Monte Carlo Methods - Fall 2017/18

Universität Bielefeld

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Exercise Nr. 5

Discussion on November 27th, 14:00-15:00

13) Metropolis-Hastings algorithm *(5+3 points)*

Generate a binomial distribution $\pi(k) = \begin{pmatrix} n \\ k \end{pmatrix} p^k(1-p)^{n-k}$ via the Metropolis-Hastings algorithm as described in the lecture. Plot $\pi(k)$, and compute the mean value and the variance for the probabilities (a) $p = 1/2$, (b) $p = 1/3$, (c) $p = 1/4$, and in each case for $n = 4, 8, 16, 32$.

14) Ising Chain *(3+3 points)*

Study the Ising chain for the ferromagnetic ($J = 1$) and anti-ferromagnetic ($J = -1$) model.

(a) Implement either the Metropolis algorithm or the Heatbath algorithm and measure the energy density.

(b) Add to the Hamiltonian an external field h coupling to the spins:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_{i=1}^{N} \sigma_i.$$

Derive the analytic solution in this more general case, by diagonalizing the corresponding transfer matrix and determine the energy density. As an intermediate step, verify that the eigenvalues are

$$\lambda_\pm = e^{\beta J} \left(\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} \right)$$

(*c) *Extra points (+3):* incorporate the external magnetic field in your simulation and measure the energy. Does it agree with the analytic result in the limit of large N?

15) Random Walk *(2+2+2)*

Implement a random walk (RW) on (a) a 1-dimensional chain, (b) a square lattice and (c) a cubic lattice and measure the root mean square distance between the starting point at the origin and the end point after N steps. For a statistical analysis you have to sample many walkers. Does your critical exponent agree with $\nu = 2$ within statistical errors?

W. Keith Hastings

(July 21, 1930 - May 13, 2016) is an Canadian statistician.

The Metropolis-Hastings algorithm (or, Hastings-Metropolis algorithm) is the most common Markov chain Monte Carlo (MCMC) method. It is extremely widely used in applied statistics (and in statistical physics and computer science), to sample from complicated, high-dimensional probability distributions. A primary source for this algorithm is the paper [right]. This paper has been cited well over two thousand times - a huge number. However, despite this paper's importance, very little information about W.K. Hastings himself is publicly available. [...] W. Keith Hastings was born on July 21, 1930, in Toronto, Ontario, Canada. He received his B.A. in Applied Mathematics from the University of Toronto in 1953, and then worked from 1955-59 as a "Consultant in Computer Applications" for the Toronto company H.S. Gellman & Co. Hastings recalls:

> Harvey Gellman was a good mentor and encouraged me to pursue my ideas. Some of the projects involved simulations and this was my first contact with statistics and generation of samples from probability distributions.

Overlapping somewhat with this, Hastings received his M.A. in 1958, and his Ph.D. in 1962, both from the University of Toronto's Department of Mathematics (which included Statistics at that time). His Ph.D. thesis title was "Invariant Fiducial Distributions". His Ph.D. supervisor was initially Don Fraser (who mentioned Hastings' thesis results in a January 10, 1962 letter to R.A. Fisher), and later Geoffrey Watson (while Fraser visited Stanford in 1961-62). After completing his Ph.D., Hastings worked briefly at the University of Canterbury in New Zealand (1962-64), and at Bell Labs in New Jersey (1964-66). Hastings writes:

> I was never comfortable working on statistical inference for my thesis. My investigations led to too many dead ends and the work seemed to involve more mathematical considerations than statistical ones. When Geoff took over as my supervisor I briefly considered changing topics, but ended up sticking with my original topic and completed my thesis. In New Zealand, I continued this work for a while but eventually gave it up, the final blow coming when I learned that Fiducial Probability was declared 'dead' in a session during a statistics conference held in Ottawa. Bell Labs provided a welcome and effective antidote to all this as I gradually turned towards the computational aspects of statistics. In effect, I was then returning to my professional roots.

From 1966 to 1971, Hastings was an Associate Professor in the Department of Mathematics at the University of Toronto. During this period, he wrote the famous paper listed above (which generalised the work of N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller (1953), "Equations of state calculations by fast computing machines", J. Chem. Phys. 21, 1087-1091). Hastings explains:

> When I returned to the University of Toronto, after my time at Bell Labs, I focused on Monte Carlo methods and at first on methods of sampling from probability distributions with no particular area of application in mind. [University of Toronto Chemistry professor] John Valleau and his associates consulted me concerning their work. They were using Metropolis's method to estimate the mean energy of a system of particles in a defined potential field. With 6 coordinates per particle, a system of just 100 particles involved a dimension of 600. When I learned how easy it was to generate samples from high dimensional distributions using Markov chains, I realised how important this was for Statistics, and I devoted all my time to this method and its variants which resulted in the 1970 paper.

[...] In 1971, Hastings joined the Department of Mathematics at the University of Victoria. [...] Hastings retired from the University of Victoria in 1992. [...] Dr. Hastings passed away peacefully in Victoria on May 13, 2016, at the age of 85.

`[from Jeffrey S. Rosenthal, http://probability.ca/hastings]`