

First-passage times for non-Markovian processes: Multivalued noise

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A new method for the calculation of first-passage times for non-Markovian processes is presented. In addition to the general formalism, some familiar examples are worked out in detail.

Recently Masoliver, Lindenberg, and West¹ have developed a technique for the solution of the first-passage-time problem related to stochastic differential equations driven by dichotomous Markovian or non-Markovian fluctuations. The method consists of an exact enumeration of stochastic trajectories to calculate the probability density function for the first-passage time out of an interval on a line. Doering² has generalized the method to situations where the noise occurs multiplicatively and nonlinearly in the stochastic differential equation. While such an analysis can in principle be extended to noise processes that are more complicated than the dichotomous fluctuations discussed in Refs. 1 and 2, the analysis would be very involved because of the many possibilities that have to be taken into account.³ Hence it is desirable to reformulate the theory in such a way as to minimize the combinatorial difficulties that accompany the exact enumeration of trajectories. This will allow us to reduce the appropriate calculations to ones that can be carried out numerically if need be, and exactly for a particular class of separable kernels to be described later on. The techniques to be developed have been anticipated in some work by Weiss and Szabo.⁴ The same techniques are applicable to problems in higher dimensions but we anticipate that only a limited number of such first-passage-time problems will be solvable in a useful way.

Let us first consider simple random motion in an interval $[0,L]$ in which the dynamics of the process is linear, in the sense that

$$\dot{X}(t) = F(t) . \tag{1}$$

We take the velocity $F(t)$ to change randomly among the members of a set of $(n + m + 1)$ constant values:

$$F(t) = (v_k; k = -m, -m + 1, \dots, n) . \tag{2}$$

The sign of v_k is determined by the sign of its index, and $v_0 \equiv 0$. Thus, for $j > 0$, v_j represents motion in the positive x direction and v_{-j} in the negative x direction. There are two further sources of randomness in our formulation of the problem. The first is the fact that $F(t)$ remains at a constant value v_k for a random length of time τ , the probability density for this time interval being denoted by $\psi_k(\tau)$. The second source of randomness is the process by which switches are made among the v_k . Here a number of possibilities suggest themselves. We make an assumption that generalizes the models discussed by Masoliver *et al.*¹: The random process $F(t)$ switches from the value v_k to the value v_l with probability β_{lk} , i.e., the switching can be characterized as a Markov chain.

The origin of the random process $X(t)$ will be denoted by $X(0) = x_0$, where $0 < x_0 < L$. Notice that even if $X(t) = 0$ [$X(t) = L$], the random process does not exit the interval $[0,L]$ at time t unless it is moving in the negative (positive) direction. The fundamental functions in our theory will be denoted by $S_k(x,t)$ ($k = -m, -m + 1, \dots, n$) and are defined as follows:

$$S_k(x,t) dx dt = \text{Probability that the random process } X(t) \text{ has not exited } [0,L] \text{ before time } t ,$$

$$\text{and that a switch in velocities to } v_k \text{ occurs during } (t, t + dt)$$

$$\text{at which time the process is in the interval } (x, x + dx) . \tag{3}$$

The $S_k(x,t)$ satisfy the set of integral equations

$$S_k(x,t) = \beta_k \delta(x - x_0) \delta(t) + \sum_{l=-m}^n \beta_{kl} \int_0^L dy \int_0^t d\tau S_l(y,\tau) \delta[x - y - v_l(t - \tau)] \psi_l(t - \tau) \tag{4}$$

for $0 \leq x \leq L$ ($k = -m, -m + 1, \dots, n$), where β_k is the probability that the initial velocity of the system is v_k . Here we have assumed that a switch occurs with certainty at time $t = 0$. Other initial conditions can also be considered.¹ One of the two integrations in Eq. (4) can be carried out directly using the δ function in the integrand. We choose to do the time integrations for $l \neq 0$ and the spatial integration for the $l = 0$ term. Equation (4) then reduces to the simpler form

$$S_k(x, t) = \beta_k \delta(x - x_0) \delta(t) + \sum'_{l=-m}^n \frac{\beta_{kl}}{|v_l|} \int_0^L dy \Theta((x-y)/v_l) S_l(y, t - (x-y)/v_l) \psi_l((x-y)/v_k) + \beta_{k0} \int_0^t d\tau S_0(x, \tau) \psi_0(t - \tau), \quad (5)$$

where $\Theta(x) \equiv 1$ for $x > 0$ and $\Theta(x) \equiv 0$ for $x < 0$, and where the prime on the summation denotes exclusion of the $l = 0$ term. It is convenient to consider the time Laplace transforms

$$\hat{S}_k(x, s) \equiv \int_0^\infty dt e^{-st} S_k(x, t). \quad (6)$$

From Eq. (5) it directly follows that these transforms obey the integral equations

$$\hat{S}_k(x, s) = \beta_k \delta(x - x_0) + \sum'_{l=-m}^n \frac{\beta_{kl}}{|v_l|} \int_0^L dy \Theta((x-y)/v_l) e^{-(x-y)s/v_l} \psi_l((x-y)/v_l) \hat{S}_l(y, s) + \beta_{k0} \frac{\lambda_0}{s + \lambda_0} \hat{S}_0(x, s). \quad (7)$$

We next consider the quantity of physical interest that motivates this development, i.e., the probability density function $f(t | x_0)$ for the first-passage time out of the interval $[0, L]$. To express this density in terms of the $S_k(x, t)$ we need to define the set of probabilities

$$\Psi_k(t) \equiv \int_t^\infty d\tau \psi_k(\tau). \quad (8)$$

$\Psi_k(t)$ thus is the probability that the velocity v_k is retained for a time interval longer than t . Then since random processes with positive velocities can only be absorbed at $x = L$, and those with negative velocities can only be absorbed at $x = 0$, it follows that

$$f(t | x_0) = \sum_{l=1}^n \int_0^L dx S_l(x, t - (L-x)/v_l) \Psi_l((L-x)/v_l) + \sum_{l=-m}^{-1} \int_0^L dx S_l(x, t - x/|v_l|) \Psi_l(x/|v_l|), \quad (9)$$

which furnishes a formal solution to our problem once the $S_l(x, t)$ are known. Here it is understood that $S_l(x, t) \equiv 0$ for negative times. The first set of terms on the right-hand side of this equation arise from a process moving to the right. If such a process with velocity $v_l > 0$ is at x a given time, then it must move towards $x = L$ for a time that is at least equal to $(L-x)/v_l$. Similarly, a process with velocity $v_l < 0$ which finds itself at x must continue moving towards $x = 0$ for at least a time $x/|v_l|$ in order

to exit the interval. This situation is embodied in the second set of terms in (9). The Laplace transform of $f(t | x_0)$ is found directly from (9):

$$\hat{f}(s | x_0) = \sum_{l=1}^n \int_0^L dx \hat{S}_l(x, s) e^{-s(L-x)/v_l} \Psi_l((L-x)/v_l) + \sum_{l=-m}^{-1} \int_0^L dx \hat{S}_l(x, s) e^{-sx/|v_l|} \Psi_l(x/|v_l|). \quad (10)$$

Equations (5) and (9) [equivalently, Eqs. (7) and (10)] complete our solution to the problem of calculating the probability density function of the first-passage time out of the interval. In the most general case in which no further simplifications can be made, Eq. (5) [Eq. (7)] is a convenient starting point for the calculation of numerical solutions for the $S_k(x, t)$ followed by substitutions of the results in Eq. (9) to find $f(t | x_0)$.

Let us consider possible simplifications of the formalism. The simplest physical problems for which useful results can be obtained in closed form are those which lead to separable kernels in the integral equation (7). To obtain a separable kernel consider the case of exponentially distributed persistence times for each velocity v_k , i.e.,

$$\psi_k(t) = \begin{cases} \lambda_k \exp(-\lambda_k t), & t \geq 0 \\ 0, & t < 0. \end{cases} \quad (11)$$

With these densities we then rewrite (7) as

$$\hat{S}_k(x, s) = \beta_k \delta(x - x_0) - \sum_{l=-m}^{-1} \frac{\beta_{kl} \lambda_l}{v_l} \int_x^L dy \hat{S}_l(y, s) e^{-(s+\lambda_l)(x-y)/v_l} + \frac{\beta_{kl} \lambda_l}{v_l} \int_0^x dy \hat{S}_l(y, s) e^{-(s+\lambda_l)(x-y)/v_l} + \frac{\beta_{k0} \lambda_0}{s + \lambda_0} \hat{S}_0(x, s). \quad (12)$$

Let $U_k(p,s)$ denote the Laplace transform of $\hat{S}_k(x,s)$ with respect to x :

$$U_k(p,s) \equiv \int_0^\infty dx e^{-px} \hat{S}_k(x,s). \quad (13)$$

Although the definition (4) is valid and physically sensible only for $0 \leq x \leq L$, we can analytically extend $\hat{S}_k(x,s)$ to larger values of x for use in Eq. (13). The Laplace transform of Eq. (12) then yields

$$U_k(p,s) = \beta_k e^{-px_0} + \sum_{l=-m}^{-1} \beta_{kl} \lambda_l \frac{[U_l(p,s) - C_l(s)]}{(pv_l + s + \lambda_l)} + \sum_{l=0}^n \beta_{kl} \lambda_l \frac{U_l(p,s)}{(pv_l + s + \lambda_l)}, \quad (14)$$

where

$$C_l(s) \equiv \int_0^L dy \hat{S}_l(y,s) e^{(s+\lambda_l)y/v}. \quad (15)$$

Equation (14) represents a set of linear coupled algebraic equations whose solution is readily obtained.

To carry this illustration of the method further, we con-

$$\hat{S}_1(x,s) = \left[(1-\beta) + \beta \frac{\lambda_0}{s+\lambda_0} \right] \left\{ \delta(x) + \frac{\lambda_1 \lambda_0}{v(s+\lambda_0)} \exp \left[-\frac{xs}{v} \left[\frac{s+\lambda_0+\lambda_1}{s+\lambda_0} \right] \right] \right\}, \quad (17a)$$

$$\hat{S}_0(x,s) = \beta \delta(x) + \frac{\lambda_1}{v} \left[(1-\beta) + \beta \frac{\lambda_0}{s+\lambda_0} \right] \exp \left[-\frac{xs}{v} \left[\frac{s+\lambda_0+\lambda_1}{s+\lambda_0} \right] \right]. \quad (17b)$$

The solution (17) can now be used to evaluate the time Laplace transform of the first-passage-time density,

$$\begin{aligned} \hat{f}(s | 0) &= \int_0^L dx \hat{S}_1(x,s) e^{-(s+\lambda_1)(L-x)/v} \\ &= \left[(1-\beta) + \beta \frac{\lambda_0}{s+\lambda_0} \right] \\ &\quad \times \exp \left[-\frac{Ls}{v} \left[\frac{s+\lambda_0+\lambda_1}{s+\lambda_0} \right] \right]. \end{aligned} \quad (18)$$

In particular, the mean first-passage time T_1 to $x=L$ is obtained from (18) via the relation¹ $T_1(x_0) = -\partial \hat{f}(s | x_0) / \partial s |_{s=0}$:

$$T_1(0) = \frac{\beta}{\lambda_0} + \left[1 + \frac{\lambda_1}{\lambda_0} \right] \frac{L}{v}. \quad (19)$$

The first term in (19) is the contribution that arises from an initially stationary phase, while the second is a simple weighted average of subsequent mobile and stationary intervals. Because the motion is strictly unidirectional, T_1 is linear in the length of the column.

consider three examples that have been discussed in the literature. One is the Giddings-Eyring model⁵ for flow in a chromatographic column. This model can be described by the formalism outlined above with one stationary state and one mobile state ($v_0=0$, $v_1 \equiv v > 0$, $\beta_0 \equiv \beta = 1 - \beta_1$, $\beta_{01} = \beta_{10} = 1$). The probability densities for sojourn times are those appropriate to first-order kinetics for transitions between mobile and stationary states as originally discussed by Giddings and Eyring,⁵ and have the negative exponential form given in Eq. (11). Since the process can only move in the positive x direction, absorption can only occur at $x=L$, and x_0 can be taken as zero. The system of equations (14) in this case reduces to

$$U_0(p,s) = \beta + \frac{\lambda_1}{pv + s + \lambda_1} U_1(p,s), \quad (16a)$$

$$U_1(p,s) = (1-\beta) + \frac{\lambda_0}{s+\lambda_0} U_0(p,s). \quad (16b)$$

By inverse Laplace transforming with respect to p , these forms lead directly to the expressions

Our second example corresponds to that analyzed by Masoliver *et al.*¹ and by others⁶⁻⁸ using different methods: We suppose that $F(t)$ is a dichotomous process that takes on one positive ($v_1=v$) and one negative ($v_{-1}=-v$) value. The transition probabilities have the value $\beta_{1,-1} = \beta_{-1,1} = 1$ and the initial velocity is v and $-v$ with probability β and $(1-\beta)$, respectively. This case differs from the previous example in that the process can now leave the interval $[0,L]$ through either end. For this example, the system of equations (14) reduces to

$$U_{-1}(p,s) = (1-\beta) e^{-px_0} + \frac{\lambda}{(pv + s + \lambda)} U_1(p,s), \quad (20a)$$

$$U_1(p,s) = \beta e^{-px_0} - \frac{\lambda}{(pv - s - \lambda)} [U_{-1}(p,s) - C(s)], \quad (20b)$$

where we have set $\lambda_1 = \lambda_{-1} = \lambda$ and

$$C_{-1}(s) \equiv C(s) = \int_0^L dy \hat{S}_{-1}(y,s) e^{-(\lambda+s)y/v}. \quad (21)$$

The solution of the set of simultaneous linear equations and their Laplace inversion with respect to p is straightforward and yields

$$\begin{aligned} \hat{S}_1(x,s) &= \beta \left[\delta(x-x_0) - \frac{\lambda^2}{2qv^2} \Theta(x-x_0) (e^{q(x-x_0)} - e^{-q(x-x_0)}) \right] + \frac{\lambda}{2qv} C(s) [(q+\alpha)e^{qx} + (q-\alpha)e^{-qx}] \\ &\quad - \frac{\lambda(1-\beta)}{2vq} \Theta(x-x_0) [(q+\alpha)e^{q(x-x_0)} + (q-\alpha)e^{-q(x-x_0)}], \end{aligned} \quad (22a)$$

$$\hat{S}_{-1}(x,s) = (1-\beta) \left[\delta(x-x_0) - \frac{\lambda^2}{2qv^2} \Theta(x-x_0) (e^{q(x-x_0)} - e^{-q(x-x_0)}) \right] + \frac{\lambda^2}{2qv^2} C(s) (e^{qx} - e^{-qx}) + (1-\beta) \frac{\lambda}{2qv} \Theta(x-x_0) [(q+\alpha)e^{q(x-x_0)} + (q-\alpha)e^{-q(x-x_0)}], \tag{22b}$$

where

$$\alpha \equiv (\lambda + s)/v, \tag{23}$$

$$q \equiv (\alpha^2 - \lambda^2/v^2)^{1/2}, \tag{24}$$

and

$$C(s) = [(q+\alpha)e^{qL} + (q-\alpha)e^{-qL}]^{-1} \{ (1-\beta)[(q+\alpha)e^{q(L-x_0)} + (q-\alpha)e^{-q(L-x_0)}] + \frac{\lambda}{v} \beta (e^{q(L-x_0)} - e^{-q(L-x_0)}) \}. \tag{25}$$

Substitution of (22)–(25) into (10) finally yields the Laplace transformed first-passage-time distribution obtained previously.¹ The mean first-passage time out of the interval $[0, L]$ starting from x_0 is¹

$$T_1(x_0) = \frac{\lambda}{v^2} (L-x_0)x_0 + \frac{(1-\beta)}{v} x_0 + \frac{\beta}{v} (L-x_0). \tag{26}$$

The first (quadratic) term in (26) is typical of diffusive motion while the remaining (linear) terms arise from the ballistic motion between velocity changes.

The third example that we consider is one in which the velocity is randomized at each switch independently of its previous value, i.e., the transition probability $\beta_{kl} = \beta_k$ is independent of l . The switching process is then no longer a Markov chain, but rather an independent process in the velocities. This model is similar in spirit to that of Gordon⁹ in his study of rotational relaxation in fluids, wherein the angular momentum is randomized at each collision. In this model it is no more difficult to deal with a continuum of velocities than with a discrete set. We define the function

$$D(x,s) \equiv - \sum_{l=-m}^{-1} \frac{\lambda_l}{v_l} \int_x^L dy \hat{S}_l(y,s) e^{-(\lambda_l+s)(x-y)/v_l} + \sum_{l=1}^n \frac{\lambda_l}{v_l} \int_0^x dy \hat{S}_l(y,s) e^{-(\lambda_l+s)(x-y)/v_l} \tag{27}$$

and note that (12) can be reexpressed entirely in terms of this density:

$$D(x,s) = \frac{s + \lambda_0}{s + (1-\beta_0)\lambda_0} \left[g(x-x_0,s)\Theta(x-x_0) + g(x_0-x,s)\Theta(x_0-x) + \int_0^x dy g(x-y,s)D(y,s) + \int_x^L dy g(y-x,s)D(y,s) \right], \tag{28}$$

where

$$g(x,s) = \sum_{k>0} \beta_k \frac{\lambda_k}{v_k} e^{-(s+\lambda_k)x/v_k}. \tag{29}$$

In writing (28) we have taken the velocity distribution to be symmetric, i.e., $m=n$, $\beta_{-k} = \beta_k$, $v_{-k} = -v_k$, and $\lambda_{-k} = \lambda_k$. The transformed mean first-passage-time density (10) then is

$$\hat{f}(s | x_0) = \sum_{k>0} \frac{2\beta_k(s + \lambda_0)}{s + (1-\beta_0)\lambda_0} \int_0^L dx e^{-(s+\lambda_k)(L-x)/v_k} \times [\delta(x-x_0) + D(x,s)]. \tag{30}$$

The integral equation (28) is in general difficult to solve analytically for arbitrary transition probabilities β_k , velocities v_k , and persistence times λ_k^{-1} . However, if one chooses

$$\frac{\lambda_k}{v_k} = c \text{ independent of } k \tag{31}$$

the problem becomes tractable. With this choice the process retains lower velocities for longer times. Since for exponentially distributed switching times only the distance traversed in a given times is of importance in calculating the first-passage time, the choice (31) together with $\beta_0=0$ reduces this problem to the second example above. In particular, with the relations

$$\sum_{k>0} \beta_k = \frac{1}{2} \tag{32a}$$

and

$$\sum_{k>0} \frac{\beta_k}{v_k} \equiv \gamma, \tag{32b}$$

and the identification $\beta = \frac{1}{2}$, $\beta/v = \gamma$, and $\lambda = c/2\gamma$ in (26), the latter result is the mean first-passage time out of $(0, L)$ in the current example.

We have developed a new approach to the problem of

calculating first-passage times for processes driven by colored noise. The method is particularly suited to numerical solution. Herein we have presented simple examples that lend themselves to analytic solution. We wish to point out some generalizations that can easily be incorporated into this technique.

Although we have concentrated on linear processes [viz., Eq. (1)], one can easily consider more general dynamical processes of the form

$$\dot{X}(t) = f(X, F(t)) , \quad (33)$$

with the random function $F(t)$ defined as in (2), as was

done in earlier work.^{1,2} A second generalization that is conceptually straightforward is to a continuum of possible velocities instead of the discrete set used in this paper. Formally, this is accomplished by the replacement $\sum_k \rightarrow \int dv \rho(v)$ where $\rho(v)$ is the distribution of velocities. Finally, one can handle forms of the switching time distributions $\psi(t)$ other than the exponentials considered in the above examples.^{1,2}

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