Statistical errors

$$I = \int_{-\infty}^{\infty} G(x) f_{\hat{\mathbf{x}}}(x)\, dx$$

$$\hat{\theta} = \frac{1}{N} \sum_{i=1}^{N} G(\hat{\mathbf{x}}_i), \qquad \langle \hat{\theta} \rangle = I$$

$$\sigma^2[\hat{\theta}] = \langle (\hat{\theta} - I)^2 \rangle$$

$$I = \hat{\theta} \pm \sigma[\hat{\theta}]$$

$$\sigma^2[\hat{\theta}] = \langle \left[\frac{1}{N} \sum_{i=1}^{N} (\hat{\mathbf{G}}_i - I) \right]^2 \rangle$$

$$= \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} < (\hat{\mathbf{G}}_i - I)(\hat{\mathbf{G}}_j - I) >$$

. . .

$$\sigma^2[\hat{\theta}] = \frac{\sigma^2[\hat{\mathbf{G}}]}{N}(2\tau_G + 1)$$

$$\tau_G = \sum_{k=1}^{N-1} \left(1 - \frac{k}{N}\right) \rho_G(k)$$

$$\rho_G(k) = \frac{\langle \hat{\mathbf{G}}_i \hat{\mathbf{G}}_{i+k} \rangle - I^2}{\sigma^2[\hat{\mathbf{G}}]}$$

If $\hat{\mathbf{x}}_i$ are independent, $\rho_G(k) = \delta_k$ and $\tau_G = 0$

$\rho_G(k)$ decays with k (exponentially)

Continuum time variable. $\delta t = 1$ MC

$$t_G = \tau_G \delta t = \sum_{k=1}^{N-1} \left(1 - \frac{k}{N}\right) \rho_G(k) \delta t \approx \int_0^{\infty} \rho_G(t)\, dt$$

$$\sigma^2[\hat{\mathbf{G}}] = \frac{\sigma^2[\hat{\mathbf{G}}]}{N}\left(2\frac{t_G}{\delta t}+1\right)$$

One measures after M Monte-Carlo steps.$\Delta t = M\delta t$

$$\sigma^2[\hat{\mathbf{G}}] = \frac{\sigma^2[\hat{\mathbf{G}}]}{N}\left(2\frac{t_G}{\Delta t}+1\right) = \frac{\sigma^2[\hat{\mathbf{G}}]}{N}\left(2\frac{\tau_G}{M}+1\right) =$$

Minimize $\sigma^2[\hat{\mathbf{G}}]$ for constant computer time.

t_1 measure time, t_2 1 MC time. Minimize:

$$\frac{1}{N}\left(2\frac{\tau_G}{M}+1\right)$$

with the constrain:

$$Nt_1 + NMt_2 = t \ \ \text{constante}$$

Solution:

$$M = \sqrt{\frac{2\tau_G t_1}{t_2}}$$

So that

$$\sigma^2[\hat{\mathbf{G}}] = \frac{\sigma^2[\hat{\mathbf{G}}]}{N}\left(1+\sqrt{\frac{2t_2\tau_G}{t_1}}\right)$$

$$\frac{\frac{M}{K}t_1}{Mt_2} = \sqrt{\frac{t_1}{2\tau_G t_2}} \neq 1!!!!$$

Near a critical point $\sigma^2[\hat{\mathbf{G}}]$ diverges.

Try to chose an algorithm that minimizes τ_G

Intrinsic correlation time of the algorithm:

$$\tau = \max_G \tau_G$$

Rule: chose parameters such that acceptance $\approx 50\%$

Why?

In most algorithms τ_G also diverges near a critical point.

If we make the (exponential) approximation:

$$\rho_G(k) = [\rho_G(1)]^k$$

then the correlation time is

$$\tau_G = \sum_{k=1}^{M-1} \left(1 - \frac{k}{M}\right) \rho_G(k) = \frac{\rho_G(1)}{1 - \rho_G(1)}$$

One can prove the (exact) formula:

$$\rho_G(1) = 1 - \frac{1}{2\sigma^2[G]} \int dx \int dy\, h(x|y) g(x|y) f_{\hat{\mathbf{x}}}(y) [G(x) - G(y)]^2$$

For the Metropolis algorithm applied to the Ising model, one gets for the magnetization m:

$$[m(x) - m(y)]^2 = \frac{4}{N^2}$$

Therefore

$$\rho_m(1) = 1 - \frac{2\epsilon}{N^2\sigma^2[m]} = 1 - \frac{2\epsilon kT}{N\chi_T}$$

(ϵ is the average acceptance probability). Therefore, we arrive at:

$$t_m = \frac{\tau_m}{N} = \frac{\chi_T}{2\epsilon kT}$$

and t_m diverges as $\left|1 - \frac{T}{T_c}\right|^\gamma$, in this approximation. In general, one expects the behavior:

$$t_G \sim \left|1 - \frac{T}{T_c}\right|^{z_G}$$

for the Metropolis algorithm applied to the Ising model, it is $z_m \approx 2.2$.

Clever algorithms have been devised to overcome this *critical slowing down* of the Montecarlo simulation. The best performing ones are the collective updates: hybrid Montecarlo and cluster algorithms (Wolff and Swendsen-Wang).

Another important improvement is that of extrapolation techniques (Ferrenberg-Swendsen) that allow one to combine simulations at different temperatures in order to obtain smoot curves as a function of temperature.

Thermalization

$$\lim_{n \to \infty} f_{\hat{\mathbf{x}}_n}(x) = f_{\hat{\mathbf{x}}}(x)$$

Discard the first M_0 values generated for $\hat{\mathbf{x}}$.

$$< G(n) >= \int_{-\infty}^{\infty} f_{\hat{\mathbf{x}}_n}(x) G(x)\, dx$$

Non-linear relaxation function:

$$\rho_G^{NL}(n) = \frac{\langle G(n) \rangle - \langle G \rangle}{\langle G(0) \rangle - \langle G \rangle}$$

Non-lineal relaxation time:

$$\tau_G^{NL} = \sum_{n=0}^{\infty} \rho_G^{NL}(n)$$

$$\tau^{NL} = \max_G \tau_G^{NL}$$

How do we know we are in the steady state?

We never know for sure!!!

But we can check:

$$\langle q(x|y) \rangle_{x,y} = 1$$

average over x in the supposed steady state

average over proposals y.

Proof:

$$\begin{aligned}
\langle q(x|y)\rangle_{x,y} &= \int dy \int dx f_{\hat{\mathbf{x}}}(x) g(y|x) q(y|x) \\
&= \int dy \int dx f_{\hat{\mathbf{x}}}(x) g(y|x) \frac{g(x|y) f_{\hat{\mathbf{x}}}(y)}{g(y|x) f_{\hat{\mathbf{x}}}(x)} \\
&= \int dy \left[\int dx g(x|y)\right] f_{\hat{\mathbf{x}}}(y) \\
&= \int dy f_{\hat{\mathbf{x}}}(y) = 1
\end{aligned}$$

If $g(x|y) = g(y|x)$ and $f_{\hat{\mathbf{x}}}(x) = \frac{\exp(-\beta\mathcal{H}(x))}{\mathcal{Z}}$ then

$$\langle \exp\left(-\beta\left[\mathcal{H}(y) - \mathcal{H}(x)\right]\right)\rangle = \langle \exp\left(-\beta\Delta\mathcal{H}\right)\rangle = 1$$

necessary condition to be verified at the equilibrium state.