Simple sampling

Configurations are generated with a uniform probability (density)

$$\langle A \rangle \approx \frac{\sum_i B(X_i) A(X_i)}{\sum_i B(X_i)}$$

where X_i are configurations that we have generated. A is the observable and B the weight factor; in our context mostly the Boltzmann factor.

Problem: Typically B only has a significant amplitude for a very small fraction of the configurations.

Importance sampling (achieved by using a Markov chain)

Configurations X_i are generated with a probability (density) proportional to $B(X_i)$. We get

$$\langle A \rangle \approx \frac{1}{N} \sum_{i=1}^{N} A(X_i)$$

(Here we assume that sufficient configurations at the beginning of the chain are discarded)

Generalization: "Reweighting"

We generate configurations with a probability (density) proportional to $B_0(X_i)$. Now we like to get expectation values of observables A with respect to weight factors B which are in some sense close to B_0

$$\langle A \rangle_B \approx \frac{\sum_i [B(X_i)/B_0(X_i)] A(X_i)}{\sum_i [B(X_i)/B_0(X_i)]}$$

Acctually known for a long time; Most researchers just did not aspect that it could have useful applications. Became popular with

Alan M. Ferrenberg and Robert H. Swendsen
New Monte Carlo technique for studying phase transitions
Phys. Rev. Lett. 61, 2635
Citing articles (1658) , Jun 17 11:28:59 CEST 2015
Erratum: Phys. Rev. Lett. 63, 1658

Simple example: We generate configurations of the ϕ^4 model with a Boltzmann factor corresponding to $\kappa = \kappa_0$ and $\lambda = \lambda_0$

Now we like to compute expectation values of observables at fixed λ for various values of κ in the neighbourhood of κ_0.

$$\frac{B([\phi])}{B_0([\phi])} = \exp(-S(\kappa, \lambda_0, [\phi]) + S(\kappa_0, \lambda_0, [\phi]) =$$

$$\exp\left(2[\kappa - \kappa_0] \sum_x \sum_\mu \phi_x \phi_{x+\hat{\mu}}\right)$$