Overview of slides 04

Stochastic processes

Stochastic process

- Random process, evolving with 'time'
- More precisely: collection of random variables, X_t, indexed by time
- 'Time' can be continuous or discrete
  We only consider discrete time.
  $\longrightarrow$ t can be thought of as 'iteration index' or 'step'
- $X \longrightarrow$ single- or multi-dimensional, discrete or continuous
  We considered examples where:
  - X is a single real variable, for MCMC generation of exponential dist.
  - X is a configuration of the Ising model, e.g., $\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\downarrow$.
- Study probability of finding particular states at particular times
  $P(x)_t$ or $P(x_t)$ or $P(xt)$ or $P(x,t)$
  May or may not depend on probabilities at prior times.

Stochastic processes

Independent random process

Simplest case. Future probability independent of present or past:

$$P(x_n t_n | x_{n-1} t_{n-1} \dots x_1 t_1) = P(x_n t_n)$$

Completely memory-less. Special case of Markov process.

Markov process

Future probability depends only on present, independent of past:

$$P(x_n t_n | x_{n-1} t_{n-1} \dots x_1 t_1) = P(x_n t_n | x_{n-1} t_{n-1})$$

Limited memory — Only most recent value counts

Markov processes

Transition probabilities

A Markov chain is described by transition probabilities

$$T(X \to Y) \quad \text{or} \quad T_{X \to Y}$$

When states space is finite:
Can represent as matrix with elements $T_{ij} = T(X_i \to X_j)$

$\longrightarrow$ stochastic matrix or transition matrix or Markov matrix

Markov processes: transition graph + transition matrix

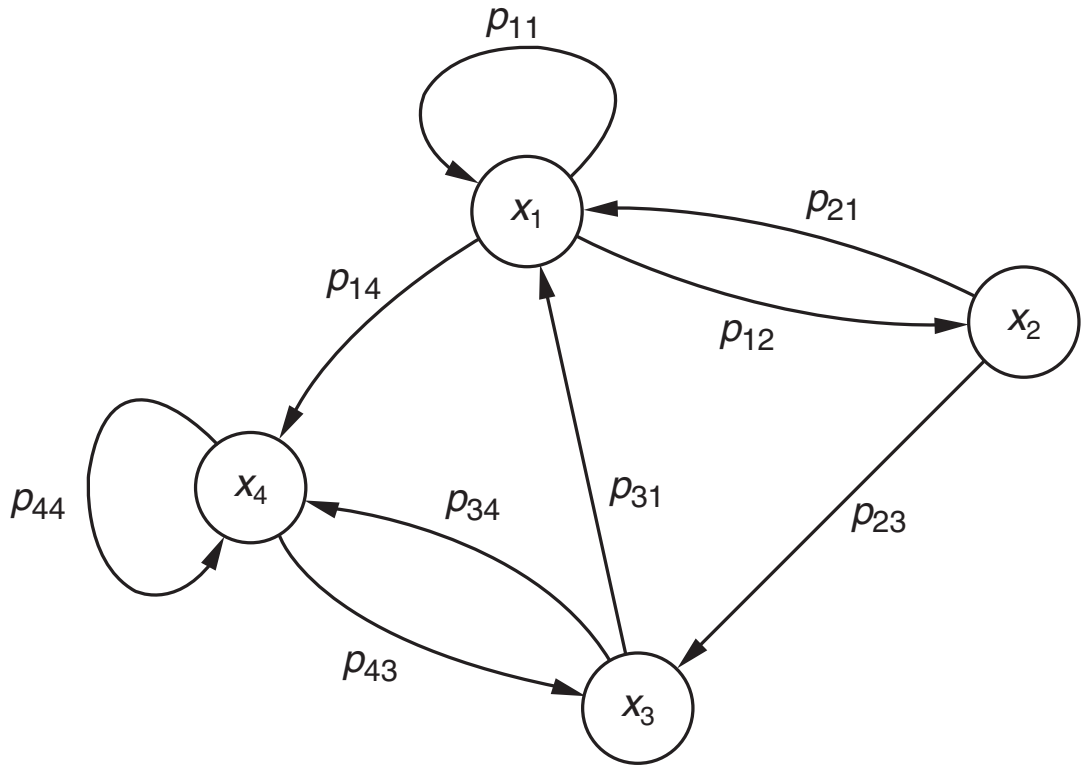


Fig. 3.1. The graph representation of a four-state Markov chain. Its corresponding transition matrix is

$$\begin{bmatrix} p_{11} & p_{12} & 0 & p_{14} \\ p_{21} & 0 & p_{23} & 0 \\ p_{31} & 0 & 0 & p_{34} \\ 0 & 0 & p_{43} & p_{44} \end{bmatrix}.$$

Transition matrix / stochastic matrix

Row stochastic matrix

Matrix with elements $T_{ij} = T(X_i \to X_j)$.

Sum of each row $= 1$ (system must end up in some state)

Has one eigenvalue exactly $=1$. All other eigenvalue magnitudes < 1.
$\to$ follows from Perron-Frobenius theorem.

If probabilities of states at step n is row vector p_n, then

$$p_{n+1} = p_n T$$

The left eigenvector corresponding to eigenvalue 1 is the stationary state

Analogy: power method

Column stochastic matrix: elements $T_{ij} = T(X_j \to X_i)$

Right eigenvectors, column vectors for probability
Row stochastic matrix is more commonly used. :-(

Markov process: Master Equation and Detailed Balance

Master equation

$$P(X, t_{n+1}) - P(X, t_n) = \sum_Y \Big[P(Y, t_n) T_{Y \to X} - P(X, t_n) T_{X \to Y} \Big]$$

Derived using:

$$\begin{cases} P(X, t_{n+1}) = \sum_Y P(Y, t_n) T_{Y \to X} \\ P(X, t_n) = P(X, t_n) \sum_Y T_{X \to Y} \end{cases}$$

Detailed balance — condition for stationary distribution

$$P(X) T(X \to Y) = P(Y) T(Y \to X)$$

Sufficient, not necessary

Markov chain Monte Carlo

Task

Generate an ergodic Markov chain of configurations which leads to the stationary distribution $P(X) \propto \exp(-\beta H(X))$

Main criterion: detailed balance

$$P(X)T(X \to Y) = P(Y)T(Y \to X)$$

Proposal step and acceptance/rejection step

Write transition probability as $T(X \to Y) = \omega_{XY} A_{XY}$

- ω_{XY} = proposal probability $P_{\text{prop.}}(Y|X)$, satisfies $\sum_Y \omega_{XY} = 1$.
- $A_{XY} \neq A_{YX}$ = acceptance probability

1. Propose a move from current state X to another state Y
2. Accept proposal with probability A_{XY}, otherwise stay put at X

Metropolis algorithm

Metropolis

Ensure symmetric proposal probability: $\omega_{XY} = \omega_{YX}$
Use acceptance probability

$$A_{XY} = \min\left(1, \frac{P(Y)}{P(X)}\right) = \begin{cases} 1 & P(X) \leq P(Y) \\ \frac{P(Y)}{P(X)} & P(X) > P(Y) \end{cases}$$

Metropolis-Hastings

More general: proposal probability need not be symmetric.
Use acceptance probability

$$A_{XY} = \min\left(1, \frac{P(Y)\omega_{XY}}{P(X)\omega_{YX}}\right)$$

Metropolis algorithm

Metropolis

Use symmetric proposal probability: $\omega_{XY} = \omega_{YX}$. Acceptance probability

$$A_{XY} = \min\left(1, \frac{P(Y)}{P(X)}\right) = \begin{cases} 1 & P(X) \le P(Y) \\ \frac{P(Y)}{P(X)} & P(X) > P(Y) \end{cases}$$

Proof of detailed balance

$$\frac{T(X \to Y)}{T(Y \to X)} = \frac{\omega_{XY} A_{XY}}{\omega_{YX} A_{YX}} = \frac{A_{XY}}{A_{YX}}$$

If $P(X) \le P(Y)$ then $A_{XY} = 1, \quad A_{YX} = P(X)/P(Y)$
If $P(X) > P(Y)$ then $A_{XY} = P(Y)/P(X), \quad A_{YX} = 1$
In either case

$$\frac{T(X \to Y)}{T(Y \to X)} = \frac{A_{XY}}{A_{YX}} = \frac{P(Y)}{P(X)} \qquad \Longrightarrow \text{ detailed balance}$$

Metropolis algorithm

Ergodicity

Depends on ω_{XY}

It must be possible to reach any Y from any X after a series of steps.

Statistical physics

$$P(X) \propto e^{-\beta H(X)} \quad \Longrightarrow \quad \frac{P(Y)}{P(X)} = e^{-\beta \Delta H}$$

Don't need to know normalization factor $Z = \sum_X e^{-\beta H(X)}$
$\rightarrow$ partition function, might be impossible to calculate

Metropolis acceptance probabilities for Statistical physics

$$A_{XY} = \begin{cases} 1 & \text{if } H(Y) \leq H(X) \\ e^{-\beta \Delta H} & \text{if } H(Y) > H(X) \end{cases}$$

Autocorrelations

Two successive configurations in Markov chain are "close" in phase space $\Longrightarrow$ any quantity will have similar values on the two configs

If ϕ is some scalar property, nearby values of ϕ are correlated.

$$\langle \Phi[X_n]\Phi[X_{n+1}]\rangle \neq \langle \Phi[X_n]\rangle\langle \Phi[X_{n+1}]\rangle \quad \text{i.e.,} \quad \neq \langle \Phi\rangle^2$$

Define autocorrelation function:

$$R(t) \;=\; \langle \Phi[X_n]\Phi[X_{n+t}]\rangle - \langle \Phi[X_n]\rangle\langle \Phi[X_{n+t}]\rangle$$

Nonzero for small t, should vanish for large t.

We want Monte Carlo samples to be statistically independent

Save Φ values spaced from each other along Markov chain.

Autocorrelations

Autocorrelation time τ

$$R(t) = \langle \Phi[X_n] \Phi[X_{n+t}] \rangle - \langle \Phi \rangle^2 \sim C e^{-t/\tau}$$

τ measures "memory" of the Markov process

Configurations separated by $t \gtrsim 2\tau$ are $\approx$ statistically independent

- How to make τ small? $\rightarrow$ improved update/proposal schemes
  E.g., cluster updates
- Autocorrelations increase dramatically near phase transitions
  $\rightarrow$ critical slowing down
- Statistical uncertainties are underestimated if autocorrelations are ignored

Alternatives to Metropolis

Reminder: Metropolis acceptance probabilities

$$A_{XY} = \begin{cases} 1 & \text{if } H(Y) \leq H(X) \\ e^{-\beta \Delta H} & \text{if } H(Y) > H(X) \end{cases}$$

Detailed balance can be satisfied by other acceptance probabilities.

1. Glauber algorithm:

$$A_{XY} = \frac{1}{1 + e^{\beta \Delta H}}$$

2. Heat-bath algorithm

Ising model

Simple model of (anti)ferromagnetism

We have a lattice of spins $\sigma_i = \pm 1$

$$H = -J \sum_{<ij>} \sigma_i \sigma_j - B \sum_i \sigma_i \, ; \qquad \sum_{<ij>} = \text{sum over nearest neighbours}$$

- $J > 0$: energy minimized by aligning spins $\rightarrow$ ferromagnet
- $J < 0$: energy minimized by anti-aligning neighboring spins $\rightarrow$ antiferromagnet
- Magnetic field $B > 0$: tries to have spins all $+1$.
- Physics depends on lattice: square, cube, triangular, honeycomb, Kagome, pyrochlore,...

Ising model

Simple model of (anti)ferromagnetism

We have a lattice of spins $\sigma_i = \pm 1$

$$H = -J \sum_{<ij>} \sigma_i \sigma_j - B \sum_i \sigma_i \, ; \qquad \sum_{<ij>} = \text{sum over nearest neighbours}$$

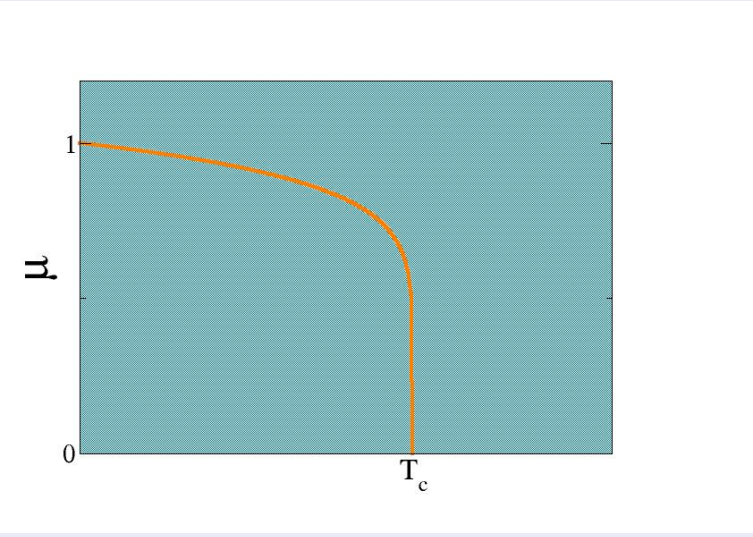
- 1D Ising chain: analytically solvable. No phase transitions.
- 2D Ising on square lattice: $B = 0$:
  "Solvable", difficult $\rightarrow$ Onsager solution.
  Has a phase transition at $T = T_c \approx 2.2692 J$
- No analytical solution is known for $d = 3$, for $B \neq 0$, other lattices.
  Many types of interesting physics in different lattices
  Even more types of interesting physics in models with continuous degrees of freedom, e.g., Heisenberg models.
  $\rightarrow$ Monte Carlo simulations are essential

Phase transition of Ising model

Focus on 2D square lattice, $B = 0$.

Phase transition

There is a second order phase transition at temperature T_c



Magnetization per site:

$$\mu = \frac{M}{\text{num.sites}} = \frac{\sum_i \sigma_i}{\text{num.sites}}$$

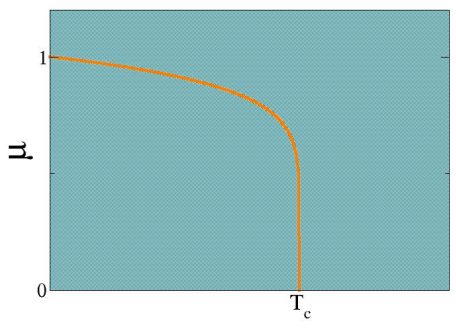
Spontaneous magnetization at low T:

$T > T_c$: $\mu = 0$

$T < T_c$: $\mu \neq 0$

Phase transition of 2D Ising model

Second-order Phase transition



2nd-order $\rightarrow$ μ vanishes continuously

Critical behaviour: with $t \equiv (T_c - T)/T_c$,

$$\mu \sim t^{\beta}, \quad \chi \sim t^{-\gamma}, \quad C_v \sim (-t)^{-\alpha}$$

The critical exponents $\alpha, \beta, \gamma, \ldots$ are universal:
Same behaviour for all systems with the same symmetries and dimensions

χ $\rightarrow$ susceptibility, $\left.\frac{\partial M}{\partial B}\right|_{B=0}$ $\quad$ C_v $\rightarrow$ spec. heat, $\frac{\partial H}{\partial T}$

Phase transition of 2D Ising model

Second-order Phase transition

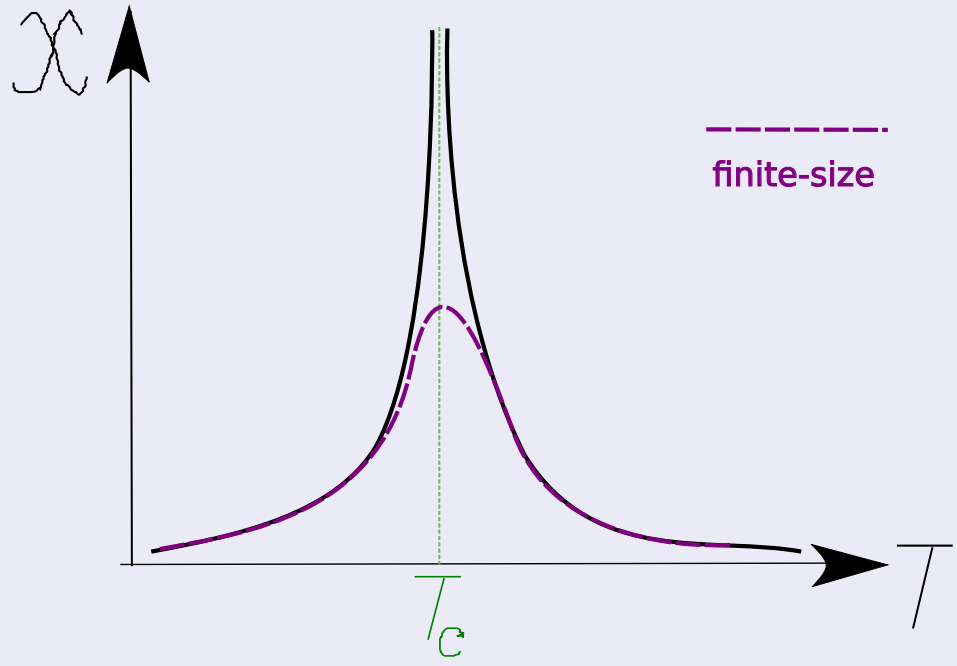
Critical behaviour: with $t \equiv (T_c - T)/T_c$,

$$\mu \sim t^{\beta}, \quad \chi \sim t^{-\gamma}, \quad C_v \sim (-t)^{-\alpha}$$

2D Ising universality class:

$\gamma = 7/4$
Susceptibility diverges at critical point!

$\alpha = 0$, but specific heat also diverges $\rightarrow$ logarithmic divergence.



Actual divergence only seen in infinite-size system.

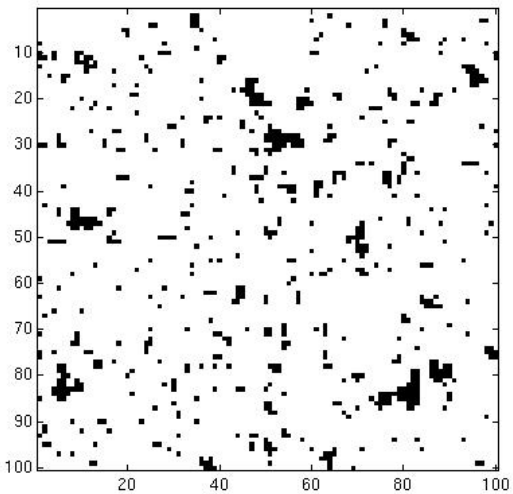
Simulation of Ising model

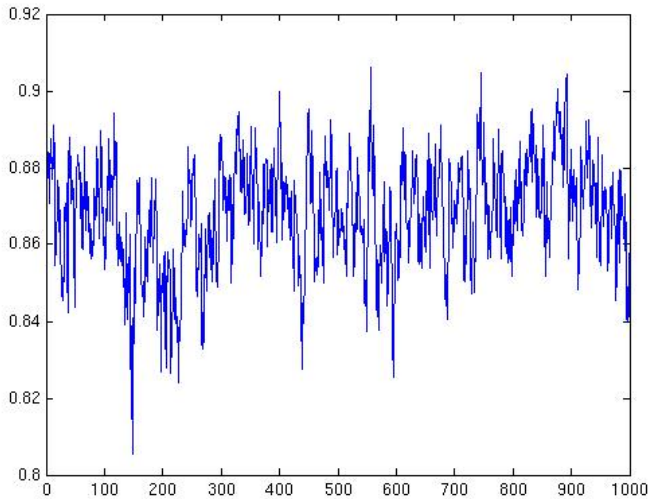
Metropolis algorithm

1. Start with all $\sigma_i = 1$ (cold start) or random ± 1 (hot start)
2. Sweep through all sites of lattice successively.
   (Or pick a site at random at each step.)
   For each site:
   - Calculate the energy difference ΔE if you flip that spin $\sigma_i \to -\sigma_i$
   - If $\Delta E < 0$ flip the spin
   - otherwise generate a uniform random $r \in (0, 1)$,
     flip the spin if $r < e^{-\beta \Delta E}$
3. Compute + save physical quantities (μ, E etc)
   maybe only every m-th step to minimize correlations
4. Repeat for N sweeps

Simulation results

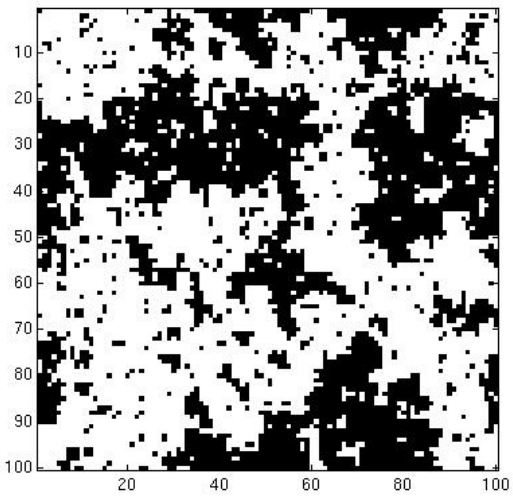
$T \approx 0.9 T_c$

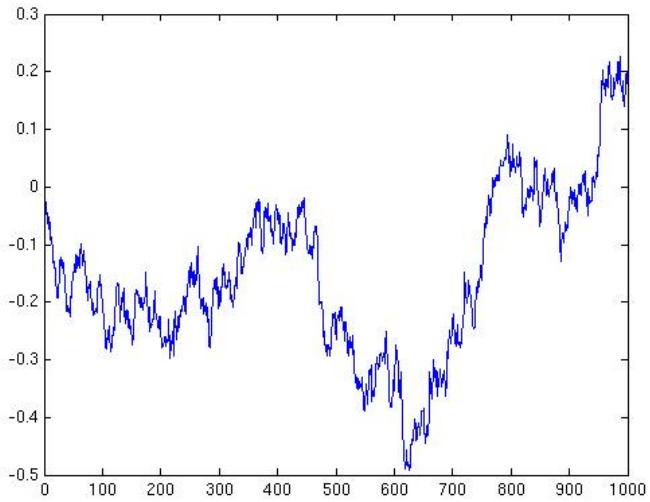




Simulation results

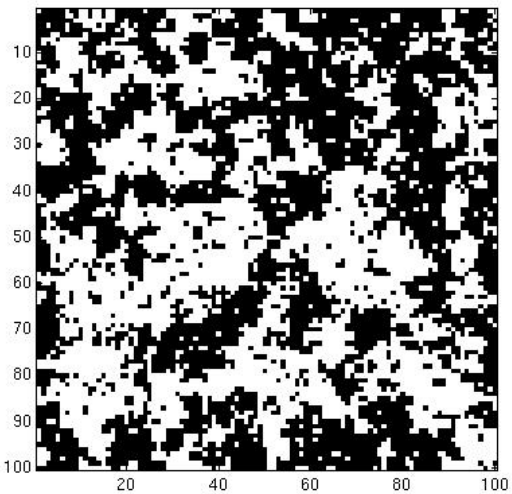
$T \approx T_c$

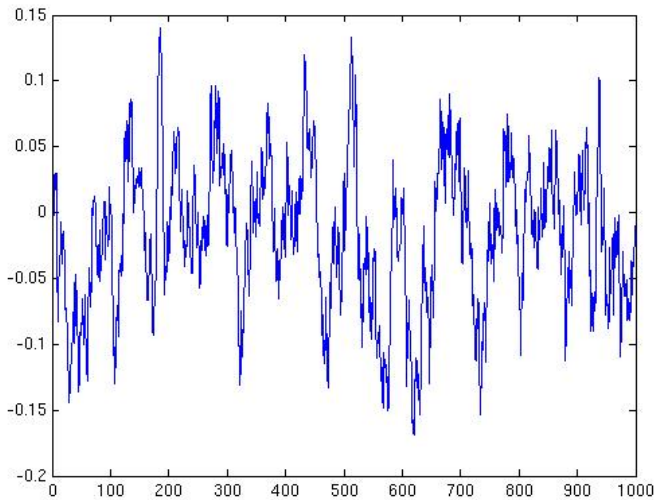




Simulation results

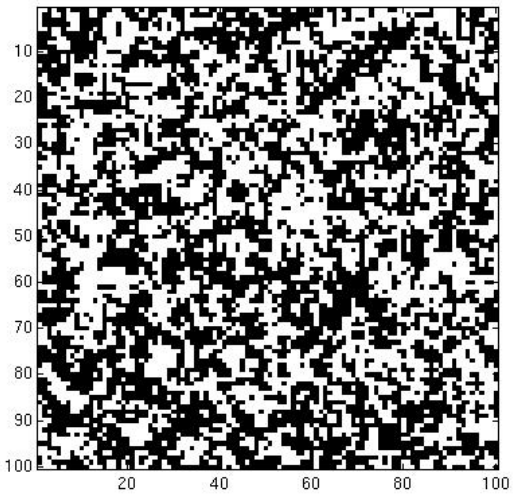
$T \approx 1.13 T_c$

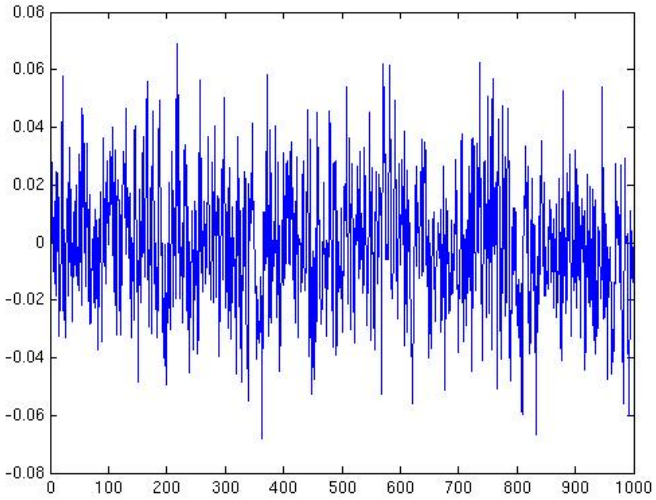




Simulation results

$T \approx 1.6\,T_c$





Finite volume issues

Boundary conditions

We want to study a macroscopic (nearly infinite) system

- the finite system we simulate is only a subsample of this
- use periodic boundary conditions to mimic surroundings

No phase transitions on a finite volume

All thermodynamic functions on finite V are smooth functions of T.

Not insurmountable: use finite volume scaling

- As V grows the crossover becomes sharper
- Extrapolate to $1/V = 0$
- There are critical exponents for finite volume scaling

Summary

Markov processes

- A Markov process is a stochastic process with no memory
- Described by transition probabilities
- All Markov processes obey the master equation
- Detailed balance is a sufficient condition for a stationary process

Markov chain Monte Carlo

- Use an ergodic Markov chain to create a statistical distribution of configurations
- Metropolis: all-purpose algorithm for Monte Carlo simulations
- Application to statistical physics (condensed matter) systems eg Ising model
- Autocorrelations need to be monitored