Monte Carlo Methods
Convergence

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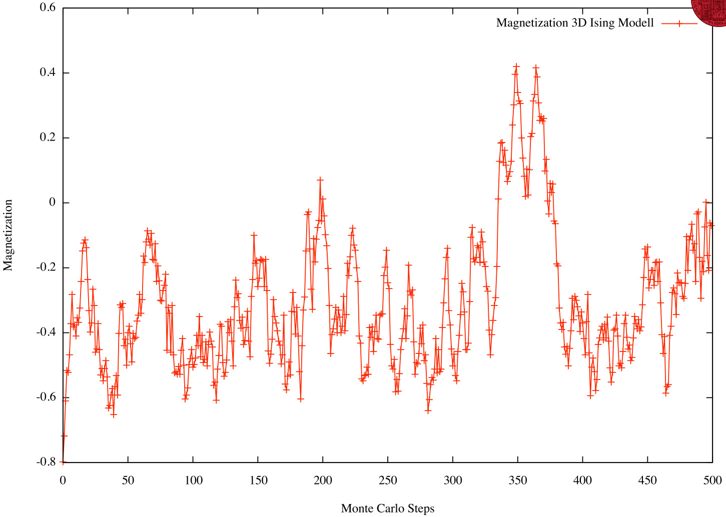
Magnetization 3D Ising Modell
Magnetization
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
50
100
150
200
250
300
350
400
450
500
Monte Carlo Steps

- What does this mean if we calculate the time average of an observable A, [...] by necessity can cover only a finite observation time?
- Let us consider the statistical error for n successive observations $A_i, i = 1, ..., n$:

$$\left\langle (\delta A)^2 \right\rangle = \left\langle \left[n^{-1} \sum_{i=1}^{n} (A_i - \langle A \rangle)^2 \right] \right\rangle \quad . \tag{1}$$

- In terms of the autocorrelation function for the observable A

$$\phi_A(t) = \frac{\langle A(0)A(t) \rangle - \langle A \rangle^2}{\langle A^2 \rangle - \langle A \rangle^2} \tag{2}$$

We define two characteristic correlation times.

- **Exponential autocorrelation time**
  - Typically we expect that (asymptotically, for large t) one gets an exponential behavior

$$\Phi_A(t) \propto \exp\left(-\frac{t}{\tau_{A,exp}}\right) \tag{3}$$

  - We do expect, though, that the complete expression involves a sum over several such terms; here we consider only the asymptotically most leading term with largest autocorrelation time.

- **Integrated autocorrelation time**

$$\tau_A^{int} = \int_0^\infty \phi_A(t)dt \quad . \tag{4}$$

- We can rewrite the statistical error as

$$\left\langle (\delta A)^2 \right\rangle \cong \frac{2\tau_A}{n\delta t} \left[\left\langle A^2 \right\rangle - \langle A \rangle^2 \right] \quad , \tag{5}$$

where δt is the time between observations, i.e., $n\delta t$ is the total observation time τ_{obs}.

- We notice that the error does not depend on the spacing between the observations but on the total observation time.
- Also the error is not the one which one would find if all observations were independent.
- The error is enhanced by the characteristic (integral) correlation time between configurations.
- Only an increase in the sample size and/or a reduction in the characteristic correlation time τ_A can reduce the error.

Critical Slowing Down

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- Problem: Critical Slowing Down
  - For local dynamics, the autocorrelation between successively generated configurations varies with the linear system size L as

$$\tau \propto L^z \tag{6}$$

with the dynamical critical exponent $z \neq 0$, while for those with non-local dynamics $z = 0$, i.e., a logarithmic behaviour can occur

- In the thermodynamic limit one finds for the intrinsic relaxation time: τ

$$\tau \sim \xi^z \sim (1 - \tau/\tau_c)^{-\nu z}$$

(Rule $\xi \leftrightarrow L$)

$$\Rightarrow \tau_{max} \sim L^z \;\; (T = T_c)$$

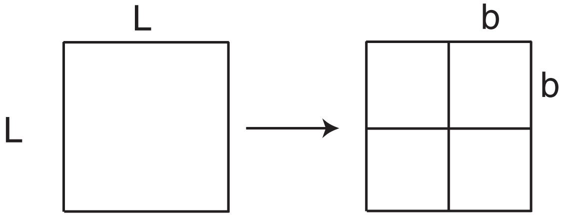
$$\begin{aligned} < (\delta M)^2 > \quad &= \quad \frac{2\tau_{max}}{t_{obs}} \left[< M^2 >_{T_c} - < |M| >^2_{T_c}\right] \\ &= \quad \frac{2\tau_{max}\chi\text{'}_{max} k_B T_c}{t_{obs} L^{\alpha}} \sim L^{z+\gamma/\nu-d}/t_{obs} \end{aligned}$$

since $L^{z+\gamma/\nu} \approx L^y$ $(d \leq 4)$ we have:
To raise the precision by a factor of 10 we need 10^y more computing time.

- Now that we know how the statistical error for an observable A depends on the finite observation time, we can ask for the dependence on the finite system size. For this we define

$$\Delta(n, L) = \sqrt{\left(\langle A^2 \rangle_L - \langle A \rangle_L^2\right) / n} \quad . \tag{7}$$

Here L is the linear dimension of the system. Note that we write $< . >_L$ for the average. This is meant as the average with respect to the finite system size. How does this error depend on L.



- Recall that for thermodynamic equilibrium, for a system of infinite size one observation suffices to obtain A.
- In other words, if $L \to \infty$ then $\Delta(n, L)$ must go to zero, regardless of n. Or, if we increase the system size then the effective number of observations should increase.
- Let L be the system size and L' the new one which we obtain by a scale factor b with $b > 1 : L' = bL$.
- The number of effective observations will change to $n' = b^{-d} n$ where d is the dimensionality.

- More formally we can express the idea by

$$\Delta(n, L) = \Delta(n', L') = \Delta(b^{-d} n, bL) \tag{8}$$

- We can work out this expression using the definition of Δ and find

$$\left\langle A^2 \right\rangle_L - \langle A \rangle_L^2 \propto L^{-x}, \quad 0 \leq x \leq d \quad . \tag{9}$$

- In the case where $x = d$ we call the observable A strongly self-averaging and in the cases $0 < x < d$, weakly self-averaging.
- As we increase L, b tends to a finite value, independent of L.