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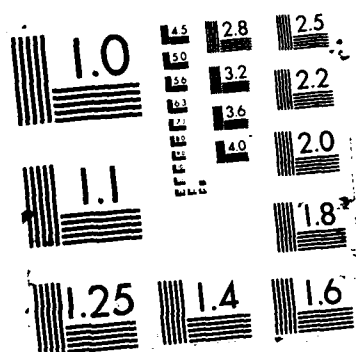
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Diffusion First Passage Times: Approximations and Related Differential Equations

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A finite spectral expansion is presented for the distribution of first passage to a fixed level, by a diffusion process with reflecting lower boundary. The n -term expansion derived here matches the first n moments of the passage time distribution. We derive also an interesting representation for the moment generating function of the first passage distribution.

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1. Introduction and Motivation

Let $\{\Omega, F, P\}$ be a probability space. Suppose that F_t is a filtration of F and that $\{W(t), t \geq 0\}$ is standard Brownian motion adapted to F_t .

Let

$$A \equiv \frac{\sigma^2(x)}{2} D^2 + \mu(x) D \quad (1.1)$$

be the infinitesimal generator of a diffusion $X(t)$ on $[0, r]$ satisfying

$$dX(t) = \sigma(x) dW(t) + \mu(x) dt,$$

with a reflecting boundary at 0 and absorption at $r < \infty$, and where $\sigma^2(x) > 0$ and $\mu(x)$ are continuously differentiable on $[0, r]$.

Define the stopping time τ_r by

$$\tau_r \equiv \inf \{s: s \geq 0, X(s) \geq r\}$$

and the moment generating function $\Psi_\theta(x, y)$ by

$$\Psi_\theta(x, y) = E\{e^{\theta \tau_r} | X(0) = x\} \equiv E^x[e^{\theta \tau_r}].$$

First Passage Times as Failure Times

Our motivation for studying first passage time distributions is their relevance to modeling of failure times. Indeed, this paper continues the line of development initiated in [9], where a stochastic process is used to model system state, ie, *wear-and-tear*, and failure occurs when either a traumatic killing event occurs (killing events happen with rate $k(x)$ in state x), or the system is retired when *wear-and-tear* reaches some predefined threshold (ie, a first passage occurs).

For example, if system state is modeled as Brownian motion with positive drift, then first passage to a specified threshold has an inverse Gaussian distribution. This first passage distribution has been successfully applied to numerous problems to obtain good fits, (cf Jorgensen [5]).

A related but parallel line of development is explored in Wenocur [12], where the killing time distribution of Brownian motion with quadratic extinction rate is calculated.

Our aim in this paper is to study first passage time distributions, where the system state process is a general diffusion with reflection at the origin and absorption at $r < \infty$. That is, the system state evolves as a diffusion, and failure occurs at the epoch of first passage (or absorption) to level r .

In future work, we intend to explore the practical ramifications of employing the computational methods suggested here to evaluate interesting first passage times statistics.

Backward Equation for First Passage Time Distribution

Let $w(x, t)$ denote the tail of the first passage time distribution, ie,

$$w(x, t) \equiv P^x\{\tau_r > t\}.$$

The backward differential equation for $w(x, t)$ is

$$\frac{\partial w(x, t)}{\partial t} = \mu(x) \frac{\partial w(x, t)}{\partial x} + \frac{\sigma^2(x)}{2} \frac{\partial^2 w(x, t)}{\partial x^2} = Aw(x, t) \quad (1.2)$$

for $(x, t) \in (0, r) \times (0, \infty)$, with boundary conditions

$$w(x, 0) = 1 \text{ for } 0 < x < r, \text{ and for all } t > 0 \text{ } w(r, t) = 0 \text{ and } \frac{\partial w(0, t)}{\partial x} = 0.$$

For a derivation of this equation and other related quantities see [6, pp 222-224].

The Spectral Representation for $w(x, t)$

The following representation for $w(x, t)$ is valid whenever $\sigma^2(x)$ and $\mu(x)$ are sufficiently smooth:

$$w(x, t) = \sum_{k=1}^{\infty} c_k e^{-\alpha_k t} \phi_k(x) \quad (1.3)$$

where α_k and ϕ_k are eigenvalues and eigenfunctions, and c_k are generalized Fourier coefficients, all defined below (This representation is proved in Section 8).

The $\{\phi_k, k \geq 1\}$ are eigenfunctions of A corresponding to the eigenvalues $\{\alpha_k, k \geq 1\}$, ie,

$$A \phi_k = -\alpha_k \phi_k,$$

and

$$c_k = \int_0^r \phi_k(x) \rho(x) dx,$$

where $\rho(x)$ is given by

$$\rho(x) = 2\pi(x)/\sigma^2(x) \quad (1.4)$$

and $\pi(x)$ is given by

$$\pi(x) = \exp \int_0^x 2\mu(u)/\sigma^2(u) du . \quad (1.5)$$

In general an arbitrary function $f \in L^2(\rho)$ will have a *Fourier* type expansion, ie,

$$f = \sum_{k=1}^{\infty} c_k \phi_k$$

where equality is interpreted in the $L^2(\rho)$ sense and

$$c_k = \int_0^r f(x) \phi_k(x) \rho(x) dx .$$

Remark: In the sequel it is assumed that A 's eigenvalues form a complete set in $L^2(\rho)$. The completeness of A 's eigenfunctions can be assured by certain regularity conditions on the infinitesimal parameters $\sigma^2(x)$ and $\mu(x)$. For example, $\sigma^2(x) > 0$ and the continuity of $\sigma^2(x)$ and $\mu'(x)$ are sufficient conditions. See [11, chap 1] for more details.

A Generalization

(previous work a generalization)
This paper is primarily concerned with computing first passage time statistics. In [9], as alluded to in (1.1), a general reliability model was proposed in which system failures occur when either system wear-and-tear reaches some maximum permissible level (ie, a first passage occurs), or when some killing event happens (such killing events occur with rate $k(x)$ in state x). Under this model $w(x,t)$ satisfies the following equation:

$$\frac{\partial w(x,t)}{\partial t} = k(x)w(x,t)\mu(x) \frac{\partial w(x,t)}{\partial x} + \frac{\sigma^2(x)}{2} \frac{\partial^2 w(x,t)}{\partial x^2} = Bw(x,t) ,$$

with the same boundary conditions as (1.2), and where

$$Bf(x) = \frac{1}{2} \sigma^2(x) f''(x) + \mu(x) f'(x) + k(x) f(x) .$$

It is possible to solve for $w(x,t)$ and related quantities with methods very similar to those presented here.

In Section 2, algorithms for approximating $w(x,t)$ are obtained. In particular, the infinite spectral expansion for $w(x,t)$ is approximated by an n -term sub-expansion which matches the first $n-1$ moments. Section 2 concludes with some remarks about our preliminary computational experience.

Proofs validating the spectral expansion and the related approximation scheme are given in the Appendix, Section 8 of this paper.

In Sections 3 and 4, methods are given for obtaining the eigenvalues and first passage moments, necessary for computing approximations to $w(x,t)$. In Section 5, computational issues related to calculating the moment generating function are considered.

Sections 6 and 7 include theoretical complements about first passage times. In particular, the moment generating function is shown to possess an interesting representation having exponential form (cf equation (7.1)). This exponential representation is related to asymptotic expansions used in analyzing perturbations of certain second-order differential equations.

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2. Approximating The First Passage Time Distribution

The preceding discussion might suggest that solving for $w(x,t)$ is fairly straightforward. Generally, eigenvalues and eigenfunctions are difficult to obtain. However the problem of approximating $w(x,t)$ can be approached by the method of moments. One technique is to calculate the first three moments, and then use the Pearson curve fitting method (cf [10]). This method is computationally feasible, and the Pearson family of curves includes some important first passage distributions, such as the gamma distribution (cf [1]). The merits of this approach will be studied in a forthcoming paper.

Given n Eigenvalues And $n-1$ First Passage Moments

A more computationally intensive approach, but one founded on stronger theoretical grounds, is the following. Suppose that n moments $\{M_k(x,r), 1 \leq k \leq n\}$ are known, where $M_k(x,r) = E^x[\tau_r^k]$, as well as the first n eigenvalues $\{\alpha_k, 1 \leq k \leq n\}$. Then use a finite sum in place of the infinite sum in equation (1.3). In particular, approximate $w(x,t)$ by

$$w_n(x,t) = \sum_{j=1}^n p_j^{(n)}(x) e^{-t/\mu_j},$$

where $\mathbf{p}^{(n)} \equiv (p_1^{(n)}, \dots, p_n^{(n)})$ satisfies for $0 \leq k \leq n-1$

$$\sum_{j=1}^n p_j^{(n)}(x) (\mu_j)^k = \frac{M_k(x,r)}{k!} \quad \text{where } \mu_j = 1/\alpha_j. \quad (2.1)$$

Ideally we want $w_n(x,t)$ to be a distribution function, ie, $w_n(x,t) \geq 0$ and $w_n(x,s+t) \geq w_n(x,t)$ whenever $s > 0$. It is not clear that solving (2.1) always produces such a function. This issue requires further investigation.

Obtaining The Weighting Factors

The weighting factors $\{p_k^{(n)}, 1 \leq k \leq n\}$ in (2.1) above are obtained by solving the following linear system:

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ \mu_1 & \mu_2 & \dots & \mu_n \\ \mu_1^2 & \mu_2^2 & \dots & \mu_n^2 \\ \vdots & \vdots & \dots & \vdots \\ \mu_1^{n-1} & \mu_2^{n-1} & \dots & \mu_n^{n-1} \end{bmatrix} \begin{bmatrix} p_1^{(n)} \\ p_2^{(n)} \\ \vdots \\ p_n^{(n)} \end{bmatrix} = \begin{bmatrix} 1 \\ m_1 \\ m_2 \\ \vdots \\ m_{n-1} \end{bmatrix} \quad (2.2)$$

where $m_k = M_k(x,r)/k!$.

Observe that the matrix $\{\mu_j^k, 1 \leq j \leq n, 0 \leq k < n\}$ is none other than the

transpose of the celebrated Vandermonde matrix. Cramer's equation gives the following formula for $p_k^{(n)}$.

$$p_k^{(n)} = \sum_{j=1}^n m_j g_{n-j}(\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n) / \prod_{\substack{j=1 \\ j \neq k}}^n (\mu_j - \mu_k) \quad (2.3)$$

where g_r are the signed symmetric functions defined as follows:

$$g_0(a_1, a_2, \dots, a_m) = 1$$

and for $r \geq 1$

$$g_r(a_1, a_2, \dots, a_m) = \sum_{1 \leq i_1 < i_2 < \dots < i_r \leq m} a_{i_1} a_{i_2} \dots a_{i_r} (-1)^r.$$

In Section 8 the following convergence theorem is proved:

Theorem

For fixed k

$$|p_k^{(n)} - c_k \phi_k(x)| = O\left(\frac{1}{n^2}\right),$$

where $c_k \phi_k(x)$ is defined by equation (1.3).

Given $2n-1$ Moments Only

Suppose that the first $2n-1$ moments have been determined. It is possible to approximately determine the first n eigenvalues by solving the following system of equations for $\mu_i, p_i^{(n)}, 1 \leq i \leq n$.

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ \mu_1 & \mu_2 & \dots & \mu_n \\ \mu_1^2 & \mu_2^2 & \dots & \mu_n^2 \\ \vdots & \vdots & \dots & \vdots \\ \mu_1^{2n-1} & \mu_2^{2n-1} & \dots & \mu_n^{2n-1} \end{bmatrix} \begin{bmatrix} p_1^{(n)} \\ p_2^{(n)} \\ \vdots \\ p_n^{(n)} \end{bmatrix} = \begin{bmatrix} 1 \\ m_1 \\ m_2 \\ \vdots \\ m_{2n-1} \end{bmatrix}$$

where $\mu_j > 0$.

One approach is to solve for $\{p_j^{(n)}, j=1, \dots, n\}$ in terms of $\{\mu_k, 1 \leq k \leq n\}$ and $\{m_0, m_1, \dots, m_{n-1}\}$ as detailed above, and then use the remaining n constraints to determine the $\{\mu_k, 1 \leq k \leq n\}$. This reduced system can then be

solved using mathematical programming techniques, eg, approximate Newton-Raphson techniques. The numerical stability and feasibility of this method merit further study.

Preliminary Computational Experience

Numerical experiments conducted in the C programming language suggest the following. For small values of t , finite difference methods are more attractive than finite spectral expansions, but the finite expansion approach is preferable for large values of t . For relatively small number of terms (less than 6), the method of moments seems to be an attractive method of computing weights, especially when moments are also to be computed. Because the Vandermonde system of equations grows increasingly unstable with its dimension (but see Bjork [2]), longer expansions require that the spectral coefficients should be computed in terms of the eigenvectors and Fourier coefficients.

Small values of t will generally be of interest for first passage distributions with small means, and conversely. Roughly speaking, if $\mu(x) > 0$ or $\sigma(x)$ is large, then first passages occur rapidly. But if $\mu(x) \ll 0$, or $\mu(x) \leq 0$ and $\sigma(x)$ is small, then first passages occur slowly. These observations should help to guide the choice of numerical method.

The following example illustrates the efficacy of the method of moments for computing the spectral weights. Let $\sigma(x) \equiv 1$, $\mu(x) \equiv 0$ and $r = 0$, ie, driftless Brownian motion with a reflecting boundary at 0 and an absorbing boundary at 1. In the following table exact and approximate values for $c_k \phi_k(0)$, $k = 1, \dots, 5$ (cf eqn (1.3) with $x = 0$).

Coefficient	Method of Moments			Exact
	3 Terms	4 Terms	5 Terms	
$c_1 \phi_1(0)$	1.2731	1.2732	1.2732	1.27324
$c_2 \phi_2(0)$	-0.4002	-0.4226	-0.4243	-0.42441
$c_3 \phi_3(0)$	0.1272	0.2228	0.2500	0.25464
$c_4 \phi_4(0)$		-0.0735	-0.1452	-0.18189
$c_5 \phi_5(0)$			0.0463	0.14147

3. Solving For The Eigenvalues

The Eigenvalue Equation

Before the eigenvalue equation can be introduced, the eigenfunction differential equation must be rewritten in more suitable form. To do so, let $Y_\theta(x)$ satisfy

$$\frac{1}{2}\sigma^2(x)Y_\theta''(x) + \mu(x)Y_\theta'(x) + \theta Y_\theta(x) = 0 \quad (3.1)$$

Multiplying (3.1) by $\rho(x)$ gives

$$\pi(x)Y_\theta''(x) + \pi'(x)Y_\theta'(x) + \theta\rho(x)Y_\theta(x) = 0, \quad (3.2)$$

where $\rho(x)$ and $\pi(x)$ are given by (1.4) and (1.5) respectively.

Now suppose that Y_θ satisfies the boundary conditions

$$Y_\theta'(0) = 0 \text{ and } Y_\theta(0) = 1.$$

Then define $\omega(\theta)$ by

$$\omega(\theta) = Y_\theta(r). \quad (3.3)$$

The eigenvalues of equation (3.1) are none other than the zeroes of ω , see [3, Chap 8] for further details.

Standardized Eigenvalue Problem

It is also possible to transform (3.1) into more standard form using the following transformation scheme. Setting

$$z = Z(x) = \int_0^x \frac{du}{(\sigma^2(u)/2)^{1/2}} \text{ reduces (3.1) to}$$

$$\frac{d^2 Y}{dz^2} + \beta(z)\frac{dY}{dz} + \theta Y = 0, \quad (3.4)$$

$$\text{where } \beta(z) = \{\mu(x(z)) - \frac{1}{4}\sigma^2(x(z))'\}/(\sigma^2(x(z))/2)^{1/2}.$$

Putting $Y(z) = g(z)y(z)$, where $g(z) = e^{\int_0^z \frac{-1}{2}\beta(u)du}$ gives

$$\frac{d^2 y}{dz^2} + (\theta - q(z))y = 0 \quad (3.5)$$

where $q(z) = \frac{1}{4}\beta^2(z) + \frac{1}{2}\beta'(z)$, and with boundary conditions $y'(0) = 0$ and $y(b) = 0$ with $b = Z(r)$.

The eigenvalues of (3.5) are the same eigenvalues as those of (3.4) and (3.2). Moreover the eigenfunctions of (3.5) are easily transformed into those of (3.2). In particular if $\psi_n(x)$ is the eigenvalue corresponding to α_n for (3.5), then $\phi_n(x) = g(Z(x))\psi_n(Z(x))$.

The following asymptotic results (as $n \rightarrow \infty$) are known about the eigenvalues and eigenfunctions of the standardized problem (cf [11, p. 19]):

$$\alpha_n = (n+1/2)^2\pi^2/b^2 + O(1); \quad (3.6)$$

$$\psi_n(x) = (2/b)^{1/2}\cos((n+1/2)\pi x/b) + O(\frac{1}{n}); \text{ and} \quad (3.7)$$

$$\psi_n'(x) = -(n+1/2)\pi(2/b^3)^{1/2}\sin(n\pi x/b) + O(1). \quad (3.8)$$

4. Obtaining First Passage Moments

To solve (2.1) we need to produce the moment-sequence $\{M_k(x, r), 1 \leq k \leq n\}$, three such methods are outlined below.

Complex Integration To Invert Moment Generating Function

Corollary 6.4 shows that $\Psi_\theta(x, r)$ is an analytic function of θ around 0, and so Cauchy's formula implies the identity

$$\frac{M_n(x, r)}{n!} = \frac{1}{2\pi i} \int_{|\theta|=\theta_0} \frac{\Psi_\theta(x, r)}{\theta^{n+1}} d\theta \quad (4.1)$$

where θ_0 is sufficiently small.

The integrals in (4.1) may be computed numerically using Gaussian quadrature to minimize the number of values of θ to be evaluated, and then taking the real part. This reduces evaluating the equation to calculating a small number of values of $\Psi_\theta(x, r)$. Evaluating $\Psi_\theta(x, r)$ may be done by either using finite differences to solve the boundary value problem (cf equation (7.6)), or by using the series method suggested in the differentiation approach, or some hybrid of series and finite differences. An important virtue of estimates of $M_n(x, r)$ based on formula (4.1) is that the accuracy of these estimates is independent of the accuracy of the $n-1$ smaller moments, unlike the methods given below.

Recursive Integration

This approach iteratively uses (6.1) to compute successive moments. This is feasible when the successive moments form a closed family of integrals (compare example 1), or when only a few moments are desired.

Example 1

Choosing parameters $\sigma^2(x) = 2(x + \sigma_0)$ and $\mu(x) = \nu$ where $\nu \neq 0$

gives rise to the iteration:

$$M_n(x) = \int_x^r \frac{n}{(w + \sigma_0)^\nu} \int_0^w M_{n-1}(u)(u + \sigma_0)^{\nu-1} du dw$$

An easy induction will show that for ν not integer $M_{n-1}(x)$ satisfies the expansion

$$M_{n-1}(x) = c[n, 0] + \sum_{k=1}^n c[n, k](x+a)^k + \sum_{k=1}^n d[n, k](x+a)^{k-\nu}$$

where the coefficients are calculated using the iteration:

$$c[n,k] = -nc[n-1,k-1]/(k(k-1)+\nu k) \quad \text{for } k \geq 1, \text{ and}$$

$$d[n,k] = -nd[n-1,k-1]/((- \nu + k)(- \nu + k - 1) + \nu(- \nu + k)) \quad \text{for } k \geq 2$$

Finally $c[n,0]$ and $d[n,1]$ are determined by solving the two-dimensional linear system arising from the boundary conditions $M_n(r) = 0$ and $M_n'(0) = 0$.

For integer ν , closed formulas for all moments are obtainable, but the calculations will be messier.

Differentiating the Moment Generating Function

Successive moments may be obtained by calculating the θ -derivatives of the moment generating function $\Psi_\theta(x,r)$ at $\theta = 0$. This approach is facilitated by Kent's observation in [8] that $\Psi_\theta(x,r) = \Upsilon_\theta(x)/\Upsilon_\theta(r)$ where $\Upsilon_\theta(x)$ satisfies

$$\frac{1}{2}\sigma^2(x)\Upsilon_\theta'(x) + \mu(x)\Upsilon_\theta'(x) + \theta\Upsilon_\theta(x) = 0 \quad (4.2)$$

with initial conditions

$$\Upsilon_\theta(0) = 0, \quad \Upsilon_\theta'(0) \neq 0. \quad (4.3)$$

To solve for the θ -derivatives of $\Psi_\theta(x,r)$ it suffices to solve for the derivatives of $\Upsilon_\theta(x)$. We can obtain $\Upsilon_\theta(x)$ using the series expansion method around $x=0$ to solve (4.2). Under certain regularity conditions, the Taylor series coefficients may be differentiated with respect to θ , and the series summed. This process is illustrated in Example 2 below.

Example 2

We indicate how the technique in (4.3) may be applied to Example 1:

$$\Upsilon_\theta(x) = \sum_{j=0}^{\infty} b_j(\theta)x^j.$$

Equation (4.2) implies that

$$\sigma^2(x) \sum_{j=0}^{\infty} \left[\frac{j+2}{2} \right] b_{j+2}(\theta)x^j + \mu(x) \sum_{j=0}^{\infty} (j+1)b_{j+1}(\theta)x^j + \theta \sum_{j=0}^{\infty} b_j(\theta)x^j = 0.$$

Since $\mu(x) = \nu$ and $\sigma(x) = 2(x+\sigma_0)$ we deduce that

$$\theta b_{j-2}(\theta) + (\nu + (j-1)(j-2))b_{j-1}(\theta) + \sigma_0 j(j-1)b_j(\theta) = 0, \quad \text{for } j \geq 2, \quad (4.4)$$

and

$b_0(\theta) = 1$ and $b_1(\theta) = 0$, for $j = 0, 1$.

Repeatedly differentiating (4.4) will give successive iterative formulas for computing the Taylor series coefficients of $\mathcal{T}_\theta^{(n)}(x)$. For example, if $n = 1$

$$\theta b'_{j-2}(\theta) + b_{j-2}(\theta) + (\nu + (j-2)(j-1))b'_{j-1}(\theta) + \sigma_0 j(j-1)b'_j(\theta) = 0, \text{ for } j \geq 2,$$

with initial condition given by equation (4.4) with $\theta = 0$.

If the above iteration diverges, we can always try renormalizing by x and calculating $b_j^{(n)}(\theta)x^n$. If r is sufficiently small then renormalization will suffice, otherwise $\mathcal{T}_\theta(x)$ can be calculated by successively moving out from 0 towards r as suggested in Section 5 below, and then using the contour integration method given in the beginning of this section.

5. Some Remarks About Computing $\Psi_\theta(x, r)$

Computing $\Psi_\theta(0, r)$

The series expansion method may not permit solving for $\Psi_\theta(0, r)$ in a single step. However, suppose the series converges for some $y \in (0, r)$, ie, it is possible to compute $\Psi_\theta(0, y)$ by the series method. We may use $\Psi_\theta(0, y)$ as a bootstrap to calculate $\Psi_\theta(y, r)$ as follows. Observe that $\Psi_\theta(0, r) = \Psi_\theta(0, y)\Psi_\theta(y, r)$. Thus

$$\Psi_\theta(y, r) = - \frac{\Psi_\theta(0, y)}{\frac{\partial \Psi_\theta(0, y)}{\partial y}} \frac{\partial \Psi_\theta(y, r)}{\partial y}.$$

Using this initial condition and Kent's normalization technique, it is possible to calculate $\Psi_\theta(y, r)$ starting from y rather than from 0.

Interpolating $\Psi_\theta(x, r)$ And A Related Boundary Value Problem

Suppose that $\Psi_\theta(x, r)$ and $\Psi_\theta(y, r)$ have been obtained ($x < y$), and it is desired to calculate $\Psi_\theta(z, r)$ for $z \in (x, y)$. The multiplicative character of $\Psi_\theta(x, r)$ implies that

$$\Psi_\theta(z, r) = \Psi_\theta(z, y)\Psi_\theta(y, r)$$

It thus suffices to determine $\Psi_\theta(z, y)$. We have $\Psi_\theta(x, y) = \Psi_\theta(x, r)/\Psi_\theta(y, r)$ and $\Psi_\theta(y, y) = 1$. Therefore it suffices to find $h_\theta(z)$ ($\equiv \Psi_\theta(z, y)$) such that

$$\frac{1}{2}\sigma^2(z)h_\theta''(z) + \mu(z)h_\theta'(z) + \theta h_\theta(z) = 0 \quad (5.1)$$

with boundary conditions $h_\theta(x) = \Psi_\theta(x, r)/\Psi_\theta(y, r)$ and $h_\theta(y) = 1$. These boundary conditions uniquely determine h_θ . To solve for h_θ , first find ξ_0 and ξ_1 satisfying (5.1), where $\xi_i'(x) = 1-i$ and $\xi_i(x) = i$, for $i = 0, 1$. Then set

$$h_\theta(z) = \Psi_\theta(x, y)\xi_1(z) + \xi_0(z)(1 - \Psi_\theta(x, y)\xi_1(y))/\xi_0(y).$$

6. Theoretical Complements

In this section some of the properties of moments of τ_x are examined, but first some new notation is introduced.

Define $M_n(x, y) \equiv E^x(\tau_y^n)$ for $x \leq y$ and $n \geq 0$, and let

$$M_n'(x, y) = \frac{\partial M_n(x, y)}{\partial x}$$

$$M_n''(x, y) = \frac{\partial^2 M_n(x, y)}{\partial x^2}$$

Recursive Equations For Moments Of τ_x

The functions $M_n(x, y)$ jointly satisfy the iterative differential equation (cf [6], p. 203, equation (3.38)) :

$$\frac{1}{2}\sigma^2(x)M_n''(x, y) + \mu(x)M_n'(x, y) + nM_{n-1}(x, y) = 0 \quad (6.1)$$

subject to $M_n'(0, y) = 0$ and $M_n(y, y) = 0$.

Lipschitz Conditions For Moments Of τ_x

Lemma

$M_n(x, y)$ is a smooth function in x and y jointly, and there exists a constant C such that

$$|M_n(x, y)| \leq C^n y^{2n-1} (y-x)n! \quad (6.2)$$

and

$$|M_n'(x, y)| \leq C^n y^{2(n-1)} n!$$

for all $x \leq y$.

Proof:

Set

$$s(x) = \exp\left\{-\int_0^x \frac{2\mu(\xi)}{\sigma^2(\xi)} d\xi\right\}$$

and

$$m(x) = 1/[\sigma^2(x)s(x)] .$$

Rewriting (6.1) as follows

$$\frac{d}{dx} \left(\frac{M_n'(x, y)}{s(x)} \right) = -2n M_{n-1}(x, y) m(x)$$

implies that

$$M_n(x, y) = 2n \int_x^y \int_0^\eta M_{n-1}(\xi, y) m(\xi) d\xi s(\eta) d\eta$$

By virtue of continuity there exists a constant K such that

$$\|s\| \equiv \sup_{0 \leq x \leq r} |s(x)| \leq K$$

and

$$\|m\| \leq K.$$

Therefore

$$\begin{aligned} |M_n(x, y)| &\leq 2n \int_x^y \int_0^\eta K^2 \|M_{n-1}\| d\xi d\eta \\ &= 2n K^2 \|M_{n-1}\| y(y-x) \leq 2K^2 y^2 n \|M_{n-1}\| \end{aligned}$$

An easy induction implies that $M_n(x, y)$ is a smooth function in x and y , moreover

$$\|M_n(x, y)\| \leq 2^n K^{2n} y^{2n-1} (y-x) n! \quad (6.3)$$

and

$$\|M_n'(x, y)\| \leq 2^n K^{2n} y^{2(n-1)} n!$$

Taking $C = (2K^2)$ completes the proof.

(6.4) Corollary

$\Psi_\theta(x, y) < \infty$ whenever $|\theta| < C^{-1} y^{-2}$, and

$$\Psi_\theta(x, y) = \sum_{n=0}^{\infty} \frac{\theta^n}{n!} M_n(x, y) \quad (6.4)$$

Infinitesimal Relations Governing First Passage Moments

Proposition

Define

$$U_n(x, y) \equiv \frac{\partial M_n(x, y)}{\partial y}$$

and

$$u_n(x) \equiv U_n(x, x)$$

Then $M_n(x, y)$, $U_n(x, y)$, $u_n(x)$ satisfy

$$M_n(0, y) = \sum_{j=0}^n \binom{n}{j} M_j(0, x) M_{n-j}(x, y) \quad (6.5)$$

$$U_n(0, x) = \sum_{j=0}^{n-1} \binom{n}{j} M_j(0, x) u_{n-j}(x) \quad (6.6)$$

Proof

Conditional on $X(0) = 0$ the strong Markov property (**SMP**) implies that $\{\tau_{a_1}, \tau_{a_2} - \tau_{a_1}, \dots, \tau_r - \tau_{a_n}\}$, where $0 < a_1 < a_2 < \dots < a_n < r$, form a set of independent random variables. In particular

$$\begin{aligned} M_n(0, y) &\equiv E^0[\tau_y^n] = E^0[(\tau_x + \tau_y - \tau_x)^n] \\ &= \sum_{j=0}^n \binom{n}{j} E^0[\tau_x^j (\tau_y - \tau_x)^{n-j}] \\ &= \sum_{j=0}^n \binom{n}{j} E^0[\tau_x^j] E^x[(\tau_y - \tau_x)^{n-j}] \end{aligned}$$

which coincides with (6.5). Using a little algebraic manipulation on (6.5) shows that

$$[M_n(0, y) - M_n(0, x)] / (y - x) = \sum_{j=0}^{n-1} \binom{n}{j} M_j(0, x) M_{n-j}(x, y) / (y - x) \quad (6.7)$$

Now letting $y \rightarrow x$ in (6.7) yields (6.6). QED

Comments

Equations (6.5) and (6.6) provide some nice intuition about the way that first passage times from x to y depend on first passage times from 0 to x .

Equations (6.5) and (6.6) are similar to (6.1), but may capture better the dependence of higher moments on lower moments. From a practical point of view equation (6.1) is certainly preferable for moment calculation. In Section 4, other methods are proposed for calculating the moments $M_n(x,y)$.

7. A Representation Result

Theorem

$$\Psi_\theta(x, y) = \exp\left\{ \sum_{n=1}^{\infty} \int_x^y u_n(z) \frac{\theta^n}{n!} dz \right\} \quad (7.1)$$

where $\{u_n(z), n \geq 1\}$ satisfy

$$\frac{1}{2} \sigma^2(x) u_1'(x) + \mu(x) u_1(x) = 1, \quad (7.2)$$

and for $n \geq 2$

$$\frac{1}{2} \sigma^2(x) u_n'(x) + \mu(x) u_n(x) = \frac{1}{2} \sigma^2(x) \sum_{k=1}^{n-1} \binom{n}{k} u_k(x) u_{n-k}(x). \quad (7.3)$$

Proof

We begin by showing that (7.1) holds for $\Psi_\theta(0, r)$.

Let $x_j = jr/L$ for $0 \leq j \leq L$. Using the **SMP** as in the proof of (6.5),

$$\Psi_\theta(0, r) = \prod_{j=0}^{L-1} \Psi_\theta(x_j, x_{j+1}).$$

Taking logarithms,

$$\log \Psi_\theta(0, r) = \sum_{j=0}^{L-1} \log \Psi_\theta(x_j, x_{j+1}).$$

Applying the proposition in Section 8 to the above yields

$$\log \Psi_\theta(0, r) = \sum_{j=0}^{L-1} [\Psi_\theta(x_j, x_{j+1}) - 1 + (\Psi_\theta(x_j, x_{j+1}) - 1)^2 g(\Psi_\theta(x_j, x_{j+1}))].$$

Since $\Psi_\theta(x, x) = 1$ it follows

$$\Psi_\theta(x_j, x_{j+1}) - 1 = \frac{\partial \Psi_\theta}{\partial y}(x_j, x_j + \alpha L^{-1}) L^{-1}$$

where $0 < \alpha < 1$. Also since $\Psi_\theta(x, y)$ is a smooth function in x and y jointly, it follows that $\frac{\partial \Psi_\theta(x, y)}{\partial y}$ is uniformly bounded on the region $0 \leq x \leq y \leq r$. So there exists a function $h(L)$ such that $h(L) \sim O(1)$

$$\log \Psi_\theta(0, r) = \sum_{j=0}^{L-1} [\Psi_\theta(x_j, x_{j+1}) - 1] + h(L) L^{-1}.$$

Replacing each $\Psi_\theta(x_j, x_{j+1})$ in the above by the expression in (6.4), yields

$$\log \Psi_\theta(0, r) = \sum_{j=0}^{L-1} \sum_{n=1}^{\infty} \frac{\theta^n M_n(x_j, x_{j+1})}{n!} + O(L^{-1}).$$

Since the summands are positive the order of summation may be permuted to get

$$\log \Psi_\theta(0, r) = \sum_{n=1}^{\infty} \sum_{j=0}^{L-1} \frac{\theta^n M_n(x_j, x_{j+1})}{n!} + O(L^{-1}).$$

The inner summation can be expressed as a Riemann sum

$$\log \Psi_\theta(0, r) = \sum_{n=1}^{\infty} \theta^n \sum_{j=0}^{L-1} \frac{M_n(x_j, x_{j+1})}{n! L^{-1}} \frac{1}{L} + O(L^{-1}). \quad (7.4)$$

Equation (6.2) implies that

$$\frac{M_n(x_j, x_{j+1})}{n! L^{-1}} \leq C^n (x_{j+1})^{2n} \leq C_0^n$$

where $C_0 = Cr^2$.

The Lebesgue dominated convergence theorem (applied to the product space $\{1, 2, \dots\} \times [0, r]$ endowed with product of the counting measure with the Lebesgue measure on $[0, r]$) implies the right side of (7.4) approaches the limit

$$\log \Psi_\theta(0, r) = \sum_{n=1}^{\infty} \frac{\theta^n}{n!} \int_0^r u_n(z) dz$$

as $L \rightarrow \infty$, or

$$\Psi_\theta(0, r) = \exp \left\{ \sum_{n=1}^{\infty} \frac{\theta^n}{n!} \int_0^r u_n(z) dz \right\}.$$

Due to the multiplicative nature of $\Psi_\theta(x, y)$ it is easy to show that

$$\Psi_\theta(x, y) = \exp \left\{ \sum_{n=1}^{\infty} \int_x^y u_n(z) \frac{\theta^n}{n!} dz \right\}. \quad (7.5)$$

The function $\Psi_\theta(x, y)$ satisfies the following differential equation (cf [6, pp 203])

$$\frac{1}{2} \sigma^2(x) \frac{\partial^2 \Psi_\theta(x, y)}{\partial x^2} + \mu(x) \frac{\partial \Psi_\theta(x, y)}{\partial x} + \theta \Psi_\theta(x, y) = 0 \quad (7.6)$$

subject to $\frac{\partial \Psi_\theta(0,y)}{\partial x} = 0$ and $\Psi_\theta(y,y) = 1$.

Substituting equation (7.5) in (7.6), shows that the exponent in (7.5) satisfies the differential equation

$$\frac{1}{2}\sigma^2(x)\left[\left(\sum_{n=1}^{\infty} \frac{\theta^n}{n!} u_n(x)\right)^2 - \sum_{n=1}^{\infty} \frac{\theta^n}{n!} u_n'(x)\right] - \mu(x) \sum_{n=1}^{\infty} \frac{\theta^n}{n!} u_n(x) + \theta = 0.$$

Since the above series converge absolutely for θ sufficiently small, we can rearrange terms to obtain a single power series in θ . Because this power series is zero for θ sufficiently small, all its coefficients must be zero. Setting the coefficients of θ to zero yields equations (7.2) and (7.3).

The initial condition that $\frac{\partial \Psi_\theta(0,y)}{\partial x} = 0$ in (7.6) implies $u_n(0) = 0$, where $n \geq 1$. This concludes the proof.

8. Appendix

Spectral Representations For First Passage Time Distributions

Theorem The right-hand-side of (1.3) is the unique function satisfying (1.2), jointly continuous in x and t on $[0, r] \times (0, \infty)$ with $\frac{\partial w(x, t)}{\partial t}$ absolutely integrable over $[0, r] \times (N^{-1}, N)$ for all $N \geq 1$.

Proof:

Suppose that $w(x, t)$ satisfies equation (1.2) and the integrability conditions. Observe that for fixed $t > 0$ $w(x, t)$ is a continuous function of x belonging to $L^2(\rho)$ (where ρ is defined by equation (1.4)). Therefore $w(x, t)$ possesses the orthogonal expansion

$$w(x, t) = \sum_{k=1}^{\infty} c_k(t) \phi_k(x)$$

where

$$c_k(t) = \int_0^r w(x, t) \phi_k(x) \rho(x) dx .$$

Multiply (1.2) by $\phi_k(x) \rho(x)$ and integrate over $[0, r]$ to get

$$\int_0^r \frac{\partial w(x, t)}{\partial t} \phi_k(x) \rho(x) dx = \int_0^r A w(x, t) \phi_k(x) \rho(x) dx .$$

Now since $A f(x) \rho(x) = \pi(x) f''(x) + \pi'(x) f'(x)$ (cf (3.1) and (3.2)), a simple integration by parts shows

$$\int_0^r A w(x, t) \phi_k(x) \rho(x) dx = \int_0^r w(x, t) A \phi_k(x) \rho(x) dx .$$

The relationship $A \phi_k(x) = -\alpha_k \phi_k(x)$ implies that

$$\int_0^r \frac{\partial w(x, t)}{\partial t} \phi_k(x) \rho(x) dx = - \int_0^r \alpha_k w(x, t) \phi_k(x) \rho(x) dx .$$

Integrating both sides with respect to t over $[u_0, u]$ and permuting the order of integration on the left-hand-side yields (permissible because Fubini's Theorem which is absolutely integrable)

$$\int_0^r \int_{u_0}^u \frac{\partial w(x, t)}{\partial t} \phi_k(x) \rho(x) dt dx = \int_{u_0}^u \int_0^r -\alpha_k w(x, t) \phi_k(x) \rho(x) dx dt .$$

Using the definition of $c_k(t)$ on the the last equation implies

$$c_k(u) + C = \int_{u_0}^u -\alpha_k c_k(t) dt ,$$

where C is an arbitrary constant.

Therefore $c_k(t) = c_k e^{-\alpha_k t}$. It remains to determine the constants c_k , but they may be derived from the boundary condition $w(x,0) = 1$ for $0 < x < r$ as follows. Since ρ is continuous, $w(x,0) = 1$ for almost all $\rho(dx)$, and $1 \in L^2(\rho)$. So

$$1 = \sum_{k=1}^{\infty} c_k \phi_k(x) \quad (8.1)$$

where

$$c_k = \int_0^r \phi_k(x) \rho(x) dx . \quad (8.2)$$

Now Theorem 1.9 of [11] implies that the right-hand-side of (8.1) converges pointwise to 1 on $(0,r)$. Therefore $w(x,t)$ has the representation

$$w(x,t) = \sum_{k=1}^{\infty} c_k e^{-\alpha_k t} \phi_k(x) . \quad (8.3)$$

To prove the converse, suppose that $w(x,t)$ is defined by (8.2) and (8.3) jointly. Equations (3.7) and (8.2) imply that the coefficients c_k , $k \geq 1$ are uniformly bounded. Hence for $t > \epsilon > 0$ the series converges uniformly to a function continuous on the product $[0,r] \times [\epsilon, \infty)$. The uniform convergence and boundary conditions on the eigenfunctions imply the boundary conditions on x . The integrability conditions on $\frac{\partial w(x,t)}{\partial t}$ follow in similar fashion. The boundary condition $w(x,0) = 1$ for $x \in (0,r)$ follows from Theorem 1.9 of [11] and equation (8.1). The differential equation (1.2) may be derived from the definition of derivatives as limits of divided differences, and the dominated convergence theorem applied to series. QED.

It should be noted that the first passage time distribution satisfies the regularity conditions of the theorem, and therefore must have representation (1.2).

Convergence Of The Finite Approximations To The Infinite Vector

It will now be shown that the solution vector to system (2.1), denoted by $\mathbf{p}^{(n)} = \{p_j^{(n)}, 1 \leq j \leq n\}$, converges at rate n^{-2} component-wise to the infinite vector $\mathbf{p} = \{p_j, j \geq 1\}$, where $p_j = c_j \phi_j(x)$.

Theorem

$$|p_{k_0}^{(n)} - p_{k_0}| = O\left(\frac{1}{n^2}\right)$$

Proof: Define $\nu_k^{(n)}$, $\delta_k^{(n)}$ and $\eta_k^{(n)}$ as follows:

$$\nu_k^{(n)} = \sum_{j=1}^n \mu_j^k p_j \quad \text{where } 0 \leq k \leq n-1$$

$$\delta_k^{(n)} = m_k - \nu_k^{(n)} = \sum_{j=n+1}^{\infty} \mu_j^k p_j \quad \text{where } 0 \leq k \leq n-1 \quad (8.4)$$

$$\eta_k^{(n)} = p_k - p_k^{(n)}$$

Observe that $\{\eta_k^{(n)}, 1 \leq k \leq n\}$ is the solution to (2.2) where $\{m_k, 1 \leq k \leq n\}$ has been replaced by $\{\delta_k^{(n)}, 1 \leq k \leq n\}$. In particular

$$\eta_k^{(n)} = \sum_{1 \leq j \leq n} \delta_j^{(n)} g_{n-j}(\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n) / \prod_{\substack{1 \leq j \leq n \\ j \neq k}} (\mu_j - \mu_k). \quad (8.5)$$

For $1 \leq j \leq n$

$$|g_{n-j}((\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n))| \leq \mu_k^{n-j-k}.$$

Also equations (3.2), (3.6) and (3.7) together imply that $|c_n| = O\left(\frac{1}{n}\right)$, thus (8.4) and (3.6) imply

$$|\delta_j^{(n)}| \leq Cn^{-2j}.$$

So

$$\begin{aligned} \left| \sum_{j=1}^n g_{n-j}((\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n)) \delta_j^{(n)} \right| &\leq \sum_{j=1}^n \mu_k^{n-j-k} |\delta_j^{(n)}| \\ &\leq \mu_k^{n-k} \sum_{j=1}^k Cn^{-2j} \mu_k^{-j} = \mu_k^{n-k-1} O\left(\frac{1}{n^2}\right). \end{aligned}$$

Thus

$$\left| \sum_{j=1}^n g_{n-j}((\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n)) \delta_j^{(n)} \right| = O\left(\frac{\mu_k^{n-k-1}}{n^2}\right).$$

Finally, the denominator of (8.5) may be written as

$$\prod_{\substack{1 \leq j \leq n \\ j \neq k}} (\mu_j - \mu_k) = \mu_k^{n-k} d_k^{(n)}$$

where

$$d_k^{(n)} = \prod_{1 \leq j \leq k-1} (\mu_j - \mu_k) \prod_{k+1 \leq j \leq n} (1 - \frac{\mu_j}{\mu_k}).$$

Now equation (3.6) and the Weierstrass Product Convergence test jointly imply that

$$\lim_{n \rightarrow \infty} d_k^{(n)} = d > 0.$$

Thus setting $k = k_0$ yields $\eta_{k_0}^{(n)} = O(\frac{1}{n^2})$ as claimed.

A Conjecture

It is interesting to note that $p_k(x)$ is linearly proportional to the eigenfunction $\phi_k(x)$, and therefore $Ap_k(x) = \alpha_k p_k(x)$. This suggests that $p_k^{(n)}(x)$ will approximately satisfy this relation. Observe that $Am_k(x) = -m_{k-1}(x)$. Thus

$$Ap_k^{(n)}(x) = \sum_{1 \leq j \leq n-1} -m_j g_{n-j-1}(\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n) / \prod_{\substack{1 \leq j \leq n \\ j \neq k}} (\mu_j - \mu_k).$$

Comparing this with (2.3) suggests that

$$\lim_{n \rightarrow \infty} \frac{g_{n-j-1}((\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n))}{g_{n-j}((\mu_1, \mu_2, \dots, \mu_{k-1}, \mu_{k+1}, \dots, \mu_n))} = \alpha_k = \frac{1}{\mu_k}$$

Proposition

For $1 \leq x < 2$

$$| \log(x) - x + 1 | = (x-1)^2 g(x)/2, \text{ where } |g(x)| < 1.$$

Proof: The mean value theorem applied to $\log(x)$ at $x=1$ gives:

$$\log(x) = \log(1+x-1) = \log(1) + (x-1) - (x-1)^2/2(1+\alpha(x-1)^{-2})$$

where $0 < \alpha < 1$. The prop now follows from $x \geq 1$ and $\alpha > 0$.

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