Monte Carlo Methods - Fall 2017/18

Universität Bielefeld

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Exercise Nr. 3

Discussion on October 30th, 14:00-15:00

7) Importance Sampling *(4+4 points)*

Sample the three-dimensional integral

$$I = 128 \frac{\int_0^1 dxdydz\, x^3 y^2 z\, e^{-x^2-y^2-z^2}}{\int_0^1 dxdydz\, e^{-x^2-y^2-z^2}}$$

by making use of importance sampling: identify the Boltzmann distribution $P(x,y,z)$ and the observable and compare the two strategies:

a) Generate the Boltzmann distribution via your procedure `gauss()` from sheet 2, exercise 5.

b) Use the Metropolis algorithm (see pseudo-code) to generate the Boltzmann distribution.

procedure `metropolis`
input $\{x, y, z\}, i$
$x' \leftarrow \texttt{ran}(0,1)$
$y' \leftarrow \texttt{ran}(0,1)$
$z' \leftarrow \texttt{ran}(0,1)$
$r \leftarrow \texttt{ran}(0,1)$
if $(P(x',y',z') > r\, P(x,y,z))$ **do**
    $x \leftarrow x',\ \ y \leftarrow y',\ \ z \leftarrow z'$
endif
$i \leftarrow i+1$
output $\{x, y, z\}, i$

8) Two proofs: Metropolis Algorithm, Variance *(2+2 points)*

a) Prove that the Metropolis algorithm fulfills the detailed balance condition.

b) Prove that the variance of the sum of independent random variables $X = \sum_{i=1}^{N} X_i$ is given by

$$\mathrm{Var[X]} = \sum_{\mathrm{i=1}}^{\mathrm{N}} \mathrm{Var[X_i]}, \qquad \mathrm{Var[X_i]} \equiv \left\langle \mathrm{X_i^2} \right\rangle - \left\langle \mathrm{X_i} \right\rangle^2 .$$

Hint: consider the function $\log \left\langle e^{it(X_1+\ldots+X_N)} \right\rangle$ and take the second derivative w.r.t. t.

9) The Pebble Game *(2+4+2 points)*

Play the pebble game, an instructive example for a Markov chain: Assume you place a pebble at some square on a 3x3 board (the initial state). Move the pebble to one of the neighbors (left, right, up, down), or leave it where it is, with probabilities which depend on the current state:

- at corners: $p_{ii} = 1/2$, $p_{ij} = 1/4$ for $j \neq i$ (two neigbors)
- at edges: $p_{ii} = 1/4$, $p_{ij} = 1/4$ for $j \neq i$ (three neigbors)
- at the center: $p_{ii} = 0$, $p_{ij} = 1/4$ for $j \neq i$ (four neigbors)

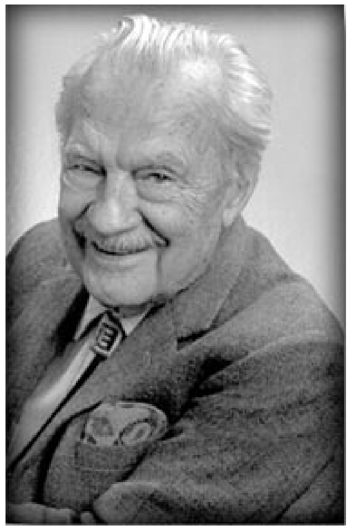
a) Label the 9 possible states and determine the transition matrix for the above probabilites. Check that it is well-defined.

b) Show by a Monte Carlo simulation that in average, each state is equally often visited (with probability 1/9), and that this is independent of the initial state.

c) What would be the rules (transition probabilities) on a 4×4 board in order to obtain a chain with uniformly distributed states?

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 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]`