Monte Carlo methods

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1. Almost any FORTRAN or C compiler provides a pseudo-random number generator that produces real numbers uniformly distributed in the interval $[0, 1]$.

    a) Find a way to check that your random numbers generator produces a uniform distribution in the interval $[0, 1]$

    b) Use your random numbers generator to implement a Monte Carlo algorithm, based in Metropolis' method, to create a sample of M real numbers distributed according to the Gaussian distribution:

    $$g(x) = \sqrt{\frac{\sigma}{\pi}} \exp\left(-\sigma x^2\right) \tag{1}$$

    The exact low order moments of the distribution are:

    $$\begin{aligned} \langle x \rangle &= \left\langle x^3 \right\rangle = 0 && (2) \\ \left\langle x^2 \right\rangle &= \frac{1}{2\sigma} && (3) \\ \left\langle x^4 \right\rangle &= 3 \left\langle x^2 \right\rangle^2 && (4) \\ & && (5) \end{aligned}$$

    Study the accuracy and convergence of the moments in your calculation when increasing the sample size M.

2. Consider a system of N spins arranged on a 2D square lattice. In the presence of a magnetic field, H, perpendicular to the lattice plane, the energy of the system is given by:

$$\mathcal{H} = -J \sum_{<ij>} s_i s_j - \sum_{i=1}^{N} H s_i \tag{6}$$

where $s_i = \pm 1$, J is called the coupling constant and the sum $(< i, j >)$ extends over nearest-neighbors. Such system is known as the Ising model and for $J < 0$ and $H = 0$ it shows spontaneous magnetisation below a temperature $T_c = 2.27 J/k_B$.

a) Implement a Monte Carlo program to sample states, $\mathbf{s} = (s_1, s_2, \cdots, s_N)$, of the Ising model consistent with the distribution:

$$P_{\mathbf{s}} \propto \exp\left(-\beta \mathcal{H}_{\mathbf{s}}\right) \tag{7}$$

Consider a periodic lattice of 20x20 spins.

b) Set $H = 0$ and run simulations at different temperatures in the interval $[J/k_B, 8J/k_B]$. Calculate the average magnetisation $\langle m \rangle = \frac{1}{M}\sum_{i=1}^{M} m_i$ and the average energy $\langle U \rangle = \frac{1}{M}\sum_{i=1}^{M} \mathcal{H}_i$, where M is the number of configurations generated and $m_i = \frac{1}{N_{spins}}\sum_{j=1}^{N_{spins}} s_j$ and $\mathcal{H}_i = -J\sum_{<ij>} s_i s_j - \sum_{i=1}^{N} H s_i$ are the instantaneous magnetisation and the configurational energy respectively. Plot $\langle m \rangle$ and $\langle U \rangle$ vs. T and discuss the results.

c) Set $H = J/3$ and repeat the previous computations. At each temperature calculate and plot the probability, $P(m)$, of observing an instantaneous magnetisation m in the system. $P(m)$ is simply a normalised histogram of the magnetisation per spin.