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LETTER TO THE EDITOR

Exact enumeration of random walks with traps

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Abstract. A new useful method of exact enumeration of random walks with traps is presented. The method is applied to the one-dimensional case and is shown to yield excellent agreement with an exact solution. The advantage of the method is that it can be applied in higher dimensions. Numerical results confirm the known asymptotic solution and can be used to estimate the time and concentration needed to approach this limit.

The problem of the trapping of random walks by randomly distributed traps on a lattice has recently been the focus of both theoretical and Monte Carlo (MC) studies (some recent references are Movaghar *et al* 1981, 1982, Grassberger and Procaccia 1982, Kayser and Hubbard 1983, Klafter *et al* 1984, Stanley *et al* 1983, Redner and Kang 1983; some older references are given in Weiss and Rubin 1983). Few theoretical results are available for quantities of interest, these being mostly in the form of asymptotic expressions for the survival probability of the random walk as a function of step number. It appears to be quite diffcult to determine the earliest times at which these asymptotic results can be expected to be reliable. Monte Carlo studies usually do not provide conclusive results on the time of onset of the asymptotic regime because of inherent fluctuations.

In this letter we present a new useful method, based on exact enumeration, for calculating the survival probabilities of random walkers on a lattice with randomly distributed traps. The utility of the method will be demonstrated by comparing the numerical results with exact results in 1D. The advantage of this method is that it is independent of dimension. Detailed results for 2D and 3D will be published elsewhere.

The method to be described provides an exact solution for the survival probability as a function of step number for an arbitrary distribution of traps. MC simulation, on the other hand, will yield only an approximate solution for the same distribution of traps. We illustrate the exact enumeration method for a nearest-neighbour 1D random walk.

The detailed procedure is illustrated in three lines shown in figure 1. The first line represents the traps distributed randomly on a 1D lattice each site being a trap with probability c. In the second line each site not occupied by traps is denoted by a 1 which represents the probability of survival of a random walker occupying that site at step $n = 0$. Every site not occupied by a trap is a starting point of a random walker.

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T . . . T . . T . . . . T .

0 1 1 1 0 1 1 0 1 1 1 1 1 0 1

0 $\frac{1}{2}$ 1 $\frac{1}{2}$ 0 $\frac{1}{2}$ $\frac{1}{2}$ 0 $\frac{1}{2}$ 1 1 $\frac{1}{2}$ 0 0

Figure 1. Demonstration of the exact enumeration on a given configuration. The dots represent regular sites, T represents a trap site. The sum of the numbers in lines 2 and 3 represent survival probability at step $n=1$ and $n=2$ respectively. Periodic boundary conditions were used for calculating line 3.

The situation at $n=1$, representing the inductive step, is illustrated in the third line of figure 1. This step, for a random walk to nearest neighbours, consists of replacing each non-trap site register by the sum of values in its neighbouring sites divided by two (in a hypercubic D-dimensional lattice the division factor is 2D) while trapping sites retain the value 0. If we call the value of site register i after the nth step, $V_i(n)$, then the survival probability after n steps is *exactly*

$$Q_n = \frac{1}{N_0} \sum_i V_i(n) \tag{1}$$

for N_0 random walkers started on a particular configuration of traps. The probability of survival of interest is $\langle Q_n \rangle$, where the average must be taken over all possible configurations. It is clearly impossible to do this exactly, but we have found that an average over relatively few configurations leads to a very good approximation as will be demonstrated below. It is also possible, in principle, to calculate statistical properties of the displacement after n steps using the present method by starting with a one at a single non-trap site and a zero at all others and proceeding as before. This calculation is necessarily longer than that needed for the survival probability since for each trap configuration the starting position of the random walkers must be varied over the entire lattice, but it is exact in the same sense as described earlier. A similar method was used previously to study diffusion on fractals (Ben-Avraham and Havlin 1982).

To study the performance of the method we compared our computed results for the survival probability with the exact result (Weiss and Havlin 1984, in preparation)

$$\langle Q_n \rangle = c^2 \delta_{n,0} + 2c^2 \sum_{l=2}^{\infty} \frac{(1-c)^{l-1}}{(l-1)} \sum_{j=0}^{[(l-1)/2]} \cos^n\left(\frac{\pi(2j+1)}{l}\right) \cot^2\left(\frac{\pi(2j+1)}{2l}\right) \tag{2}$$

where the square brackets means 'largest integer contained in.' Asymptotic results derived by Donsker and Varadhan (1979) indicate that $\ln\langle Q_n \rangle$ for large n should scale as

$$\ln\langle Q_n \rangle = -K\left(\ln\frac{1}{1-c}\right)^{2/3} n^{1/3} \tag{3}$$

where K is a constant. To apply the present computational technique to the 1D trapping problem we used a lattice consisting of 50 000 sites and calculated the survival probability as a function of n for several values of c. Typical results are shown in figure 2 where results of the exact solution in equation (2) are compared with those obtained by the present method as well as by direct simulation. The excellent agreement between the numerically calculated and exact values up to 2000 steps is evident, while the MC simulations with 5×10^4 trials give much poorer results, the survival probability actually

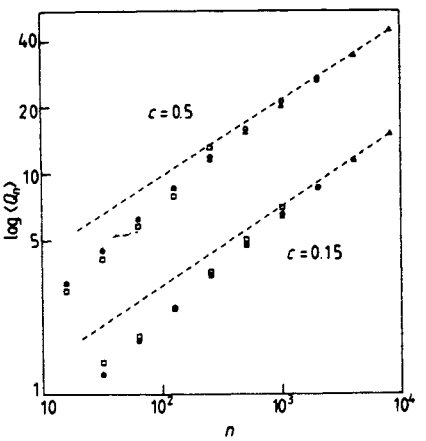

Figure 2. Comparison of the results for probability of survival between the exact solution equation (2) triangles, the enumeration method circles, and MC method squares. The broken lines represent the slope corresponding to $\alpha = \frac{1}{3}$.

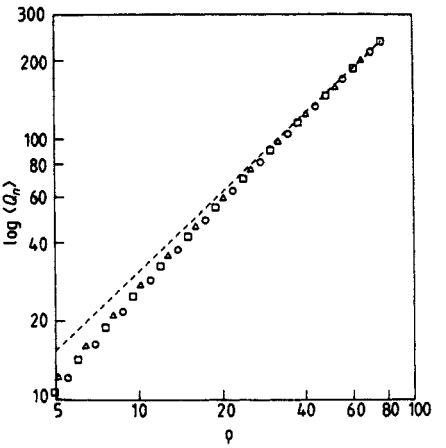

Figure 3. Results for $\log\langle Q_n\rangle$ for different concentrations and time plot as a function of $\rho = \{\log[1/(1-c)]^{2/3}\, n^{1/3}$. The symbols denote different trap concentrations as follows: △ corresponds to 0.3; □ to 0.5; and ○ to 0.8. The broken line represents the slope corresponding to $\alpha = \frac{1}{3}$.

going to zero at greater than 1000 steps. The agreement between our enumeration method and the exact solution is an order of magnitude better than the agreement between the MC results and equation (2).

The interesting question of the ranges of time and of concentration in which the asymptotic result (3) is expected to be useful is clear from figure 3. This figure shows a plot of $\log\langle Q_n\rangle$ for several values of c and for values of n up to 10^7. The data which consist of the exact solution and results of our enumeration method have been plotted as a function of $\rho = \{\log[1/(1-c)]^{2/3}\, n^{1/3}\}$ and appear to lie on a universal curve. This suggests that the Donsker–Varadhan (1979) scaling form is correct even in the transient regime. Since the slope decreases and approaches one only for large values of ρ, one can estimate the range in which the exponents $\frac{2}{3}$ and $\frac{1}{3}$ appearing in ρ give a useful approximation using our results.

Figure 4 shows results of a direct calculation of the exponent α by assuming (2) to have the form $A\, e^{-Bn^{\alpha}}$ for several values of c. The results illustrate again that only for relatively high values of c and $n > 10^4$ does one begin to see a good approximation to the theoretical expected value of $\alpha = \frac{1}{3}$. This should be compared with the correction term of the order of $n^{-1/3}$ predicted by theory in 1D (Weiss and Havlin 1984).

To conclude, we have suggested a new useful numerical technique for calculating survival probabilities in trapping problems that is the equivalent of replacing one of the two parts of a simulation by an exact calculation. We have shown that in 1D the results are in excellent agreement with theoretically known results and the precision far exceeds that of the commonly used simulation methods. For a single configuration of traps the number of random walks for $n = 1000$ is of the order of $2^{1000} \times 10^5$ rather than 10^5 as is typical in such studies. It should also be noted that the computer time used in obtaining the MC results is about an order of magnitude more than the time for the exact enumerations for the same number of sites. The technique can be modified to deal with partially absorbing traps by simply replacing the value of zero at these

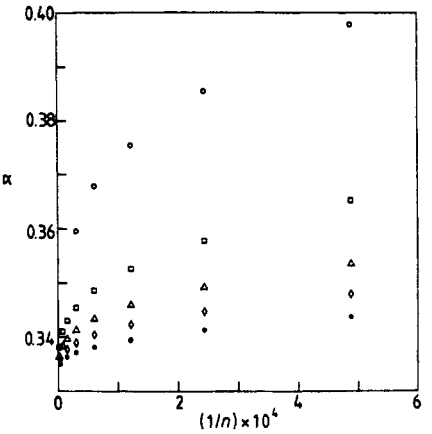

Figure 4. Values of the exponent α for different values of n and c. The symbols denote different trap concentrations as follows: ○ corresponds to 0.1; □ to 0.3; △ to 0.5; ◇ to 0.7, and ● to 0.9.

sites by an appropriate trapping probability. It can also be modified to deal with random walks with jumps to further neighbours, but here one must be careful about edge effects. One other model that can be analysed by a similar technique is that of moving traps.

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