = \frac{1}{N}\mathrm{Tr}(U^k)$$

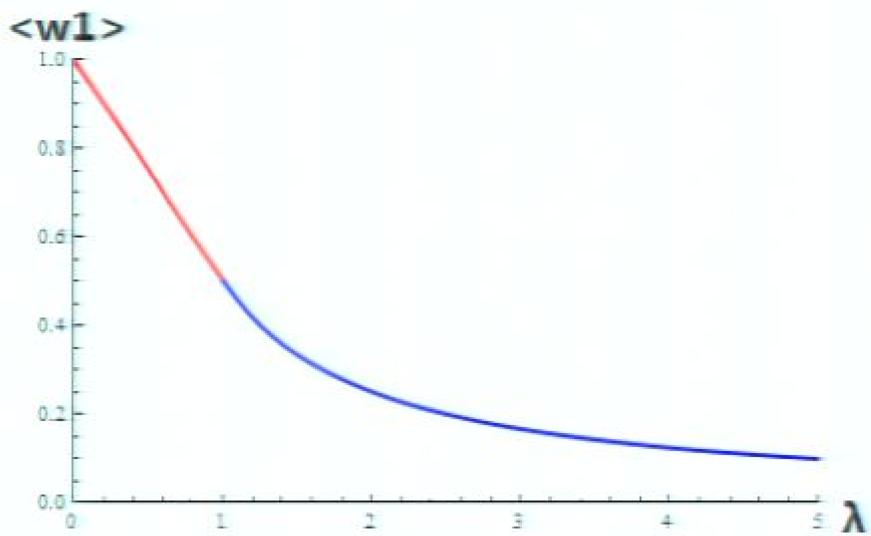
Then

$$\langle W_k \rangle = \frac{1}{Z}\int \mathrm{d}U \frac{\mathrm{Tr}(U^k)}{N} e^{\frac{N}{\lambda}\mathrm{Re}(\mathrm{Tr}U)}$$

Application in Lattice Gauge Theories
One matrix in SU(N)

We have the analytical result about W_1:
when $N \to \infty$

$$\langle W_1 \rangle = \begin{cases} \frac{1}{2\lambda}, & \lambda > 1 \\ 1 - \frac{\lambda}{2}, & \lambda < 1 \end{cases}$$



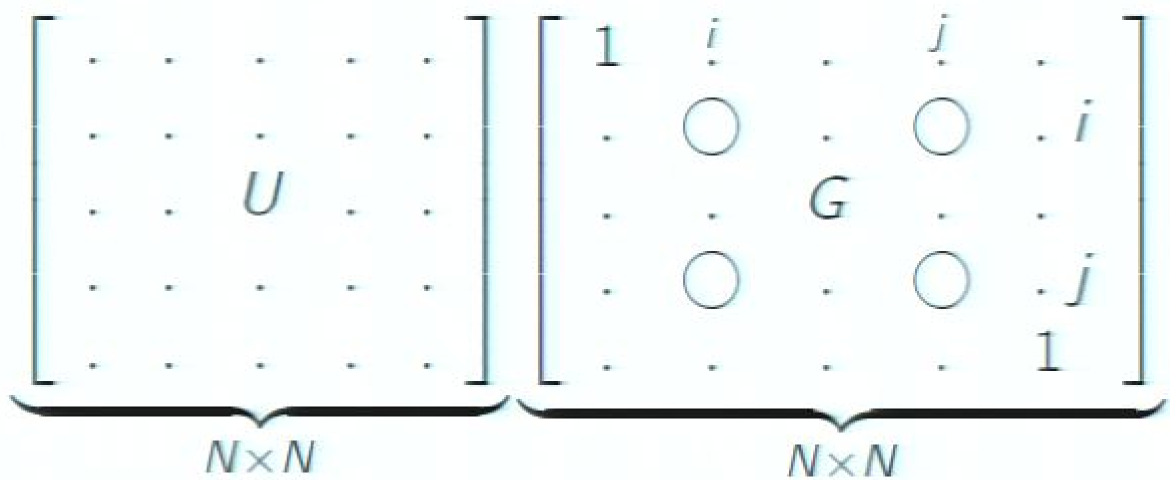
Application in Lattice Gauge Theories

One matrix in SU(N)

Metropolis Monte-Carlo method in SU(N)

Topology

1.Pick a matrix $G \in SU(N)$



Application in Lattice Gauge Theories

One matrix in SU(N)

Metropolis Monte-Carlo method in SU(N)

(a).Pick up two random integers i and j, where $1 \leq i < j \leq N$.

(b).Replace $\begin{pmatrix} \bigcirc & \bigcirc \\ \bigcirc & \bigcirc \end{pmatrix}$ by an arbitrary $SU(2)$ matrix $\equiv g$.

1. Choose a_0 from uniform distribution between $[\gamma, 1]$, where $\gamma \sim 1$, which makes g not very far away from $\mathbb{I}$.
2. Choose a_1, a_2, a_3 uniformly from the sphere $a_1^2 + a_2^2 + a_3^3 = 1 - a_0^2$.
    1. $|\vec{a}|^2 = 1 - a_0^2$
    2. $\vec{a} = |\vec{a}| (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$
    3. Make sure the distribution is uniform on area element $dA = \sin\theta \; \mathrm{d}\theta\mathrm{d}\phi$.
        - ϕ uniformly in $[0, \; 2\pi]$.
        - θ with distribution $p(\theta) \propto \sin\theta$.
3. Construct the unitary matrix g with identity determinant: $g = a_0\sigma_0 + i\sum_{i=1}^{3} a_i\sigma_i$.

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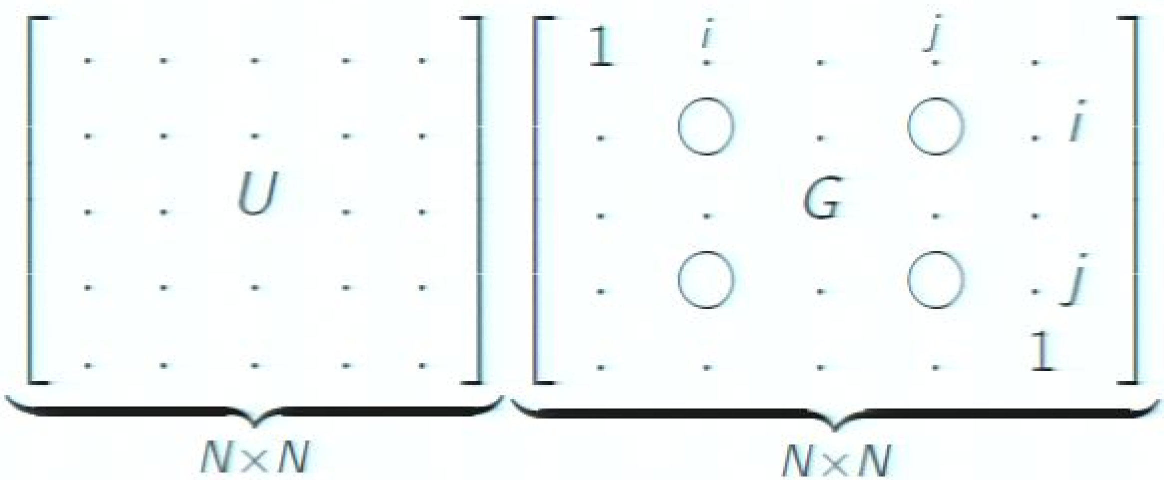

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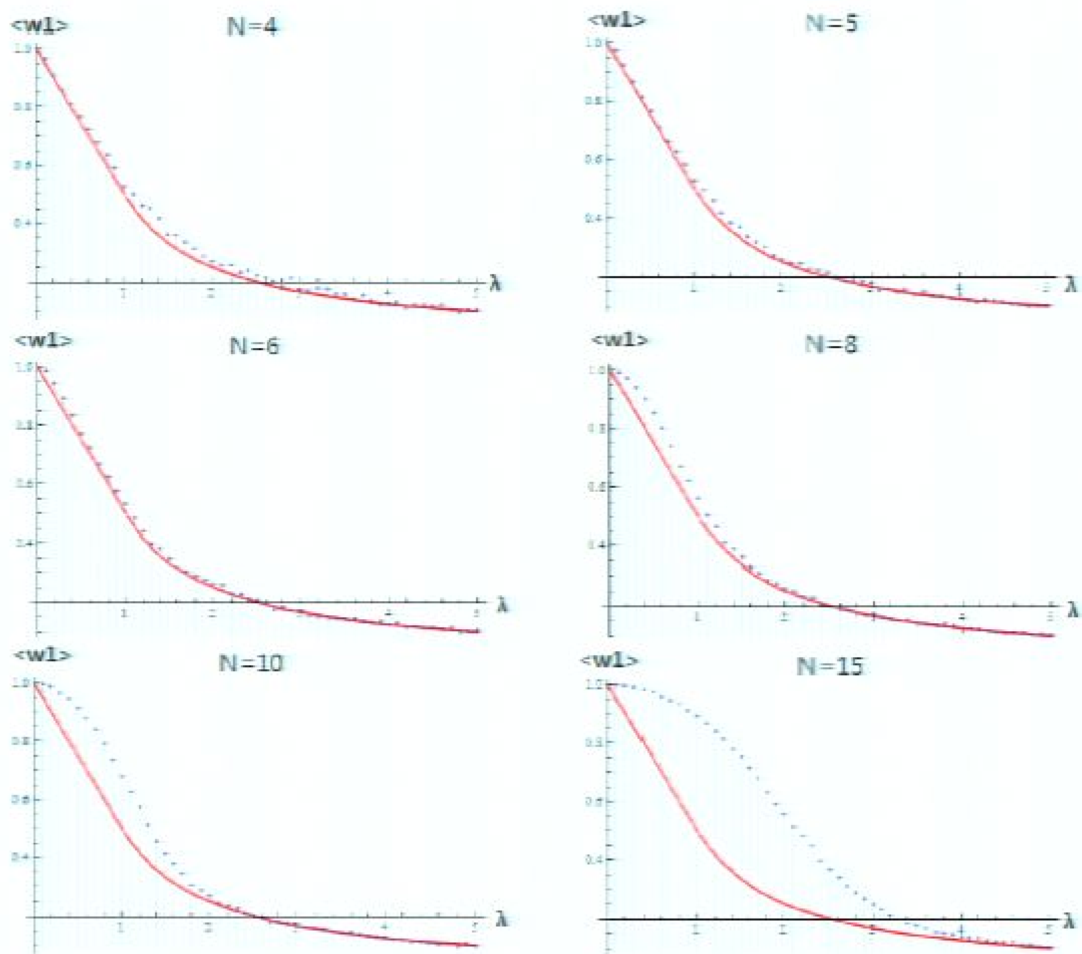
Metropolis Monte-Carlo method in SU(N)



Application in Lattice Gauge Theories

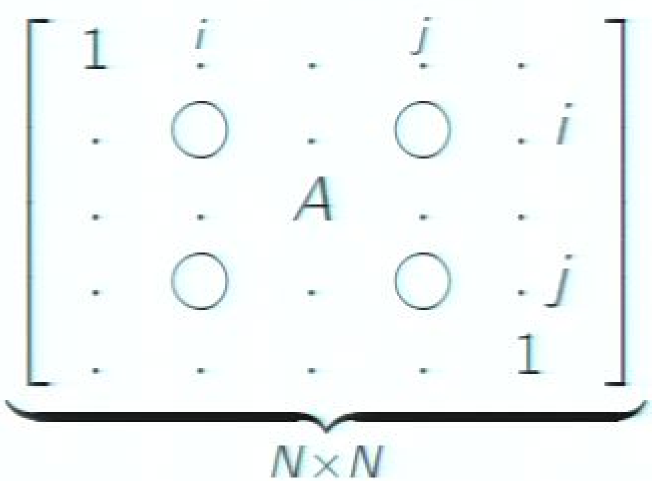
One matrix in SU(N)

Heat bath Monte-Carlo method in SU(N)[Creutz 80'][Cabibbo & Marinari 82']

Topology

1.Pick a matrix

$A \in SU(N)$



2.Change U to

$U(t+1) = U(t) \cdot A$.

- Pick up two random integers i and j, where $1 \leq i < j \leq N$.
- Read of $k \in \mathbb{R}$, $v \in SU(2)$.

$$u_t = \begin{pmatrix} \bigcirc & \bigcirc \\ \bigcirc & \bigcirc \end{pmatrix} = u_0 \mathbb{I} + i \sum_{j=1}^{3} u_j \sigma_j$$

$$k \cdot v = (\mathrm{Re} u_0)\mathbb{I} + i \sum_{j=1}^{3} (\mathrm{Re} u_j)\sigma_j$$

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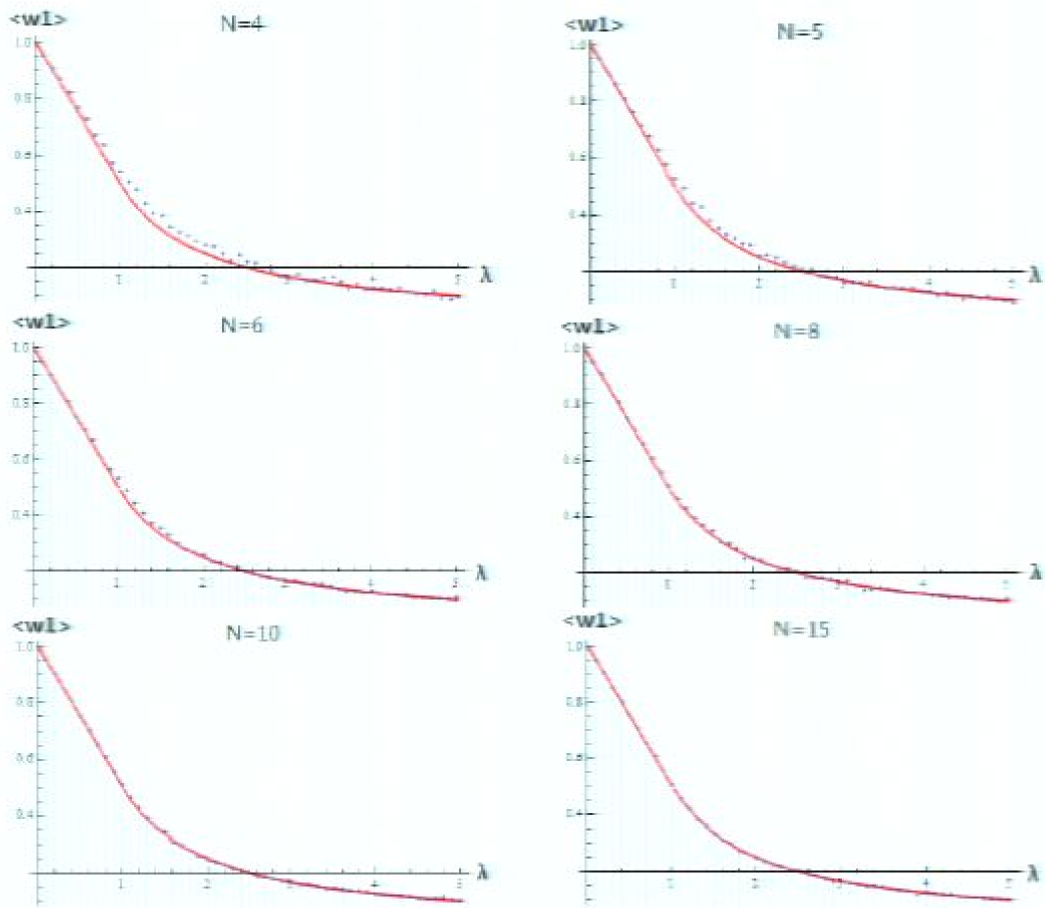
Application in Lattice Gauge Theories

One matrix in SU(N)

Heat bath Monte-Carlo method in SU(N)[Creutz 80'][Cabibbo & Marinari 82']



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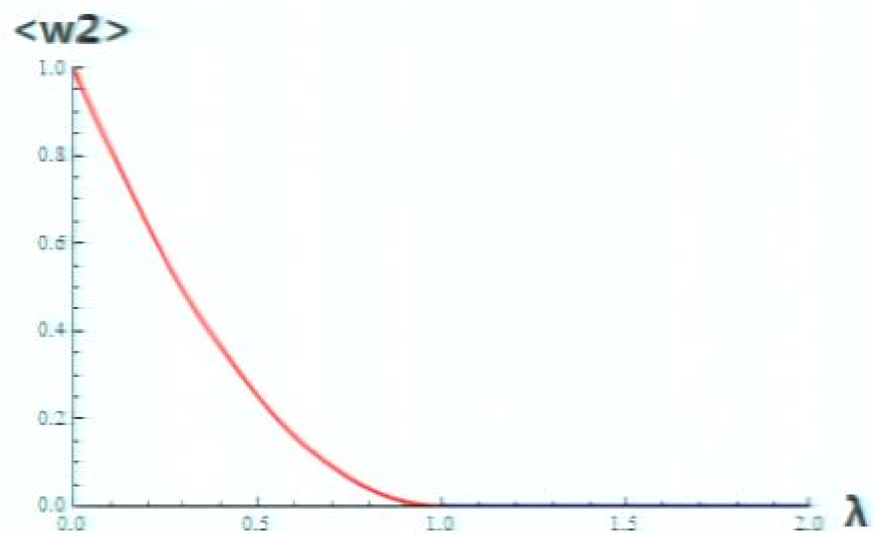

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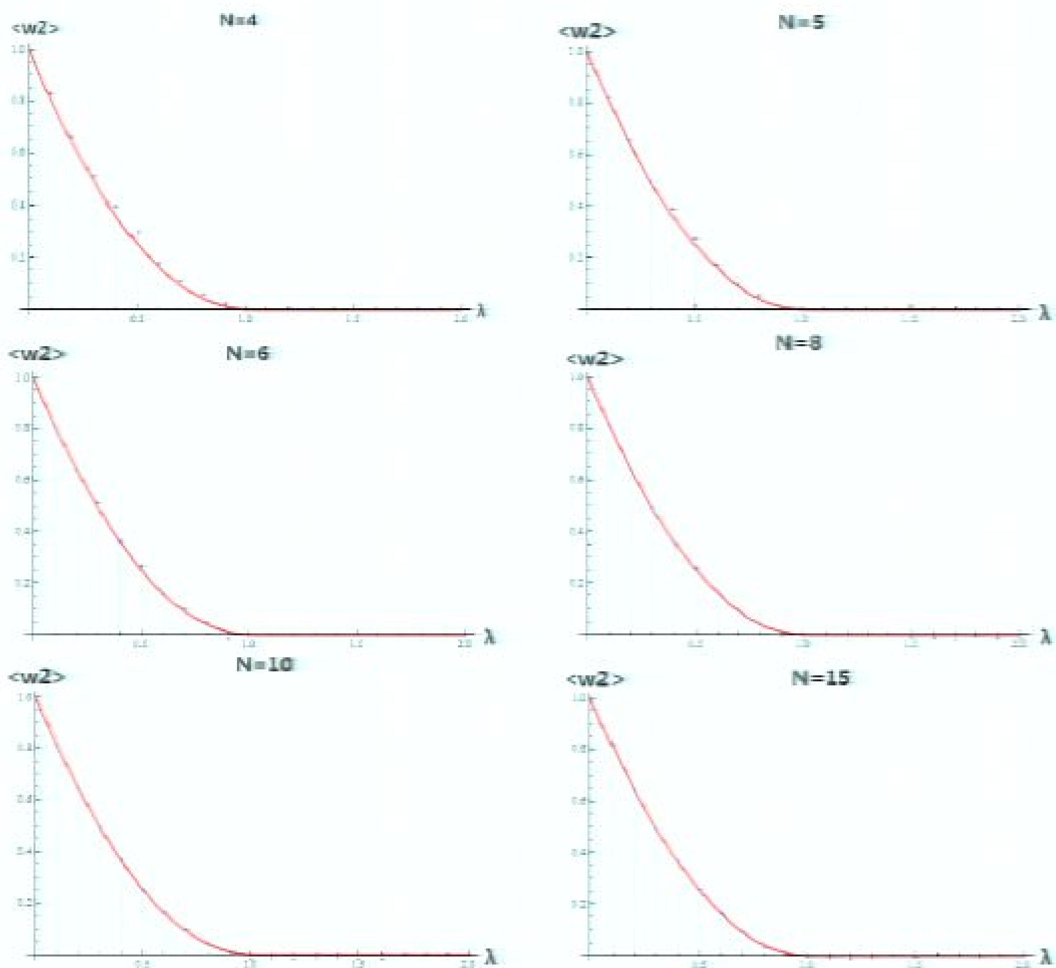

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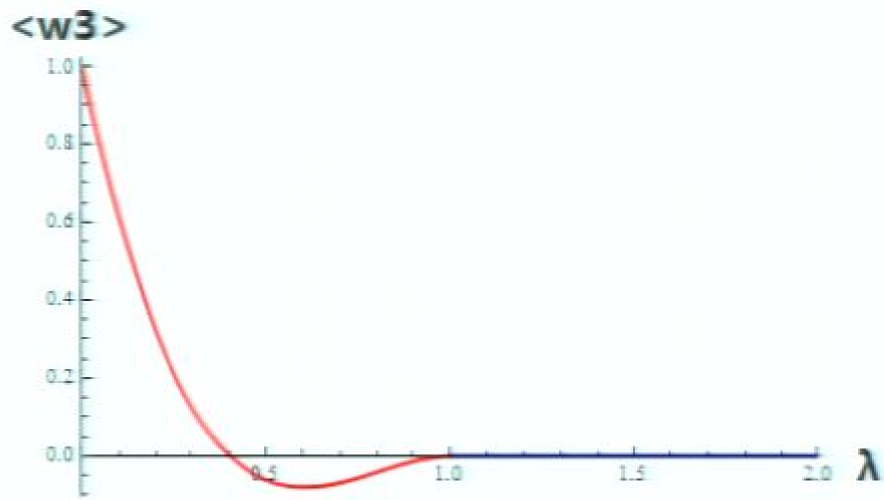

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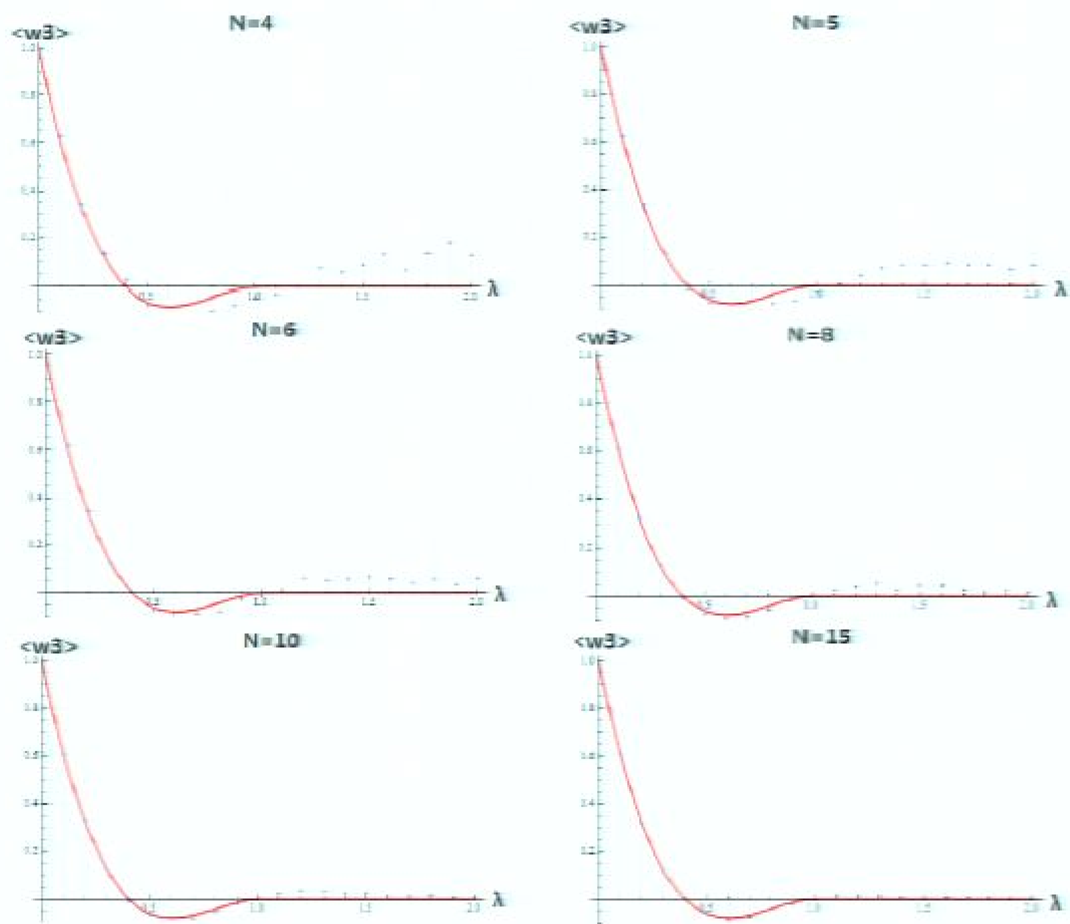

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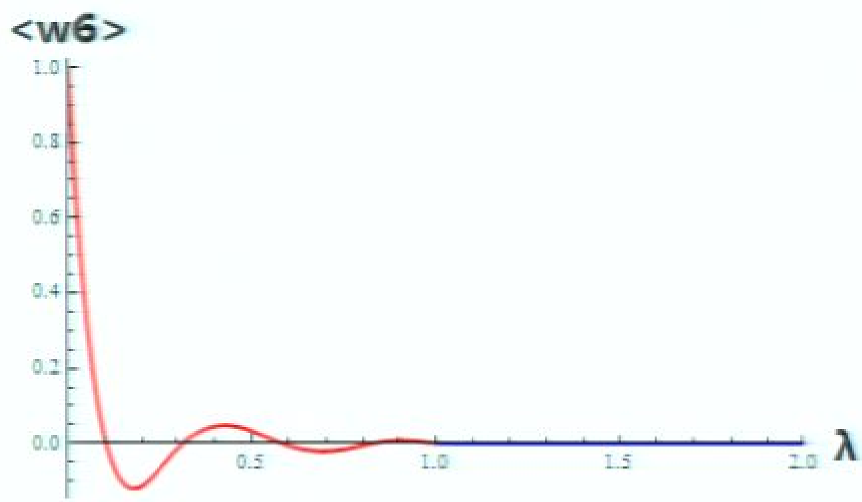

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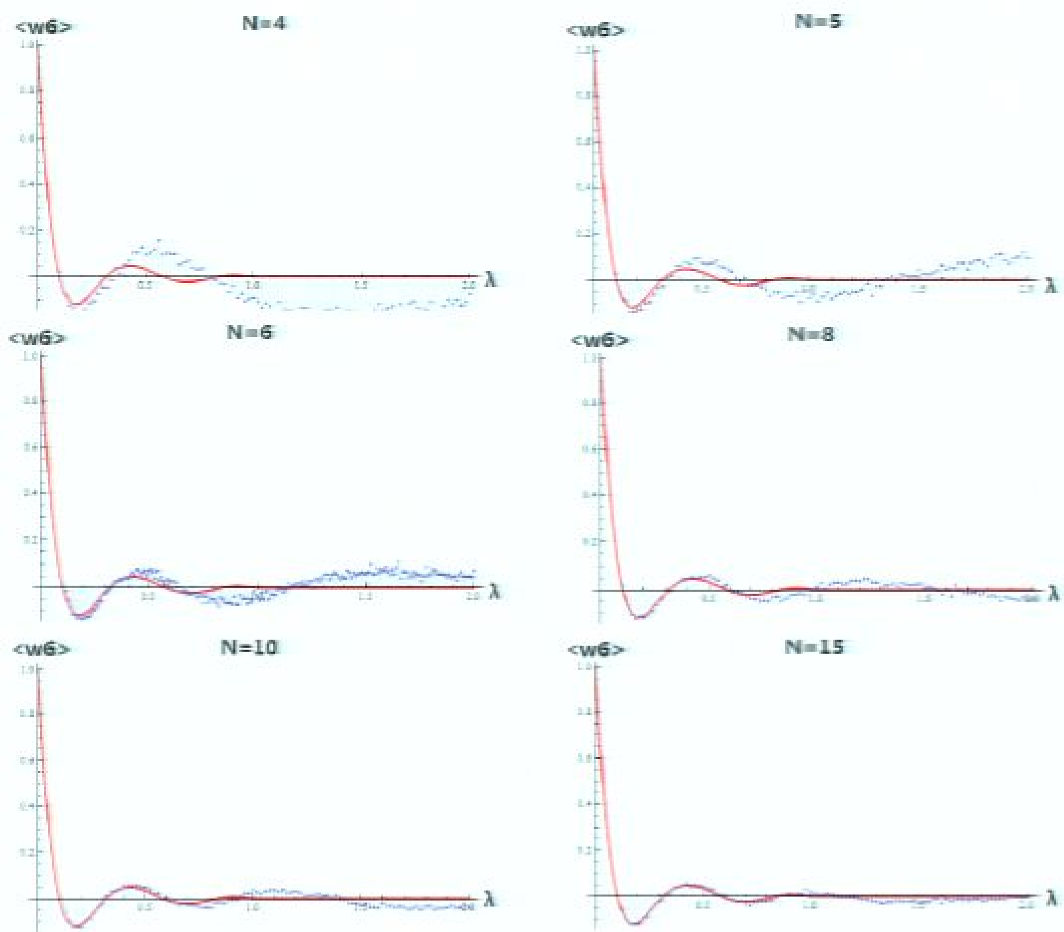


Application in Lattice Gauge Theories

One matrix in SU(N)

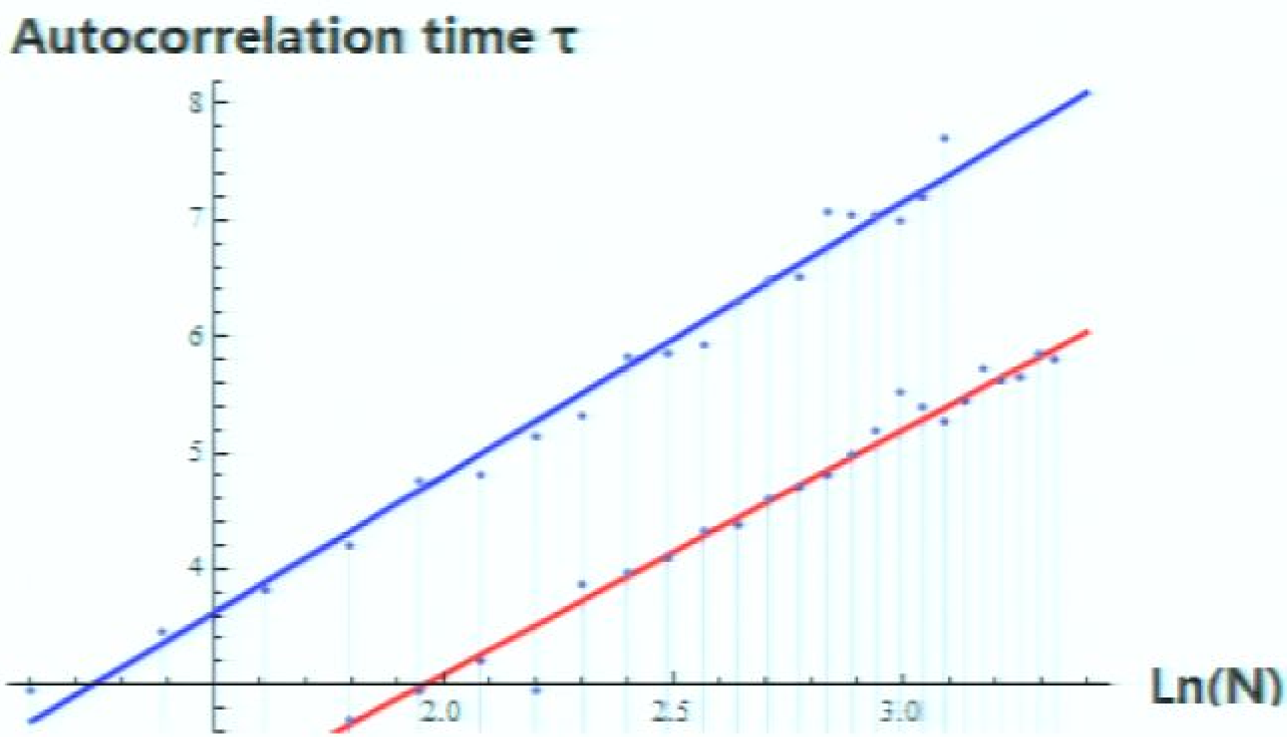
Considerations — Auto-correlation time

- Metropolis

$$\text{Ln}\ \tau = 0.109184 + 2.34945\ \text{Ln}N$$

- Heat bath

$$\text{Ln}\ \tau = -1.09774 + 2.09913\ \text{Ln}N$$



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Considerations — Acceptance ratio

The parameter γ in our program will affect the **acceptance ratio**,

$$\text{Acceptance ratio} = \frac{U \text{ is changed to a new state } U \cdot G}{U \text{ remains the same state } U}$$

Application in Lattice Gauge Theories

One matrix in SU(N)

Considerations — Acceptance ratio

For small γ

- $\Rightarrow$ U_{t+1} is far away from U_t
- $\Rightarrow$ Δs tends to be very large.
- $\Rightarrow$ $e^{-\Delta s}$ is then extremely small at least for low "temperature"
- $\Rightarrow$ Acceptance ratio tends to be very small.
- $\Rightarrow$ the state does not move.
- $\Rightarrow$ Auto-correlation time is large.
- $\Rightarrow$ $\langle W_1 \rangle$ is not reliable.

For large γ

- $\Rightarrow$ g is close to $\mathbb{I}$
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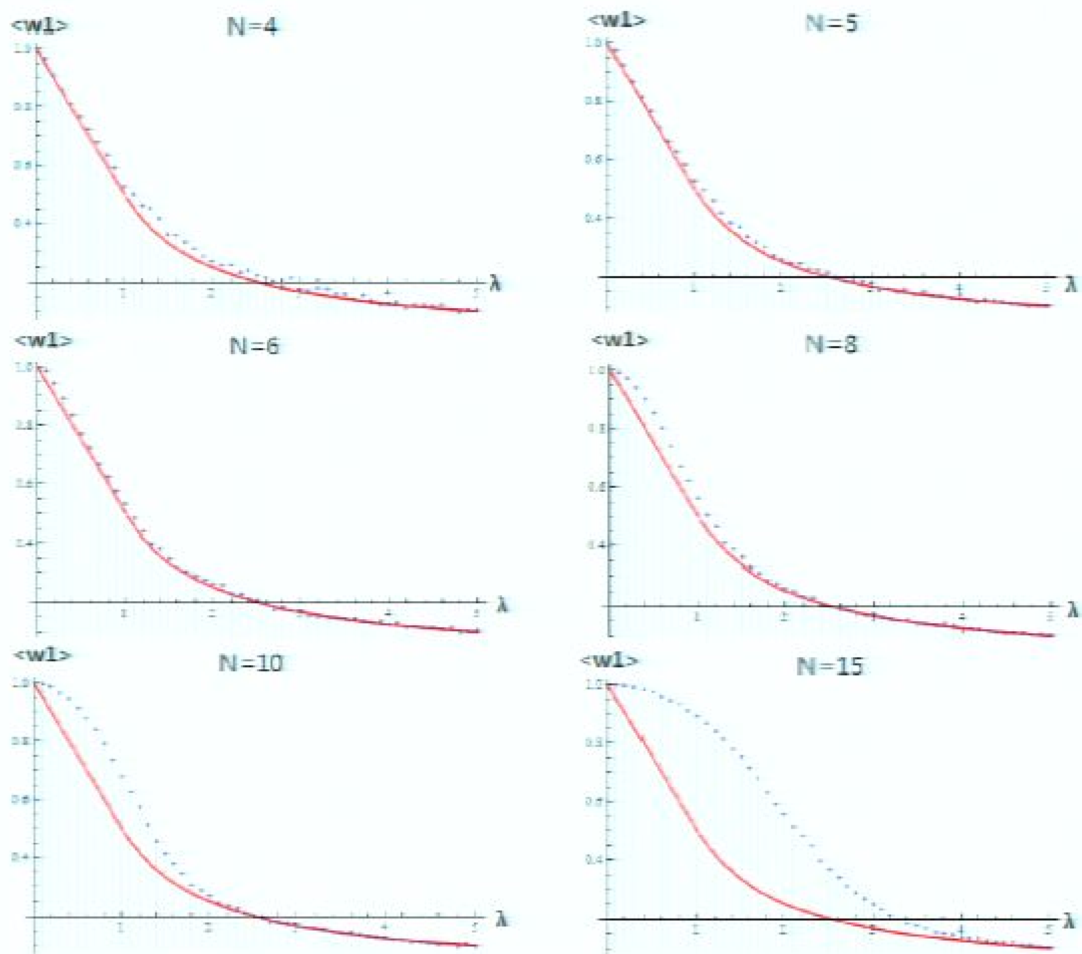
Application in Lattice Gauge Theories

One matrix in SU(N)

Metropolis Monte-Carlo method in SU(N)



Application in Lattice Gauge Theories

One matrix in SU(N)

Heat bath Monte-Carlo method in SU(N)[Creutz 80'][Cabibbo & Marinari 82']

Topology

1.Pick a matrix $A \in SU(N)$

$$\underbrace{\begin{bmatrix} 1 & \overset{i}{\vdots} & . & \overset{j}{\vdots} & . & \\ . & \bigcirc & . & \bigcirc & . & i \\ . & . & A & . & . & \\ . & \bigcirc & . & \bigcirc & . & j \\ . & . & . & . & 1 & \end{bmatrix}}_{N \times N}$$

2.Change U to $U(t+1) = U(t) \cdot A$.

- Pick up two random integers i and j, where $1 \leq i < j \leq N$.
- Read of $k \in \mathbb{R}$, $v \in SU(2)$.

$$u_t = \begin{pmatrix} \bigcirc & \bigcirc \\ \bigcirc & \bigcirc \end{pmatrix} = u_0 \mathbb{I} + i \sum_{j=1}^{3} u_j \sigma_j$$

$$k \cdot v = (\mathrm{Re} u_0)\mathbb{I} + i \sum_{j=1}^{3} (\mathrm{Re} u_j)\sigma_j$$

- Pick matrix $b \in SU(2)$ with $P(b_0) \propto \sqrt{1 - b_0^2} e^{2\frac{N}{\lambda} k b_0}$
- Complete the big unitary matrix A with $a = b \cdot v^{-1}$

Application in Lattice Gauge Theories
One matrix in SU(N)
Metropolis Monte-Carlo method in SU(N)

(a).Pick up two random integers i and j, where $1 \leq i < j \leq N$.

(b).Replace $\begin{pmatrix} \bigcirc & \bigcirc \\ \bigcirc & \bigcirc \end{pmatrix}$ by an arbitrary $SU(2)$ matrix $\equiv g$.

1. Choose a_0 from uniform distribution between $[\gamma, 1]$, where $\gamma \sim 1$, which makes g not very far away from $\mathbb{I}$.
2. Choose a_1, a_2, a_3 uniformly from the sphere $a_1^2 + a_2^2 + a_3^3 = 1 - a_0^2$.
    1. $|\vec{a}|^2 = 1 - a_0^2$
    2. $\vec{a} = |\vec{a}| (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$
    3. Make sure the distribution is uniform on area element $dA = \sin\theta \; \mathrm{d}\theta\mathrm{d}\phi$.
        - ϕ uniformly in $[0, \; 2\pi]$.
        - θ with distribution $p(\theta) \propto \sin\theta$.
3. Construct the unitary matrix g with identity determinant: $g = a_0\sigma_0 + i\sum_{i=1}^{3} a_i\sigma_i$.

Application in Lattice Gauge Theories
One matrix in SU(N)
Considerations — Acceptance ratio

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$$W_{\mathrm{EK}}[C] = \left\langle \frac{1}{N} \mathrm{Tr} \left[(U_2^\dagger)^T (U_1^\dagger)^R U_2^T U_1^R \right] \right\rangle$$

Application in Lattice Gauge Theories

Multiple matrices in SU(N)

For $N \to \infty$,

$$W_{\mathrm{EK}}(T, R) \xrightarrow{T \to \infty} c(R) e^{-V(R)T}$$

At large R, we expect linear behavior of we are in a confining regime:

$$\frac{dV(R)}{dR} \xrightarrow{R \to \infty} \sigma$$

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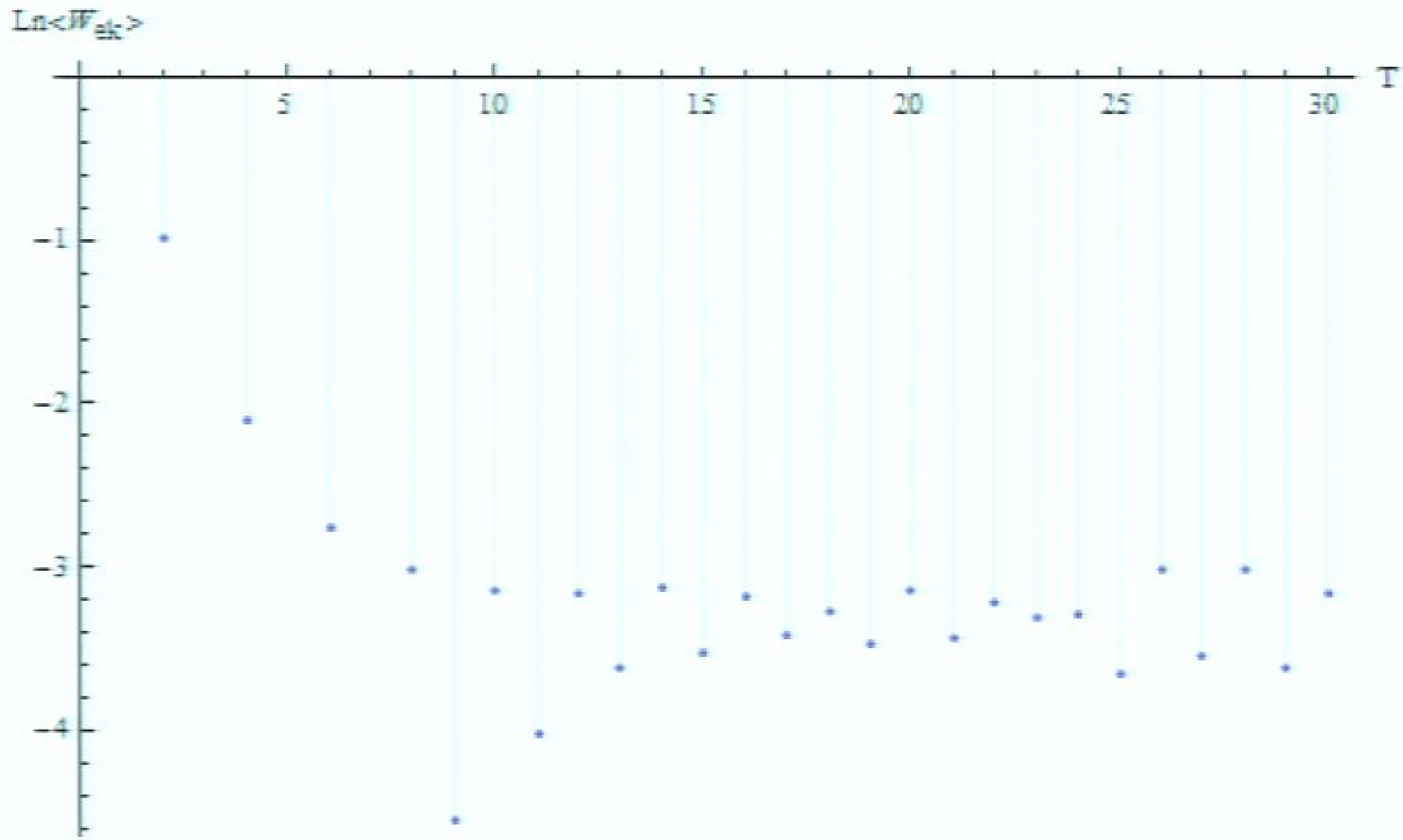

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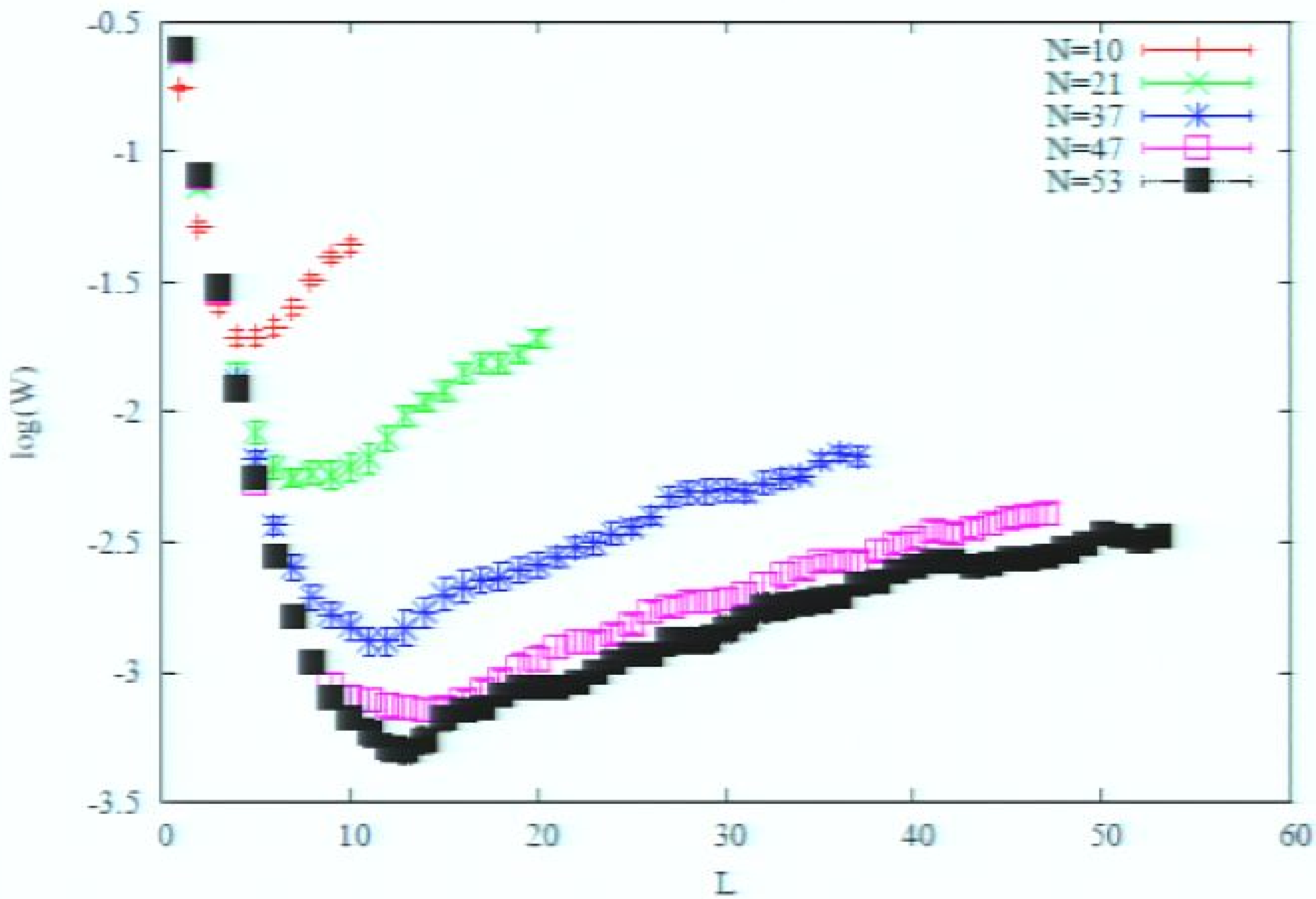

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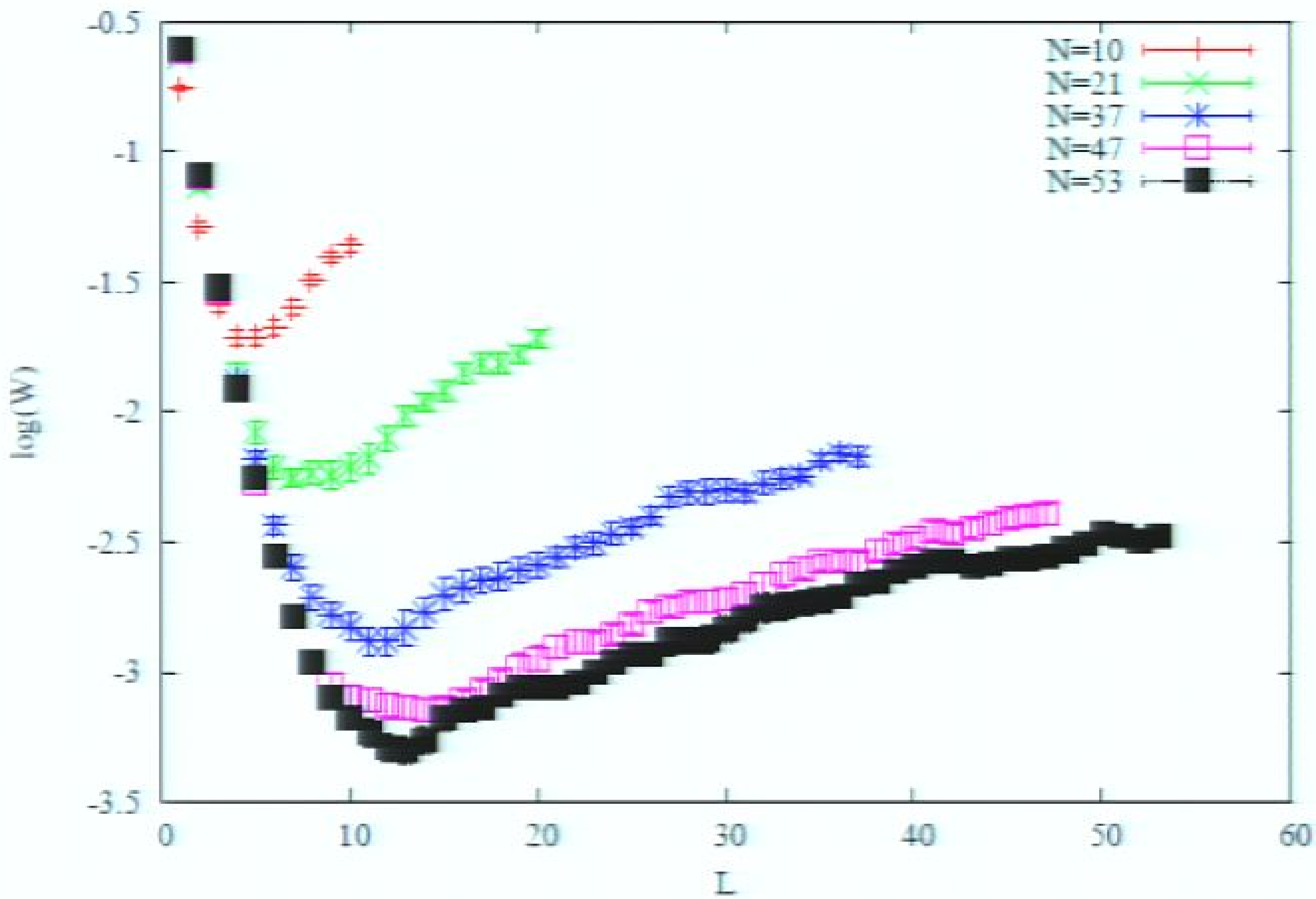

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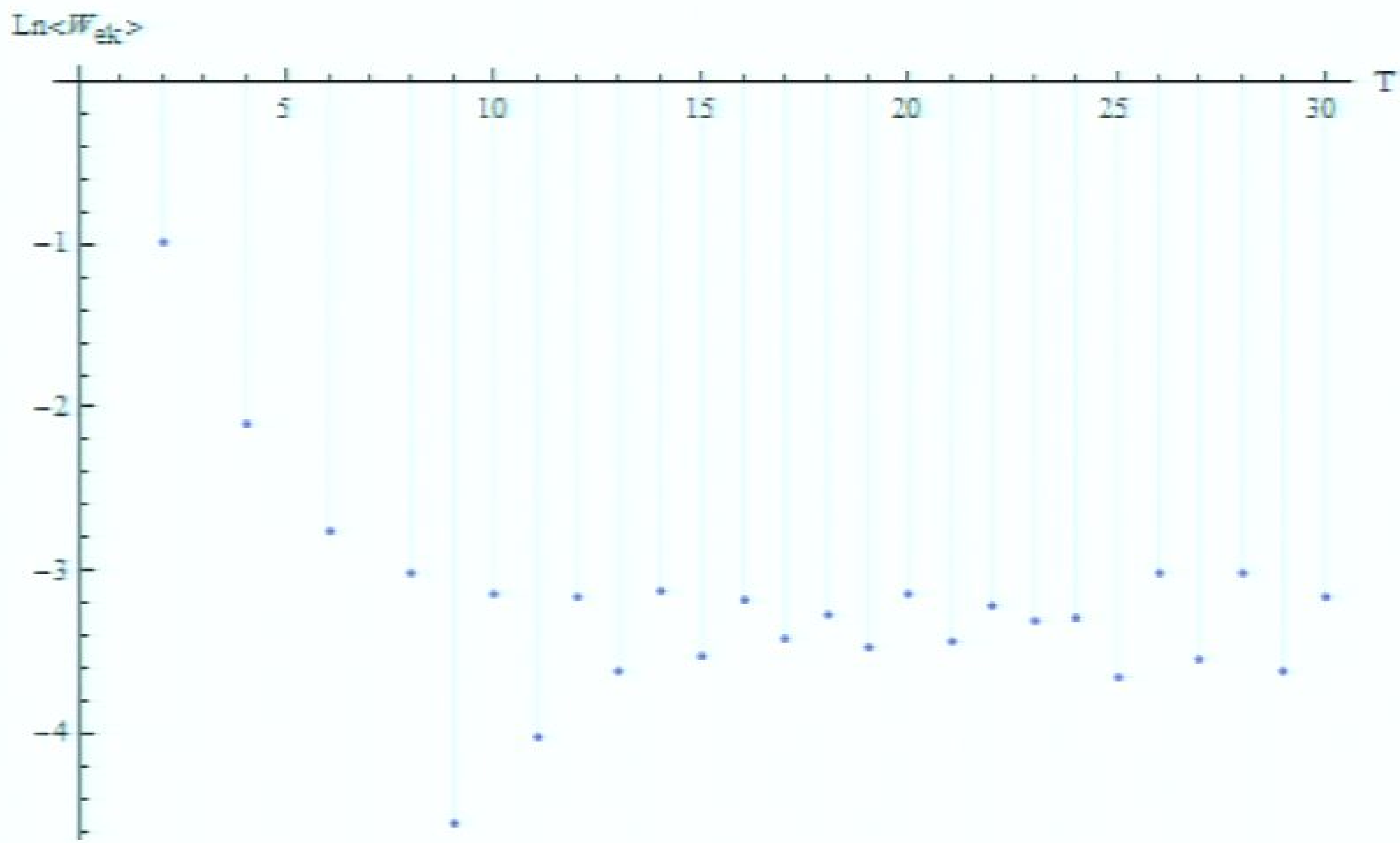

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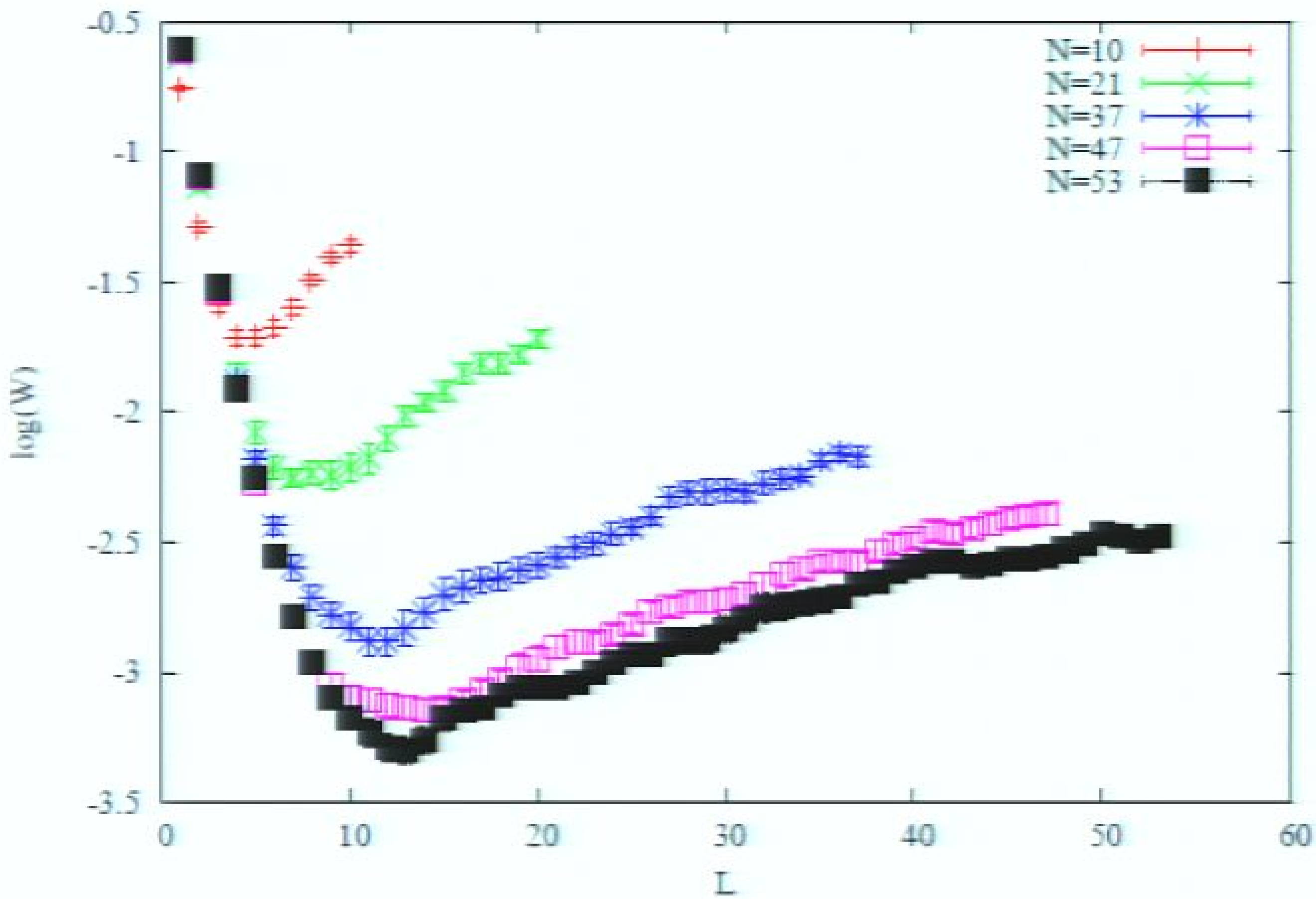

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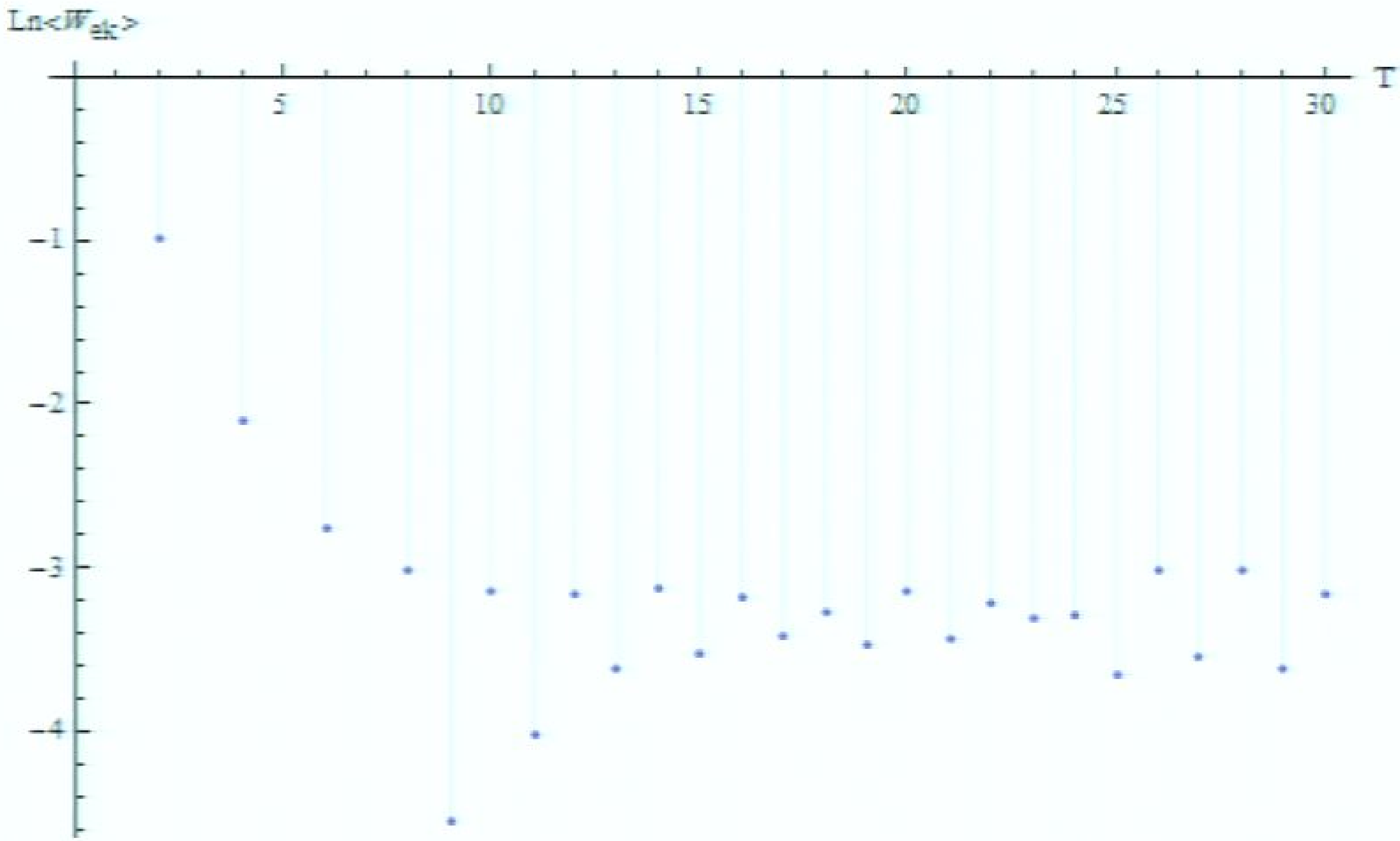

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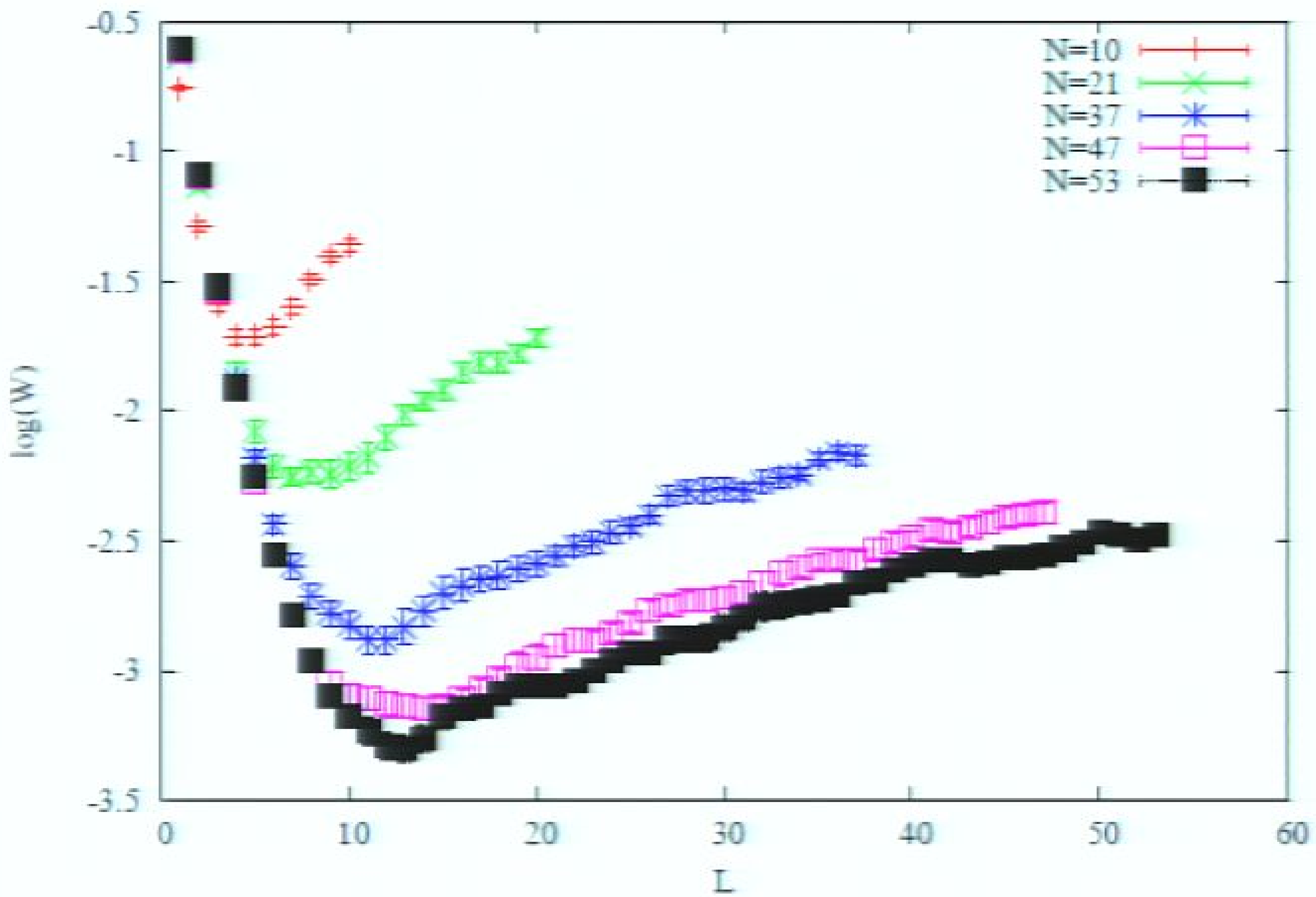

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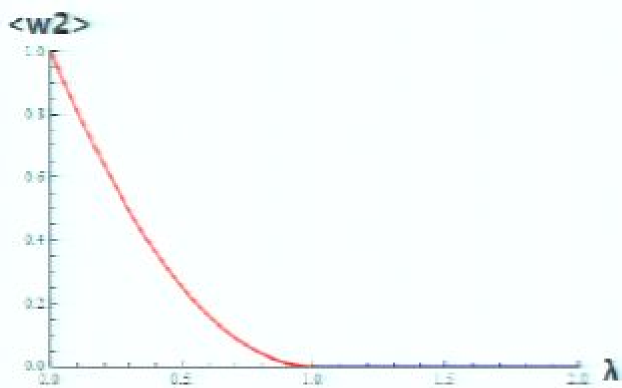

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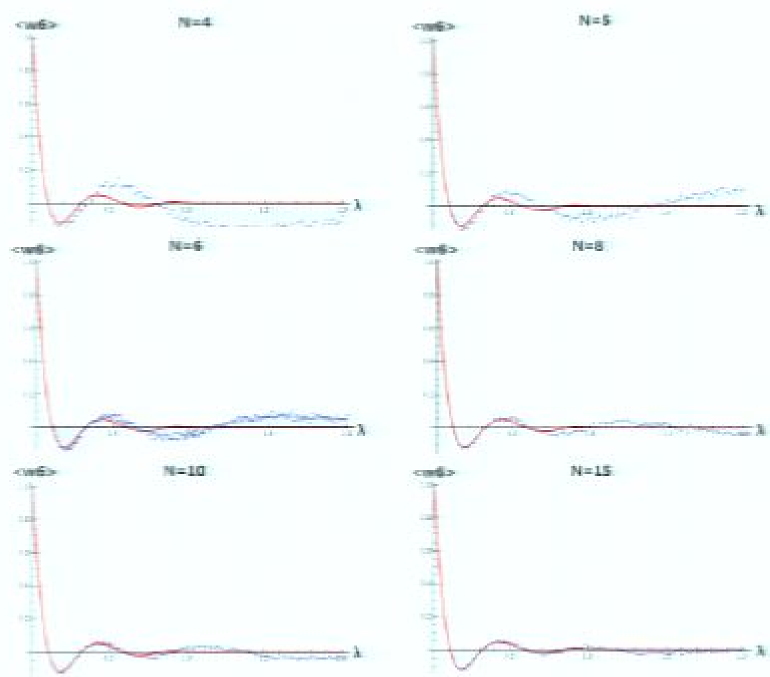

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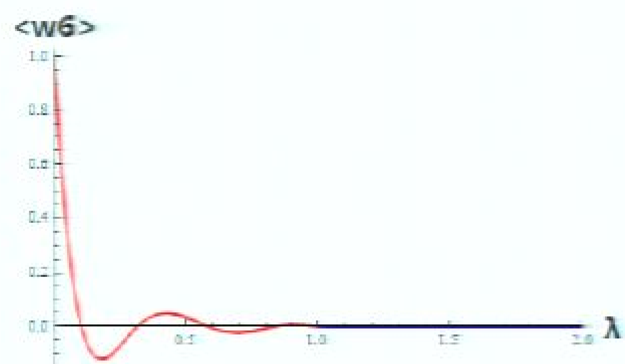

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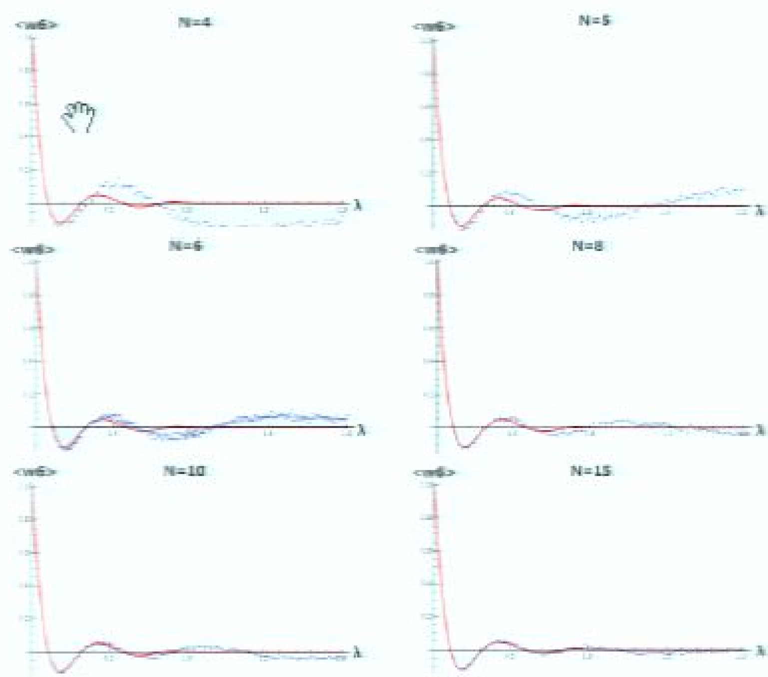

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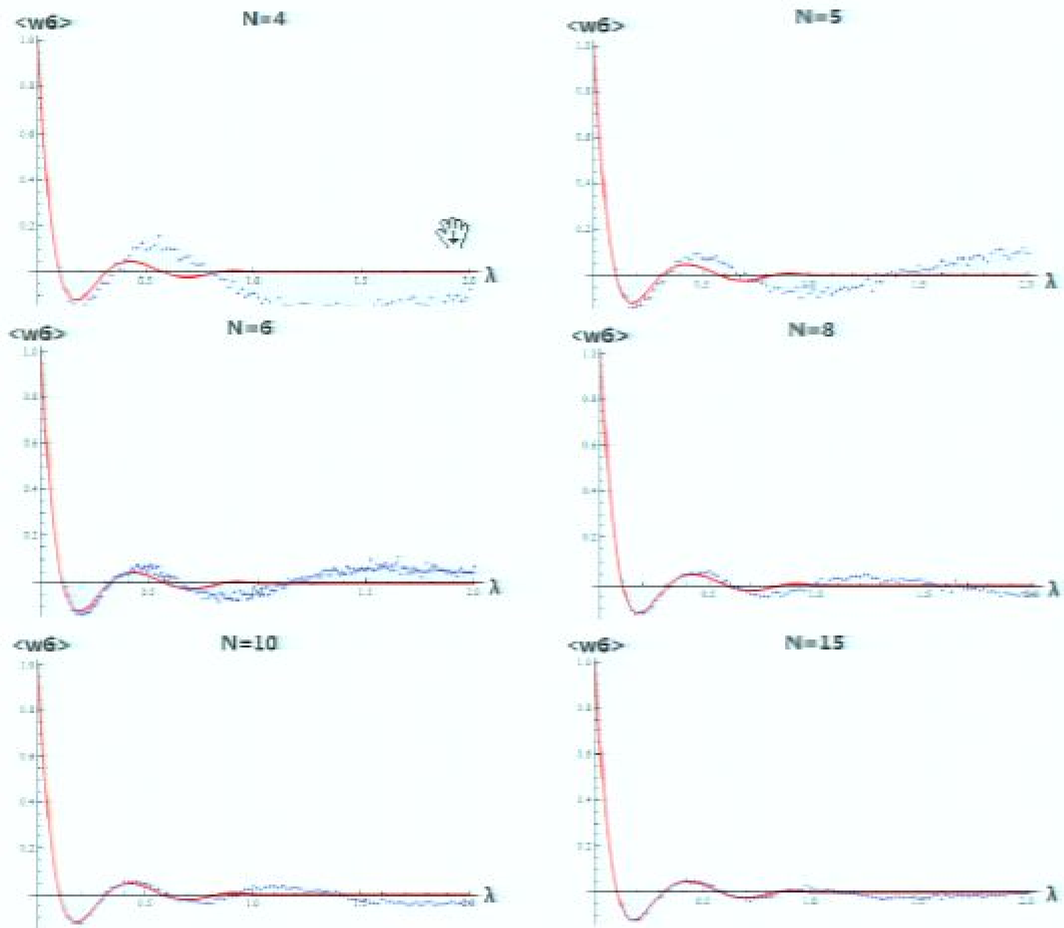

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