Detailed Balance for Metropolis Monte Carlo method

Probability distribution on $\{\vec{\sigma}\}$: $P(\vec{\sigma}, t)$

"Master Equation" $\frac{\partial P(\sigma,t)}{\partial t} = \sum_{\sigma'} \{ \underbrace{W_{\sigma' \to \sigma} P(\sigma', t)}_{\text{enter state } \sigma} - \underbrace{W_{\sigma \to \sigma'} P(\sigma, t)}_{\text{leave state } \sigma} \}$

$W_{\sigma \to \sigma'}$ = rate of transitions to $\vec{\sigma}'$ given initial state $\vec{\sigma}$

Equilibrium: distribution $P_{eq}(\vec{\sigma})$ independent of time t

Sufficient condition for $\frac{\partial P}{\partial t} = 0 \Rightarrow W_{\sigma' \to \sigma} P_{eq}(\sigma') = W_{\sigma \to \sigma'} P_{eq}(\sigma)$

"Detailed Balance" (equal net rates $\sigma' \to \sigma$ and $\sigma \to \sigma'$)

$\therefore$ need $\frac{W_{\sigma' \to \sigma}}{W_{\sigma \to \sigma'}} = \frac{P_{eq}(\sigma)}{P_{eq}(\sigma')} = \frac{e^{-\beta E(\sigma)}/Z}{e^{-\beta E(\sigma')}/Z} = e^{-\beta(E(\sigma) - E(\sigma'))}$

Note: $W_{\sigma \to \sigma'}$ contains two factors : $W_{\sigma \to \sigma'} = F_{\sigma \to \sigma'} P_{\sigma \to \sigma'}$

1) Attempt frequency $F_{\sigma \to \sigma'}$ given initial state σ

2) Acceptance probability given that $\sigma \to \sigma'$ has been attempted

Metropolis: $F_{\sigma \to \sigma'} = F_{\sigma' \to \sigma}$ $\forall \sigma, \sigma'$ $\Rightarrow P_{\sigma' \to \sigma} / P_{\sigma' \to \sigma} = P_{eq}(\sigma) / P_{eq}(\sigma')$

Glauber: Single spin flip dynamics: choose spin σ_k flip $\to -\sigma_k$

accept if random number $r \in (0,1)$ is $r < e^{-\beta \Delta E}$, else reject

note: Sequential update can violate detailed balance