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RANDOM WALK PROBABILITIES IN TERMS OF LEGENDRE POLYNOMIALS

M. A. EL-SHEHAWAY

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ABSTRACT. Asymmetric random walk on non-negative integers S , with one or two absorbing boundaries is considered.

The probability distribution $(p_n(x|x_0))$ of being at any position $x \in S$ after n steps, given an initial position $x_0 \in S$, from their generating function is obtained in terms of derivatives of Legendre polynomials. This derivation is different from the standard approach.

1. Introduction

Anomalous diffusion in random systems has received wide attention in the last decade. In spite of considerable progress, many important problems are still open. One of the models, intensively studied in the earlier works is a one-dimensional discrete-time random walk on the random lattice (see for example, Neuts [6], Cox and Miller [1], Feller [5], Srinivasan and Mehata [8], Weiss and Havlin [9], Raykin [7], EL-Shehaway [2], El-Shehaway and Matrafi [3], and El-Shehaway [4]). The determination of explicit expressions for random walk probabilities from their generating functions is effected by partial fractions. However, it is generally quite difficult. In this paper we seek explicit expressions for obtaining the n -step probability $p_n(x|x_0)$ that the particle is at location $x \in S$ after n steps given that its initial position was $x_0 \in S$. These are easily derived from their generating function expansion involving derivatives of Legendre polynomials.

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2. The generating function for the n th step occupation probability

Let $p_n(x|x_0)$ be the n -step occupation probability that the particle reaches the position $x \in S$ at time n given that its initial position was $x_0 \in S$; and α , β and γ are respectively the probabilities of moving one step to the right, one to the left and remaining in position, $\alpha + \beta + \gamma = 1$. The boundary points 0 and L are absorbing barriers. Then, $p_n(x|x_0)$ must satisfy the following difference equations.

For $n \geq 1$

$$p_n(x|x_0) = \alpha p_{n-1}(x-1|x_0) + \gamma p_{n-1}(x|x_0) + \beta p_{n-1}(x+1|x_0),$$

$$x \in \{2, 3, \dots, L-2\} \quad (2.1)$$

$$p_n(1|x_0) = \gamma p_{n-1}(1|x_0) + \beta p_{n-1}(2|x_0) \quad (2.2)$$

$$p_n(0|x_0) = \beta p_{n-1}(1|x_0) \quad (2.3)$$

$$p_n(L-1|x_0) = \alpha p_{n-1}(L-2|x_0) + \gamma p_{n-1}(L-1|x_0) \quad (2.4)$$

$$p_n(L|x_0) = \alpha p_{n-1}(L-1|x_0) \quad (2.5)$$

with the initial condition

$$p_0(x|x_0) = \delta_{x,x_0}, \quad (2.6)$$

where δ_{x,x_0} denotes the Kronecker delta.

Introduce the generating functions

$$G(z; x|x_0) = \sum_{n=0}^{\infty} z^n p_n(x|x_0), \quad x, x_0 \in S, \quad |z| < 1. \quad (2.7)$$

The Equations (2.1)–(2.5) reduce to

$$G(z; x|x_0) = \frac{1}{1-\gamma z} \left[\delta_{x,x_0} + z(\alpha G(z; x-1|x_0) + \beta G(z; x+1|x_0)) \right],$$

$$x \in \{2, 3, \dots, L-2\}, \quad (2.8)$$

with the boundary conditions

$$G(z; x|x_0) = \begin{cases} \delta_{0,x_0} + \beta z G(z; 1|x_0), & x = 0, \\ \frac{1}{1-\gamma z} [\delta_{1,x_0} + \beta z G(z; 2|x_0)], & x = 1, \\ \frac{1}{1-\gamma z} [\delta_{L-1,x_0} + \alpha z G(z; L-2|x_0)], & x = L-1, \\ \delta_{L,x_0} + \alpha z G(z; L-1|x_0), & x = L. \end{cases} \quad (2.9)$$

Solving (2.8) and (2.9) systematically (see El-Shehawey [2]) we deduce that

$$G(z; x|x_0) = \begin{cases} \left(\sqrt{\frac{\beta}{\alpha}} \right)^{x_0} \left[\frac{\theta_1^{L-x_0} - \theta_2^{L-x_0}}{\theta_1^L - \theta_2^L} \right], & x_0 \in S, \quad x = 0, \\ \frac{\left(\sqrt{\frac{\beta}{\alpha}} \right)^{x_0-x}}{z\sqrt{\alpha\beta}} \left(\frac{\theta_1^x - \theta_2^x}{\theta_1 - \theta_2} \right) \left[\frac{\theta_1^{L-x_0} - \theta_2^{L-x_0}}{\theta_1^L - \theta_2^L} \right], & x_0 \in S \setminus \{0, L\}, \\ & x \in \{1, 2, \dots, x_0\}, \end{cases} \quad (2.10)$$

$$G(z; x|x_0) = \begin{cases} \frac{\left(\sqrt{\frac{\alpha}{\beta}} \right)^{x-x_0}}{z\sqrt{\alpha\beta}} \left(\frac{\theta_1^{x_0} - \theta_2^{x_0}}{\theta_1 - \theta_2} \right) \left[\frac{\theta_1^{L-x} - \theta_2^{L-x}}{\theta_1^L - \theta_2^L} \right], & x_0 \in S \setminus \{0, L\}, \\ & x \in \{x_0, x_0+1, \dots, L-1\}, \\ \left(\sqrt{\frac{\alpha}{\beta}} \right)^{L-x_0} \left[\frac{\theta_1^{x_0} - \theta_2^{x_0}}{\theta_1^L - \theta_2^L} \right], & x_0 \in S, \quad x = L \end{cases} \quad (2.11)$$

and $G(z; x|x_0) = 0$ for $x_0 = 0$ or L , $x \in S \setminus \{0, L\}$, where $\theta_1(z)$ and $\theta_2(z)$ are given by

$$\begin{aligned} \theta_1(z) &= \left(2z\sqrt{\alpha\beta} \right)^{-1} \left[1 - \gamma z + \sqrt{1 - 2\gamma z + (\gamma^2 - 4\alpha\beta)z^2} \right], \\ \theta_2(z) &= \left(2z\sqrt{\alpha\beta} \right)^{-1} \left[1 - \gamma z - \sqrt{1 - 2\gamma z + (\gamma^2 - 4\alpha\beta)z^2} \right]. \end{aligned} \quad (2.12)$$

With the convention that the square roots are positive we have $\theta_1(z) > \theta_2(z)$ and hence, if $w_n(x|x_0)$ denotes the n -step occupation probability that the particle is at location x after n steps, given that its initial position was $x_0 \in S$ for the case L infinite, the generating function expression (2.10) is easily modified to the one-boundary case.

$$\tilde{G}(z; x|x_0) = \begin{cases} \left(\sqrt{\frac{\beta}{\alpha}} \right)^{x_0} \theta_2^{x_0}, & x = 0, \\ \frac{\left(\sqrt{\frac{\alpha}{\beta}} \right)^{x-x_0}}{z\sqrt{\alpha\beta}} \left(\frac{\theta_1^{x-x_0} - \theta_2^{x-x_0}}{\theta_1 - \theta_2} \right), & x_0 \in S \setminus \{0, L\}, \\ & x = \{1, 2, \dots, x_0\}. \end{cases} \quad (2.13)$$

On using $\theta_1(z)\theta_2(z) = 1$ and expanding the denominator of (2.10) as a geometric series in $\frac{\theta_2(z)}{\theta_1(z)}$ we can deduce that

$$\begin{aligned} & p_n(x|x_0) \\ &= w_n(x|x_0) + \lim_{M \rightarrow \infty} \sum_{j=1}^M \left(\frac{\alpha}{\beta} \right)^{jL} \left[w_n(x|2jL+x_0) - \left(\frac{\beta}{\alpha} \right)^{x_0} w_n(x|2jL-x_0) \right] \end{aligned} \quad (2.14)$$

in the two cases

- (1) $x = 0, x_0 \in S,$
- (2) $x = 1, 2, \dots, x_0, x_0 \in S \setminus \{0, L\}.$

Thus the problem of identifying the coefficient of z^n in (2.10) can be reduced to that of determining the coefficient of z^n in (2.13). In the following section we state some fundamental concepts and notions needed.

3. Basic notions and fundamental concepts

Let us introduce the notation

$$u = z\sqrt{\gamma^2 - 4\alpha\beta} \quad \text{and} \quad v = \frac{\gamma}{\sqrt{\gamma^2 - 4\alpha\beta}} \tag{3.1}$$

with the assumption $\gamma^2 > 4\alpha\beta$, we see that $\theta_2(z)$ becomes

$$\theta_2(z) = \frac{\sqrt{\gamma^2 - 4\alpha\beta}}{2\sqrt{\alpha\beta}u} \left[1 - uv - \sqrt{1 - 2uv + u^2} \right]. \tag{3.2}$$

From Whittaker and Watson [10; p. 336],

$$\left[1 - uv - \sqrt{1 - 2uv + u^2} \right]^m = m(v^2 - 1)^m \sum_{n=m}^{\infty} \frac{(n-1)!}{(n+m)!} P_n^{(m)}(v) u^{n+m} \tag{3.3}$$

where $P_n^{(m)}(y)$ denotes the m th derivative with respect to y of the Rodrigues formula for Legendre polynomials $p_n(y)$ defined by

$$p_n(y) = \frac{1}{n!2^n} \frac{d^n}{dy^n} (y^2 - 1)^n, \quad n \geq 0. \tag{3.4}$$

We need the following results for Legendre polynomials,

$$P_n^{(m)}(v) = \frac{(n+m)!}{\pi n!(v^2 - 1)^{\frac{m}{2}}} \int_0^\pi \left[v + \sqrt{v^2 - 1} \cos \varphi \right]^n \cos m\varphi \, d\varphi \tag{3.5}$$

(see Whittaker and Watson [10; p. 325–326]), and

$$P_n^{(m)}(0) = \frac{(-1)^{\frac{n-m}{2}}}{2^n} \frac{(n+m)!}{\left(\frac{n+m}{2}\right)! \left(\frac{n-m}{2}\right)!}. \tag{3.6}$$

Formula (3.6) is derived from the generating function for Legendre polynomials, namely

$$\frac{1}{\sqrt{1 - 2uv + u^2}} = \sum_{n=0}^{\infty} p_n(v) u^n \tag{3.7}$$

by differentiation with respect to v and then setting $v = 0$, and then equating coefficients of u .

We shall also need the trigonometric identity

$$\sum_{m=0}^M \cos 2m\psi = \frac{1}{2} + \frac{\sin(2M+1)\psi}{2\sin\psi}, \quad (3.8)$$

as well as the result given by Whittaker and Watson [10; p. 180]

$$\lim_{M \rightarrow \infty} \int_0^\pi \frac{\sin(2M+1)\psi}{\sin\psi} f(\psi) d\psi = \frac{\pi}{2} [f(0) + f(\pi)], \quad (3.9)$$

provided that $f(\psi)$ is continuously differentiable in the range $(0, \pi)$.

4. The one-boundary case ($L \rightarrow \infty$)

In the case L infinite, from (2.13), (3.2) and (3.3) we can deduce that

$$w_n(0|x_0) = x_0(2\beta)^{x_0} \frac{(n-1)!}{(x+x_0)!} (\gamma^2 - 4\alpha\beta)^{\frac{n-x_0}{2}} p_n^{(x_0)} \left(\frac{\gamma}{\sqrt{\gamma^2 - 4\alpha\beta}} \right), \quad (4.1)$$

$$n \geq x_0,$$

and for $x \in \{1, 2, \dots, x_0\}$, $x_0 \in S \setminus \{0, L\}$

$$w_n(x|x_0) = \sum_{k=0}^{x-1} (2k-x+x_0+1) 2^{2k-x+x_0+1} \alpha^k \beta^{k-x+x_0} \frac{n!}{(n+2k-x+x_0+2)!} \cdot (\gamma^2 - 4\alpha\beta)^{\frac{n-2k+x-x_0}{2}} p_{n+1}^{(2k-x+x_0+1)} \left(\frac{\gamma}{\sqrt{\gamma^2 - 4\alpha\beta}} \right), \quad (4.2)$$

$$n \geq 2k - x + x_0,$$

and zero elsewhere.

Formulae (4.1), (4.2) and (3.5) enable us to find after integration by parts alternative expressions for $w_n(x|x_0)$, namely

$$w_n(x|x_0) = \begin{cases} \frac{x_0}{n\pi} \left(\frac{\beta}{\alpha}\right)^{\frac{x_0}{2}} \int_0^\pi (\gamma + 2\sqrt{\alpha\beta} \cos \varphi)^n \cos x_0 \varphi d\varphi, & x = 0, \\ \frac{1}{\pi} \left(\frac{\alpha}{\beta}\right)^{\frac{x-x_0}{2}} \int_0^\pi (\gamma + 2\sqrt{\alpha\beta} \cos \varphi)^n \sin x_0 \varphi \sin x \varphi d\varphi, & x \in \{1, 2, \dots, x_0\}, \\ & x_0 \in S \setminus \{0, L\}. \end{cases} \quad (4.3)$$

Formulae (4.1)–(4.3) generalize those of Feller [5; p. 353] to the case γ and x are non-zero. In fact the case $\gamma = 0$ can be formally deduced from (4.1),

(4.2) using (3.6). We obtain,

$$w_n(x|x_0) = \begin{cases} \frac{x_0}{n} \binom{n}{\frac{n+x_0}{2}} \alpha^{\frac{n-x_0}{2}} \beta^{\frac{n+x_0}{2}}, & x = 0, \quad n \geq x_0, \\ 2^{n+1} \alpha^{\frac{n+x-x_0}{2}} \beta^{\frac{n-x+x_0}{2}} \int_0^1 \cos^n \pi\varphi \sin x_0 \pi\varphi \sin x \pi\varphi \, d\varphi, & n \geq x - x_0, \\ & x \in S \setminus \{0, L\}, \\ & x_0 \in S \setminus \{0, L\}. \end{cases} \tag{4.4}$$

This obviously agrees with the well-known result for the infinite random walk with absorbing barrier at the origin (see for example F e l l e r [5], S r i n i v a s o n and M e t h a t a [8]).

5. Random walk with two absorbing boundaries

Using (4.3) and performing an integration by parts we can verify that

$$\begin{aligned} \left(\frac{\alpha}{\beta}\right)^{jL} \left[w_n(x|2jL + x_0) - \left(\frac{\beta}{\alpha}\right)^{x_0} w_n(x|2jL - x_0) \right] \\ = \int_0^{L\pi} F_n(\psi; x|x_0) \cos 2m\varphi \, d\varphi \end{aligned} \tag{5.1}$$

where the function $F_n(\psi; x|x_0)$ is given by

$$F_n(\psi; x|x_0) = \frac{4}{\pi L} \begin{cases} \sqrt{\alpha\beta} \left(\sqrt{\frac{\beta}{\alpha}}\right)^{x_0} \left(\gamma + 2\sqrt{\alpha\beta} \cos \frac{\psi}{L}\right)^{n-1} \sin \frac{\psi}{L} \sin \frac{x_0\psi}{L}, & x = 0, \\ \left(\frac{\alpha}{\beta}\right)^{\frac{x-x_0}{2}} \left(\gamma + 2\sqrt{\alpha\beta} \cos \frac{\psi}{L}\right)^n \sin \frac{x\psi}{L} \sin \frac{x_0\psi}{L}, & x \in \{1, 2, \dots, x_0\}, \\ & x_0 \in S \setminus \{0, L\}. \end{cases} \tag{5.2}$$

From (2.14) and (5.1) we have

$$p_n(x|x_0) = \lim_{M \rightarrow \infty} \int_0^{L\pi} F_n(\psi; x|x_0) \frac{\sin(2M+1)\psi}{2 \sin \psi} \, d\psi, \tag{5.3}$$

where we have used the trigonometric identity (3.8). But clearly we have

$$\begin{aligned} \int_0^{L\pi} F_n(\psi; x|x_0) \frac{\sin(2M+1)\psi}{\sin \psi} \, d\psi \\ = \sum_{m=0}^{L-1} \int_0^{\pi} f_n(\Psi+m\pi; x|x_0) \frac{\sin(2M+1)\Psi}{\sin \Psi} \, d\Psi \end{aligned} \tag{5.4}$$

by employing a result given in Whittaker and Watson [10; p. 180].

Thus from (3.9), (5.3) and (5.4) we have

$$p_n(x|x_0) = \frac{\pi}{2} \sum_{m=1}^{L-1} F_n(m\pi; x|x_0), \tag{5.5}$$

and therefore finally using (5.2) we obtain

$$p_n(0|x_0) = \frac{2\sqrt{\alpha\beta}}{L} \left(\sqrt{\frac{\beta}{\alpha}} \right)^{x_0} \sum_{m=1}^{L-1} \left(\gamma + 2\sqrt{\alpha\beta} \cos \frac{m\pi}{L} \right)^{n-1} \cdot \sin\left(\frac{m\pi}{L}\right) \sin\left(\frac{x_0 m\pi}{L}\right), \quad x_0 \in S, \tag{5.6}$$

$$p_n(x|x_0) = \frac{1}{L} \left(\sqrt{\frac{\beta}{\alpha}} \right)^{\frac{x_0-x}{2}} \sum_{m=1}^{L-1} \left(\gamma + 2\sqrt{\alpha\beta} \cos \frac{m\pi}{L} \right)^n \cdot \sin\left(\frac{xm\pi}{L}\right) \sin\left(\frac{x_0 m\pi}{L}\right), \tag{5.7}$$

$x \in \{1, 2, \dots, x_0\}, \quad x_0 \in S \setminus \{0, L\}.$

Observing (2.10) and (2.11) we can conclude that $p_n(L|x_0)$ can be obtained directly from $p_n(0|x_0)$ using the transformation

$$\alpha \leftrightarrow \beta \quad \text{and} \quad x_0 \mapsto L - x_0.$$

Therefore $p_n(L|x_0)$ is of the form

$$p_n(L|x_0) = \frac{2\sqrt{\alpha\beta}}{L} \left(\sqrt{\frac{\beta}{\alpha}} \right)^{L-x_0} \sum_{m=1}^{L-1} \left(\gamma + 2\sqrt{\alpha\beta} \cos \frac{m\pi}{L} \right)^{n-1} \cdot \sin\left(\frac{m\pi}{L}\right) \sin\left(\frac{m\pi(L-x_0)}{L}\right), \quad x_0 \in S. \tag{5.8}$$

The explicit expressions for $p_n(x|x_0)$, $x \in \{x_0, x_0+1, \dots, L-1\}$, $x_0 \in S \setminus \{0, L\}$ can be similarly obtained from (5.7) using the transformation

$$\alpha \leftrightarrow \beta \quad \text{and} \quad x_0 \leftrightarrow x.$$

Therefore, the explicit formula for $p_n(x|x_0)$ for any $x \in S \setminus \{0, L\}$, $x_0 \in S \setminus \{0, L\}$

$$p_n(x|x_0) = \frac{2}{L} \left(\frac{\beta}{\alpha} \right)^{\frac{x_0-x}{2}} \sum_{m=1}^{L-1} \left(\gamma + 2\sqrt{\alpha\beta} \cos \frac{m\pi}{L} \right)^n \sin\left(\frac{xm\pi}{L}\right) \sin\left(\frac{x_0 m\pi}{L}\right). \tag{5.9}$$

We see that with the appropriate change of notation formula, (5.6) is similar to a formula given by Cox and Miller [1; p. 353] and generalizes that of Feller [5; p. 353] and formula (5.9) generalizes that of Weiss and Havlin [9] to the case $\alpha \neq \beta$, γ non-zero. Unfortunately, however, the expression in Neuts [6; Equation (20)] corresponding to (5.6) is erroneous. A comparison leads to the necessity of a correction in Neuts [6]. The expression

$$T_\rho = \frac{1}{b} \sin \rho \frac{b-j}{b} \pi \frac{1}{[d\gamma/du]_{u=u_\rho}}$$

$$= b^{-1} (4pq)^{\frac{1}{2}} \cos \frac{\rho\pi}{b} \sin \frac{\rho\pi(b-j)}{b} \left[r + (4pq)^{\frac{1}{2}} \cos \frac{\rho\pi}{b} \right]^{-2}$$

should be

$$T_\rho = \frac{1}{b} \sin \rho \frac{b-j}{b} \pi \frac{1}{[d\gamma/du]_{u=u_\rho}} (\cos \rho\pi)^{-1}$$

$$= -b^{-1} (4pq)^{\frac{1}{2}} (\cos \rho\pi)^{-1} \sin \frac{\rho\pi}{b} (b-j) \sin \frac{\rho\pi}{b} \left[r + (4pq)^{\frac{1}{2}} \cos \frac{\rho\pi}{b} \right]^{-2}$$

$$= b^{-1} (4pq)^{\frac{1}{2}} \sin \frac{\rho\pi}{b} \sin \frac{j\rho\pi}{b} \left[r + (4pq)^{\frac{1}{2}} \cos \frac{\rho\pi}{b} \right]^{-2}$$

in which $\gamma = \arccos(4pq)^{-\frac{1}{2}}(u^{-1} - r)$, and formula (20) should corrected accordingly to agree with our result (5.6).

A glance at the sums in (5.6), (5.8) and (5.9) show that the terms corresponding to the summation indices $m = k$ and $m = L - k$ are of the same absolute value, they are of the same sign when n , x and x_0 are of the same parity and cancel otherwise. Accordingly $p_n(x|x_0) = 0$ when $n + x - x_0$ is odd while for even $n + x - x_0$ and $n > 1$

$$p_n(x|x_0) =$$

$$= \frac{4}{L} \begin{cases} \sqrt{\alpha\beta} \left(\frac{\beta}{\alpha}\right)^{\frac{x_0}{2}} \sum_{m < \frac{L}{2}} (\gamma + 2\sqrt{\alpha\beta} \cos \frac{m\pi}{L})^{n-1} \sin \frac{m\pi}{L} \sin \frac{x_0 m\pi}{L}, & x_0 \in S, x = 0, \\ \left(\frac{\beta}{\alpha}\right)^{\frac{x_0-x}{2}} \sum_{m < \frac{L}{2}} (\gamma + 2\sqrt{\alpha\beta} \cos \frac{m\pi}{L})^n \sin \frac{xm\pi}{L} \sin \frac{x_0 m\pi}{L}, & x, x_0 \in S \setminus \{0, L\}, \\ \sqrt{\alpha\beta} \left(\frac{\alpha}{\beta}\right)^{\frac{L-x_0}{2}} \sum_{m < \frac{L}{2}} (\gamma + 2\sqrt{\alpha\beta} \cos \frac{m\pi}{L})^{n-1} \sin \frac{m\pi}{L} \sin \frac{m\pi(L-x_0)}{L}, & x_0 \in S, x = L, \end{cases}$$

(5.10)

the summation extending over the positive integers $< \frac{L}{2}$. This form is more natural than (5.6), (5.8) and (5.9) because now the coefficients form a decreasing sequence and so for large n it is essentially only the first term that counts.

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Finally we observe that (4.3), (5.6)–(5.9) are well defined for $\gamma^2 \leq 4\alpha\beta$ and by straight forward modifications of the above we can more rigorously deduce these expressions for these cases.

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