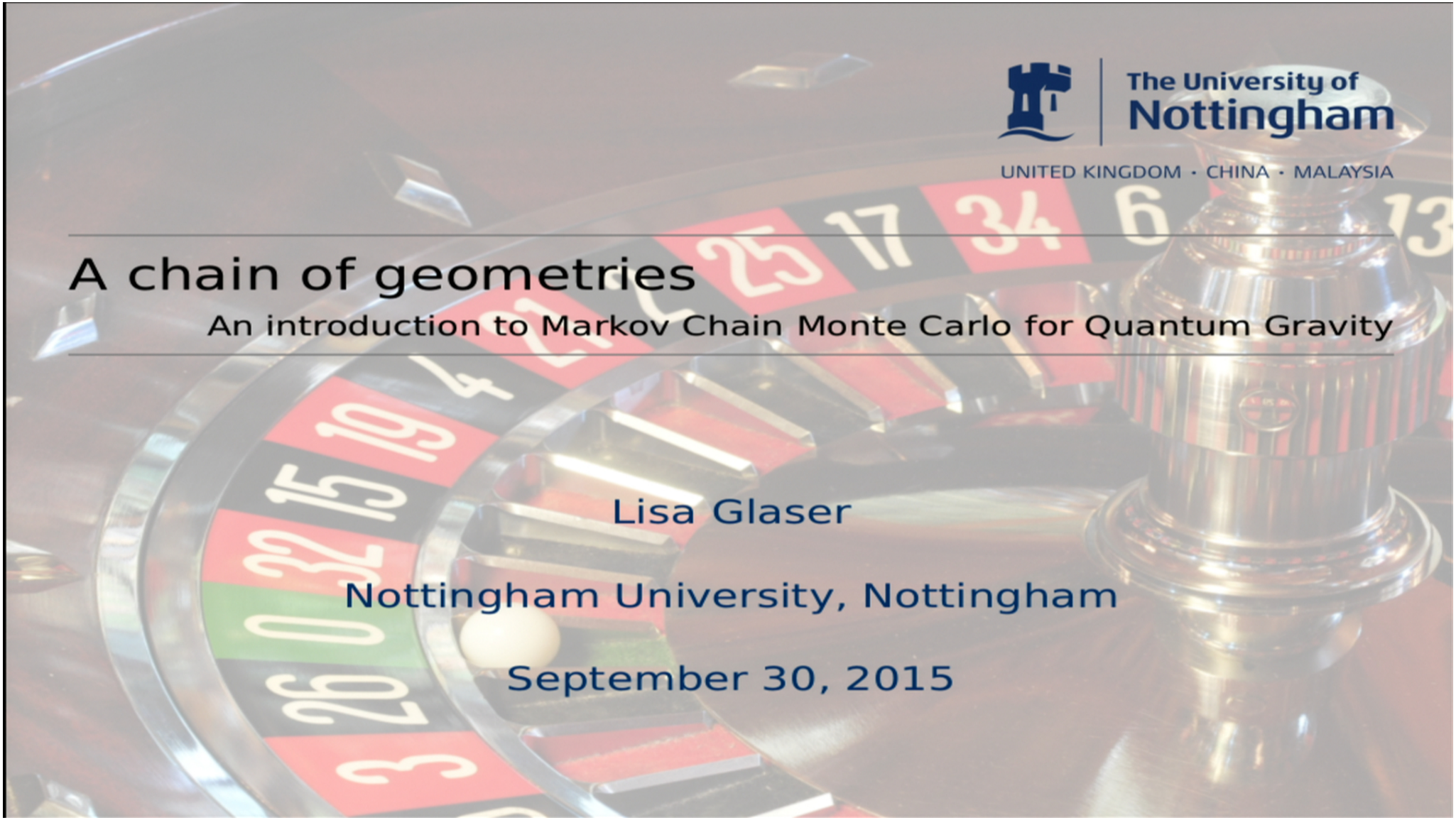
Title: A chain of geometries

Date: Sep 30, 2015 11:00 AM

URL: http://pirsa.org/15090083

Abstract: The path integral is a very elegant formulation of quantum theory. It can also be an incredibly useful one, since it allows us to use methods of statistical physics, like computer simulations.
In this talk I will introduce the subject of Markov Chain Monte Carlo simulations to solve the path integral over geometries. This general introduction will use examples from Causal Dynamical Triangulations, Causal Set Theory and Non Commutative geometry to show how different issues can be explored in this manner.


The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA
A chain of geometries
An introduction to Markov Chain Monte Carlo for Quantum Gravity
Lisa Glaser
Nottingham University, Nottingham
September 30, 2015

Outline

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

What is Markov Chain Monte Carlo?

The (Markov Chain) Monte Carlo algorithm

Measuring things in Monte Carlo simulations

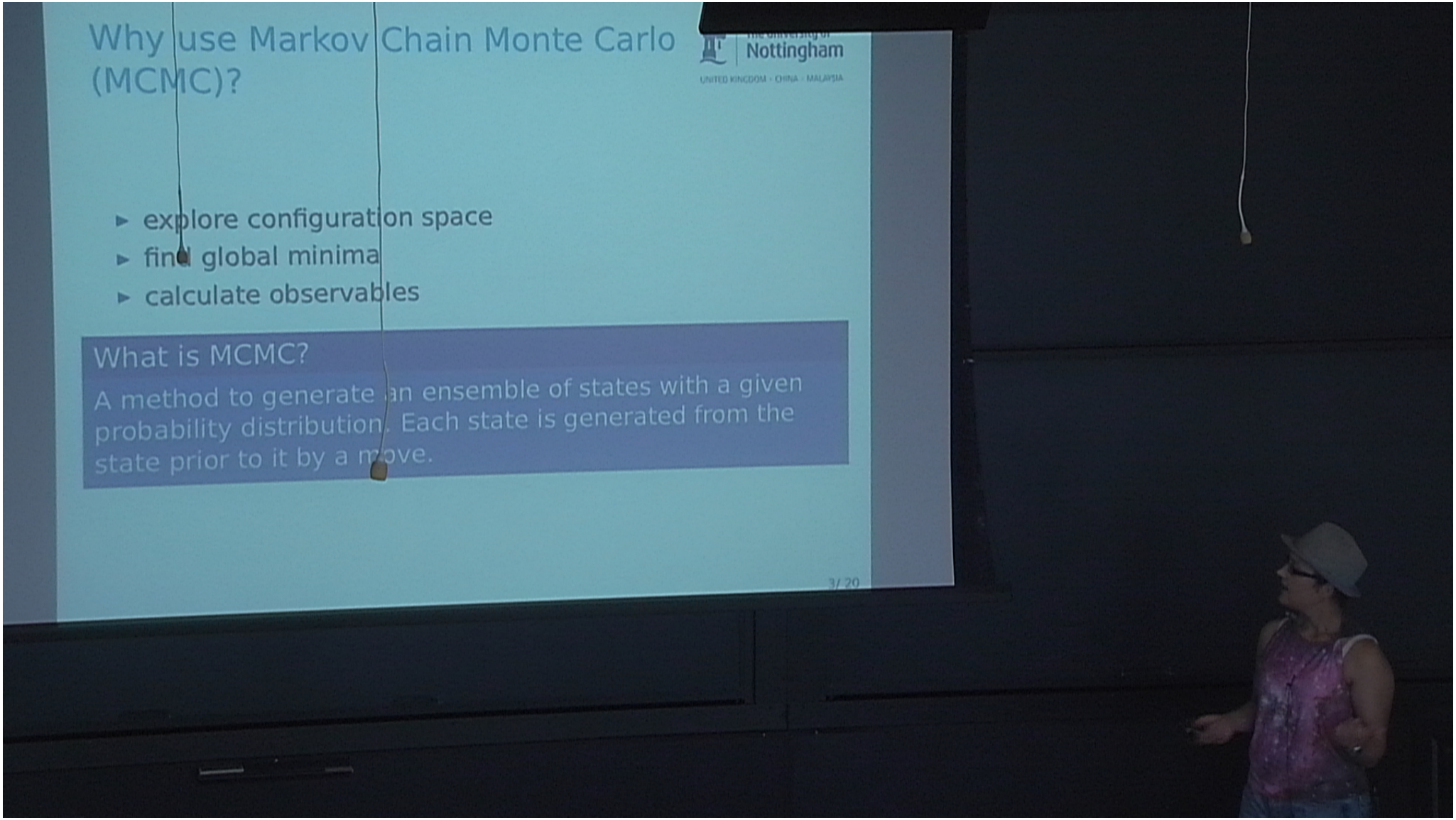
Why use Markov Chain Monte Carlo (MCMC)?

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

- explore configuration space
- find global minima
- calculate observables

What is MCMC?

A method to generate an ensemble of states with a given probability distribution. Each state is generated from the state prior to it by a move.


Why use Markov Chain Monte Carlo (MCMC)?
The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA
explore configuration space
find global minima
calculate observables
What is MCMC?
A method to generate an ensemble of states with a given probability distribution. Each state is generated from the state prior to it by a move.
3/ 20

Why use Markov Chain Monte Carlo (MCMC)?

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

- explore configuration space
- find global minima
- calculate observables

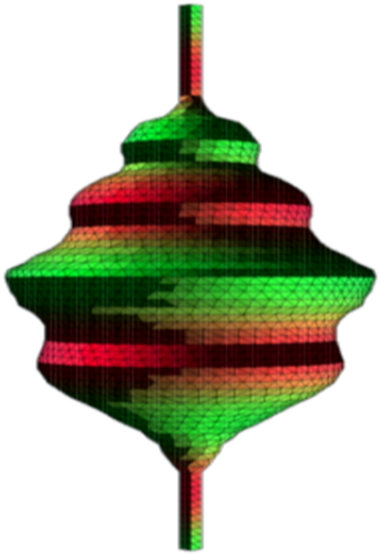
What is MCMC?

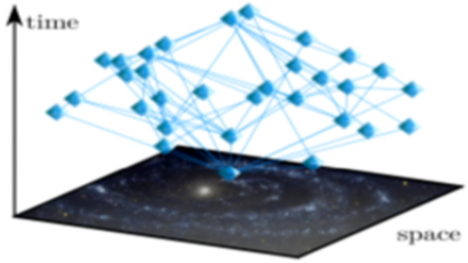
A method to generate an ensemble of states with a given probability distribution. Each state is generated from the state prior to it by a move.

What do we need for MCMC?

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

- a space of states
- a probability for each state i
- a move on the state space





What do we need for MCMC?

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

- a space of states
- a probability for each state i
- a move on the state space

$$e^{-\mathcal{S}(i)}$$

What do we need for MCMC?

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

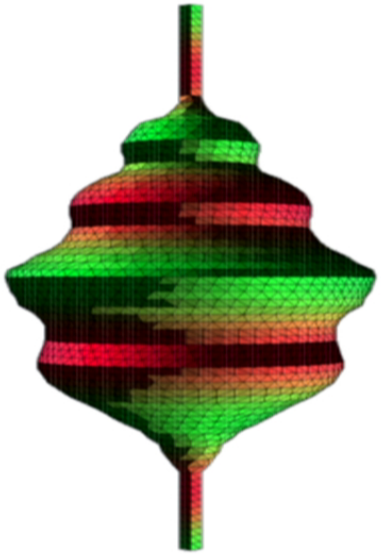
- a space of states
- a probability for each state i
- a move on the state space

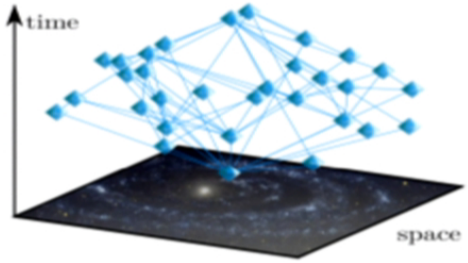
- Pacher moves in (Causal) dynamical triangulation
- adding links in Causal set theory
- adding random matrices in non commutative geometry Monte Carlo

What do we need for MCMC?

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

- a space of states
- a probability for each state i
- a move on the state space





We then move through the state space, according to the probability distribution by using the moves.

Markov chain

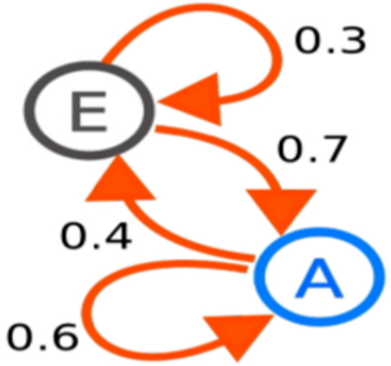
The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Markov chain:

A memoryless sequence of random variables.

$$P(X_{n+1} = x \mid X_1 = x_1, \ldots, X_n = x_n) = P(X_{n+1} = x \mid X_n = x_n)$$

Each step only depends on the current state.



Path integral on the computer

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$Z = \int \mathcal{D}(\phi) e^{-S[\phi]} \qquad \langle \mathcal{O}(\phi) \rangle = \frac{1}{Z} \int \mathcal{D}(\phi) \mathcal{O}(\phi) e^{-S[\phi]}$$

Feynman diagrams are a perturbative expansion of this, can we do better?

Path integral on the computer

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$Z = \sum_{\phi} e^{-S[\phi]} \qquad \langle \mathcal{O}(\phi) \rangle = \frac{1}{Z} \sum_{\phi} \mathcal{O}(\phi)\, e^{-S[\phi]}$$

Sum over regular set of field configurations.

$$\phi(n), n = 0, \ldots, N$$

Problem

Needs very large N, mostly samples low probability regions

Can we do even better?

Path integral on the computer

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$Z = \sum_{\phi} e^{-S[\phi]} \qquad \langle \mathcal{O}(\phi) \rangle = \frac{1}{Z} \sum_{\phi} \mathcal{O}(\phi)\, e^{-S[\phi]}$$

Generate statistically independent field configurations

$$\phi(n), n = 0, \ldots, N$$

w. probability distribution

$$P(\phi(n)) = Z^{-1} e^{-S[\phi(n)]}$$

Then

$$\langle \mathcal{O}(\phi) \rangle_N = \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}(\phi(n)) \xrightarrow[N \to \infty]{} \langle \mathcal{O}(\phi) \rangle$$

Outline

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

What is Markov Chain Monte Carlo?

The (Markov Chain) Monte Carlo algorithm
Examples

Measuring things in Monte Carlo simulations

Transition probability

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

The transition probability

$$\mathcal{T}(\phi \to \phi') = g(\phi \to \phi')\, A(\phi \to \phi')$$

can be split into two parts

- Selection probability $\Rightarrow$ determined by moves
- Acceptance rate $\Rightarrow$ adjusted

Transition probability

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

The transition probability

$$\mathcal{T}(\phi \to \phi') = g(\phi \to \phi')\, A(\phi \to \phi')$$

can be split into two parts

- Selection probability $\Rightarrow$ determined by moves
- Acceptance rate $\Rightarrow$ adjusted

Transition probability

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

The transition probability

$$\mathcal{T}(\phi \to \phi') = g(\phi \to \phi') A(\phi \to \phi')$$

needs to satisfy

- depends only on ϕ and ϕ' only, no time, or further state dependence
-

$$\sum_{\phi'} \mathcal{T}(\phi \to \phi') = 1$$

- ergodic, any ϕ can be reached in finite # of steps
- Probability distribution converges towards $Z^{-1} e^{-S[\phi(n)]}$
- Usually $\mathcal{T}(\phi \to \phi') \neq 0$ only if ϕ, ϕ' are close

Detailed Balance

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$\frac{P(\phi')}{P(\phi)} = \frac{\mathcal{T}(\phi \to \phi')}{\mathcal{T}(\phi' \to \phi)} = \frac{g(\phi \to \phi')A(\phi \to \phi')}{g(\phi' \to \phi)A(\phi' \to \phi)}$$

Ensures that the probablity distribution converges

$$P_{n+1}(\phi) = \sum_{\phi'} P_n(\phi')\mathcal{T}(\phi' \to \phi) \xrightarrow[n\to\infty]{} P(\phi) = Z^{-1}\, e^{-S[\phi(n)]}$$

Detailed Balance

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$\frac{P(\phi')}{P(\phi)} = \frac{\mathcal{T}(\phi \to \phi')}{\mathcal{T}(\phi' \to \phi)} = \frac{g(\phi \to \phi')A(\phi \to \phi')}{g(\phi' \to \phi)A(\phi' \to \phi)}$$

Ensures that the probablity distribution converges

The transition probability $g(\phi \to \phi')$ is fixed by the moves, so we adjust the acceptance rate $A(\phi \to \phi')$ to fullfill detailed balance.

Metropolis Hastings algorithm

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

The Metropolis Hastings algorithm is one particular algorithm to generate a Markov Chain.

- generate a new state ϕ' according to $g(\phi \to \phi')$
- automatically accept it if $P(\phi') > P(\phi)$
- else accept it with probability $P(\phi')/P(\phi)$

Metropolis Hastings algorithm

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

The Metropolis Hastings algorithm is one particular algorithm to generate a Markov Chain.

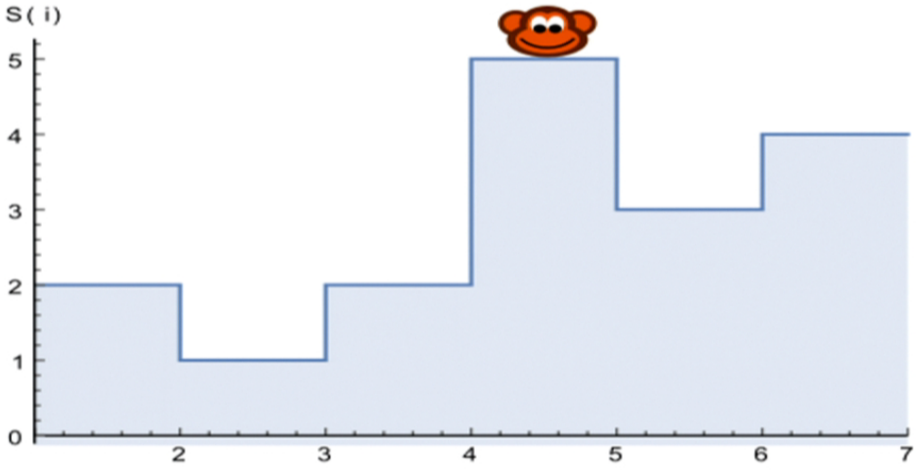
- generate a new state ϕ' according to $g(\phi \to \phi')$
- automatically accept it if $P(\phi') > P(\phi)$
- else accept it with probability $P(\phi')/P(\phi)$

A toy model

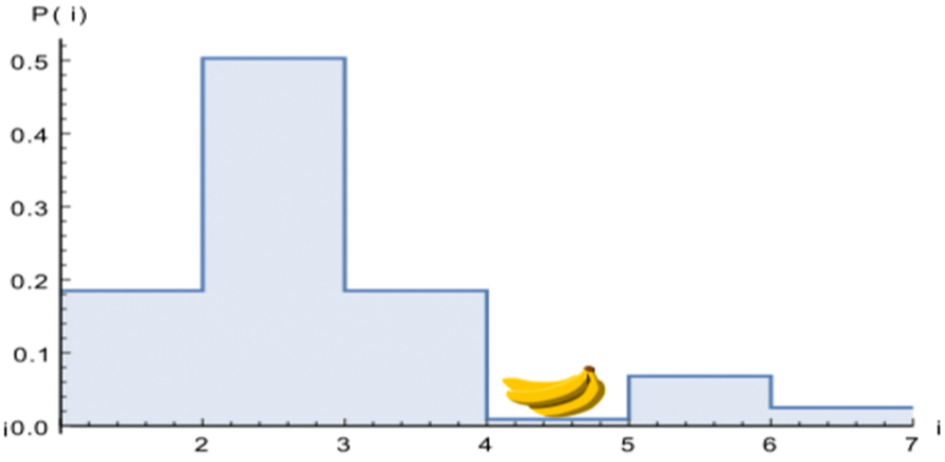
The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$g(i \to i') = \begin{cases} \frac{1}{2} \text{ if } i' = i \pm 1 \\ 0 \text{ else} \end{cases}$$

In this case $g(i \to i') = g(i' \to i)$
We need to adjust $A(i \to i')$ to get the right probabilities.



Real space

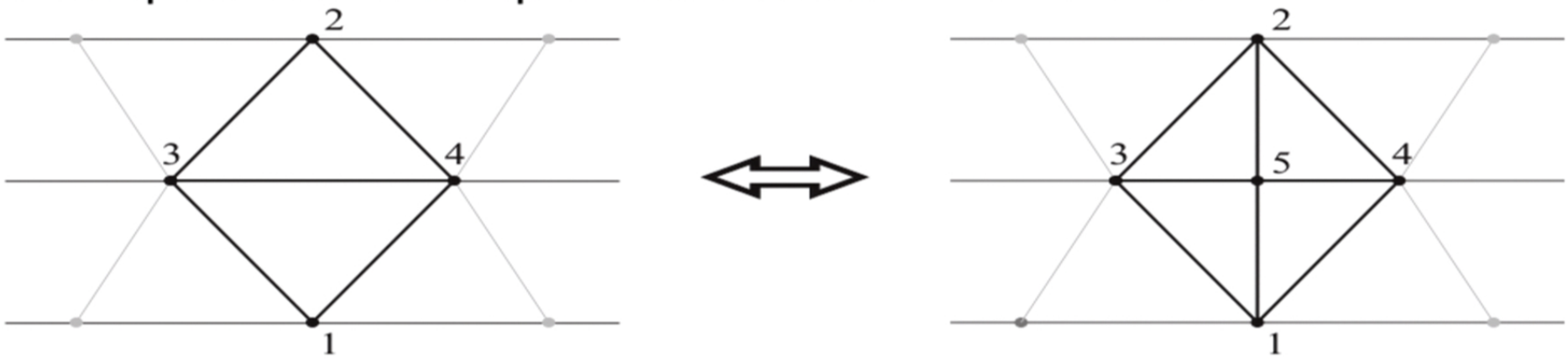


Probability space

A CDT example

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

We will adjust the accpetance rate for one simple CDT example. The example will use the $2 \to 4$ move



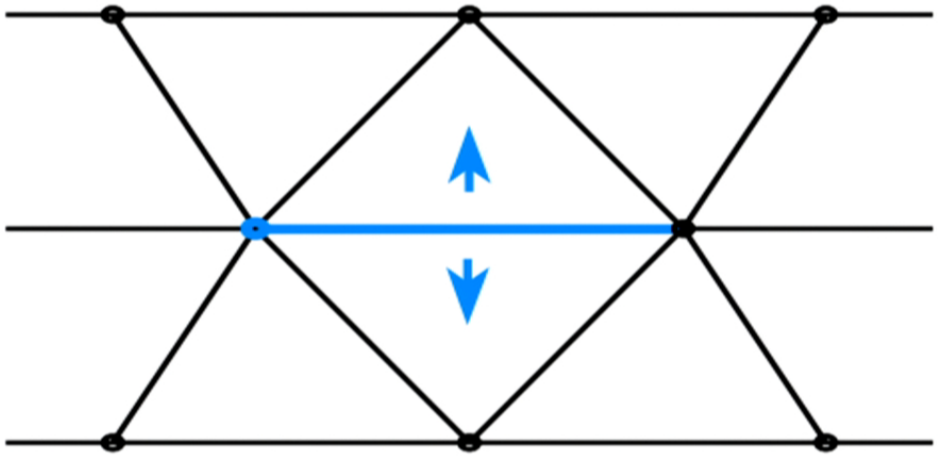
$$134 + 234 \quad \leftrightarrow \quad 135 + 145 + 235 + 245$$

On the computer we work with labeled triangulations!

Detailed Balance example

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$N_2(T) = 2N_0(t)$$



Detailed Balance example

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

for the $(2,4)$ move (or the $(4,2)$ move)

Choose selection probability

For $T_{N_0} \to T_{N_0+1}$ pick a vertex at random

$$g(T_{N_0} \to T_{N_0+1}) = \frac{1}{N_0}$$

For $T_{N_0+1} \to T_{N_0}$ remove vertex N_0+1 (if it is of order 4)

$$g(T_{N_0+1} \to T_{N_0}) = 1$$

Detailed Balance example

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

The acceptance ratios are then given by

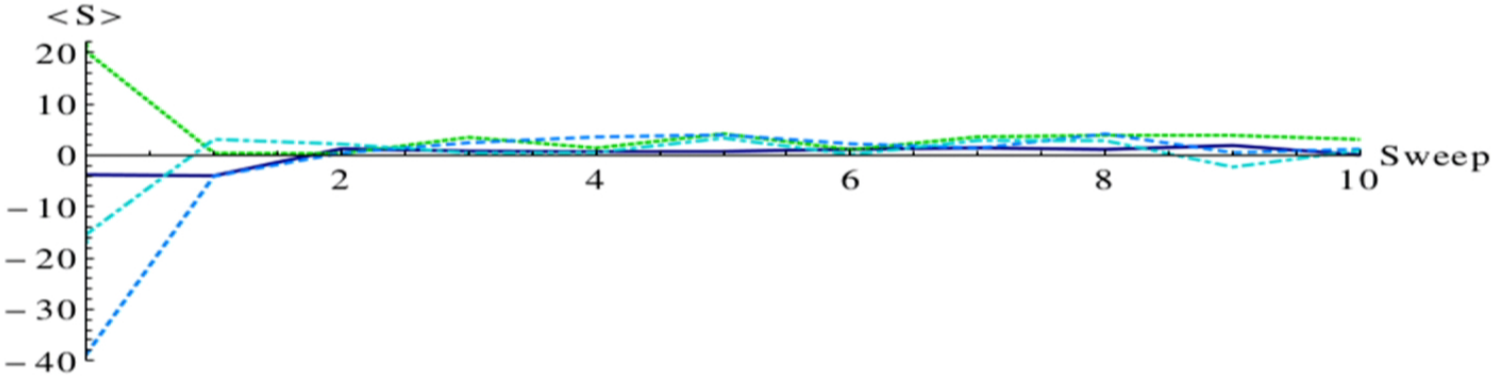
$$A(T \to T') = min(1, \frac{g(T' \to T)}{g(T \to T')} \frac{P(T')}{P(T)})$$

$$\text{and} \quad P(T) = \frac{1}{Z} \frac{1}{N_0(T)!} e^{-2\lambda N_0(T)}$$

$$A(T_{N_0} \to T_{N_0+1}) = min(1, \frac{N_0}{N_0+1} e^{-2\lambda})$$

$$A(T_{N_0+1} \to T_{N_0}) = min(1, \frac{N_0+1}{N_0} e^{2\lambda})$$

Thermalisation



Gold standard

Convergence of different initial conditions

Outline

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

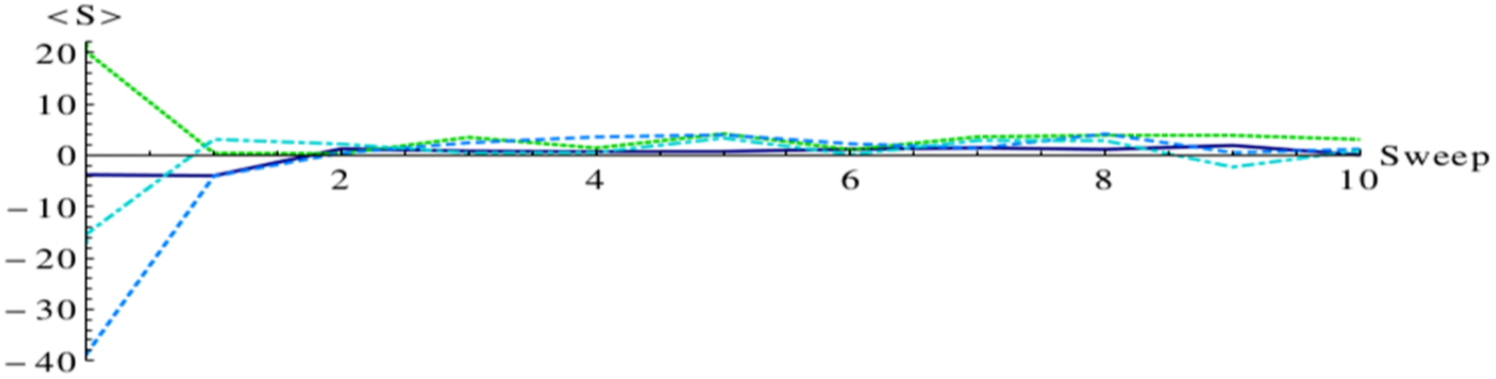
What is Markov Chain Monte Carlo?

The (Markov Chain) Monte Carlo algorithm

Measuring things in Monte Carlo simulations

Thermalisation

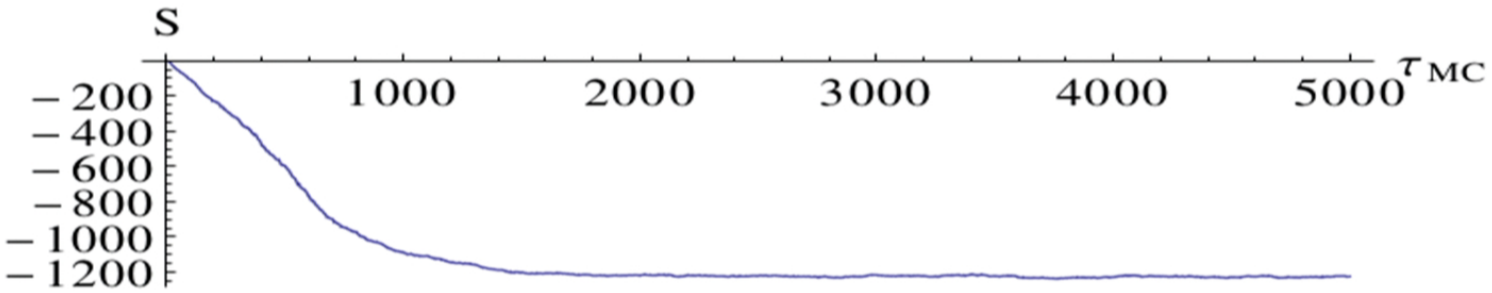
The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA



Gold standard

Convergence of different initial conditions

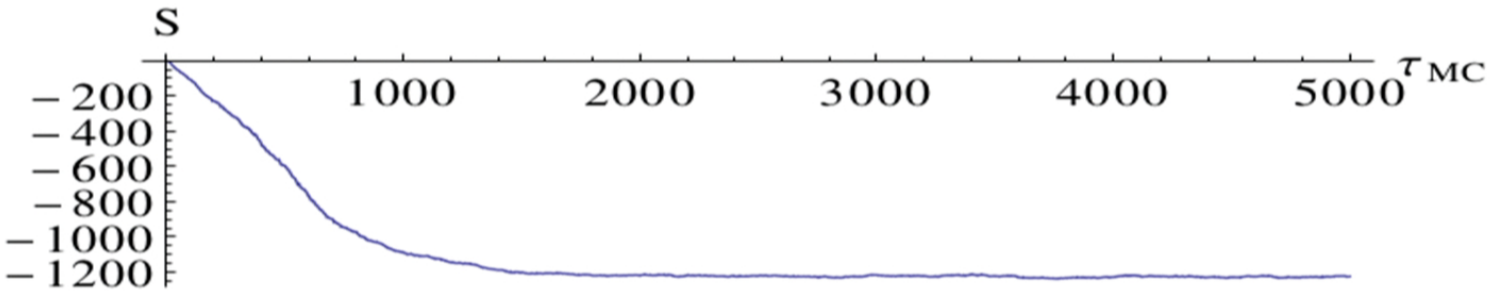
Thermalisation



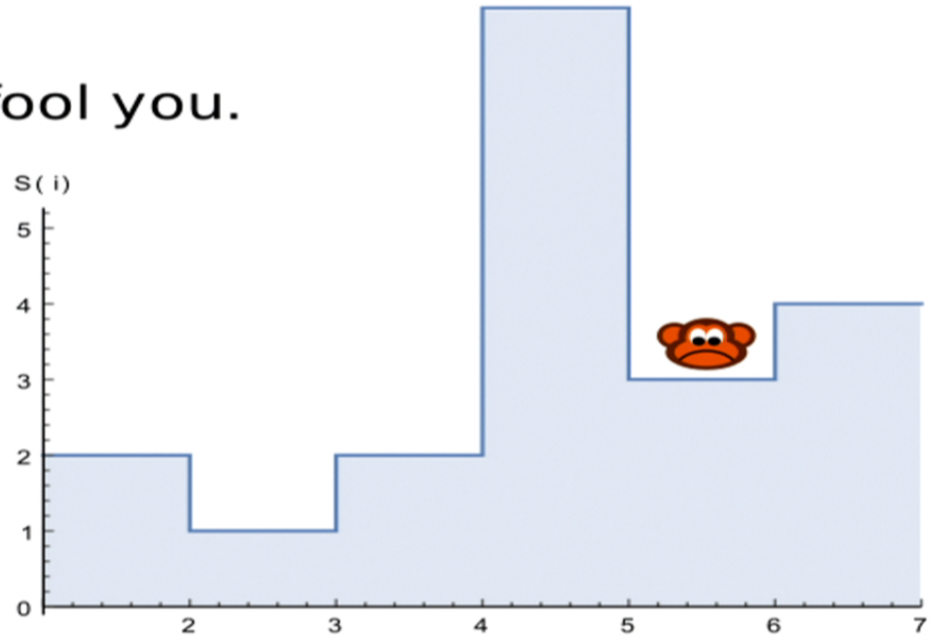
Other option

Monitor behavior of observables, if they ‘settle down’ the configuration is probably thermalized.

Thermalisation



Careful, local minima can fool you.

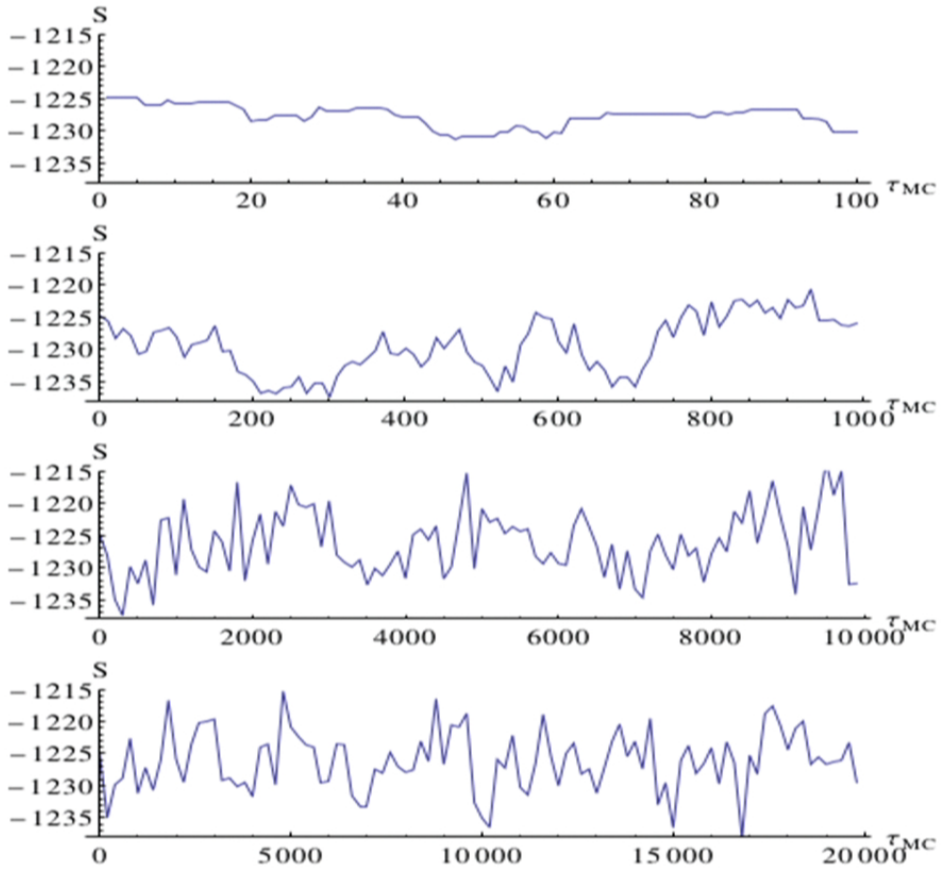


Autocorrelation

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Successive steps are correlated

We need to correct for this correlation when calculating errors.



Autocorrelation time

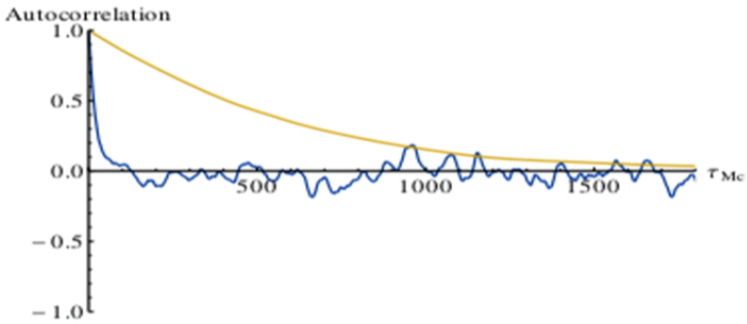
The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$\chi(t) = \frac{1}{N-t}\sum_{t'=0}^{N-t} S(t')S(t'+t)$$
$$- \frac{1}{N-t}\sum_{t'=0}^{N-t} S(t')\frac{1}{N-t}\sum_{t'=0}^{N-t} S(t'+t)$$

correlation after t steps with N measurements taken in total

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

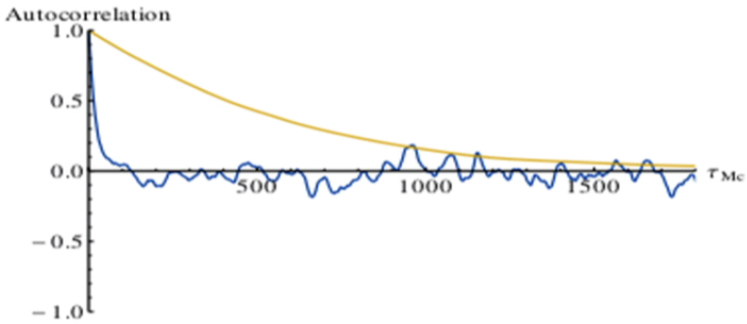
τ is the autocorrelation time



Autocorrelation time

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

$$\chi(t) = \frac{1}{N-t}\sum_{t'=0}^{N-t} S(t')S(t'+t)$$
$$- \frac{1}{N-t}\sum_{t'=0}^{N-t} S(t')\frac{1}{N-t}\sum_{t'=0}^{N-t} S(t'+t)$$



correlation after t steps with N measurements taken in total

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

τ is the autocorrelation time

Good Observables

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Very important in Monte Carlo. What are good observables?

- make sense (generally covariant)
- can be easily averaged over configurations
- do not take too long to measure
- physical interpretation

Good Observables

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Very important in Monte Carlo. What are good observables?

- make sense (generally covariant)
- can be easily averaged over configurations
- do not take too long to measure
- physical interpretation

Good Observables

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Very important in Monte Carlo. What are good observables?

- make sense (generally covariant)
- can be easily averaged over configurations
- do not take too long to measure
- physical interpretation

Good or bad observables?

- Two point function on the manifold
- Spectral dimension
- Curvature (at a point/ integrated)
- 3-Volume in time steps/ size of antichains
- hausdorff dimensions


e^{-S}
$S^3 \times \mathbb{R}$
$t_0 = 1$
$t_0 = 2$

Summary

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Markov Chain Monte Carlo

- sample space of geometries according to P
- converges (proven, for infinite process)

Move from configuration to configuration through small change.

Summary

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Markov Chain Monte Carlo

- sample space of geometries according to P
- converges (proven, for infinite process)

Move from configuration to configuration through small change.

Practical advice:

- check for thermalisation
- check for autocorrelation
- find good observables

Thank you for your attention

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Literature suggestions

- **Newman and Barkema, Monte Carlo Methods in statistical Physics**
  If you want a more thourough introduction to Monte Carlo methods in general
- **Ambjørn et.al. ,Quantum Geometry, A statistical field theory approach**
  Has a nice chapter explaining Monte Carlo for dynamical triangulations
- **Ambjørn et.al. , Nonperturbative Quantum Gravity (arXiv/1203.3591)**
  Not about Monte Carlo per se, but introduces the CDT Pachner moves and much more

Fixed Volume simulations

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

A computer can not sum over all possible volumes.

$$S_{4D} = -(\kappa_0 + 6\Delta)N_0 + \kappa_4(N_4^{(4,1)} + N_4^{(3,2)}) + \Delta(2N_4^{(4,1)} + N_4^{(3,2)})$$

Two options:

- $\kappa_4 \to \kappa_{4,crit}$ the closer the larger $\langle N_4 \rangle$
- add volume fixing term $\epsilon(N_4 - \bar{N}_4)^2$