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First passage time distributions for finite one-dimensional random walks

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Abstract. We present closed expressions for the characteristic function of the first passage time distribution for biased and unbiased random walks on finite chains and continuous segments with reflecting boundary conditions. Earlier results on mean first passage times for one-dimensional random walks emerge as special cases. The divergences that result as the boundary is moved out to infinity are exhibited explicitly. For a symmetric random walk on a line, the distribution is an elliptic theta function that goes over into the known Lévy distribution with exponent 1/2 as the boundary tends to ∞.

Keywords. Biased random walks; Markov processes; first passage time; finite chains.

1. Introduction

There is considerable current interest (Weiss 1966, 1981; Montroll and West 1979; Seshadri *et al* 1980; Gillespie 1981; Seshadri and West 1982) in the classic problem of the first passage time in one-dimensional random walks owing to its diverse applications in physical problems: for example, the calculation of reaction rates in chemical processes, chemical dissociation induced by surface catalysis, optical bistability, decay of metastable states, etc. In general, such applications require the estimation of the mean first passage time for diffusion in the presence of specific potentials. In this paper, our aim is to present *exact* results for a simpler situation that takes account, however, of certain physical circumstances common to most applications. Thus, we study a random walk on a bounded set with perfectly reflecting boundaries, so that there is no 'leakage of probability'. We consider both discrete and continuous sets (finite chains or line segments). Further, we allow for an arbitrary uniform bias in the random walk — thus simulating the effect of a constant external field, or a finite temperature in the case of spectral diffusion, etc. Finally, we present closed-form expressions for the *characteristic function* of the first passage time distribution. The corresponding mean and variance can be deduced from this. The known results for the mean first passage time on the (semi-) infinite chain or line emerge, of course, as special cases of the expressions obtained here. Our primary result for the characteristic function follows from a lengthy calculation the outlines of which are sketched in the Appendix; the structure of the final result will be seen to comply with that required by a formal theorem on the first passage time problem for Markov processes (Darling and Siegert 1953). Our result facilitates an analytic examination of the effects of the finite 'probability-conserving' boundary and of the superposed drift on the distribution of the first passage time.

The standard procedure (Pontryagin *et al* 1933; Stratonovich 1963) used in solving first passage time problems for a continuous Markov process whose conditional density satisfies a Fokker-Planck equation is *via* the solution of the adjoint equation. Our procedure, however, will be to present first the results for random walk on a discrete chain (a somewhat more difficult case), and then to pass to the continuum limit. We shall exploit for this purpose our recent exact solution (Khantha and Balakrishnan 1983) of the biased random walk problem on finite chains, obtained in the context of the frequency-dependent hopping conductivity in a bond-percolation model as well as the study of a spectral diffusion problem.

2. Biased random walk on a finite chain

We consider first a biased random walk on a finite chain with site label $m = 0, 1, \ldots, N$ (the lattice constant a being set equal to unity for convenience), *via* nearest-neighbour jumps at an average rate $2W$ and respective *a priori* probabilities $(1+g)/2$ and $(1-g)/2$ for jumps to the right and left, with $-1 < g < 1$. The end points of the chain are reflecting boundaries. Let $Q(m, t\,|\,m_0)\,\mathrm{d}t$ be the probability of reaching m for the first time in the time interval $(t, t+\mathrm{d}t)$ starting from m_0 at $t=0$, where $0 \leqslant m_0 < m \leqslant N$. (The solution for $m_0 > m$ can be deduced from this with the help of a symmetry present in the problem.) Let $P(m, t\,|\,m_0)$ denote the conditional probability of finding the walker at the point m at time t, given that she starts from m_0 at $t = 0$. Then, *because* the simple random walk under consideration is a *Markov chain**, Q is related to P *via* the Siegert equation (Siegert 1951; Montroll and West 1979)

$$P(m_1, t\,|\,m_0) = \int_0^t P(m_1, t-t'\,|\,m)\, Q(m, t'\,|\,m_0)\,\mathrm{d}t', \quad m_0 < m \leqslant m_1. \tag{1}$$

Hence, in terms of the corresponding Laplace transforms,

$$\tilde{Q}(m, u\,|\,m_0) = \tilde{P}(m_1, u\,|\,m_0)\,/\,\tilde{P}(m_1, u\,|\,m), \quad m_0 < m \leqslant m_1, \tag{2}$$

where u is the transform variable. Analytic continuation to $u = i\omega$ will now yield the characteristic function of the distribution $Q(m, t\,|\,m_0)$ since the latter is defined only for positive values of t. The first passage to the point m from a point $m_0 < m$ (with $0 \leqslant m_0 < m < N$) involves the consideration of a random walk in the restricted range $[0, m]$ with an absorbing barrier at m. (We have already specified that 0 is a reflecting barrier.) Though $\tilde{P}(m_1, u\,|\,m_0)$ depends explicitly on m_1 and N (the loca-

*The non-Markov case, in particular the one in which the sequence of steps exhibits a memory in time as governed by a renewal process with a non-exponential pausing time distribution, is of interest in its own right. Some results for mean first passage times in such 'continuous time random walks' on an infinite chain have been given in Weiss (1981) using a generalised master equation. We have recently obtained an exact solution for $\tilde{Q}$ in the case of a general CTRW by other methods. These results will be reported separately (Balakrishnan and Khantha 1983).

tion of the boundary on the right), one would expect the dependence on m_1 and N to cancel out in the ratio on the right side of (2): $\tilde{Q}(m, u \mid m_0)$ must depend only on m_0, m and the reflecting barrier at the origin; as $0 \leqslant m_0 < m$, the effects of any boundary at a site to the right of m will not appear in $Q(m, t \mid m_0)$.

The mean first passage time from m_0 to m is given by

$$E\,[(t\,(m_0 \to m)] = -\lim_{u \to 0}\, \partial\, \tilde{Q}\,(m, u \mid m_0)\, /\, \partial\, u, \tag{3}$$

while the second moment is

$$E\,[t^2\,(m_0 \to m)] = \lim_{u \to 0}\, \partial^2\, \tilde{Q}\, /\, \partial\, u^2, \tag{4}$$

provided these limits exist. As $E\,[t]$, $E\,[t^2]$, etc. diverge in certain simple situations corresponding to random walks on an infinite chain (see below), it is advantageous and instructive to derive first the exact results for a finite chain and then pass to the appropriate limit carefully so as to bring out the origin of these divergences.

As already mentioned in § 1, we now employ in (2) the solution we have obtained for $\tilde{P}\,(m, u \mid m_0)$ (Khantha and Balakrishnan 1983). The derivation of this solution is outlined in the Appendix. It turns out that the result can be written very compactly if we identify certain convenient variables. Accordingly, let us characterise the bias by the parameter $\alpha = \text{arc tanh}\, g$, so that the ratio of the probability of a jump to the right to that of a jump to the left is $(1 + g)/(1 - g) = \exp(2\alpha) = f$. We further define the quantity $\xi_0 = \text{arc cosh}\,(1 + u/2W)$, and finally introduce the variable ξ defined by $\cosh \xi = \cosh \xi_0 \cosh \alpha = (1 + u/2W)/(1 - g^2)^{1/2}$. (As the Laplace transform is initially defined (is analytic) in a right half plane in u, it is appropriate to use hyperbolic functions. Note also that $\xi \to \xi_0$ when there is no bias). Then, for $0 \leqslant m, m_0 \leqslant N$, our answer for $\tilde{P}$ reads

$$\tilde{P}\,(m, u \mid m_0) = f^{(m-m_0)/2}\,[\sinh\,(N - m_> + 1)\,\xi - \sqrt{f} \sinh\,(N - m_>)\xi]$$
$$\times\,[\sqrt{f} \sinh\,(m_< + 1)\,\xi - \sinh m_<\,\xi]/[u \sinh \xi \sinh\,(N + 1)\,\xi], \tag{5}$$

where $m_> = \max\,(m, m_0)$ and $m_< = \min\,(m, m_0)$. This representation of $\tilde{P}$ is in conformity with a general theorem on the structure of the Laplace transform of the conditional probability density for a temporally homogeneous Markov process (Darling and Siegert 1953; Siegert 1951). According to this thorem, $\tilde{P}\,(m, u \mid m_0)$ for such a process can always be written as a product of a function of m and a function of m_0. The proof of the theorem is based on the Siegert equation given earlier, and is valid for solutions on finite or infinite intervals. Our solution for $\tilde{P}\,(m, u \mid m_0)$ in (5) is explicitly a product of two such factors: one of them is a function of $m_>$ (and the right boundary at N), while the other is a function of $m_<$ (and the left boundary at 0).

Substitution of (5) in (2) yields, for $0 \leqslant m_0 < m \; (\leqslant N)$,

$$\tilde{Q}(m, u \mid m_0) = f^{(m-m_0)/2} \left[\frac{\sqrt{f} \sinh (m_0 + 1)\, \xi - \sinh m_0\, \xi}{\sqrt{f} \sinh (m+1)\, \xi - \sinh m\, \xi} \right]. \tag{6}$$

This is (after a straightforward analytic continuation to $u = i\omega$) the desired result for the characteristic function of the first passage time distribution in the presence of a reflecting barrier at the point 0. For a first passage from m_0 to m with $0 \leqslant m_0 < m < N$, the barrier at N is irrelevant, as already stated. The effect of the bias is measured by the deviation of the quantity f from unity, or, more accurately, of α from zero (recall that $f = \exp(2\alpha)$). For instance, in the application of the random walk model to the problem of spectral diffusion (Alexander *et al* 1978, 1981) at a finite temperature T, involving the non-radiative transfer of energy among a set of energy levels in a system with level spacing Δ, the parameter α is equal to Δ/KT. The unbiased case then corresponds to the $T \to \infty$ limit in which all the levels have equal occupation probabilities.

The mean first passage time corresponding to the characteristic function (6) is, using (3),

$$E\,[t\,(m_0 \to m)] = \frac{1}{2W} \frac{(f+1)}{(f-1)} \left[(m - m_0) - \frac{(f^{-m} - f^{-m_0})}{(f-1)} \right], \; (0 \leqslant m_0 < m). \tag{7}$$

A result equivalent to (7) is already known (see, *e.g.*, Parzen 1962)* for a discrete-time random walk on the set $\{0, 1, .., N\}$.

3. The continuum limit

The solution to the first passage time problem for diffusion on a finite segment $(0 \leqslant x \leqslant L)$ with reflecting boundary conditions can be obtained by proceeding to the continuum limit of the foregoing. Let the lattice spacing $a \to 0$, the bias factor $g \to 0$, the jump rate $W \to \infty$ and the number of sites $N \to \infty$ such that the following quantities are finite. the segment length $L = \lim Na$, the diffusion constant $D = \lim Wa^2$, and the drift velocity $c = \lim 2\,Wag$. ($c > 0$ signifies a drift to the right, $c < 0$ a drift to the left. We use the term bias for a random walk on a discrete chain, and drift when referring to diffusion on a continuous line. Further, in the discrete case, $D = Wa^2$ is the static diffusion constant on an infinite chain). Alternatively, one may employ the continuum version of (2) after solving for the Laplace transform $\tilde{P}(x, u \mid x_0)$ of the conditional probability density from the Smoluchowski equation

$$(D\, d^2/dx^2 - c\, d/dx - u)\, \tilde{P} = -\,\delta\,(x - x_0), \tag{8}$$

*In Parzen 1962 (see equation (7.29) therein), this result has been derived by solving the recursion relation obeyed by $E[t(m_0 \to m)]$ in the variable m_0. (The numerator of the first factor on the right in that equation should read p instead of q.)

with the reflecting boundary conditions

$$(D\,d/dx - c)\,\tilde{P} = 0, \tag{9}$$

at $x = 0$ and L for all u. Let $Q\,(x, t\,|\,x_0)\,dt$ be the probability of reaching the point x for the first time in the interval $(t, t + dt)$ starting from the point $x_0 < x$ at $t = 0$. We find the following solution for $\tilde{Q}$:

$$\tilde{Q}\,(x, u\,|\,x_0) = \left[\frac{R\,\cosh\,(Rx_0) + (c/2D)\,\sinh\,(Rx_0)}{R\,\cosh\,(Rx) + (c/2D)\,\sinh\,(Rx)}\right] \times$$

$$\exp\,[c\,(x - x_0)/2\,D]\ \ (0 \leqslant x_0 < x), \tag{10}$$

where $R = R(u) = (c^2 + 4\,u\,D)^{1/2}/2D$. This last quantity can be recast in the form $R = (1 + 2\,u\,\tau)^{1/2}\,/\lambda$, where $\tau = 2D/c^2$ $(= \lim 1/(2W\,g^2))$ and $\lambda = 2D/c$ $(= \lim a/g)$ respectively define natural time and length scales for diffusion with drift. $\tilde{Q}(x, i\omega\,|\,x_0)$ is the characteristic function of the first passage time distribution from x_0 to x $(0 \leqslant x_0 < x)$ in the presence of a reflecting barrier at the origin. As in the discrete case, the barrier on the right at L is irrelevant in this context, and (10) is valid even for a first passage from x_0 to x on a semi-infinite line $[0, \infty]$ with a reflecting barrier at the origin.

Using (3) and (4), the mean and variance of the distribution $Q\,(x, t\,|\,x_0)$ are found to be respectively

$$E\,[t\,(x_0 \to x)] = \frac{(x - x_0)}{c} + \tfrac{1}{2}\,\tau\,[\exp\,(-\,2x/\lambda) - \exp\,(-\,2x_0/\lambda)] \tag{11}$$

and

$$\mathrm{Var}\,[t\,(x_0 \to x)] = \tau\left[\left\{\frac{x}{c} + \left(\tau + \frac{2x}{c}\right)\exp\,(-\,2x/\lambda)\right.\right.$$

$$\left.\left.+\,\tfrac{1}{4}\,\tau\,\exp\,(-\,4x/\lambda)\right\} - \{x \to x_0\}\right]. \tag{12}$$

4. Infinite random walks

According to Polya's classic result (Polya 1921), the mean first passage time from m_0 to m $(m_0 < m)$, or from x_0 to x $(x_0 < x)$, for a random walk on a (semi-)infinite chain or line is *infinite* if the bias (or drift) is zero; it is finite if the bias or drift is to the right. (We shall comment shortly on what happens when the bias is to the left.) For the discrete chain the emergence of these results is conveniently exhibited with the help of the general formula in (7) if we first translate the origin to the point $-M$ and eventually let $M \to +\infty$. When the bias is to the right $(0 < g < 1$, or $1 < f < \infty$, or $0 < \alpha < \infty)$, we find

$$E\,[t\,(m_0 \to m)] = (m - m_0)/(2Wg) + O\,[\exp\,(-\,2M\alpha)]$$

$$\underset{M \to \infty}{\to}\ (m - m_0)/(2Wg) \qquad (-\,\infty < m_0 < m). \tag{13}$$

The corresponding variance in the limit $M \to \infty$ is

$$\mathrm{Var}\,[t\,(m_0 \to m)] = (m - m_0)/(4W^2 g^3) \qquad (-\infty < m_0 < m). \tag{14}$$

The continuum analogues of (13) and (14) for diffusion with a drift to the right ($c > 0$) on an infinite line are obtained similarly, using (11) and (12). We find

$$E\,[t\,(x_0 \to x)] = (x - x_0)/c \qquad (-\infty < x_0 < x), \tag{15}$$

and

$$\mathrm{Var}\,[t\,(x_0 \to x)] = 2D\,(x - x_0)/c^3 \qquad (-\infty < x_0 < x). \tag{16}$$

When the bias is zero ($g = 0, f = 1, \alpha = 0$), we find

$$E\,[t\,(m_0 \to m)] \to M\,(m - m_0)/W \qquad (-M \ll m_0 < m), \tag{17}$$

which diverges *linearly* as $M \to \infty$. On the other hand, for a bias to the left ($-1 < g < 0$, or $0 < f < 1$, or $-\infty < \alpha < 0$),

$$E\,[t\,(m_0 \to m)] \to O\,[\exp\,(2M\,|\,\alpha\,|)] \qquad (-M \ll m_0 < m), \tag{18}$$

which diverges *exponentially* as the boundary is moved out to infinity on the left. What is happening is best understood as follows. The characteristic function for first passage on the (semi-) infinite chain is found from (6) by replacing m and m_0 by $m + M$ and $m_0 + M$ respectively, and then taking the limit $M \to +\infty$. We obtain

$$\tilde{Q}(m, u\,|\,m_0) = f^{(m-m_0)/2}\left[\frac{u + 2\,W - (u^2 + 4\,u\,W + 4\,W^2 g^2)^{1/2}}{2\,W(1 - g^2)^{1/2}}\right]^{m-m_0}, \tag{19}$$

which is *apparently* valid for all f in $0 < f < \infty$, or $-1 < g < +1$, *i.e.* for left, right, or zero bias. Now, an examination of the general formula of (2) in the limit $u \to 0$ immediately reveals that

$$\tilde{Q}\,(m, 0\,|\,m_0) = \lim_{u \to 0} \left\{\frac{u^{-1} P^{\mathrm{st}}\,(m_1)}{u^{-1} P^{\mathrm{st}}\,(m_1)}\right\} = 1, \tag{20}$$

so that the Siegert equation ensures that the first passage time distribution is *inherently* normalised according to

$$\int_0^\infty Q(m, t\,|\,m_0)\,\mathrm{d}t = 1. \tag{21}$$

On the other hand, taking the limit $u \to 0$ carefully in (19) yields

$$\tilde{Q}(m, 0\,|\,m_0) = \begin{cases} 1, \text{ for } f > 1 \text{ (or } g > 0) \\ f^{m-m_0}\,(< 1), \text{ for } f < 1 \text{ (or } g < 0). \end{cases} \tag{22}$$

The distribution is therefore not normalised to unity when the bias is to the left. The resolution of the paradox lies in the fact that, when the bias is to the left, a passage to the right (equivalently, absorption at a site $m > m_0$) is not a *certain* event if the chain extends infinitely far to the left: *i.e.*,

$$\int_0^\infty Q(m, t \mid m_0)\, \mathrm{d}t < 1 \tag{23}$$

in that case. Therefore the first passage time from m_0 to $m > m_0$ is not a proper random variable in the sense of Darling and Siegert (1953), and its moments do not exist. This circumstance appears to have been overlooked by Montroll and West (1979), and hence the distribution function $Q(m, t \mid m_0)$ and the mean first passage time obtained from it (see equations (6.14) and (6.16) in Montroll and West 1979) are not valid when the bias is to the left.* For the sake of completeness, let us record the (known) expression for the first passage time distribution on the (semi-) infinite chain when the bias is to the right or is absent. This is the inverse transform of (19):

$$\begin{aligned} Q(m, t \mid m_0) = {} & [(m - m_0)/t]\, f^{(m-m_0)/2} \\ & \exp(-2\,W t)\, I_{m-m_0}\,[2\,Wt\,(1 - g^2)^{1/2}] \quad (-\infty < m_0 < m). \end{aligned} \tag{24}$$

Here I_r is the modified Bessel function of order r, and $1 \leqslant f < \infty$ or $0 \leqslant g < 1$, as already explained. One may verify that the first moment of this distribution is $(m - m_0)/(2Wg)$ when $0 < g < 1$ and infinite when $g = 0$, in accord with the preceding remarks.

4. Symmetric random walks

Going back to the finite chain considered earlier, taking the limit $g \to 0$ ($f \to 1$) gives very simple answers for unbiased or symmetric random walks. We find (for $0 \leqslant m_0 < m$ as usual)

$$\begin{aligned} E[t(m_0 \to m)] &= [(m + \tfrac{1}{2})^2 - (m_0 + \tfrac{1}{2})^2]/(2\,W), \\ \mathrm{Var}\,[t(m \to m)] &= [(m + \tfrac{1}{2})^4 - (m_0 + \tfrac{1}{2})^4]/(6\,W^2), \end{aligned} \tag{25}$$

and so on. The continuum analogues are, again with $0 \leqslant x_0 < x$,

$$\begin{aligned} E[t(x_0 \to x)] &= (x^2 - x_0^2)/(2\,D), \\ \mathrm{Var}\,[t(x_0 \to x)] &= (x^4 - x_0^4)/(6\,D), \text{ etc.} \end{aligned} \tag{26}$$

*There are also typographical errors in (6.10) and (6.13)-(6.16) of that reference: *e.g.*, $\eta/(1 - \eta)$ should be replaced by its reciprocal in several places.

The characteristic function $\tilde{Q}$ in (6) itself reduces in this case to

$$\tilde{Q}(m, u \mid m_0) = \cosh (m_0 + \tfrac{1}{2})\xi_0 / \cosh (m + \tfrac{1}{2})\xi_0 \quad (0 \leqslant m_0 < m), \tag{27}$$

where $\cosh \xi_0 = (1 + u/2W)$ as already defined. The first passage time distribution can then be written as

$$Q(m, t \mid m_0) = (1/t) \exp(-2Wt) \sum_{r=0}^{\infty} (-1)^r [a_r \{I_{a_r}(2Wt) + I_{b_r}(2Wt)\} + (2m_0 + 1) I_{b_r}(2Wt)], \tag{28}$$

where $\quad a_r = (m - m_0) + (2m + 1) r, \; b_r = a_r + 2m_0 + 1.$ (29)

The continuum version of (27) is

$$\tilde{Q}(x, u \mid x_0) = \cosh (ux_0^2/D)^{1/2} / \cosh (ux^2/D)^{1/2} \quad (0 \leqslant x_0 < x). \tag{30}$$

Inversion of the transform yields (Oberhettinger and Badii 1973)

$$Q(x, t \mid x_0) = \frac{D}{x} \frac{\partial}{\partial x_0} \theta_1 \left(\frac{x_0}{2x} \middle| \frac{Dt}{x^2} \right), \quad (0 \leqslant x_0 < x), \tag{31}$$

where θ_1 is the elliptic theta function of the first kind. As before. if we shift the origin to the point $-L$ and let L become very large, we can find the form of the 'correction' to the known result for an infinite line (see, *e.g.*, Feller 1966; Itô and McKean 1974) owing to the introduction of a (distant) boundary. We get

$$Q(x, t \mid x_0) = (x - x_0)(4\pi Dt^3)^{-1/2} \exp[-(x - x_0)^2/(4Dt)] + O[\exp(-L^2/Dt)], \quad (-L \ll x_0 < x). \tag{32}$$

The term that survives when $L \to +\infty$ is the familiar one-sided Lévy distribution (in the *time* t) with exponent 1/2, all of whose moments diverge. To get an idea of the effect of introducing a reflecting barrier, we have plotted in figure 1 the first passage time distribution function for drift-free diffusion on a line. Curve (a) is the Lévy distribution that applies when the line extends infinitely far to the left of the starting point x_0. Curve (b) represents the other extreme in which the confining barrier is at x_0 itself. All other intermediate cases, in which the barrier is at a finite distance to the left of x_0, fall in between these two extremes.* The *exponential* fall off as $t \to \infty$ in the case of a finite barrier changes to a power law ($\sim t^{-3/2}$) when the barrier is moved out to infinity—causing, incidentally, the divergence of the moments of the distribution.

*For numerical accuracy, in the case of a finite boundary (as in figure 1b) one must use different representations for the θ_1 function in different time regimes: for small t, an expansion in terms of the form $t^{-3/2} \exp(-\mu_n/t)$; for large t, of the form $\exp(-\lambda_n t)$.

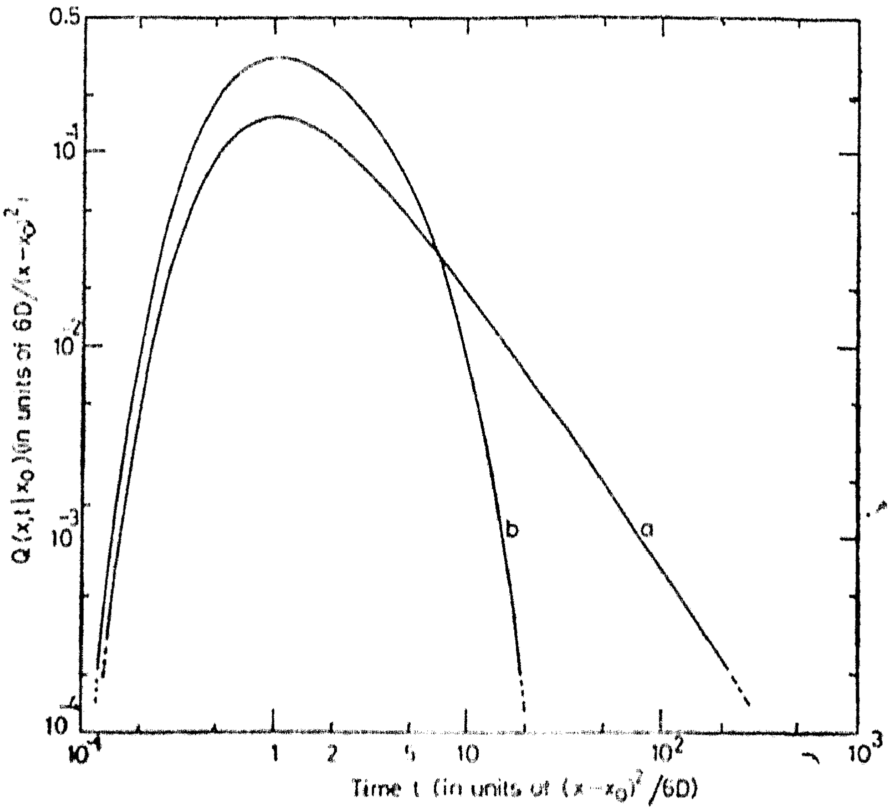

Figure 1. The normalized first passage time distribution function $Q(x, t|x_0)$ for unbiased diffusion on a line. Curve (a) (a Lévy distribution) corresponds to diffusion on an infinite line. Curve (b), related to an elliptic theta function, corresponds to a reflecting barrier at the starting point x_0 itself. Both distributions are unimodal, with the peak at $t = (x - x_0)^2/(6D)$. The total area under each curve is unity. Curve (b) falls off exponentially as $t \to \infty$, while (a) decays according to a power law. Both the abscissa and the ordinate in this figure are on logarithmic scales, to highlight this fact.

Finally, it is noteworthy that the Lévy distribution given in (32) [or its discrete counterpart in (24), with $f = 1$ and $g = 0$)] is just $(x - x_0)/t$ [or $(m - m_0)/t$] times the corresponding conditional probability density $P(x, t|x_0)$ [probability $P(m, t|m_0)$] for drift-free diffusion [symmetric random walk] on the infinite line [chain]. One may ask whether this property is shared by any other type of random walk on the infinite line or chain. We have been able to show* that, of the entire class of 'continuous time random walks', this property holds good only in the Markov case, *i.e.* only if the distribution of the pausing time between the steps of the random walk is an exponential one, the situation considered in this paper. Remarkably enough, however, there exist even more general types of temporally-correlated random walks for which the property does hold good. And there are, too, 'temporally fractal' continuous time random walks for which a simple generalisation of the property obtains. These results will be presented elsewhere.

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*See footnote on p. 112

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Appendix

P(m, t | m$_0$) for a biased random walk on a finite chain

We indicate in brief how the result quoted in (5) is derived. The conditional probability $P(m, t\,|\,m_0)$ for a standard random walk on a chain *via* nearest-neighbour jumps obeys the master equation for a Markov process, namely,

$$\frac{\partial}{\partial t}P(m, t\,|\,m_0) = W_{m,m+1}\; P(m+1, t\,|\,m_0) + W_{m,m-1}\; P(m-1, t\,|\,m_0)$$
$$- (W_{m+1,m} + W_{m-1,m})\, P(m, t\,|\,m_0), \tag{A1}$$

where $W_{m,m'}$ is the transition rate for a jump from m' to m. We now specialise to a biased random walk on the bounded set $\{0, 1, \ldots, N\}$, with reflecting boundaries at 0 and N, and the initial condition $P(m, 0\,|\,m_0) = \delta_{m,m_0}$. The Laplace transform of the master equation can then be written in the matrix form

$$\mathbf{A}\,\tilde{\boldsymbol{P}}(u; m_0) = \boldsymbol{\delta}(m_0). \tag{A2}$$

Here the mth element of the column vector $\tilde{\boldsymbol{P}}(u; m_0)$ [or $\boldsymbol{\delta}(m_0)$] is $\tilde{P}(m, u\,|\,m_0)$ [or δ_{m,m_0}]. The elements of the asymmetric, tridiagonal matrix $\mathbf{A}$ are given by

$$\left.\begin{aligned} A_{mm'} &= (u + 2W)\,\delta_{mm'} - W(1-g)\,\delta_{m+1,m'} - W(1+g)\,\delta_{m-1,m'} \\ A_{0m'} &= [u + W(1+g)]\,\delta_{0m'} - W(1-g)\,\delta_{1m'} \\ A_{Nm'} &= -W(1+g)\,\delta_{N-1,m'} + [u + W(1-g)]\,\delta_{Nm'}, \end{aligned}\right\} \tag{A3}$$

where $1 \leqslant m \leqslant N$, $0 \leqslant m' \leqslant N$, and the bias is parametrised by g, with $-1 < g < 1$. The $(N+1)$ eigenvalues of $\mathbf{A}$ are

$$\lambda_0 = u,\; \lambda_r = u + 2W\,[1 - (1-g^2)^{\frac{1}{2}} \cos\{r\pi/(N+1)\}],\; r = 1, \ldots, N, \tag{A4}$$

with λ_0 corresponding to the steady-state solution. Using the right and left eigenvectors of the asymmetric matrix $\mathbf{A}$, we can construct a matrix that diagonalises $\mathbf{A}$, and thence the inverse $\mathbf{A}^{-1}$. This procedure yields, after all the algebra is done, the result

$$\tilde{P}(m, u \mid m_0) = \frac{1}{u}\frac{(1-f)\, f^m}{(1-f^{N+1})} + \frac{2}{(N+1)} f^{(m-m_0)/2}.$$

$$\cdot \sum_{r=1}^{N} \frac{\left\{\sqrt{f}\sin\left(\frac{(m+1)\,r\pi}{N+1}\right) - \sin\left(\frac{m\,r\,\pi}{N+1}\right)\right\}\{m \to m_0\}}{\left(1 - 2\sqrt{f}\cos\frac{r\pi}{N+1} + f\right)\left[u + 2W(1-g^2)^{1/2}\cos\left(\frac{r\pi}{N+1}\right)\right]},$$

$$(0 \leqslant m, m_0 \leqslant N), \tag{A5}$$

where $f = (1+g)/(1-g)$. The first term on the right represents, as may be guessed, the transform of the steady-state solution. It is expedient to split this term into partial fractions and to combine it with the second term, to obtain

$$\tilde{P}(m, u \mid m_0) = \frac{1}{u}\delta_{N,m}\,\delta_{N,m_0} + \frac{2}{(N+1)} f^{(m-m_0)/2}$$

$$\sum_{r=1}^{N}\left[u + 2W(1-g^2)^{1/2}\cos\left(\frac{r\pi}{N+1}\right)\right]^{-1}.$$

$$\cdot\left[\sin\left(\frac{(m+1)\,r\pi}{N+1}\right)\sin\left(\frac{(m_0+1)r\pi}{N+1}\right) + \frac{2W}{u(1+f)}\sin\left(\frac{r\pi}{N+1}\right).\right.$$

$$\left.\left\{\sin\left(\frac{(m+m_0+1)\,r\pi}{N+1}\right) - \sqrt{f}\sin\left(\frac{(m+m_0+2)\,r\pi}{N+1}\right)\right\}\right]. \tag{A6}$$

To find a closed form for $\tilde{P}(m, u \mid m_0)$, we must carry out the finite summations in (A6). We have done this, with the help of several auxiliary trigonometric summation formulas we have derived in a straightforward manner, and also the following formulas (Hansen 1975):

$$\sum_{k=1}^{[(N-1)/2]} \frac{\cos(2\pi\,k\,m/N)}{\cosh x - \cos(2\pi\,k/N)} = \frac{N}{2}\operatorname{cosech} x \operatorname{cosech}(Nx/2)$$

$$\cosh\left\{\left(\frac{N}{2} - m + N\left[\frac{m}{N}\right]\right)x\right\} - \frac{1}{4}\operatorname{cosech}^2(x/2) - \frac{1}{8}(-1)^m$$

$$(1 + (-1)^N)\operatorname{sech}^2(x/2), \tag{A7}$$

$$\sum_{k=1}^{[(N-2)/2]} \frac{\cos((2k+1)\,m\pi/N)}{\cosh x - \cos((2k+1)\pi/N)} = (-1)^{[m/N]}\frac{N}{2}\operatorname{cosech} x \operatorname{sech}(Nx/2).$$

$$\cdot\sinh\left\{\left(\frac{N}{2} - m + N\left[\frac{m}{N}\right]\right)x\right\} + \frac{1}{8}(-1)^m((-1)^N - 1)\operatorname{sech}^2(x/2). \tag{A8}$$

Here $[a/b]$ stands for the largest integer less than (a/b). A great deal of algebra is involved, but the end result is simply

$$\tilde{P}(m, u\,|\,m_0) = \frac{f^{(m-m_0)/2}}{\sinh\,(N+1)\,\xi}\left[\frac{(1+f)}{2W\sqrt{f}}\,\frac{\sinh\;(N-m_>)\xi\,\sinh\;(m_<+1)\xi}{\sin h\;\xi}\right.$$
$$\left. + \frac{1}{u}\left\{\frac{1}{\sqrt{f}}\sinh\,(N-m_>-m_<)\xi - \sinh\,(N-m_>-m_<-1)\xi\right\}\right], \tag{A9}$$

where $m_> = \max\,(m, m_0)$, $m_< = \min\,(m, m_0)$, and $\xi = \cosh^{-1}\,[(1 + u/2W\;1 - g^2)^{-1/2}]$, as defined in the text. Further simplification leads to the surprisingly compact answer quoted in (5), namely,

$$\tilde{P}(m, u\,|\,m_0) = (\sqrt{f})^{m-m_0}\,[\sinh\,(N - m_> + 1)\xi - \sqrt{f}\sinh\,(N - m_>)\xi]$$
$$\times\;[\sqrt{f}\sinh\,(m_< + 1)\xi - \sinh\,m_<\xi]/[(u\sinh\,\xi\,\sinh\,(N+1)\xi]. \tag{A10}$$

When there is no bias ($g = 0$, or $f = 1$), this becomes even simpler:

$$\tilde{P}(m, u\,|\,m_0) = \frac{\cosh\,(N - m_> + \frac{1}{2})\xi_0\;\cosh\,(m_< + \frac{1}{2})\xi_0}{W\sinh\,\xi_0\;\sinh\,(N+1)\xi_0}, \tag{A11}$$

where $\xi_0 = \cosh^{-1}\,(1 + u/2W)$. This is, incidentally, the closed-form result for the sum obtained as a solution for $\tilde{P}$ in the bias-free case by Odagaki and Lax (1980) in the study of a bond-percolation model.

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