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One-Dimensional Non-Nearest-Neighbor Random Walks in the Presence of Traps

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A one-dimensional lattice random walk in the presence of m equally spaced traps is considered. The step length distribution is a symmetric exponential. An explicit analytic expression is obtained for the probability that the random walk will be trapped at the jth trapping site.

KEY WORDS: One-dimensional random walk; non-nearest-neighbor step distribution; traps, conditioned first passage time; generating functions.

1. INTRODUCTION

In this note we calculate the probability that a random walker whose step distribution function is exponential will be trapped at one of a set of regularly spaced trapping sites. In our analysis we utilize a result of Rubin and Weiss[(1)] (RW). RW obtained a general expression for the generating function for the probability of random walks which start at the origin in a d-dimensional lattice and reach lattice point $\mathbf{R}$ at step N having visited each of a set of m lattice points $\{\mathbf{R}_i\}$, where $\mathbf{R}_i$ is visited s_i times and where $s_i \geqslant 0$. The RW generating function is expressed in terms of the generating function for the probability of random walks which start at $\mathbf{R}_i$ and reach $\mathbf{R}_j$ at step N, $P[\mathbf{R}_j - \mathbf{R}_i; z]$. The explicit form of $P[\mathbf{R}_j - \mathbf{R}_i; z]$ for the one-dimensional lattice with exponentially distributed step length has been obtained by Lakatos-Lindenberg and Shuler[(2)] (LS).

In Section 2 we define the one-dimensional random walk model with trapping sites, present the explicit results from RW[(1)] and LS[(2)] which we use in our analysis, and outline the results of our calculation. Details of the calculation are given in the Appendix.

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2. ONE-DIMENSIONAL LATTICE WITH TRAPS

We consider a one-dimensional random walk on a lattice with m equally spaced trapping sites located at lattice points b, $2b$,..., mb, where b is a positive integer. RW[1] have given an expression for $\xi(jb; x_1,..., x_m; z)$, the generating function of the probability of random walks which start at the origin and reach lattice point $R_j = jb$ at step N, having visited lattice $R_i = ib$, s_i times, where $s_i \geq 0$ and $i = 1,..., m$. When we use this result in our trapping problem, we will require that all s_i are equal to zero. In this way, we assure that all trapping sites have been avoided until trapping site R_j is reached for the first time.

The RW generating function is expressed as the ratio of two $m \times m$ determinants [Eq. (17b) in ref. 1]

$$\xi(jb; x_1,..., x_m; z) = x_j D^{(j)}(x_1,..., x_m; z)/D(x_1,..., x_m; z) \tag{1}$$

where

$$D(x_1,..., x_m; z) = \begin{vmatrix} x_1 + (1-x_1) P[0; z] & (1-x_2) P[-b; z] & \cdots & (1-x_m) P[-(m-1)b; z] \\ (1-x_1) P[b; z] & x_2 + (1-x_2) P[0; z] & \cdots & (1-x_m) P[-(m-2)b; z] \\ \vdots & \vdots & & \vdots \\ (1-x_1) P[(m-1)b; z] & (1-x_2) P[(m-2)b; z] & \cdots & x_m + (1-x_m) P[0; z] \end{vmatrix} \tag{2}$$

and where the $m \times m$ determinant $D^{(j)}(x_1,..., x_m; z)$ is obtained from $D(x_1,..., x_m; z)$ by replacing its jth column by the column

$$\begin{pmatrix} P[b; z] \\ P[2b; z] \\ \vdots \\ P[mb; z] \end{pmatrix} \tag{3}$$

The function $P[R_j - R_i; z]$ is the generating function of the probability of random walks which start at R_i and reach R_j at step N. In this note we only consider symmetric random walks with an exponential step distribution. For the case of random walks with the normalized step distribution

$$p(l_j - l_i) = \begin{cases} \frac{1}{2}(e^a - 1) \exp[-|l_i - l_j| a], & l_i \neq l_j \\ 0, & l_i = l_j \end{cases} \tag{4}$$

LS[2] obtained an explicit formula for $P[R_j - R_i; z]$ [see Eq. (74) in ref. 2]:

$$P[R_j - R_i; z] = \begin{cases} \dfrac{X^{|R_j - R_i|} z(e^{2a} - 1)}{[2 + z(z^a - 1)]\mathscr{D}}, & |R_j - R_i| \geqslant 1 \\ \dfrac{z(e^{2a} - 1) + 2\mathscr{D}}{[2 + z(e^a - 1)]\mathscr{D}}, & R_j = R_i \end{cases} \tag{5}$$

where

$$\mathscr{D} = \{(e^a + 1)[e^a + 1 + z(e^a - 1)](1 - z)\}^{1/2} \tag{6}$$

and

$$X = \frac{e^{2a} + 1 + z(e^a - 1) - (e^a - 1)\mathscr{D}}{e^a[2 + z(e^a - 1)]} \tag{7}$$

The symmetric nature of the random walk is evident in the dependence of $P[R_j - R_i; z]$ on $|R_j - R_i|$ in Eq. (5).

Finally, the generating function of the probability of random walks which start at $R = 0$ and reach $R = jb$, having visited lattice point $R_i = ib$, s_i times, where $i = 1,\ldots,$ is $\Pi[jb; s_1,\ldots,s_m; z]$, the coefficient of $x_1^{s_1} x_2^{s_2} \cdots x_m^{s_m}$ in the expansion of $\xi(jb; x_1,\ldots,x_m; z)$ in a multiple power series

$$\xi(jb; x_1,\ldots,x_m; z) = x_j \sum_{s_1=0} \cdots \sum_{s_m=0} \Pi(jb; s_1,\ldots, s_m; z) x_1^{s_1} \cdots x_m^{s_m} \tag{8}$$

We have now assembled all the explicit formulas which we require in our trapping problem. If we wish to calculate the probability that a random walker starting at the origin will be trapped at lattice site $R_j = jb$, one of the trapping sites $\{ib\}$, $i = 1,\ldots, m$, we can simply calculate it from the conditioned first-passage probability-generating function [Eqs. (1) and (8)]

$$\Pi(jb; 0,\ldots, 0; z) = D^{(j)}(0,\ldots, 0; z)/D(0,\ldots,0;z) \tag{9}$$

The coefficient of z^N in the expansion of $\Pi(jb; 0,\ldots, 0; z)$ in powers of z, $F(jb; 0,\ldots, 0; N)$, is the probability of first passage to lattice site jb at step N conditioned on the walker never having visited any of the other trapping sites prior to step N (i.e., $s_i = 0$ for all i)

$$\Pi(jb; 0,\ldots, 0; z) = \sum_{N=0}^{\infty} F(jb; 0,\ldots, 0; N) z^N \tag{10}$$

The probability $\Pi^{(j)}$ that the random walker will be trapped eventually at $R_j = jb$ is, according to Eqs. (9) and (11),

$$\begin{aligned}\Pi^{(j)} &= \Pi(jb; 0,..., 0; 1)\\ &= \sum_{N=0}^{\infty} F(jb; 0,..., 0; N)\\ &= \lim_{z\to 1} \{D^{(j)}(0,..., 0; z)/D(0,..., 0; z)\}\end{aligned} \tag{11}$$

The determinant $D(0,..., 0; z)$ which appears in Eqs. (9) and (11) has a simpler form than that in Eq. (2), namely

$$D(0,..., 0; z) = \begin{vmatrix} P[0; z] & P[b; z] & \cdots & P[(m-1)b; z] \\ P[b; z] & P[0; z] & \cdots & P[(m-2)b; z] \\ \vdots & \vdots & & \vdots \\ P[(m-1)b; z] & P[(m-2)b; z] & \cdots & P[0; z] \end{vmatrix} \tag{12}$$

The determinant $D(0,..., 0; z)$ is symmetric for symmetric random walks because $P[R_j - R_i; z]$ is an even function of its first argument. All elements of the determinants $D(0,..., 0; z)$ and $D^{(j)}(0,..., 0; z)$ are singular, containing a factor $(1-z)^{-1/2}$, so care must be taken in evaluating the limit $z \to 1$ in Eq. (11). The details of this calculation are given in the Appendix; we merely list the results here. The probaibility $\Pi^{(j)}$ in Eq. (11) that the random walker will be trapped eventually at $R = jb$ is [Appendix, Eq. (A30)]

$$\Pi^{(j)} = [\sinh(m-j+1)\Gamma - \sinh(m-j)\Gamma]/\sinh m\Gamma \tag{13}$$

where

$$\sinh(\Gamma/2) = b^{1/2} \sinh(a/2) \tag{14}$$

It follows from the form of $\Pi^{(j)}$ in Eq. (13) that Π, the probability that the random walker will be trapped eventually at one of the m trapping sites, is a certainty, i.e.,

$$\Pi = \sum_{j=1}^{m} \Pi^{(j)} = 1 \tag{15}$$

We next consider the form of $\Pi^{(j)}$ in two limiting cases: (a) first the limit in which the average step length is large compared to the spacing between traps; and (b) the opposite limit of a small average step length. The average magnitude of the step length of the exponential step distribution, Eq. (4), is

$$\langle l \rangle = (1 - e^{-a})^{-1} \tag{16}$$

The limit $\langle l\rangle \gg b$ corresponds to $a \ll 1$, in which case

$$\langle l\rangle \cong a^{-1} \tag{17}$$

and from Eq. (14)

$$\Gamma \cong b^{1/2} a \tag{18}$$

Thus in case (a), Eq. (13) for $\Pi^{(j)}$ yields

$$\lim_{a\to 0} \{\Pi^{(j)}\} = m^{-1} \tag{19}$$

the same value for all trapping sites.

LS[2] have note that in the opposite limit [our case (b)], where $a \to \infty$, the exponential-step-distribution random walk, Eq. (4), behaves like a nearest-neighbor random walk. According to Eq. (14), in the limit of large a,

$$\Gamma/a = 1, \qquad a \to \infty \tag{20}$$

In the limit where $\Gamma \gg 1$, it is convenient to rewrite Eq. (13) as

$$\Pi^{(j)} = e^{-(j-1)\Gamma}\left(\frac{1 - e^{-\Gamma} - e^{-2(m-j+1)\Gamma} + e^{-[2(m-j)+1]\Gamma}}{1 - e^{-2m\Gamma}}\right) \tag{21}$$

Thus, for $\Gamma \gg 1$,

$$\Pi^{(1)} \cong 1 - e^{-\Gamma}$$

$$\Pi^{(m)} \cong e^{(m-1)\Gamma}$$

and

$$\lim_{\Gamma\to\infty} \{\Pi^{(j)}\} = \begin{cases} 1, & j = 1 \\ 0, & j > 1 \end{cases}$$

Thus in the limiting case (b), it is seen that the probability of trapping at site $j = 1$, closest to the starting point, is a certainty, the result expected for a nearest-neighbor one-dimensional random walk.

Finally, we make two remarks suggesting interesting generalizations of the model treated in this paper. First, it is possible to repeat the calculation of trapping probabilities for a biased exponential step distribution since LS[2] have obtained the generating function in this case. Second, it would be of interest to consider the trapping problem for Weierstrass random walks.

APPENDIX. EVALUATION OF $\lim_{z\to 1}\{D^{(j)}(0,..., 0; z)/D(0,..., 0; z)\}$

Each of the elements in the determinants $D(0,..., 0; z)$ and $D^{(j)}(0,..., 0; z)$, Eqs. (2), (3), and (12), is expressed in terms of the generating function for the exponential-step random walk, Eq. (5). In this calculation it is convenient to isolate the singular part of the generating function which is located at $z=1$:

$$P[R_j - R_i; z] = \begin{cases} \alpha g(1-z)^{-1/2} X^{b|j-i|}, & |j-i| \geqslant 1 \\ \alpha[1+g(1-z)^{-1/2}], & j=i \end{cases} \tag{A1}$$

where

$$\alpha = 2[2+z(e^a-1)]^{-1} \tag{A2}$$

$$g = z(e^{2a}-1)/(2h) \tag{A3}$$

$$h = \{(e^a-1)[e^a+1+z(e^a-1)]\}^{1/2} \tag{A4}$$

and

$$X = \frac{e^{2a}+1+z(e^a-1)-(e^a-1)(1-z)^{-1/2}h}{e^a[2+z(e^a-1)]} \tag{A5}$$

The diagonal and off-diagonal elements of $P[R_j - R_i; z]$ in Eq. (A1) can be represented by the single expression

$$P[R_j - R_i; z] = \alpha[\delta_{ij} + g(1-z)^{1/2} X^{b|j-i|}] \tag{A6}$$

where δ_{ij} is the Kronecker delta:

$$\delta_{ij} = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}$$

Each element of the $m \times m$ determinant $D(0,..., 0; z)$ contains a factor α. Therefore $D(0,..., 0; z)$ can be written as

$$D(0,..., 0; z) = \alpha^m d_m \tag{A7}$$

where the i, j element of the $m \times m$ determinant d_m is

$$\delta_{ij} + g(1-z)^{-1/2} X^{b|j-i|} \tag{A8}$$

We next show that the determinant $D^{(j)}(0,..., 0; z)$ can be expressed as a simple combination of a pair of determants d_{m-j+1} and d_{m-j}. Each element of $D^{(j)}(0,..., 0; z)$ is proportional to α, so

$$D^{(j)}(0,..., 0; z) = \alpha^m d_m^{(j)} \tag{A9}$$

where $d_m^{(j)}$ is the $m \times m$ determinant which is obtained from d_m, Eqs. (A7) and (A8), by replacing its jth column by

$$\begin{pmatrix} g(1-z)^{-1/2}X^b \\ g(1-z)^{-1/2}X^{2b} \\ \vdots \\ g(1-z)^{-1/2}X^{mb} \end{pmatrix} \tag{A10}$$

First note that when a factor X^b is removed from column j, its elements are identical with those of column 1 [see Eq. (A8)], except for the first element of column 1, which contains a contribution from δ_{11}. Thus, by subtracting column j from column 1 and expanding by elements of the first column, one obtains

$$d_m^{(j)} = X^b d_{m-1}^{(j-1)} \tag{A11}$$

This procedure can be repeated until

$$d_m^{(j)} = X^{(j-1)b} d_{m-j+1}^{(1)} \tag{A12}$$

Next note that after removing one additional factor X^b from the first column of $d_{m-j+1}^{(1)}$ the 1, 1 element of Eq. (A12) can be written as

$$1 + g(1-z)^{-1/2}X^b - 1$$

It therefore follows that

$$d_{m-j+1}^{(1)} = X^b[d_{m-j+1} - d_{m-j}] \tag{A13}$$

Finally, we have

$$D^{(j)}(0,..., 0; z) = \alpha^m X^{jb}[d_{m-j+1} - d_{m-j}] \tag{A14}$$

The conditioned first-passage probability generating function, Eq. (9), is reduced with the aid of Eqs. (A7) and (A14) to

$$\Pi(jb; 0,..., 0; z) = X^{jb}(d_{m-j+1} - d_{m-j})/d_m \tag{A15}$$

We next obtain an explicit expression for the determinant d_m. Consider the following pair of operations: (1) multiply the rth row by X^b and subtract it from the $r+1$th row; (2) then repeat this operation for the rth and $(r+1)$th columns. If this pair of operations is performed in the order $r = m-1$, $m-2$,..., 1, the determinant d_m assumes the tridiagonal form

$$d_m = \begin{vmatrix} 1+g(1-z)^{-1/2} & -X^b & & & & \\ -X^b & \Omega & -X^b & & & \\ & -X^b & \Omega & & & \\ & & & \ddots & & \\ & & & & \Omega & -X^b \\ & & & & -X^b & \Omega \end{vmatrix} \tag{A16}$$

where

$$\Omega = 1 + g(1-z)^{-1/2} + [1 - g(1-z)^{-1/2}]X^{2b} \tag{A17}$$

It follows from Eq. (A16) that d_m satisfies the recurrence, or difference equation,

$$d_m = \Omega d_{m-1} - X^{2b} d_{m-2} \tag{A18}$$

where

$$d_0 = 1$$

and

$$d_1 = 1 + g(1-z)^{-1/2}$$

The recurrence equation can be solved by the method of generating functions. Multiply Eq. (A17) by t_m and sum from $m = 2$ to ∞ and obtain

$$G(t) - 1 - t[1 - g(1-z)^{-1/2}] = \Omega t[G(t) - 1] - X^{2b} t^2 G(t) \tag{A19}$$

where

$$G(t) = \sum_{m=0}^{\infty} d_m t^m \tag{A20}$$

Solving Eq. (A19) for $G(t)$,

$$G(t) = \frac{1 + t[1 + g(1-z)^{-1/2} - \Omega]}{1 - 2(\frac{1}{2}\Omega X^{-b})(X^b t) + (X^b t)^2} \tag{A21}$$

The denominator of Eq. (A21) has been cast in the form of the generating function for Tchebychef polynomials,[3] so that

$$G(t) = \{1 + t[1 + g(1-z)^{-1/2} - \Omega]\} \sum_{m=0}^{\infty} U_m(\cos\theta)(X^b t)^2 \tag{A22}$$

where

$$\cos\theta = \tfrac{1}{2}\Omega X^{-b}$$
$$= \tfrac{1}{2}(X^b + X^{-b}) - \tfrac{1}{2}g(1-z)^{-1/2}(X^b - X^{-b}) \quad \text{(A23)}$$

and

$$U_m(\cos\theta) = \sin(m+1)\theta/\sin m\theta \quad \text{(A24)}$$

Combining Eqs. (A20) and (A22) and the definition of Ω, Eq. (A17), we find that the explicit formula for d_m is the coefficient of t^m:

$$d_m = X^{mb}\{U_m(\cos\theta) + [g(1-z)^{-1/2} - 1]X^b U_{m-1}(\cos\theta)\} \quad \text{(A25)}$$

We are now prepared to consider the limit $z \to 1$ in Eq. (A15) using Eq. (A25). First note that $\cos\theta$, which appears in Eq. (A25) and is defined in Eq. (A23), approaches a well-defined limit as $z \to 1$, namely

$$\lim_{z\to 1}\{\cos\theta\} = 1 + 2b\sinh^2(a/2) \quad \text{(A26)}$$

Since the limiting value of $\cos\theta$ in Eq. (A26) is greater than one, the limiting value of θ is $i\Gamma$, where Γ is real and

$$\cosh\Gamma = 1 + 2b\sinh^2(a/2) \quad \text{(A27)}$$

As a consequence of this fact, a Tchebychef polynomial such as $U_m(\cos\theta)$ approaches the limit

$$\lim_{z\to 1}\{U_m(\cos\theta)\} = \sinh(m+1)\Gamma/\sinh\Gamma \quad \text{(A28)}$$

In obtaining the limit for $\cos\theta$ in Eq. (A26), we have used the fact that X also approaches a limit,

$$\lim_{z\to 1}\{X\} = 1 \quad \text{(A29)}$$

We thus conclude that the only singular component of d_m in the limit $z \to 1$ is the factor $(1-z)^{-1/2}$. Thus, the $z \to 1$ limit of $\Pi(jb; 0,..., 0; z)$ in Eq. (A15) is

$$\Pi^{(j)} = \lim_{z\to 1}\{\Pi(jb; 0,..., 0; z)\}$$
$$= [U_{m-j}(\cosh\Gamma) - U_{m-j-1}(\cosh\Gamma)]/U_{m-1}(\cosh\Gamma)$$
$$= [\sinh(m-j+1)\Gamma - \sinh(m-j)\Gamma]/\sinh m\Gamma \quad \text{(A30)}$$

It follows from the form of Eq. (A30) that the probability that the random walker will be trapped at one of the trapping sites is

$$\sum_{j=1}^{m} \Pi^{(j)} = 1 \tag{A31}$$

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