An Investigation of Markov Chain Monte Carlo Methods

Supervised by Prof. Stefan Sint; Group size: 1; Year: Junior Sophister

Background

Throughout statistical mechanics, the properties of a system are often determined by multi-dimensional integrals. For example, in the canonical ensemble, the expected value $\langle A \rangle$ of a thermodynamic quantity A in a system of N particles governed by a Hamiltonian H is given by

$$\langle A \rangle = \frac{1}{Z} \int_{\Gamma} d^N \vec{p}\, d^N \vec{q}\, e^{-\beta H(\vec{p},\vec{q})} A(\vec{p},\vec{q}), \tag{1}$$

where Z is the partition function for the system, Γ is the coordinate-momentum phase space of the system, and $\beta \equiv \frac{1}{k_B T}$. While these integrals can sometimes be analytically calculated for a simple Hamiltonian, this is often not possible for more complex systems containing a large number of interacting particles.

In order to deal with this problem, numerical techniques are often employed to approximate these integrals to a high degree of accuracy. One such technique is Monte Carlo integration, where a function to be integrated is evaluated at a number of randomly chosen points in order to estimate its expected value. A particular version of this technique uses Markov processes to determine a sequence of sample points, where each point in the sequence is determined solely by the preceding point in the sequence. These methods are called Markov Chain Monte Carlo (MCMC) methods, and are prevalent not only in statistical physics but also in fields such as quantum mechanics,[1] quantum field theory,[2] and computational biology.[3]

Although MCMC methods tend to converge to a desired distribution, their main drawback is the so-called autocorrelation of data, whereby pairs or clusters of generated sample points are dependent on each other, which can drastically affect results in certain instances. For this reason, care must be taken when deciding to implement these methods.

Objectives

The main objective of this project will be to investigate the efficiency, accuracy, and applicability of MCMC methods. This will be done by computing integrals using a wide range of numerical methods and comparing the results to MCMC methods. In order to properly investigate these methods, such examples will include integrals of varying complexity encountered in the study of physical systems, such as the aforementioned expectation value (1).

Another goal of the project is to analyse the autocorrelation of data obtained from MCMC methods. This can be done by repeating algorithms under different parameters, recording any changes in results.

The final main objective of this project will be to represent the change of a physical system in time in graphical form. This will be another approach to interpret and explain the logistics of MCMC methods.

Tasks

The first task of this project will be to become familiar with the basic constituents of MCMC methods; Monte Carlo integration and Markov processes. This will primarily consist of researching the theory and motivation behind these ideas as outlined in texts such as those recommended by the project supervisor.[4]

The next task of the project will be to implement various common integration techniques (i.e. trapezoidal rule, Simpson's rule, Runge-Kutta method) in Python, including MCMC methods (i.e. Metropolis algorithm), and decide upon a variety of problems to solve using these methods.

Once these problems have been tackled using the different numerical techniques, the investigation of the MCMC methods will begin. This will be done by comparing the computational cost between the methods and the difference from computed results to analytic or experimental values, where possible.

The data obtained from MCMC methods will also be analysed for autocorrelation by adjusting various parameters, such as run time and initial Markov chain point, and from this the applicability of the methods will be deduced on a case-by-case basis.

The final task of this project will be to take a molecular dynamics approach and implement MCMC methods to simulate physical systems in time (i.e. Ising model), creating a series of images corresponding to points in the Markov chain to visualise the evolution of the system.

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[1] M. Creutz, B. Freedman, "A Statistical Approach to Quantum Mechanics," *Annals of Physics* **132** (2), pp. 427-462, 1981.

[2] C. Morningstar, "The Monte Carlo Method in Quantum Field Theory," `https://arxiv.org/abs/hep-lat/0702020`, 2007.

[3] A. Gupta, J. B. Rawlings, "Comparison of paramter estimation methods in stochastic chemical kinetic models: Examples in systems biology," *AIChE Journal* **60** (4), pp. 1253-1268, 2014.

[4] I. Sachs, S. Sen, J. C. Sexton, "5. Monte Carlo integration" in *Elements of Statistical Mechanics: With an Introduction to Quantum Field Theory and Numerical Simulation*, Cambridge University Press, Cambridge, 1st ed., pp. 82-111, 2006.