Journal of Statistical Physics, Vol. 24, No. 4, 1981

First Passage Time Problems for One-Dimensional Random Walks

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Received October 15, 1979

This note contains a development of the theory of first passage times for one-dimensional lattice random walks with steps to nearest neighbor only. The starting point is a recursion relation for the densities of first passage times from the set of lattice points. When these densities are unrestricted, the formalism allows us to discuss first passage times of continuous time random walks. When they are negative exponential densities we show that the resulting equation is the adjoint of the master equation. This is the lattice analog of a correspondence well known for systems describable by a Fokker–Planck equation. Finally we discuss first passage problems for persistent random walks in which at each step the random walker continues in the same direction as the preceding step with probability α or reverses direction with probability $1 - \alpha$

KEY WORDS: Random walks; first passage time problems; continuous time random walks; adjoint equation; persistent random walks.

1. INTRODUCTION

The theory of first passage times for systems with at least one absorbing boundary whose development in time is described by a Fokker–Planck (FP) equation was first given by Pontryagin, Andronow, and Witt.[1] They showed that the probability density for the first passage time to absorption from a given point r satisfies the adjoint to the FP equation. This allowed them to write down readily solvable equations for the moments of time to absorption for one-dimensional systems. It does not seem to be generally known that the theory of lattice systems that allow for nearest-neighbor transitions only can be described by equations entirely analogous to the FP equation, although van Kampen[2] has recently pointed this out. In this note we show that for these systems one has the analogous result that the

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0022-4715/81/0400-0587$03.00/0

probability density of first passage times satisfies a fairly simple equation that allows one to find discrete analogs to the continuum results. In particular it will allow us to calculate moments of first passage times for one-dimensional systems in a much simpler way than the recursive technique suggested in Ref. 3. For simplicity we discuss the one-dimensional case only since the most useful results are obtained for it. We will also discuss the theory of first passage times for so-called persistent random walks. This theory does not appear to have been dealt with in the literature before. The fundamental equations of the present development, Eqs. (1) and (25), can be regarded as analogs of the renewal equation used by Darling and Siegert[4] in the context of first passage time problems.

2. CONTINUOUS TIME RANDOM WALKS

Suppose that $Q_r(t)$ is the probability density function for absorption of a random walker on a lattice interval $(0, N)$ given the initial position r. At least one of the points, 0 or N, is absorbing, and the other can be absorbing or reflecting. Let $a_r(t)\,dt$ $[b_r(t)\,dt]$ be the joint probability that the sojourn time at r is between t and $t + dt$, and that the succeeding transition is a step to the right (left). Then it is easily verified that the $Q_r(t)$ satisfy

$$Q_r(t) = \int_0^t a_r(\tau) Q_{r+1}(t-\tau)\,d\tau + \int_0^t b_r(\tau) Q_{r-1}(t-\tau)\,d\tau \tag{1}$$

subject to $Q_N(t) = \delta(t)$ for N an absorbing point. Different definitions can be used for a reflecting point. For example if $r = 0$ is reflecting such that when a random walker reaches it the walker is instantaneously transferred to $r = 1$, then the relevant boundary condition is $Q_0(t) = Q_1(t)$. Other definitions of reflection may be more natural and lead to boundary conditions that can be dealt with fairly easily. When the state probabilities, which we denote by $P_r(t)$, satisfy an ordinary master equation, the $a_r(t)$ and $b_r(t)$ can be given as

$$a_r(t) = \alpha_r \exp\big[-(\alpha_r + \beta_r)t\big], \qquad b_r(t) = \beta_r \exp\big[-(\alpha_r + \beta_r)t\big] \tag{2}$$

where α_r and β_r are rate constants. In all cases $a_r(t) + b_r(t) = \psi_r(t)$ is the probability density of sojourn time at r.

If we use the *ansatz* in Eq. (2) and substitute this into Eq. (1), we can use Laplace transforms to show that the $Q_r(t)$ satisfy the set of differential equations

$$\dot{Q}_r = \alpha_r \Delta^2 Q_{r-1} + (\alpha_r - \beta_r)\Delta Q_{r-1} \tag{3}$$

where $\Delta Q_{r-1} \equiv Q_r - Q_{r-1}$. In this case the master equation itself can be written

$$\dot{P}_r = \Delta\big[\Delta(\beta_{r-1} P_{r-1}) - (\alpha_{r-1} - \beta_{r-1}) P_{r-1}\big] \tag{4}$$

analogous to the FP equation. It is easily verified that Eq. (3) is the adjoint of the master equation just given. When the state probabilities satisfy a generalized master equation we must return to Eq. (1) and take Laplace transforms. If we denote the Laplace transform of a function by that same function with an asterisk, i.e., $\mathcal{L}[f(t)] = f^*(s)$, then Eq. (1) is readily transformed into

$$\left[1 - \psi_r^*(s)\right] Q_r^*(s) = a_r^*(s)\Delta^2 Q_{r-1}^* + \left[a_r^*(s) - b_r^*(s)\right]\Delta Q_{r-1}^* \tag{5}$$

Both Eqs. (1) and (3) allow us to write down and solve equations for the moments rather simply. Suppose that the mean time to absorption starting from r is T_r. Then we note that

$$T_r = \int_0^\infty t Q_r(t)\, dt = -\left.\frac{dQ_r^*}{ds}\right|_{s=0} \tag{6}$$

which allows us to work with the Laplace transforms in Eq. (5). To develop the formalism, let us set

$$a_r^*(0) = \int_0^\infty a_r(t)\, dt = \theta_r \leqslant 1 \tag{7}$$

so that $b_r^*(0) = 1 - \theta_r$. Notice that θ_r is the probability of moving to the right starting from r. Then Eq. (5), together with the obvious identity

$$\int_0^\infty Q_r(t)\, dt = Q_r^*(0) = 1 \tag{8}$$

allows us to write

$$\theta_r \Delta^2 T_{r-1} + (2\theta_r - 1)\Delta T_{r-1} = -\mu_r \tag{9}$$

where μ_r is the mean sojourn time for a single sojourn in state r,

$$\mu_r = \int_0^\infty t\psi_r(t)\, dt \tag{10}$$

assumed to be finite. In the special case in which the generalized master equation is an ordinary master equation, Eq. (9) takes the slightly simpler form

$$\alpha_r \Delta^2 T_{r-1} + (\alpha_r - \beta_r)\Delta T_{r-1} = -1 \tag{11}$$

but the more general Eq. (9) is as readily solved as is this one. A solution to Eq. (9) is found by rewriting the left-hand side as

$$\theta_r \Delta^2 T_{r-1} + (2\theta_r - 1)\Delta T_{r-1} = A_r \Delta(B_r \Delta T_{r-1}) \tag{12}$$

where A_r and B_r are chosen to ensure that the coefficients of the difference terms are in agreement. One finds in this way that

$$\frac{B_{r+1}}{B_r} = \frac{\theta_r}{1 - \theta_r} \tag{13}$$

or $B_r = \lambda_{r-1} B_1$ where

$$\lambda_{r-1} = \prod_{j=1}^{r-1} \frac{\theta_j}{1-\theta_j} \tag{14}$$

Similarly we have $A_r = \theta_r/(\lambda_r B_1)$. Since nearest-neighbor equations automatically satisfy detailed balance θ_r can also be written as a ratio of equilibrium probabilities for a lattice without absorbing sites.[2,5] Since the parameters A_r and B_r in Eq. (12) appear in multiplicative form, the parameter B_1 cancels and may be set equal to 1. Equation (9) is therefore equivalent to

$$\Delta(\lambda_{r-1} \Delta T_{r-1}) = -\mu_r \lambda_r / \theta_r \tag{15}$$

A general solution to this equation can be obtained by summing both sides of this equation. This yields

$$\Delta T_r = \frac{B}{\lambda_r} - \frac{1}{\lambda_r} \sum_{j=1}^{r} \frac{\mu_i \lambda_j}{\theta_i} \tag{16}$$

where B is an arbitrary constant. A second summation leads to

$$T_r = A + B \sum_{s=1}^{r} \frac{1}{\lambda_s} - \sum_{s=1}^{r} \frac{1}{\lambda_s} \sum_{i=1}^{s} \frac{\mu_i \lambda_i}{\theta_i} \tag{17}$$

where A is an arbitrary constant and it is understood that both sums are set equal to 0 when $r = 0$. We now have an expression analogous to that obtained for processes described by a FP equation, except that the integrals are replaced by sums. Let us suppose that $r = N$ is always absorbing so that $T_N = 0$. If $T_0 = 0$ we find from this last equation that $A = 0$ and

$$B = \left(\sum_{s=1}^{N} \frac{1}{\lambda_s} \sum_{i=1}^{s} \frac{\mu_i \lambda_i}{\theta_i} \right) \Big/ \sum_{s=1}^{N} \frac{1}{\lambda_s} \tag{18}$$

This form is obtained by setting $T_0 = 0$ first followed by setting $T_N = 0$. If we reverse the order in calculating the disposable constants we find the alternate expression

$$T_r = \sum_{s=r+1}^{N} \frac{1}{\lambda_s} \sum_{i=1}^{s} \frac{\mu_i \lambda_i}{\theta_i} - \left[\frac{\displaystyle\sum_{s=1}^{N} \frac{1}{\lambda_s} \sum_{i=1}^{s} \frac{\mu_i \lambda_i}{\theta_i}}{\displaystyle\sum_{s=1}^{N} \frac{1}{\lambda_s}} \right] \sum_{i=r+1}^{N} \frac{1}{\lambda_i} \tag{19}$$

which is easily shown to be equal to Eq. (17). When $r = 0$ is reflecting the expression obtained for T_r depends on the rule imposed when the random walker reaches $r = 0$. If we suppose that the random walker remains at $r = 0$ for an average time μ_0 and is then transferred to $r = 1$, the arbitrary

constants are determined from the requirement that $T_N = 0$ and $T_0 = T_1 + \mu_0$, which allows us to write

$$T_r = \sum_{s=r+1}^{N} \frac{1}{\lambda_s} \left(\lambda_1 \mu_0 + \sum_{i=2}^{s} \frac{\mu_i \lambda_i}{\theta_i} \right) \tag{20}$$

A similar expression is easily derived when we assume that the random walker is transferred to position r_0 after a mean time μ_0, or indeed if it is transferred to a random lattice point with a known distribution.

One can use Eq. (5) to generate equations for the higher moments. For example, if the variance of the first passage time is denoted by σ_r^2 and the variance of a single sojourn time at lattice point r is v_r then the σ_r^2 satisfy

$$\begin{aligned} \theta_r \Delta^2 \sigma_{r-1}^2 + (2\theta_r - 1)\Delta\sigma_{r-1}^2 = &-\theta_r(1-\theta_r)(T_{r+1} - T_{r-1})^2 \\ &+ 2\left[\nu_r(-)\theta_r - \nu_r(+)(1-\theta_r) \right](T_{r+1} - T_{r-1}) - v_r \end{aligned} \tag{21}$$

where $\nu_r(+)$ and $\nu_r(-)$ are

$$\nu_r(+) = \int_0^\infty t a_r(t)\, dt, \qquad \nu_r(-) = \int_0^\infty t b_r(t)\, dt \tag{22}$$

The boundary condition corresponding to an absorbing point is $\sigma_N^2 = 0$, and that corresponding to a reflecting point depends on the specific model of reflection used, but is analogous to the boundary condition for mean first passage times. Details of the solution are exactly the same as that for the mean. The same formalism can be applied to the calculation of the probability of absorption by a particular absorbing point in one dimension. If we suppose that both $r = 0$ and $r = N$ are absorbing and let Ω_r be the probability that absorption occurs at N starting from r, then one can easily show that the Ω_r satisfy

$$\theta_{r+1} \Delta^2 \Omega_r + (2\theta_{r+1} - 1)\Delta\Omega_r = 0 \tag{23}$$

subject to $\Omega_0 = 0$, $\Omega_N = 1$. The general solution to this equation is given in Eq. (17) with all of the $\mu_i = 0$. It is easy to show from that relation that

$$\Omega_r = \sum_{s=1}^{r} \frac{1}{\lambda_s} \Big/ \sum_{s=1}^{N} \frac{1}{\lambda_s} \tag{24}$$

3. PERSISTENT RANDOM WALKS

Finally, we point out that the preceding analysis can also be carried out for different generalizations of so-called persistent random walks. These were originally introduced by Taylor[6,7] as a model for diffusion, and in the continuum limit lead to a telegraph, rather than a diffusion equation.

Several generalizations of these are possible[8] but there is no discussion of first passage time problems for these processes in the literature. In a persistent random walk on a lattice one specifies the probability of a step continuing in the same direction as the preceding one or of reversing direction. We consider a simple model for persistence in which the time between successive steps is a random variable, the probability density for time of a single sojourn at lattice site r being $a_r(t)$ independent of the direction of motion. Let $U_r(t)$ be the probability density function of the first passage time starting from r, conditional on the first step being from r to $r+1$, let $V_r(t)$ be the analogous quantity when the first step is to $r-1$, let α be the probability that the following step will be in the same direction as one preceding, while $\beta = 1 - \alpha$ is the probability of reversing direction. In place of Eq. (1) we now have

$$U_r(t) = \int_0^t a_r(t)\left[\alpha U_{r+1}(t-\tau) + \beta V_{r+1}(t-\tau)\right] d\tau$$

$$V_r(t) = \int_0^t a_r(t)\left[\beta U_{r-1}(t-\tau) + \alpha V_{r-1}(t-\tau)\right] d\tau \tag{25}$$

In particular, when $a_r(t) = \lambda_r \exp(-\lambda_r t)$, these relations can be replaced by

$$\dot{U}_r + \lambda_r U_r = \lambda_r\left[\alpha U_{r+1} + \beta V_{r+1}\right]$$

$$\dot{V}_r + \lambda_r V_r = \lambda_r\left[\beta U_{r-1} + \alpha V_{r-1}\right] \tag{26}$$

If $r = N$ is an absorbing point Eq. (25) must be supplemented by the boundary condition $U_{N-1}(t) = a_{N-1}(t)$ while if $r = 0$ is absorbing the appropriate boundary condition is $V_1(t) = a_1(t)$. Reflecting boundary conditions, as before, depend on the particular model of reflection used.

The convolution form of Eq. (25) suggests that it would be advantageous to introduce Laplace transforms. If we do so we can convert Eq. (25) to a first-order relation

$$U^*_{r+1}(s) = \left[\frac{1 - \beta^2 a^*_{r+1}(s) a^*_r(s)}{\alpha a^*_r(s)}\right] U^*_r(s) - \beta a^*_{r+1}(s) V^*_r(s)$$

$$V^*_{r+1}(s) = \beta a^*_{r+1}(s) U^*_r(s) + \alpha a^*_{r+1}(s) V^*_r(s) \tag{27}$$

Alternatively we can eliminate of the variables to find second-order recurrence relations for the $U^*_r(s)$ and $V^*_r(s)$ separately. If we set $\Gamma_r(s) = 1/a^*_r(s)$ these recurrence relations are

$$\alpha\Gamma_{r+1}(s) U^*_{r+1}(s) + \left[1 - 2\alpha - \Gamma_r(s)\Gamma_{r+1}(s)\right] U^*_r(s) + \alpha\Gamma_{r-1}(s) U^*_{r-1}(s) = 0$$

$$\alpha\Gamma_{r+1}(s) V^*_{r+1}(s) + \left[1 - 2\alpha - \Gamma_r(s)\Gamma_{r-1}(s)\right] V^*_r(s) + \alpha\Gamma_{r-1}(s) V^*_{r-1}(s) = 0 \tag{28}$$

Equation (27) provides a slightly more convenient starting point for the calculation of moments. If we use the following notation:

$$\mu_r = \int_0^\infty t a_r(t)\, dt$$

$$A_r = \int_0^\infty t U_r(t)\, dt, \qquad B_r = \int_0^\infty t V_r(t)\, dt \tag{29}$$

and differentiate Eq. (27), setting $s = 0$ thereafter, we find

$$\begin{aligned} \Delta A_r &= \beta(A_r - B_r) - (1/\alpha)(\mu_r + \beta\mu_{r+1}) \\ \Delta B_r &= \beta(A_r - B_r) + \mu_{r+1} \end{aligned} \tag{30}$$

with the boundary conditions $A_{N-1} = \mu_{N-1}$, $B_1 = \mu_1$. By subtraction of these two equations we find that

$$\Delta(A_r - B_r) = -(1/\alpha)(\mu_r + \mu_{r+1}) \tag{31}$$

or

$$\begin{aligned} A_r - B_r &= A_1 - B_1 - (1/\alpha)(\mu_1 + 2\mu_2 + 2\mu_3 + \cdots + 2\mu_{r-1} + \mu_r) \\ &= A_1 - B_1 - C_r \end{aligned} \tag{32}$$

where C_r is the known sum on the right side. Hence it follows that

$$\Delta A_r = \beta(A_1 - B_1) - \beta C_{r+1} - \mu_r \tag{33}$$

where the right-hand side does not depend on the A_r. The solution to this last equation is easily seen to be

$$A_r = A_1 + (r-1)\beta(A_1 - B_1) - \sum_{i=1}^{r-1} (r-i)(\beta C_{i+1} + \mu_i) \tag{34}$$

The parameter B_1 is known to be μ_1, so that all that is needed for a complete solution is the parameter A_1. But this can be calculated from the second condition $A_{N-1} = \mu_{N-1}$. In this way we find

$$A_1 = \frac{\mu_{N-1} + (N-2)\beta\mu_1 + \sum_{i=1}^{N-2} (\beta C_{i+1} + \mu_i)(N-1-i)}{1 + (N-2)\beta} \tag{35}$$

which, together with Eqs. (32) and (34), completes the formal solution for the mean first passage times.

Further generalizations of the preceding results are easily developed for one-dimensional problems. One trivial generalization is to allow for different pausing time densities that depend on the direction of motion. All of the preceding theory can be formally generalized to multidimensional nearest-neighbor random walks, but just as in the case of systems described by a Fokker–Planck equation no general solutions to the relevant equations are available for these more complicated systems.

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