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Properties of Noninteger Moments in a First Passage Time Problem

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We calculate the moments $\langle t^q \rangle$, where q is not necessarily an integer, of the first passage time to trapping for a simple diffusion problem in one dimension. If a characteristic length of the system is L and $\langle t^q \rangle \sim L^{\tau(q)}$ as $L \to \infty$, then we show that there is a phase transition at $q = q_c$ such that when $q < q_c$, $\tau(q) = 0$, and for $q > q_c$, $\tau(q)$ is a linear function of q. These analytical results can be used to explain results for large moments for diffusion on a hierarchic structure. We also show how to calculate noninteger moments in terms of characteristic functions.

KEY WORDS: Trapping problems; hierarchic structures; survival probabilities.

One of the most frequently used characterizing features of a probability distribution is the set of its integer moments. However, it is also possible to define moments of arbitrary order. These may arise in a more or less natural way when, for example, no integer moments are finite. For example, the Cauchy density $p(x) = [\pi(1 + x^2)]^{-1}$, $-\infty < x < \infty$, has no integer moments other than the zeroth, but it is nevertheless possible to calculate moments of the form $\langle x^q \rangle$ for all $q < 1$. One of the earliest examples in which noninteger moments (NIM) were calculated related to the spans of random walks,[(1)] but more recently the properties of noninteger moments have found application in the study of random resistor networks,[(2,3)] chaos,[(4)] and diffusion-limited aggregation.[(5)]

In the present paper we examine a very simple example of trapping on a line in which the behavior of the moments of the first passage time exhibits a kind of phase transition as a function of q. We interpret this as

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indicating an absence of uniform scaling in the underlying physical problem as might be expected from diffusion on multifractal structures. Specifically, if L is a characteristic length of the system and the qth moment of the first passage time $\langle t^q \rangle$ is expressed as $\langle t^q \rangle \sim L^{\tau(q)}$ for large L, then we show that the derivative of $\tau(q)$ with respect to q is discontinuous. This suggests that the nonlinear dependence of an exponent of the qth moment on a typical size parameter of the system may sometimes be used to indicate lack of scaling. Our results exhibit in a simple and explicit form qualitative behavior similar to that found in a recent numerical study of the first passage time to reach traps at the extremities of a one-dimensional hierarchic structure.[6] Indeed, we show that there is even excellent quantitative agreement with that analysis. Finally, we show how to calculate NIMs from the characteristic function. It will be shown that NIMs reflect nonlocal properties of the characteristic function, in contrast to integer moments, which depend only on properties of the characteristic function near the origin of the transform parameter.

The model to be analyzed is that of simple diffusion on a line of length L in which $x = 0$ is a trapping point and $x = L$ is a reflecting point. We calculate the NIMs of the first passage time to absorption of a diffusing particle initially located at x_0. The calculation is most easily carried out by first finding the probability that the particle survives until time t or greater, $S(t \mid x_0)$, and then calculating the probability density function for absorption at time t, $r(t \mid x_0) = -\partial S(t \mid x_0)/\partial t$. One readily verifies that the survival function can be expressed as

$$S(t \mid x_0) = \frac{4}{\pi} \sum_{j=0}^{\infty} \frac{\sin[\theta(2j+1)]}{2j+1} \exp\left[-\pi^2(2j+1)^2 \frac{Dt}{4L^2}\right] \tag{1}$$

in which $\theta = \pi x_0/(2L)$ and D is the diffusion constant. The corresponding probability density function is

$$r(t \mid x_0) = \frac{\pi D}{L^2} \sum_{j=0}^{\infty} (2j+1) \sin[\theta(2j+1)] \exp\left[-\pi^2(2j+1)^2 \frac{Dt}{4L^2}\right] \tag{2}$$

The qth moment of the first passage time to absorption calculated from this density function is therefore

$$\langle t^q \rangle = KL^{2q} \sum_{j=0}^{\infty} \frac{\sin[\theta(2j+1)]}{(2j+1)^{2q+1}} = KL^{2q} g(\theta) \tag{3}$$

where K is the constant

$$K = \frac{4^{q+1} \Gamma(q+1)}{\pi^{2q+1} D^q} \tag{4}$$

and $g(\theta)$ is the Fourier series in Eq. (3).

We examine the behavior of $\langle t^q \rangle$, as calculated from Eq. (3), as a function of q on the assumption that the parameter L is a characteristic parameter of the system which we let grow indefinitely large, and x_0 is held fixed. It is crucial to notice that L appears both explicitly in the representation of Eq. (3) and implicitly in the parameter θ. An analysis of the series similar to one originally given by Gillis and Weiss[7] yields the asymptotic results

$$\begin{aligned} \langle t^q \rangle &\sim K, && q < 1/2 \\ &\sim K'' \ln L, && q = 1/2 \\ &\sim K' L^{2q-1}, && q > 1/2 \end{aligned} \tag{5}$$

This example can be slightly expanded by posing the same problem in terms of a different set of variables which are suggested by the analysis of diffusion on hierarchic structures given by Havlin and Matan.[6] Suppose that we set $L = x_0 + x_1$, where x_0 is the initial position, allowing x_0 to grow indefinitely large, at the same time setting $x_1 = x_0^\gamma$, where $\gamma > 1$. In this formulation x_0 will be the parameter chosen to characterize the system size. It follows from Eq. (3) that when we express the moments, both integer and noninteger, as $\langle t^q \rangle \sim L^{\tau(q)}$, then

$$\tau(q) \sim 2q, \qquad q < 1/2 \tag{6a}$$

$$\sim 1 + (2q-1)\gamma, \qquad q > 1/2 \tag{6b}$$

with a logarithmic dependence again appearing at $q = 1/2$. These results are useful in the interpretation of numerical results of the study of first passage times on a one-dimensional hierarchic comb structure[6] in which $\langle t^q \rangle$ was calculated as a function of q. The magnification of tooth length on that structure was represented by a parameter R. If one assumes that for $q \geqslant 1$ the major contribution to the survival probability comes from delays along the longest tooth, then we may identify the parameter γ in Eq. (6b) with the fractal dimension d. We therefore have $\gamma = d_f = \ln R/\ln 2$. When $R = 3$, which is the parameter used in the numerical calculations in ref. 6, $\tau(1) = 2.58$ and $d\tau(q \gg 1)/dq = 3.08$, in excellent agreement with the values 2.58 and 3.06 found by Havlin and Matan. Further unpublished numerical calculations for $R = 4$ show the same degree of agreement with Eq. (6b). If the asymptotic behavior of the survival probability is expressed as $S(t) \sim \exp(-t/t^*)$, then $t^* \sim x_0^{2.08}$, also in agreement with the cited reference. Kahng and Redner[8] obtained Eq. (6) for first passage times on hierarchic structures using a renormalization group analysis.

In the simple example just treated, the critical moment $\langle \tau^{1/2} \rangle$ is a positive one. If we consider an analogous problem of internal diffusion in a sphere with an absorbing surface, we find that the critical moment is a negative one. In that case a calculation of $\langle t^q \rangle$ in terms of the sphere radius shows that, in contrast to the one-dimensional case, there is no transition in the behavior of $\langle t^q \rangle$ as a function of q for $q > 0$, but that there is such a transition at $q = -1/2$.

As a final parenthetical remark, we note that the use of characteristic functions allows one to calculate moments in terms of derivatives of the characteristic function at the origin, i.e., it is a local property. One can also calculate NIMs in terms of the characteristic function, but these are now *nonlocal* properties of this function. To see this, consider the calculation of $\langle t^q \rangle$ for $0 < q < 1$. Let the Laplace transform of the first passage time density be denoted by $\hat{r}(s)$, and write $t^q = t/t^{1-q}$. Then we have

$$\langle t^q \rangle = \int_0^\infty \frac{t}{t^{1-q}} r(t)\, dt \tag{7}$$

We can use an integral representation of t^{q-1} to transform this into

$$\begin{aligned}\langle t^q \rangle &= \frac{1}{\Gamma(1-q)} \int_0^\infty s^{-q}\, ds \int_0^\infty tr(t) e^{-st}\, dt \\ &= -\frac{1}{\Gamma(1-q)} \int_0^\infty s^{-q} \hat{r}'(s)\, ds \end{aligned}\tag{8}$$

where $\hat{r}(s)$ is the Laplace transform, or characteristic function, corresponding to the probability density $r(t)$, and $\hat{r}'(s)$ is the derivative of $\hat{r}(s)$. Thus, the calculation of $\langle t^q \rangle$ samples all values of $\hat{r}(s)$ rather than just its value at $s = 0$. One can readily derive similar expressions for $\langle t^q \rangle$ for values of $q > 1$. A representation of negative moments can also be found in terms of the characteristic function $\hat{r}(s)$. Consider, for example, the problem of calculating $\langle t^{-q} \rangle$, $q > 0$. We write

$$\frac{1}{t^q} = \frac{1}{\Gamma(q)} \int_0^\infty s^{q-1} e^{-st}\, ds \tag{9}$$

which, after substitution into the expression defining the moments and an interchange of the orders of integration, leads to the representation

$$\langle t^{-q} \rangle = \frac{1}{\Gamma(q)} \int_0^\infty s^{q-1} \hat{r}(s)\, ds \tag{10}$$

As is true in the case of noninteger moments, this is a nonlocal function of $\hat{r}(s)$.

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