ESTIMATE OF THE AUTOCORRELATION FUNCTION

The autocorrelation function in equilibrium is

$$C_f(|n-m|) = \langle f(X_n) f(X_m) \rangle_{MC,eq} - F^2 \qquad F = \langle f \rangle_\pi$$

where $\langle \ \rangle_{MC,eq}$ is the average over the MC repetitions in which we start from a "typical" configuration.

We can rewrite it (n is dummy)

$$C_f(k) = \langle f(X_n) f(X_{n+k}) \rangle_{MC,eq} - F^2 \qquad k \geq 0$$

Of course we estimate F with $\bar{f} = \frac{1}{N+1} \sum_{k=0}^{N} f_k$

(sample mean)

$$\langle f(X_n) f(X_{n+k}) \rangle_{MC,eq} = \frac{1}{N-k+1} \sum_{n=0}^{N-k} f(X_n) f(X_{n+k})$$

Example: $N=10$ (11 data). We set $F = \frac{1}{11} \sum_{k=0}^{10} f_k \qquad f_i = f(X_i)$

$$C(0) = \frac{1}{11} \sum_{n=0}^{10} f_n^2 - F^2$$

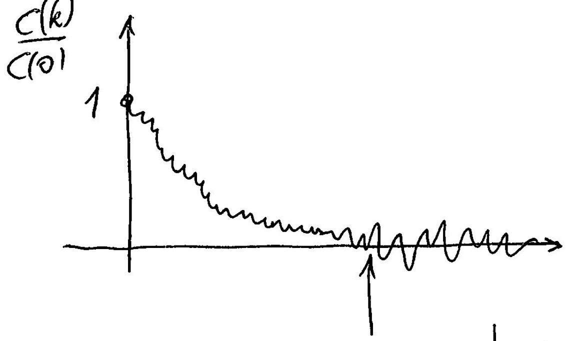
$$C(1) = \frac{1}{10} \sum_{n=0}^{9} f_n f_{n+1} - F^2$$

$$C(2) = \frac{1}{9} \sum_{n=0}^{8} f_n f_{n+2} - F^2$$

$$C(3) = \frac{1}{8} \sum_{n=0}^{7} f_n f_{n+3} - F^2$$

etc.

Typical graph



t_{max} : here $C(k)$ starts to fluctuate around zero

Compute τ_{int} as $\frac{1}{2} + \sum_{k=1}^{t_{max}} C(k) = \tau_{int}$

There is no point in summing additional values of $C(k)$: in $C(k)$ for $k > t_{max}$ there is only noise and no signal