Monte Carlo Methods - Fall 2013/14

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Exercise Nr. 12

Discussion on February 5, after the lecture

34) Hopping Parameter Expansion I

In the lecture you have learned about the hopping parameter expansion, i.e. the high temperature expansion in $\kappa \ll 1$. The partition function is expanded as follows

$$\begin{aligned}
\mathcal{Z} &= \int \prod_x \left\{ d\phi(z) e^{-u(\phi(z))} \right\} \prod_{\langle x,y \rangle} e^{2\kappa\phi(x)\phi(y)} \\
\prod_{\langle x,y \rangle} e^{2\kappa\phi(x)\phi(y)} &= \prod_{\langle x,y \rangle} \left\{ 1 + 2\kappa\phi(x)\phi(y) + \frac{1}{2!}(2\kappa)^2(\phi(x)\phi(y))^2 + \dots \right\} \\
&= \sum_{\mathcal{G}} (2\kappa)^{L(\mathcal{G})} c(\mathcal{G}) \prod_{b \in \mathcal{G}} [\phi(x_b)\phi(y_b)]
\end{aligned}$$

where the last expression sums over all graphs $\mathcal{G}$ of order $(2\kappa)^{L(\mathcal{G})}$, characterized by the number of bonds $L(\mathcal{G})$, and the vertices x_b, y_b that touch the bond $b \in \mathcal{G}$. Show that the above expansion only admits closed loops, which can visit sites several times. Show also that the coefficients $c(\mathcal{G})$ are given by $c(\mathcal{G}) = \prod_{\langle x,y \rangle} \frac{1}{m(x,y)!}$ with $m(x,y)$ the multiplicity of the bonds.

In the partition function, for given potential $u(\phi) = \phi^2 + \lambda(\phi^2 - 1)^2 - \lambda$, the integrals $\int d\phi(z)\phi^k e^{-u(\phi(z))}$ have to be carried out at each site z. They also show up in the one-point expectation values

$$\gamma_k \equiv \langle \phi^k \rangle_1 = \frac{1}{Z_0} \int d\phi \, \phi^k e^{-u(\phi)},$$

where $Z_0 = \int d\phi e^{-u(\phi)}$ is the one-point partition function at $\kappa = 0$ (notice that the full partition function at $\kappa = 0$ is given by $\mathcal{Z}_0 = Z_0^V$, with V the number of lattice sites). Explain why $\gamma_{2n+1} = 0$.

Show that the partition function can be rewritten as

$$\mathcal{Z} = \mathcal{Z}_0 \sum_{\mathcal{G}} (2\kappa)^{L(\mathcal{G})} c(\mathcal{G}) \prod_{z \in \mathcal{G}} \gamma_{N(z)},$$

with $N(z)$ the number of bonds in $\mathcal{G}$ touching site z. Calculate the explicit expansion of $\mathcal{Z}$ in a finite lattice volume V in d dimensions, up to order κ^4, in terms of the coefficients γ_k, i.e. consider each of the five graphs given in the lecture. Take care when counting the available bonds on the lattice for each graph, they are not proportional to Vd for extended graphs! Note also that there is a disconnected graph at order κ^4.

35) Hopping Parameter Expansion II

The hopping parameter expansion for the ϕ^4 theory will depend on the λ-dependent coefficients $z_{2n}(\lambda)$:

$$\mathcal{Z}(\lambda) = \mathcal{Z}_0(\lambda)\left\{1 + z_2(\lambda)\kappa^2 + z_4(\lambda)\kappa^4 \ldots\right\}.$$

Similarly, the negative free energy density defined by

$$-f = \Omega(\kappa, \lambda) \equiv \frac{1}{V}\log \mathcal{Z}(\kappa, \lambda) - \log \mathcal{Z}_0(\lambda)$$

can be expressed by the coefficients c_{2n}:

$$\Omega(\kappa, \lambda) = \sum_{n=0}^{n_{\max}} c_{2n}(\lambda)\kappa^{2n}.$$

Now consider the potential $u(\phi)$ for the free case $\lambda = 0$ and in the Ising limit $\lambda = \infty$. Calculate Z_1 and γ_{2k} for both cases. Also calculate the coefficients $c_2(\lambda = 0)$ and $c_4(\lambda = 0)$ for the free case.

In general, the critical point can be estimated from the radius of convergence (if all coefficients are positive):

$$\kappa_c(\lambda) = \lim_{n\to\infty}\sqrt{\frac{c_{2n}(\lambda)}{c_{2n+2}(\lambda)}}$$

Check whether it is a good idea to esimate the value of $\kappa_c(0)$, which we know is $1/2d$, from the lowest coefficients $c_2(0)$ and $c_4(0)$.

36) Monte Carlo for ϕ^4

Simulate the one-component ϕ^4 model via the Metropolis algorithm (similar to the one for the anharmonic oscillator) and approach the limit $\lambda \to \infty$. Check that you find κ_c in accordance with the Ising model value, by measuring the susceptibility of the modulus: $\chi = \langle\phi^2\rangle - \langle|\phi|\rangle^2$.