The Metropolis–Hastings algorithm

We have seen that simple random-number integration and also importance sampling can be used for numerical integration.

However, to integrate over the multidimensional phase space we need an even more powerful technique which is a further improvement over importance sampling by going from independent random numbers to so-called random number (=Markov) chains.

A Markov chain Monte Carlo method for obtaining a sequence of random samples from a probability distribution for which direct sampling is difficult.
The sequence can be used to approximate the distribution (i.e., to generate a histogram), or to compute an integral (such as an expected value).

History

Named after
- Nicholas Metropolis, author of
Equation of State Calculations by Fast Computing Machines (1953)
who proposed the algorithm for the specific case of the Boltzmann distribution

and W. Keith Hastings who extended it to the more general case in 1970.

There is controversy over the credit for discovery of the algorithm. Edward Teller states in his memoirs that the five authors of the 1953 paper worked together for "days (and nights)". M. Rosenbluth, in an oral history recorded shortly before his death credits E. Teller with posing the original problem, himself with solving it, and A.W. Rosenbluth (his wife) with programming the computer. According to M. Rosenbluth, neither Metropolis nor A.H. Teller participated in any way. Rosenbluth's account of events is supported by other contemporary recollections. (from *Wikipedia*)

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Equation of State Calculations by Fast Computing Machines

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A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

- see the metropolis-et-al-1953 original paper

The Metropolis–Hastings algorithm

Use a Markov chain that, at sufficiently long times, generates states that obey the distribution P(x).
The Markov chain must fulfill the conditions **ergodicity** and **balance**.
A Markov chain generates a new state $\mathbf{X}_{t+1}$ that depends only on the previous state $\mathbf{X}_t$.
The algorithm uses a *proposal density* which depends on the current state $\mathbf{X}_t$, to generate a new proposed sample **X**'.
Then **X**' Is accepted as $\mathbf{X}_{t+1}$ if a random number α (uniform between 0 and 1) satisfies:

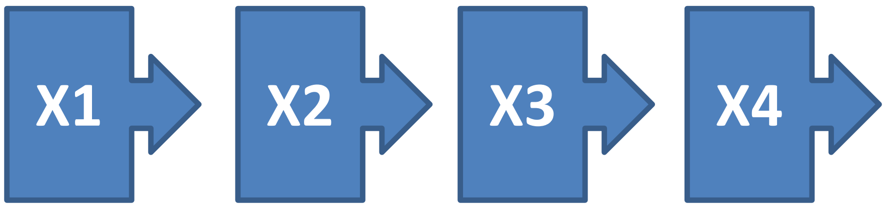
$$\alpha < P(\mathbf{X}') \, Q(\mathbf{X}_t;\mathbf{X}') \, / \, P(\mathbf{X}_t) \, Q(\mathbf{X}_t;\mathbf{X}')$$

otherwise the new state is the old state: $\mathbf{X}_{t+1} = \mathbf{X}_t$
The procedure is then repeated, $\mathbf{X}_{t+1}$ is renamed to $\mathbf{X}_t$.

The configuration space

A system of particles.
A state of the particles is described by a configuration ω taken from the configuration space Ω (infinite/finite, continuous/discrete)
Example 1 :
N interacting particles described by position and velocity of each in 3D.
Ω is an part of of R^{6N}.
Example 2:Surface with M adsorption sites that are occupied or free.

Markov-chain



dependent random variables

Our circle example:

$X_t = (x_t, y_t)$ in $[0\ 1]^2$
$X' = X_t + \Delta x$
If X' in $[0\ 1]^2$, $X_{t+1} = X'$, else $X_{t+1} = X_t$

Reminder: Accept uphill moves

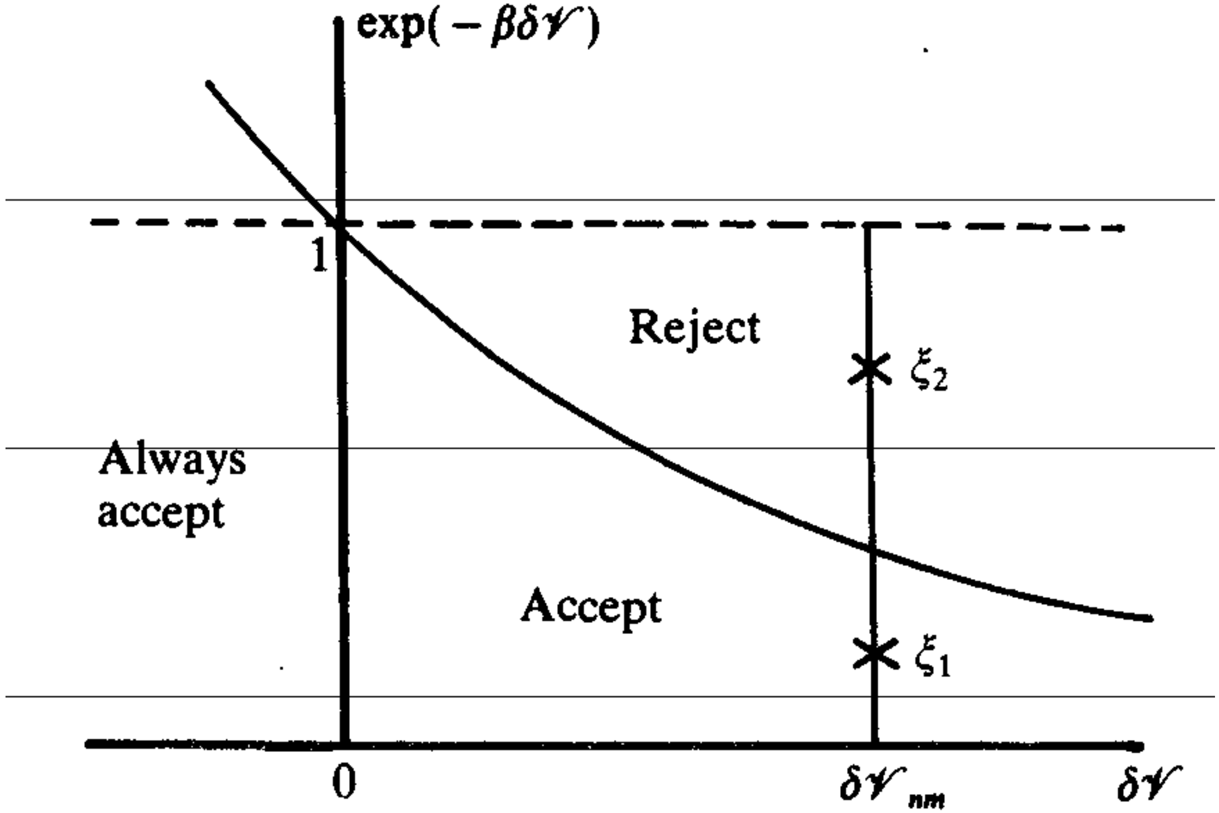


Fig. 4.5 Accepting uphill moves in the MC simulation.

END of Metropolis lecture notes