Contents of Lecturenotes IV

The $O(3)$ σ Model and the Heat Bath Algorithm

We give an example of a model with a continuous energy function. The $2d$ version of the model is of interest to field theorists because of its analogies with the four-dimensional Yang-Mills theory. In statistical physics the d-dimensional model is known as the Heisenberg ferromagnet. Expectation values are calculated with respect to the partition function

$$Z = \int \prod_i ds_i \; e^{-\beta E(\{s_i\})} \; . \tag{1}$$

$$\text{The spins } \; \vec{s}_i = \begin{pmatrix} s_{i,1} \\ s_{i,2} \\ s_{i,3} \end{pmatrix} \; \text{ are normalized to } \; (\vec{s}_i)^2 = 1 \tag{2}$$

$$\text{and the measure } ds_i \text{ is defined by } \int ds_i = \frac{1}{4\pi} \int_{-1}^{+1} d\cos(\theta_i) \int_0^{2\pi} d\phi_i \; , \tag{3}$$

where the polar (θ_i) and azimuth (ϕ_i) angles define the spin s_i on the unit sphere.

The energy is

$$E \;=\; \sum_{\langle ij \rangle} (1 - \vec{s}_i \vec{s}_j) \;, \tag{4}$$

where the sum goes over the nearest neighbor sites of the lattice. We would like to update a single spin $\vec{s}$. The sum of its $2d$ neighbors is

$$\vec{S} = \vec{s}_1 + \vec{s}_2 + \ldots + \vec{s}_{2d-1} + \vec{s}_{2d} \;.$$

Hence, the contribution of spin $\vec{s}$ to the action is $2d - \vec{s}\vec{S}$. We propose a new spin $\vec{s}^{\,\prime}$ with the measure (3) by drawing two uniformly distributed random numbers

$$\phi^r \in [0, \pi) \;\; \text{for the azimuth angle and}$$
$$\cos(\theta^r) = x^r \in [-1, +1) \;\; \text{for the cosine of the polar angle.}$$

This defines the probability function $f(\vec{s}^{\,\prime}, \vec{s})$ of the Metropolis process, which

accepts the proposed spin $\vec{s}\,'$ with probability

$$w(\vec{s} \to \vec{s}\,') \;=\; \begin{cases} 1 & \text{for} \quad \vec{S}\vec{s}\,' > \vec{S}\vec{s}, \\ e^{-\beta(\vec{S}\vec{s}-\vec{S}\vec{s}\,')} & \text{for} \quad \vec{S}\vec{s}\,' < \vec{S}\vec{s}. \end{cases}$$

If sites are chosen with the uniform probability distribution $1/N$ per site, where N is the total number of spins, it is obvious that the procedure fulfills detailed balance. It is noteworthy that the procedure remains valid when the spins are chosen in the systematic order $1, \ldots, N$, then $1, \ldots, N$ again, and so on. Balance still holds, whereas detailed balance is violated (exercise).

The heath bath algorithm

Repeating the Metropolis algorithm again and again for the same spin $\vec{s}$ leads to the equilibrium distribution of this spin, which reads

$$P(\vec{s}\,'; \vec{S}) = \text{const}\, e^{\beta \vec{S}\vec{s}\,'} \quad \text{with} \quad \int P(\vec{s}\,'; \vec{S})\, ds' = 1 \; .$$

One would prefer to choose $\vec{s}^{\,\prime}$ directly with the probability

$$W(\vec{s} \to \vec{s}^{\,\prime}) \;=\; P(\vec{s}^{\,\prime}; \vec{S}) \;=\; \text{const}\, e^{\beta\, \vec{s}^{\,\prime}\, \vec{S}} \;,$$

as $\vec{s}^{\,\prime}$ is then immediately Boltzmann distributed with respect to its neighbor spins. The algorithm, which creates this distribution, is called the **heat bath algorithm.**

Implementation of this algorithm becomes feasible when the energy function is sufficiently simple to allow for an explicit calculation of the probability $P(\vec{s}^{\,\prime}; \vec{S})$.

This is an easy task for the $O(3)$ σ-model. Let

$$\alpha = \text{angle}(\vec{s}^{\,\prime}, \vec{S}), \quad x = \cos(\alpha) \;\; \text{and} \;\; S = \beta |\vec{S}| \;.$$

For $S = 0$ a new spin $\vec{s}^{\,\prime}$ is simply obtained by random sampling. We assume in the following $S > 0$. The Boltzmann weight becomes $\exp(xS)$ and the normalization

constant follows from

$$\int_{-1}^{+1} dx\, e^{xS} \;=\; \frac{2}{S}\,\sinh(S)\;.$$

Therefore, the desired probability is

$$P(\vec{s}\,';\vec{S}) \;=\; \frac{S}{2\sinh(S)}\,e^{xS} \;=:\; f(x)$$

and the method of the first lecture can be used to generate events with the probability density $f(x)$. With

$$y = F(x) = \int_{-1}^{x} dx'\, f(x') = \int_{-1}^{x} dx'\, \frac{S}{2\sinh(S)}\,e^{x'S} = \frac{\exp(+xS) - \exp(-S)}{2\,\sinh(S)}$$

a uniformly distributed random number $y^r \in [0,1)$ translates into

$$x^r = \cos\alpha^r = \frac{1}{S}\ln\left[\exp(+S) - y^r\,\exp(+S) + y^r\,\exp(-S)\right]\,. \tag{5}$$

Finally, one has to give $\vec{s}^{\,\prime}$ a direction in the plane orthogonal to S. This is done by choosing a random angle β^r uniformly distributed in the range $0 \le \beta^r < 2\pi$. Then, $x^r = \cos\alpha^r$ and β^r completely determine $\vec{s}^{\,\prime}$ with respect to $\vec{S}$. Before storing $\vec{s}^{\,\prime}$ in the computer memory, we have to calculate coordinates of $\vec{s}^{\,\prime}$ with respect to a Cartesian coordinate system, which is globally used for all spins of the lattice. This is achieved by a linear transformation. We define

$$\cos\theta = \frac{S_3}{S},\ \sin\theta = \sqrt{1-\cos^2\theta},\ \cos\phi = \frac{S_1}{S\,\sin\theta}\quad\text{and}\quad \sin\phi = \frac{S_2}{S\,\sin\theta}\,.$$

Unit vectors of a coordinate frame K', with $\hat{z}$ in the direction of $\hat{S}$ and $\hat{y}$ in the $x-y$ plane, are then defined by

$$\hat{z}' = \begin{pmatrix} \sin\theta\,\cos\phi \\ \sin\theta\,\sin\phi \\ \cos\theta \end{pmatrix}, \quad \hat{x}' = \begin{pmatrix} \cos\theta\,\cos\phi \\ \cos\theta\,\sin\phi \\ -\sin\theta \end{pmatrix} \quad \text{and} \quad \hat{y}' = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix}.$$

Expanding $\vec{s}^{\,\prime}$ in these units vectors, we have

$$\vec{s}^{\,\prime} = \sin\alpha^r\,\cos\beta^r\,\hat{x}^{\,\prime} + \sin\alpha^r\sin\beta^r\,\hat{y} + \cos\alpha^r\,\hat{z}^{\,\prime}$$

$$= \begin{pmatrix} \sin\alpha^r\cos\beta^r\,\cos\theta\,\cos\phi - \sin\alpha^r\sin\beta^r\,\sin\phi + \cos\alpha^r\,\sin\theta\,\cos\phi \\ \sin\alpha^r\cos\beta^r\,\cos\theta\,\sin\phi + \sin\alpha^r\cos\beta^r\,\cos\phi + \cos\alpha^r\,\sin\theta\,\sin\phi \\ -\sin\alpha^r\cos\beta^r\,\sin\theta + \cos\alpha^r\,cos\theta \end{pmatrix} \qquad (6)$$

and the three numbers of the column vector (6) are stored in the computer.

Self-Averaging Illustration for the $2d$ $O(3)$ model

We compare the peaked distribution function of the mean action per link for different lattice sizes. The property of **self-averaging** is observed: The larger the lattice, the smaller the confidence range. The other way round, the peaked distribution function is very well suited to exhibit observables for which self-averaging does not work, as for instance encountered in spin glass simulations.

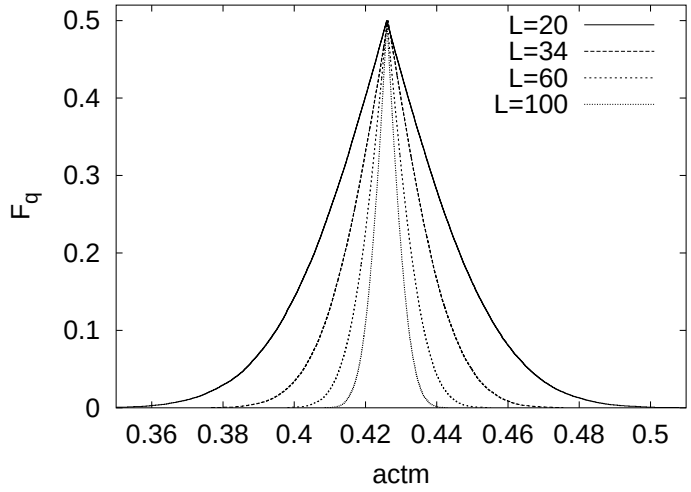

Figure 1: $O(3)$ σ-model at $\beta = 1.1$ (assignments a0304_06 and a0304_08).