16a) Example of Monte-Carlo algorithm

Metropolis algorithm

spin configuration $c_{n,i}$ $i = 1, \dots, N$

$$c_{n,i} = S_i$$

i) do local update at site i

$$c'_i = c_{n,i} + \delta c_i$$
$$c'_j = c_{nj} \text{ for } j \neq i$$

e.g. for the Ising model δc_i is a spin flip at site i

ii) choose a random # $x \in [0, 1]$

then

$$c_{n+1,i} = c_{n,i} \text{ if } e^{-\beta H(c') + \beta H(c)} < x$$

$$c_{n+1,i} = c'_i \text{ if } e^{-\beta H(c') + \beta H(c)} > x$$

If done for all lattice sites start again at the beginning

11 Monte Carlo simulations

In many fields of physics we have to evaluate multidimensional integrals

Examples: Lattice QCD
Statistical Mechanics
Green's function Monte-Carlo in solid state and nuclear physics

Riemann integration: # points is N^d for a d-dimensional integral

Monte Carlo simulation: Choose N points at random, then the error is $\sim \sqrt{N}$

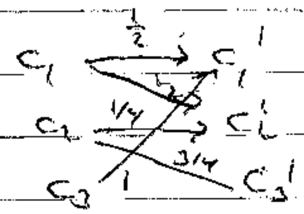
problem: Typically the integrand is negligible in most of its domain. We wish to choose the points mainly in the region where the integrand is large. This is the aim of Monte-Carlo algorithm's

Theorem: $\sum_{c'} T(c,c') = 1$

a state has to go somewhere

but $\sum_{c} T(c,c') \neq 1$ in general

example



We define $\rho_n(c)$ as the probability to find the configuration c after n steps.

Evolution $\rho_{n+1}(c') = \sum_c T(c,c')\,\rho_n(c)$

stationary solution: $\bar{\rho}(c') = \sum_c T(c,c')\,\bar{\rho}(c)$

Theorem: In a Markov process with detailed balance $\bar{\rho}(c) = e^{-\beta H(c)}$ is a stationary solution

Proof: sum over c' in detailed balance

$$e^{-\beta H(c')} = \sum_c T(c,c')\, e^{-\beta H(c)}$$

$$\left(\sum_c T(c',c) = 1\right)$$

This theorem is the basis of many Monte-Carlo algorithms. We have to construct a Markov chain that satisfies detailed balance.

Sometimes it is useful to have an evolution by a Hermitean matrix

Define $u_n(c) = \rho_n(c)\, e^{\frac{\beta}{2} H(c)}$

then $u_{n+1}(c') = \sum_c \underbrace{e^{-\frac{\beta}{2} H(c)}\, T(c,c')\, e^{\frac{\beta}{2} H(c')}}_{R(c,c')} u_n(c)$

$$R(c,c') = e^{-\frac{\beta}{2} H(c)}\, T(c,c')\, e^{\frac{\beta}{2} H(c')}$$

$$= e^{-\frac{\beta}{2} H(c)}\, e^{\beta H(c)}\, T(c',c)\, e^{-\beta H(c') + \frac{\beta}{2} H(c')}$$

$$= R(c',c)$$

R is Hermitean $\Rightarrow$ For $n \to \infty$ u_n converges to the eigenvector with the largest eigenvalue (if it is nondegenerate

$u_{eq}(c) = e^{-\beta H(c)/2}$ is an eigenvector of $R(c,c')$, corresponding to $\rho_{eq}(c) = e^{-\beta H(c)}$