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First-Passage Times in a Critical Stochastic Model

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Average first-passage times for a single-variable stochastic model with a critical fixed point at the origin are computed by exact enumeration. The numerical measurements show excellent agreement with analytical results. The scaling function approaches the predicted asymptotic dependence.

KEY WORDS: Scaling theory; relaxation times; epidemiology; exact enumeration.

This short communication addresses the relation[1] between microscopic stochastic dynamics and macroscopic equations; in particular, it is a numerical study of the times scales for which a simple stochastic model is no longer properly described by its governing macroscopic equation. The study is followed by comparison with analytical predictions for the exact value of the first-passage time and the asymptotic behavior of the scaling function for the first-passage time.

In particular, I consider a family of models also studied by Privman *et al.*[2]: particles are allowed to exist at integer sites ($n = 0, 1, 2, \ldots, N$), and have transition probabilities for microscopic time steps $\Delta t \sim 1/N^2$,

$$\begin{aligned} p(n \to n-1) &= (1-y)\rho + y\rho^2 \\ p(n \to n+1) &= (1-y)\,\rho(1-\rho) \end{aligned} \tag{1}$$

Otherwise they do not move from position n; the fluctuating density variable is $\rho \equiv (n/N)$.

These transition probabilities approximate the macroscopic ($N \to \infty$) evolution equation

$$\frac{d\bar{\rho}}{dt} = -\bar{\rho}^2$$

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which has a critical fixed point at the origin, and should show slower-than-exponential relaxation for the average density $\bar{\rho}$. This equation is of interest in epidemiology,[3,4] where the "particle" position represents the number of sick individuals, and may also be relevant to the understanding of self-organized criticality.[5]

Starting with particles placed randomly and uniformly over all allowed sites, the expectation value T of the first-passage time to $n=0$ (after which particles remain at the origin forever) determines a characteristic time for which the detailed microscopic process starts deviating significantly from the macroscopic, average process.

While it is often difficult to derive simple closed-form results for this type of model and quantity, an analytical expression [6] has been obtained for $T(y=1)$. The result, in macroscopic time steps ($N^2\Delta t$), is given by

$$T=\frac{N}{N+1}\sum_{n=1}^{N}\frac{N+1-n}{n^2} \tag{2}$$

which can be expanded to yield

$$T=\frac{\pi^2}{6}N-\frac{N}{N+1}\ln N-(\gamma+1)+\mathcal{O}\left(\frac{1}{N}\right) \tag{3}$$

where γ is Euler's constant. It appears[6] that numerical confirmation of Eqs. (2) and (3) is beyond the capability of present-day computers using traditional Monte Carlo simulations. The problem is this case seems to be the exponential distribution of the arrival probabilities. The first purpose of this communication is to confirm numerically these two equations.

Here the problem is approached with the exact enumeriation technique,[7] originally developed for random walks, but which has also been applied recently to several lattice-gas cellular automata models.[8,9] This method consists in evolving particle probabilities according to the respective transition probabilities. Denoting by $c(n, t)$ the probability of a particle being at position n and microscopic time step t, the evolution equation for probabilities corresponding to Eq. (1) is

$$\begin{aligned} c(n, t+1)=&\, c(n+1, t)\, p(n+1\to n)+c(n-1, t)\, p(n-1\to n)\\ &+c(n, t)\, p(n\to n) \end{aligned} \tag{4}$$

Equation (4) is exact for the numerical simulation; no additional averaging over disorder configurations is necessary, unlike in previous applications of the technique. Furthermore, this equation is not a disguised finite-difference form of the macroscopic evolution equation.

Defining τ to be the (probability) flux of particles reaching the origin at time t,

$$\tau(t) = c(1, t-1)\, p(1 \to 0) \tag{5}$$

one obtains

$$T = \sum_{t=0}^{\infty} t\tau(t) \tag{6}$$

as the quantity of interest.

The case $y = 1$ was studied in more detail, since Eqs. (2) and (3) are available for comparison. To make a connection between Eqs. (2) and (3) and Eq. (6), one needs an initially uniform distribution of particles between $n = 0$ and $n = N$.

Equations (4)–(6) have been iterated for lattice sizes going from 6 to 96 in factors of two. Double-precision arithmetic has been used, and simulations have been carried until the changes in T and in the sum of particle fluxes reaching to origin become smaller than machine precision.

Figure 1 is a plot of $\ln(\tau)$ against t for $N = 96$, with t given in units of 10^5 time steps. The cumulative sum of probabilities at $n = 0$ and T stopped changing after 23.8 million microscopic time steps, shortly before

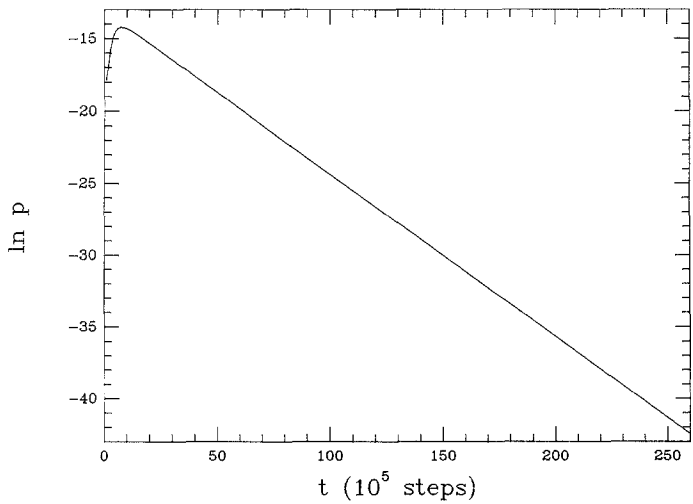

Fig. 1. Semilogarithmic plot of passage probability versus time (in units of 10^5 microscopic time steps) for $y = 1$, $N = 96$. The straight line indicates the exponentially decaying probability of arrivals to the origin.

the end of the simulation. It is clear that, after a maximum flux of particles at around 800,000 time steps, the flux starts decaying exponentially with time.

Table I contains results for five lattice sizes, differing successively by factors of two. The average first-passage time is given to six decimal places for both theory [Eq. (2)] and simulations [Eq. (6)]. It has been normalized by N, so that entries are of the same order of magnitude. Several points are worth noting. The relative error between simulations and theory diminishes with increasing lattice size, from -0.0034 to -7×10^{-7} for the values examined. The simulation value is consistently below theory, which could be explained by the fact that not all particles have arrived at the origin a finite time, and therefore the numerical estimate is always low. (See column 5 of Table I.) The times (both macroscopic and microscopic) required for convergence to machine precision grow with N: column 4 of Table I refers to the macroscopic times, $N^2\Delta t$. Therefore, even with exact enumeration it is difficult to treat large lattices: microscopic times increase roughly by a factor of eight for each size doubling; the estimate for convergence for $N=192$ is about 180 million time steps.

Privman *et al.*[2] have proposed $z\equiv N(1-y)$ as the relevant scaling variable for the scaling function defined by $T\sim N\mathcal{G}(z)$. The second purpose of this communication is to study the asymptotic behavior of the scaling function for large z.

Equation (3) suggests that T/N should be of the form $T/N\sim\mathcal{G}(z)+bw$, with $w=(\ln N)/(N+1)$. For $y\neq1$, Eq. (4) has been iterated until at most 1/1000 of all particles have not reached the origin. Values of y and N were picked so that $y\geqslant0.8$ and $N\leqslant400$. For each value

Table I. Lattice Size, Analytical Value for First-Passage Time (from Eq. (2)], Exact Enumeration Value, Number of Macroscopic Time Steps Required for Convergence, and Fraction of Particles Not Yet at the Origin after Convergence Time

	T/N			
N	From Eq. (2)	From Eq. (6)	t	p
6	1.141388	1.137420	222	$<7\times10^{-4}$
12	1.326268	1.325734	403	$<5\times10^{-5}$
24	1.453083	1.453016	745	$<3\times10^{-5}$
48	1.533320	1.533311	1396	$<2\times10^{-7}$
96	1.581512	1.581511	2582	$<2\times10^{-8}$

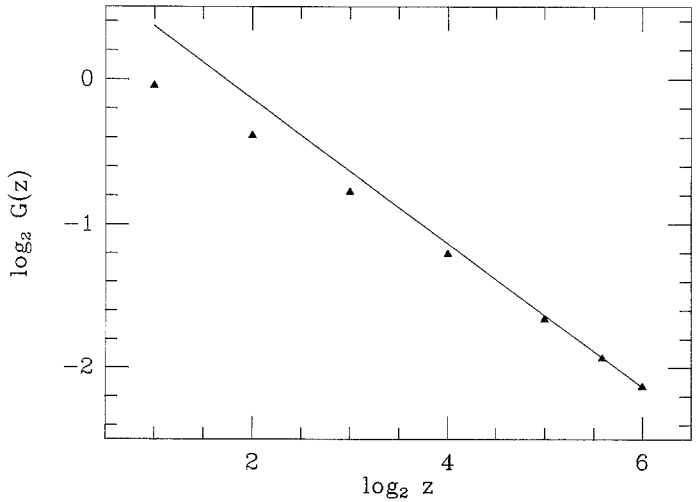

Fig. 2. Logarithmic plot (base 2) of the scaling function vs. z. The solid line has slope $-1/2$, corresponding to the predicted $\mathscr{G}(z) \sim 1/\sqrt{z}$ dependence.

of z, the scaling function has been estimated by extrapolating T/N to $w \to 0$. A logarithmic plot of the extrapolated scaling function versus z is shown in Fig. 2. For large enough z, this function seems to approach an asymptote $\mathscr{G} \sim 1/\sqrt{z}$, in agreement with the predictions of Privman *et al.*[2]

In summary, this communication reports a numerical study of a family of stochastic models governed by a macroscopic equation with a critical fixed point. Exact enumeration results confirm the exponential nature of particle arrivals to the origin, an analytical result for first-passage times, and the asymptotic form of the scaling function for the relaxation time in these models.

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