Note

On the acceptance ratio in Monte Carlo computer simulations

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The functional form of acceptance probabilities in Monte Carlo algorithms bears a resemblance to the distance functions which are specifically defined to be bracketed by the unit interval. This observation led us to seek the average distance between any two points on the unit interval and this by analogy resulted in a suggestion of an upper and a lower bound of 1/2 and 1/3, respectively, for the acceptance ratio or the average acceptance probability in Monte Carlo computer simulations.

Monte Carlo computer simulations are now routinely used to probe structural and thermodynamic properties of chemical and biochemical systems [1]. Investigations on the methodological front however, have not kept pace with the popularity that this simulation technique enjoys. One such area is the acceptance ratios. Each Monte Carlo simulation requires that the acceptance ratio be monitored and a decision be made whether a given ratio is satisfactory or not. The number of particles to be moved and the size of the displacement are dictated by the acceptance ratio. Typically, a value of 0.5 is considered to be optimal [1]. In the following, we seek an analogy between the acceptance probabilities and distances on the unit interval which quite interestingly leads to a lower and an upper bound for the acceptance ratio.

It is well known [2] that if a function $f(x_i, x_j)$ is a metric on a set X with x_i, x_j belonging to X, then

$$\min\{1, f(x_i, x_j)\} \tag{1}$$

is also a metric on X and so is

$$f(x_i, x_j)/[1 + f(x_i, x_j)]\,. \tag{2}$$

The above two metrical forms (1) and (2) may be interpreted as ensuring bounded-

ness for the function $f(x_i, x_j)$. The two metrics in expressions (1) and (2) lie in the unit interval (0, 1).

The parallel between Metropolis choice [1,3] for the acceptance probability α_{ij} defined as

$$\alpha_{ij} = \min[1, P_j/P_i] \tag{3}$$

and expression (1) cannot be missed. $f(x_i, x_j)$ is identified with (P_j/P_i), where P_i and P_j are the Boltzmann probabilities for states i and j. α_{ij} as defined by eq. (3) is confined to the unit interval. In the same vein,

$$\alpha_{ij} = P_j/[P_i + P_j]\,, \tag{4}$$

which is analogous to expression (2), is nothing but Barker's choice [4] for the acceptance probability.

Pursuing the idea that α_{ij} has the semblance of a distance function and further noting that α_{ij} is restricted to the unit interval, it is interesting to seek the average distance between any two points on the unit interval when infinite number of such points are generated. The motivation behind such an investigation being the existence of a proposed correlation between the optimal ensemble average of acceptance probability $\langle\alpha_{ij}\rangle$ in a Monte Carlo simulation and the average distance between any two points $\langle d\rangle$ on the unit interval. The ensemble average of the acceptance probability and the acceptance ratio are used interchangeably here as both carry the same information [1,5].

Consider the unit interval as a discrete lattice consisting of n segments and $(n+1)$ equally spaced points including 0 and 1. This lattice involves $(n+1)^2$ pairs of points and $(n+1)^2$ distances. This includes the distance from any arbitrary point to itself. The average distance $\langle d\rangle$ then is obtained as

$$\langle d\rangle = \frac{2}{(n+1)^2}\frac{1}{n}[n\cdot 1 + (n-1)\cdot 2 + (n-2)\cdot 3 + \ldots + 2\cdot(n-1) + 1\cdot n]\,,$$

$$\langle d\rangle = \frac{2}{n(n+1)^2}\sum_{r=1}^{n}[(n+1-r)\cdot r] = \frac{1}{3}\,\frac{(n+2)}{(n+1)}\,. \tag{5}$$

If $n = 1$, i.e. when there are just two points (or two states), namely 0 and 1, the average distance from eq. (5) is

$$\langle d\rangle = (1/3)\{(1+2)/(1+1)\} = 0.5\,.$$

Traditionally, it is this value of 0.5 which has been adopted for the acceptance ratio in Monte Carlo simulations [1,5]. As $n \to \infty$, $\langle d\rangle$ converges to a value of (1/3). This was quite unanticipated. Average distance is thus seen to span the interval (1/2, 1/3), establishing, by analogy, an upper and a lower bound for the acceptance ratio.

A random lattice as opposed to a discrete lattice described above is probably more suitable to discuss the average distances in the context of acceptance ratios.

This can be accomplished via a numerical experiment. Several points are generated randomly on the unit interval using a computer. The computed average distance between any two points is 0.330 with 10 points, 0.348 with 10^2 points, 0.326 with 10^3 points, 0.333 with 10^4 points, 0.334 with 10^5 points, and 0.333 with 10^6 points. It may be recalled that 10^6 points on the unit interval translate to 10^{12} distances and it is the average of all these distances which is computed. It is once again seen that as the number of points increases, the average distance converges to a value of (1/3). Thus an acceptance ratio of (1/3) appears to correspond to the realization of an infinite number of states during the course of a Monte Carlo simulation.

Lastly, a rigorous mathematical approach would involve a demonstration that P_i and P_j are probability measures, that P_j/P_i also defines a measure, that transition probabilities can be considered as metrics and that each satisfactory prescription for the acceptance probability generates a topology consistent with Boltzmann distribution, etc. Much of this, while being useful, is not likely to alter our conclusions regarding the upper and lower bounds of the acceptance ratios. It is hoped that the information provided here will stimulate further work on transition probabilities for more efficient simulations.

References

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