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First Passage Time for a Class of One-Dimensional Stochastic Systems

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We consider the time evolution of a class of stochastic systems of finite size with polynomial nearest neighbor transition rates. We obtain analytical expressions for the first passage time (FPT) and its moments. We show that the mean FPT, averaged over a uniform initial distribution, shows a simple asymptotoc behavior with the system size and the parameters of the transition rates.

KEY WORDS: First passage time; stochastic systems; phase transitions.

1. INTRODUCTION

The time evolution of stochastic systems plays a major role in many phenomena in diverse fields, such as semiconductors, reaction kinetics, and the spread of infection in a healthy population.[1-3] In this paper we study a class of one-dimensional stochastic systems with polynomial transition rates. In this class of systems the time evolution of a discrete random variable $X(t)$ restricted to integer values in $[0, N]$ is governed by the transition rates $A(n, N)$ and $B(n, N)$, which are, respectively, the rates of transition per unit time from states $n \rightarrow n-1$ and $n \rightarrow n+1$. The transition rates $A(n, N)$ and $B(n, N)$ are given by

$$\begin{aligned} B(n, N) &= \sum_{i=1}^{l} a_i n^i / N^{i-1} \\ A(n, N) &= B(n, N) + C n^l / N^{l-1} \end{aligned} \qquad (1)$$

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where the a_i and C are finite constants with the further restrictions

$$B(n, N) \geqslant 0 \qquad \text{for} \quad n = 0, 1, ..., N$$

$$a_1 > 0, \qquad C > 0, \qquad l > 1, \qquad \sum_{i=1}^{l} a_i = 0$$

The last condition is imposed so as to make the system closed. Note that with this condition $B(N, N) = 0$. Both $A(0, N)$ and $B(0, N)$ are also zero.

Such systems can serve as useful models of reaction kinetic systems (without diffusion) as well as of population epidemics. In the population epidemic case, N will be the total number of individuals (which remains constant with time) and $X(t)$ the number of infected individuals at any time t. The only stable state of these systems is $n = 0$. The mean first passage time (MFPT) is a useful quantity for characterizing the behavior of such systems. The random variable $\tau(i)$ denoting the FPT to reach the stable state $n = 0$ from the initial state $n = i$ is defined as

$$\tau(i) = \min[t \mid 0 < t < \infty; X(t) = 0; X(0) = i] \qquad (2)$$

Further we define

$$t_m(i) = \langle \tau^m(i) \rangle \qquad \text{for} \quad m = 1, 2, ...$$

and

$$\bar{t}_m = (1/N) \sum_{i=0}^{N} t_m(i) \qquad (3)$$

That is, $t_1(i) = \langle \tau(i) \rangle$ defines the mean first passage time (MFPT) and $\bar{t}_1$ the average MFPT starting from an initial uniform distribution. We prove the following theorem.

Theorem. Let $X(t)$ be a random variable restricted to $[0, N]$ whose time evolution is governed by the transition rates given by Eq. (1). Then the average MFPT $\bar{t}_1$ defined in Eq. (3) is given by

$$\lim_{N \to \infty} \bar{t}_1/(N')^{(l-1)/l} = \phi_l \qquad (4)$$

where $N' = (N/a_1)(1/C)^{1/(l-1)}$ and ϕ_l is given by the improper integral

$$\phi_l = l^{1/l} \int_0^\infty dz_1 \int_{z_1}^\infty (dz_2/z_2) \exp(-z_2^l + z_1^l) \qquad (5)$$

A special case of this type of system was studied by Privman *et al.*[4] with the transition rates

$$A(n, N) = (1-y)\,n + yn^2/N$$
$$B(n, N) = (1-y)\,n - (1-y)\,n^2/N \tag{6}$$

They found that even though the bulk behavior is independent of y and the system is critical for all values of y (the relaxation time goes to ∞ for $N \to \infty$), the system showed interesting finite-size effects which depend on y. They obtained the relaxation time numerically and showed that it goes as $[N/(1-y)]^{0.5}$ for $y \neq 1$ and as N for $y = 1$, thus exhibiting a phase transition at $y = 1$.

It can be proved that in the case of a system given by Eq. (1) when $a_1 = 0, a_2 > 0$, and $l > 2$, $\bar{t}_1$ goes as $N \log N/a_2$ and if $a_1, a_2, ..., a_i = 0$, $a_{i+1} > 0$, and $l > i+1$, $\bar{t}_1$ goes as N^i. However, for want of space we do not give the proof.

2. FORMULATION

Let $Q(n, t)\,dt$ represent the probability density function of the FPT $\tau(n)$ defined in Eq. (2). Then $Q(n, t)$ satisfies the equation

$$dQ(n, t)/dt = A_n Q(n-1, t) + B_n Q(n+1, t) - (A_n + B_n)\,Q(n, t) \tag{7}$$

Note that the equation for $Q(n, t)$ is adjoint to the master equation for $P(n, t)$, the probability that $X(t) = n$. Here $A(n, N)$ and $B(n, N)$ have been written as A_n and B_n for brevity. The moments $\langle t_m(n) \rangle$ of $Q(n, t)$ are defined as

$$\langle t_m(n) \rangle = \int_0^\infty dt\, t^m Q(n, t)$$

and are obtained from Eq. (7) as

$$(A_n + B_n)\langle t_m(n)\rangle = A_n\langle t_m(n-1)\rangle + B_n\langle t_m(n+1)\rangle + m\langle t_{m-1}(n)\rangle$$

For the MFPT, which is nothing but $\int_0^\infty tQ(n, t)\,dt$, the equation is simply

$$(A_n + B_n)\,t_1(n) - A_n t_1(n-1) - B_n t_1(n+1) = 1$$

Defining differences $\Delta t_1(n) = t_1(n) - t_1(n+1)$, we get

$$A_n \Delta t_1(n-1) - B_n \Delta t_1(n) = -1 \tag{8}$$

The values of A_n and B_n at $n=0$ and N (*i.e.*, $A_0=B_0=0$, $B_N=0$) impose the following boundary conditions:

$$t_1(0)=0 \quad \text{and} \quad \Delta t_1(N)=0$$

The set of equations (8) may be solved recursively from N downward to yield

$$\Delta t_1(n) = -\sum_{i=n}^{N-1} (1/A_{i+1})\,\beta_{n+1,i}$$

where

$$\beta_{i_1,i_2} = \prod_{J=i_1}^{i_2} (B_j/A_j)$$

Since $t_1(0)=0$, $t_1(n) = -\sum_{i=0}^{n-1} \Delta t_1(i)$; therefore

$$t_1(n) = \sum_{i=0}^{n-1} \sum_{J=i}^{N-1} (1/A_{J+1})\,\beta_{i+1,J} \tag{9}$$

This equation has also been derived using a different method by Murthy and Kehr[5] and Le Doussal.[6] The quantity of interest is the average MFPT $\bar{t}_1$ given that the system was initially in any of the states 1 to N with equal probability:

$$\bar{t}_1 = (1/N)\sum_{i=1}^{N} t_1(i) = -(1/N)\sum_{i=1}^{N}\sum_{n=0}^{i-1} \Delta t_1(n) = -(1/N)\sum_{n=0}^{N-1} (N-n)\,\Delta t_1(n)$$

Therefore

$$\bar{t}_1 = (1/N)\sum_{n=0}^{N-1} (N-n) \sum_{i=n}^{N-1} (1/A_{i+1})\,\beta_{n+1,i} \tag{10}$$

Similarly the higher moments of the FPT may be obtained stepwise, using the known values of the lower ones. In general $\bar{t}_m$ is given by

$$\bar{t}_m = (1/N)\sum_{n=0}^{N-1} (N-n) \sum_{i=n}^{N-1} (m t_{m-1}(i+1)/A_{i+1})\,\beta_{n+1,i} \tag{11}$$

The basis of the proof of Eq. (4) is the fact that the bias toward the stable state keeps on increasing as n increases. This leads to the contribution to $\bar{t}_1$ from values of $i \gg N^{(l-1)/l}$ being negligible. It can be shown that $\bar{t}_1(n)$ goes as n for $n \ll n_0$ and as n_0 for $n \gg n_0$, where $n_0 = N^{(l-1)/l}$. Using these observations, we find that $\bar{t}_1 \approx n_0$.

However, for a more exact proof of the theorem we make use of the relations (12a)–(12d) given below.

$$\text{if} \quad N_1 = N^{(l-1)/l}(\log N)^{(l+1)/(l-1)}$$

$$\text{and} \quad f_1 = (1/N) \sum_1^N (N-n) \sum_{N_2}^N (1/A_{i+1})\, \beta_{n+1,i} \tag{12a}$$

$$\text{then} \quad f_1/N^{(l-1)/l} = O(1/\log N), \qquad \text{where } N_2 = \max(N_1, n)$$

$$\begin{aligned} f_2 &= (1/N) \sum_1^{N_1} (N-n) \sum_n^{N_1} (1/A_{i+1})\, \beta_{n+1,i} \\ &= \sum_1^{N_1} \sum_n^{N_1} (1/a_1 i) \exp[-C(i^l - n^l)/a_1 l N^{l-1}][1 + O(N_1/N)] \qquad (12\text{b}) \\ &\quad \times \sum_1^{N_1} \sum_n^{N_1} (1/a_1 i) \exp[-C(i^l - n^l)/a_1^l N^{l-1}] \\ &= \int_1^{N_1} dy \int_y^{N_1} (dx/a_1 x) \exp[-C(x^l - y^l)/(a_1 l N^{(l-1)})] + O(\log N_1) \end{aligned}$$

(12c)

and

$$\begin{aligned} &\int_1^{N_1} dy \int_y^{N_1} dx (1/a_1 x) \exp[-C(x^l - y^l)/a_1 l N^{l-1}] \\ &\quad = \left\{ \int_0^{\infty} dy \int_y^{\infty} dx (1/a_1 x) \exp[-C(x^l - y^l)/a_1 l N^{l-1}] \right\} \\ &\qquad \times [1 + O(1/\log N)] \end{aligned} \tag{12d}$$

Now we give the proof of the above relations. To prove (12a), we first note that for $k \leqslant N/\log N$, $A_k \geqslant B_k \geqslant a_1 k(1 - S/\log N)$, where $S = \sum_{m=2}^{l} |a_m|$, and for $k > N/\log N$, $A_k = Ck^l/N^{l-1} \geqslant CN/(\log N)^l$. Therefore,

$$1/A_k \leqslant 1/a_1 k(1 - S/a_1 \log N) + (\log N)^l/CN \qquad \text{for} \quad 1 \leqslant k \leqslant N$$

Also

$$\begin{aligned} \beta_{n+1,i} &= \prod_{n+1}^{i} \frac{1}{1 + Ck^l/(B_k N^{l-1})} \\ &\leqslant \prod_{n+1}^{i} \frac{1}{1 + (C/S)(k/N)^{l-1}} \end{aligned}$$

$1/[1+(C/S)(k/N)^{l-1}]$ monotonically decreases with k. Therefore for both $n \leqslant N_1$ and $n > N_1$

$$\beta_{n+1,i} \leqslant \left[\frac{1}{1+(C/S)(N_1/N)^{l-1}}\right]^{i-N_2+1}$$

So

$$\begin{aligned} f_1 &\leqslant \sum_{i=1}^{N} \sum_{N_2}^{N} \left[\frac{1}{a_1 n(1-S/\log N)} + \frac{(\log N)^l}{CN}\right]\left[\frac{1}{1+(C/S)(N_1/N)^{l-1}}\right]^{i-N_2+1} \\ &\leqslant \sum_{i=1}^{N} \left[\frac{1}{a_1 n(1-S/\log N)} + \frac{(\log N)^l}{CN}\right]\left[\frac{1+(C/S)(N_1/N)^{l-1}}{(C/S)(N_1/N)^{l-1}}\right] \\ &\leqslant \frac{S}{C}\left[\frac{\log N}{a_1} + \frac{(\log N)^l}{C}\right]\left(\frac{N}{N_1}\right)^{l-1}\left[1+O\left(\frac{1}{\log N}\right)\right] \end{aligned}$$

Substituting the value of N/N_1, we get the relation (12a).

To prove (12b), we use the relations

$$(N-n)/N = 1 + O(N_1/N) \qquad \text{for} \quad n \leqslant N_1 \tag{13}$$

and

$$\begin{aligned} 1/A_i &= 1\Big/\left\{a_1 i\left[1+\sum_{j=2}^{l} (a_j/a_1)(i/N)^{j-1}\right]\right\} \\ &= (1/a_1 i)[1+O(N_1/N)] \end{aligned} \tag{14}$$

and

$$\beta_{n+1,i} = \prod_{k=n+1}^{i} \frac{1}{1+Ck^l/(B_k N^{l-1})}$$

along with the inequalities

$$\exp(-x+x^2) \geqslant 1/(1+x) \geqslant \exp(-x) \qquad \text{for} \quad x \geqslant 0 \tag{15}$$

This leads to

$$\exp\left[\sum_{k=n+1}^{i}\left(-\frac{Ck^l/N^{l-1}}{B_k} + \frac{C^2k^{2l}/N^{2l-2}}{B_k^2}\right)\right] \geqslant \beta_{n+1,i}$$

Now for $i \leqslant N_1$

$$\begin{aligned} \sum_{k=n+1}^{i} \frac{Ck^l}{B_k N^{l-1}} &= \frac{C}{a_1} \sum_{k=n+1}^{i} \frac{k^{l-1}/N^{l-1}}{1+\sum_{j=2}^{l} (a_j/a_1)(k/N)^{j-1}} \\ &= \frac{c}{a_1}\frac{i^l - n^l}{lN^{l-1}}\left[1+O\left(\frac{N_1}{N}\right)\right] \end{aligned} \tag{16}$$

Similarly,

$$\sum_{k=n+1}^{i} C^2 k^{2l}/B_k^2 N^{2l-2} = O(1/N_1) \tag{17}$$

Combining Eqs. (15)–(17) and making use of the fact that $i \leqslant N_1$, we have

$$\beta_{n+1,i} = \exp\left[\left(\frac{-c}{a_1}\right)\frac{i^l - n^l}{lN^{l-1}}\right]\left[1 + O\left(\frac{N_1}{N}\right)\right] \tag{18}$$

Combining Eqs. (13), (14), and (18), we have

$$f = \sum_{n=1}^{N_1} \sum_{i=n}^{N_1} \frac{1}{a_1 i} \exp\left[\left(\frac{-c}{a_1}\right)\frac{i^l - n^l}{lN^{l-1}}\right]\left[1 + O\left(\frac{N_1}{N}\right)\right]$$

For relation (12c) we first prove that for a positive, monotonically decreasing function $f(x)$ in the range $a \leqslant x \leqslant b$

$$f(a) \geqslant \sum_{i=a}^{b} f(i) - \int_a^b f(x)\,dx \geqslant f(b) \tag{19}$$

$$\int_a^b f(x)\,dx = \sum_{i=a}^{b-1} \int_i^{i+1} f(x)\,dx \tag{20}$$

Therefore

$$\sum_{a}^{b-1} f(i) \geqslant \int_a^b f(x)\,dx \geqslant \sum_{a+1}^{b} f(i) \tag{21}$$

Using Eqs. (20) and (21) and Eq. (19) twice, we get that

$$\begin{aligned}&\sum_1^{N_1} \sum_n^{N_1} (1/a_1 i) \exp[-C(i^l - n^l)/a_1 lN^{l-1}]\\ &\qquad - \int_1^{N_1} dy \int_y^{N_1} (dx/a_1 x) \exp[-C(x^l - y^l)/a_1 lN^{(l-1)}]\\ &= O(\log N_1)\end{aligned}$$

Coming to the proof of (12d), we note that

$$\begin{aligned}&\int_1^\infty dy \int_y^\infty dx\, F(x, y) - \int_1^{N_1} dy \int_y^{N_1} dx\, F(x, y)\\ &\quad = \int_0^1 dy \int_y^\infty dx\, F(x, y) + \int_1^N dy \int_{N_2}^\infty dx\, F(x, y) + \int_N^\infty dy \int_y^\infty dx\, F(x, y)\end{aligned}$$

where $F(x, y)$ stands for $(1/a_1 x) \exp[-C(x^l - y^l)/a_1 lN^{l-1}]$.

We now show that the contribution due to each of the individual terms on the right-hand side can be neglected when $N \to \infty$.

First,

$$\int_0^1 dy \int_y^\infty dx(1/a_1 x) \exp[-C(x^l - y^l)/a_1 l N^{l-1}]$$

$$\leqslant \int_0^1 dy \int_y^N (dx/a_1 x) + \int_0^1 dy \int_N^\infty (dx/a_1 N)$$

$$\times \exp(-Cx/a_1 l)] \exp(C/a_1 l N^{l-1})$$

$$= O(\log N)$$

Second,

$$\int_1^N dy \int_{N_2}^\infty dx\, (1/a_1 x) \exp[-C(x^l - y^l)/a_1 l N^{l-1}]$$

$$\leqslant \int_1^N dy \int_0^\infty dx'(1/a_1 y) \exp[-CN_1^{l-1} x'/(a_1^{l-1} x'/(a_1^l N^{l-1})]$$

$$= (lN^{l-1}/CN_1^{l-1}) \log N$$

$$= N^{(l-1)/l}/C(\log N)^l$$

Lastly,

$$\int_N^\infty dy \int_y^\infty dx(1/a_1 x) \exp[-C(x^l - y^l)/a_1 l N^{l-1}]$$

$$\leqslant \int_N^\infty dy \int_0^\infty (dx'/a_1 y) \exp(-Cy^{l-1} x'/a_1 N^{l-1})$$

$$= O(1)$$

Further, it is easy to see that

$$\int_0^\infty dy \int_y^\infty dx(1/a_1 x) \exp[-C(x^l - y^l)/a_1 l N^{l-1}]$$

$$= (N/a_1)^{(l-1)/l} (1/C)^{1/l} \phi_l \tag{22}$$

Using this (22) along with (12b)–(12d), we have

$$\frac{(1/N) \sum_1^{N_1} (N-n) \sum_n^{N_1} (1/A_i)\, \beta_{n+1,i}}{(N/a_1)^{(l-1)/l} (1/C)^{1/l}} = \phi_l \left[1 + O\left(\frac{1}{\log N}\right)\right] \tag{23}$$

where ϕ_l is the improper integral given by Eq. (5). Using Eqs. (23) and (12a) in Eq. (10), we have

$$\lim_{N \to \infty} \frac{\bar{t}_1}{(N/a_1)^{(l-1)/l} (1/C)^{1/l}} = \phi_l$$

thus proving the theorem.

3. RESULTS AND DISCUSSION

If we substitute the values $l = 2$, $a_1 = 1 - y$, $a_2 = -(1 - y)$, and $C = 1$ in Eq. (1), our system reduces to the one considered by Privman *et al.*[4] The asymptotic average MFPT in this case goes as $[N/(1 - y)]^{0.5}$ for $y \neq 1$, in agreement with the results obtained by Privman *et al.* using numerical methods. They obtain a phase transition for $y = 1$ with the average MFPT going as N. Our model also shows a phase transition for $a_1 = 0$. However, there is a slight difference between the cases $y = 1$ in Eq. (6) and $a_1 = 0$ in Eq. (1). In the former case $\bar{t}_1$ goes as N, whereas in the latter it goes as $N \log N/a_2$. This difference arises out of the fact that in the case considered by Privman *et al.* $B(n, N) = 0$ for all n, whereas it is greater than zero in our case.

Some numerical computations were done to verify Eq. (4). The average MFPT and the higher moments of the FPT distribution were computed using Eq. (11) in the range $N = 400$–40000 and for $l = 2, 3, 4, \ldots, 8$. For $a_1 \neq 0$ the exponents of N for $l = 2$, 3, and 4 come out to be 0.51, 0.68, and 0.77, respectively, which are close to the values of 0.5, 0.67, and 0.75 predicted by Eq. (4). For higher l's the agreement was slightly poorer. For $l = 8$, for example, the numerical value was 0.91, as against 0.875 from Eq. (4). This discrepancy was most likely because the asymptotic region had not yet been reached. In fact, the exponent shows a gradually decreasing trend with increasing range of N values. Similarly, for $a_1 = 0$ and $a_2 \neq 0$ and for $l = 3, 4$ the $N \log N$ behavior was verified.

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