Monte Carlo Methods - Fall 2017/18

Universität Bielefeld

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Exercise Nr. 8

Discussion on January 8th, 14:00-15:00

22) 2-dimensional Ising Model, local update *(6 points)*

Implement the Metropolis or heatbath algorithm for the 2-dimensional Ising model by modifying the Ising chain to higher dimensions. It will be advantegous for later applications to construct a lattice container and a method to implement the nearest neighbor relation for any dimension. Measure the Binder cumululant $B_L(\beta)$ as a function of the inverse temperature β for three different lattice volumes, 8×8, 16×16 and 32×32.

23) Cluster algorithm *(8 points)*

Implement the cluster algorithm for the Ising model as discussed in the lecture and compare with the local update by again measuring the Binder cumulant.

24) Integrated autocorrelation time *(6 points)*

Compare the Cluster algorithm and the local update by studying the autocorrelation function for some observable $\mathcal{O}$:

$$C_{\mathcal{O}}(t) = \frac{\langle \mathcal{O}_i \mathcal{O}_{i+t} \rangle - \langle \mathcal{O}_i \rangle^2}{\langle \mathcal{O}_i^2 \rangle - \langle \mathcal{O}_i \rangle^2}$$

where $\mathcal{O}_i = \mathcal{O}\{C_i\}$ is the evaluation of the observable of the ith step of the Markov chain. The decay of the autocorrelation function is usually given by a sum of exponential decays:

$$C_{\mathcal{O}}(t) \propto \sum_k c_k(\mathcal{O}) e^{-t/\tau_k^{(\mathcal{O})}}$$

with $\tau_i^{(\mathcal{O})}$ the autocorrelation time, which is specific to the observable. One can define the exponential autocorrelation time

$$\tau_{\text{exp}}^{(\mathcal{O})} = \lim_{t\to\infty} \sup \frac{t}{-\log C_{\mathcal{O}}(t)},$$

which is the relaxation time of the slowest mode in the Monte Carlo update with respect to $\mathcal{O}$. The statistical error of $\mathcal{O}$ is underestimated by the standard error $\sqrt{\text{Var}(\mathcal{O})/\text{N}}$, and it is controlled by the integrated correlation time

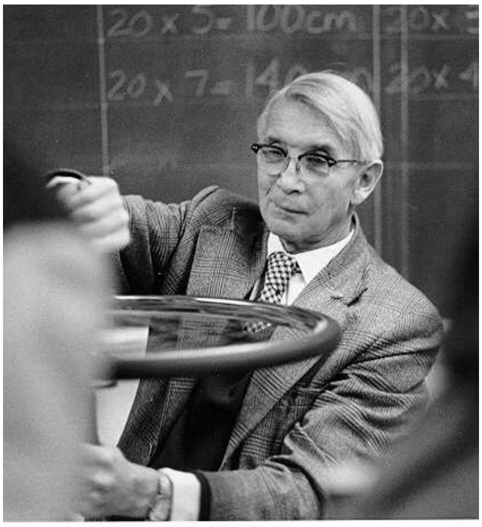
$$\tau_{\text{int}}^{(\mathcal{O})} = \frac{1}{2} + \sum_{t=1}^{N} C_{\mathcal{O}}(t)$$

which gives a better estimate for the error: $\Delta\mathcal{O} = \sqrt{\text{Var}(\mathcal{O})/\text{N}^*}$ with $N^* = N/(2\tau_{\text{int}}^{(\mathcal{O})})$.

Determine the integrated autocorrelation time and the improved error of the energy density $e = \frac{\langle E \rangle}{N}$ both for the local update and the Cluster algorithm, for three different lattice volumes 8×8, 16×16 and 32×32, at the critical inverse temperature $\beta_c = \log(1+\sqrt{2})/2$ (with $J = 1, H = 0$).

Ernst Ising

(May 10, 1900, - May 11, 1998) was a German physicist.



He is best remembered for the development of the Ising model. He was a professor of physics at Bradley University until his retirement in 1976. After school, he studied physics and mathematics at the University of Göttingen and University of Hamburg. In 1922, he began researching ferromagnetism under the guidance of Wilhelm Lenz. He earned a Ph.D in physics from the University of Hamburg in 1924. His doctoral thesis studied a problem suggested by his teacher, Wilhelm Lenz. He investigated the special case of a linear chain of magnetic moments, which are only able to take two positions, "up" and "down," and which are coupled by interactions between nearest neighbors. Mainly through following studies by Rudolf Peierls, Hendrik Kramers, Gregory Wannier and Lars Onsager the model proved to be successful explaining phase transitions between ferromagnetic and paramagnetic states.

After earning his doctorate, Ernst Ising worked for a short time in business before becoming a teacher, in Salem, Strausberg and Crossen, among other places. In 1930, he married the economist Dr. Johanna Ehmer (born February 2, 1902). As a young German-Jewish scientist, Ising was barred from teaching and researching when Hitler came to power in 1933. In 1934, he found a position, first as a teacher and then as headmaster, at a Jewish school in Caputh near Potsdam for Jewish students who had been thrown out of public schools. Ernst and his wife Dr. Johanna Ising, née Ehmer, lived in Caputh near the famous summer residence of the Einstein family. In 1938, the school in Caputh was destroyed by the Nazis, and in 1939 the Isings fled to Luxembourg, where Ising earned money as a shepherd and railroad worker. After the German Wehrmacht occupied Luxembourg, Ernst Ising was forced to work for the army. In 1947, the Ising family emigrated to the United States. Though he became Professor of Physics at Bradley University in Peoria, Illinois, he never published again. Ising died at his home in Peoria in 1998, just one day after his 98th birthday.

The Ising model is defined on a discrete collection of variables called spins, which can take on the value 1 or -1. The spins S_i interact in pairs, with energy that has one value when the two spins are the same, and a second value when the two spins are different. The energy of the Ising model is defined to be $E = -\sum_{ij} J_{ij} S_i S_j$, where the sum counts each pair of spins only once. Notice that the product of spins is either +1 if the two spins are the same (aligned), or -1 if they are different (anti-aligned). J is half the difference in energy between the two possibilities. Magnetic interactions seek to align spins relative to one another. Spins become randomized when thermal energy is greater than the strength of the interaction. For each pair, if $J_{ij} > 0$ the interaction is called ferromagnetic, if $J_{ij} < 0$ the interaction is called antiferromagnetic, and if $J_{ij} = 0$ the spins are noninteracting. A ferromagnetic interaction tends to align spins, and an antiferromagnetic tends to antialign them. The spins can be thought of as living on a graph, where each node has exactly one spin, and each edge connects two spins with a nonzero value of J. If all the Js are equal, it is convenient to measure energy in units of J. Then a model is completely specified by the graph and the sign of J. The antiferromagnetic one-dimensional Ising model has the energy function: $E = \sum_i S_i S_{i+1}$, where i runs over all the integers. This links each pair of nearest neighbors.

In his 1925 PhD thesis, Ising solved the model for the 1D case. In one dimension, the solution admits no phase transition. On the basis of this result, he incorrectly concluded that his model does not exhibit phase behaviour in any dimension. It was only in 1949 that Ising knew the importance his model attained in scientific literature, 25 years after his Ph.D thesis. Today, each year, about 800 papers are published that use the model to address problems in such diverse fields as neural networks, protein folding, biological membranes and social behavior.

[from http://en.wikipedia.org/wiki/Ernst_Ising]