Lattice Gauge Theory - Fall 2017 ETH Zürich

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Exercise Nr. 1

Discussion on September 26th, 14:45

1) Literature

Read the article by M. Creutz and B. Freedman (Annals of Physics 132, 1981) on the statistical approach to quantum mechanics. After reading in particular section III, please write down in your own words:

- what *importance sampling* is,
- what the *detailed balance condition* is,
- how the *Metropolis algorithm* works and how it is implemented.

2) Metropolis Algorithm in Statistical Mechanics

Try to implement the Metropolis algorithm in your favorite programming language for the 2-dimensional Ising model and verify that the critical coupling that you evaluate with the Monte Carlo program is close to the analytic solution given by L. Onsager: $T_c = 2J/\log(1+\sqrt{2})$ (Phys. Rev. 65, 1944). The Ising model Hamiltonian is given by

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

where $\langle i,j \rangle$ denotes the nearest neighbors on the planar square lattice and the spin degrees of freedom $\sigma_i \in \{-1,+1\}$, $i = 1, \ldots N = N_s \times N_s$ can only take two values (+ for up, − for down) and N_s is the extension in lattice units in each direction. The partition function is hence

$$\mathcal{Z} = \sum_{\{\sigma\}} \exp(-\beta H)$$

with $\beta = 1/T$ the inverse temperature. Due to the lack of other terms in the Hamiltonian, we can set $J = 1$ in the simulation and the nearest neighbor coupling is controlled solely by β.

The center piece of the Monte Carlo simulation is the *Metropolis acceptance test* which flips the sign of a spin with a probability min(1,exp($-\beta\Delta_E$)), where Δ_E is the energy difference induced by the spin flip according to the Hamiltonian H. The pseudo-code for the Metropolis algorithm is:

procedure `markov-ising`
input $\{\sigma_1, \ldots \sigma_N\}$, E
$k \leftarrow \text{nran}(1, N)$
$h \leftarrow \sum_l \sigma_{\text{Nbr}(l,k)}$
$\Delta_E \leftarrow 2h\sigma_k$
if (ran(0,1) < exp($-\beta\Delta_E$) **then**
    $\sigma_k \leftarrow -\sigma_k$
    $E \leftarrow E + \Delta_E$
endif
output $\{\sigma_1, \ldots \sigma_N\}$, E

Explanation of the Pseudo-Code:

- `nran`$(1, N)$: uniformly distributed integer random number between 1 and N
- `ran`$(0, 1)$: uniformly distributed real random number in interval [0,1[
- k denotes a lattice site, $N = N_s \times N_s$ is the lattice volume
- $Nbr(l, k)$ denotes site l if l is nearest neighbor to k (there are $2d$ n.n. on a d-dimensional lattice)
- h is the sum of the spin of all nearest neighbors

This procedure has to be called very often until the lattice is *thermalized* i.e. thermal equilibrium is reached (starting from an ordered or random configuration of spins), according to the inverse temperature β. Each call gives a new configuration in the Markov chain.

The transition region is the temperature region where the energy drops rapidly with increasing temperature, from this narrow region the approximate value of the critical temperature can be estimated. Plot the average energy per spin $\langle E/N \rangle$ for a set of β close to β_c on a 16×16 lattice with periodic boundary conditions. You will have to produce a Markov chain for various values of β, calling for each β the procedure `markov-ising` about 10^5 times from your main program

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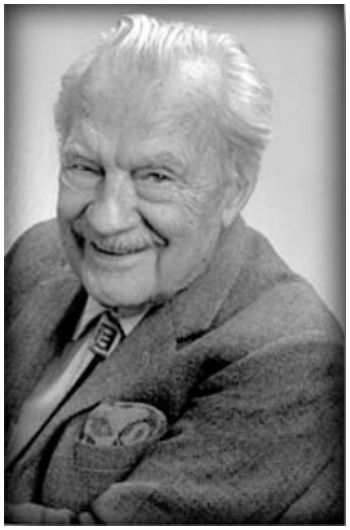
Nicholas Constantine Metropolis
(June 11, 1915 - October 17, 1999) was a Greek American physicist.



Metropolis received his B.Sc. (1937) and Ph.D. (1941) degrees in physics at the University of Chicago. Shortly afterwards, Robert Oppenheimer recruited him from Chicago, where he was at the time collaborating with Enrico Fermi and Edward Teller on the first nuclear reactors, to the Los Alamos National Laboratory. He arrived in the Los Alamos, on April 1943, as a member of the original staff of fifty scientists.
After the World War II he returned to the faculty of the University of Chicago as an Assistant Professor. He came back to Los Alamos in 1948 to lead the group in the Theoretical (T) Division that designed and built the MANIAC I computer in 1952 and MANIAC II in 1957. [...] From 1957 to 1965 he was Professor of Physics at the University of Chicago and was the founding Director of its Institute for Computer Research. In 1965 he returned to Los Alamos where he was made a Laboratory Senior Fellow in 1980.

In the 1950s, a group of researchers lead by Metropolis developed the Monte Carlo method. Generally speaking, the Monte Carlo method is a statistical approach to solve deterministic many-body problems. In 1953 Metropolis co-authored the first paper on a technique that was central to the method now known as simulated annealing. This landmark paper showed the first numerical simulations of a liquid. Although credit for this innovation has historically been given to Metropolis, the entire theoretical development in fact came from Marshall Rosenbluth, who later went on to distinguish himself as the most dominant figure in plasma physics during the latter half of the 20th century. The algorithm – the Metropolis algorithm or Metropolis-Hastings algorithm – for generating samples from the Boltzmann distribution was later generalized by W.K. Hastings. He is credited as part of the team that came up with the name Monte Carlo method in reference to a colleague's relative's love for the Casinos of Monte Carlo. Monte Carlo methods are a class of computational algorithms that rely on repeated random sampling to compute their results. In statistical mechanics applications prior to the introduction of the Metropolis algorithm, the method consisted of generating a large number of random configurations of the system, computing the properties of interest (such as energy or density) for each configuration, and then producing a weighted average where the weight of each configuration is its Boltzmann factor, $\exp(-E/kT)$, where E is the energy, T is the temperature, and k is the Boltzmann constant. The key contribution of the Metropolis paper was the idea that

> "Instead of choosing configurations randomly, then weighting them with $\exp(-E/kT)$, we choose configurations with a probability $\exp(-E/kT)$ and weight them evenly."
>
> (Metropolis et al., Journal of Chemical Physics 21 (1953)

Metropolis was a member of the American Academy of Arts and Sciences, the Society for Industrial and Applied Mathematics and the American Mathematical Society. In 1987 he became the first Los Alamos employee honored with the title "emeritus" by the University of California. Metropolis was also awarded the Pioneer Medal by the Institute of Electrical and Electronics Engineers, and was a fellow of the American Physical Society. [...]

`[from http://en.wikipedia.org/wiki/Nicholasa_Metropolis]`