

ON THE INVERSE FIRST-PASSAGE-TIME PROBLEM FOR A WIENER PROCESS^{1,2}

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The inverse first-passage problem for a Wiener process $(W_t)_{t \geq 0}$ seeks to determine a function $b: \mathbb{R}_+ \rightarrow \mathbb{R}$ such that

$$\tau = \inf\{t > 0 | W_t \geq b(t)\}$$

has a given law. In this paper two methods for approximating the unknown function b are presented. The errors of the two methods are studied. A set of examples illustrates the methods. Possible applications are enlightened.

1. Introduction. Many phenomena can be modeled as first passage time of suitable Markov processes through constant or time varying boundaries. The first-passage problem has a long history and a large number of applications that range from finance to engineering and biology [see, e.g., Ricciardi and Sato (1990) for some references]. Yet explicit solutions to the first-passage problem are known only in a limited number of special cases (including linear or quadratic boundaries).

In modeling generally one describes the dynamics of the involved variables via a suitable stochastic process $\{X_t, t \geq 0\}$ constrained by an assigned boundary $b: (0, \infty) \rightarrow \mathbb{R}$ satisfying $b(0+) \geq 0$ and investigates distribution features of the first passage time (FPT)

$$(1.1) \quad \tau_b = \inf\{t > 0 | W_t \geq b(t)\}$$

of X_t over b . This is the direct FPT problem. However, there are also instances when the underlying stochastic process is assigned, one knows or estimates the FPT distribution F_b and wishes to determine the corresponding boundary shape. This is the inverse first passage time (IFPT) problem. Different applications of

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the IFPT problem can be listed. In a reliability context one could compare performances of alternative objects, characterized by their lifetime distribution comparing the shapes of the boundaries. In this case one should assume the same underlying stochastic process to describe the evolution toward the crash of the object and to identify the crash time as an observed FPT of the process through an unknown boundary. Other interesting applications can arise when the resulting boundary exhibits a periodic behavior. This fact can suggest particular features of the modeled phenomenon in a finance or in a neurobiological context. Despite its importance in applications, the literature focuses only on specific problems [cf. Sacerdote and Zucca (2003a, 2003b) and Sacerdote, Villa and Zucca (2006)] while there is a lack of mathematical results. Here we try to cover this gap focusing on the inverse first passage time problem for the Wiener process.

The IFPT problem was brought to our attention by Professor Goran Peskir, who presented us its first formulation by A. Shiryayev in 1976 (during a Banach center meeting). The original Shiryayev question considered the case when F_b is an exponential distribution. There exist two early papers dealing with the existence problem written by Dudley and Gutmann (1977) and Anulova (1980). These papers provide the existence of *some* stopping times for given F_b ; however, these stopping times are not of the form (1.1) for some *function* b . Furthermore, in Capocelli and Ricciardi (1972) the properties characterizing the FPT distribution in the case of the constant boundary are discussed.

The problem of the existence and uniqueness of b is still open. Through the paper we do not enter into the question of the existence of b but assume that such a boundary exists, is unique and sufficiently regular (continuous or C^1).

The main aim of the present paper is to propose two algorithms for approximating the unknown function b when F_b is given. After some preliminaries presented in Section 2, in Section 3 we introduce a first approach to the IFPT problem. It is based on the idea to approximate b by a piecewise-linear boundary c for which the law of τ_c can be computed. It leads to a Monte Carlo method for determining c . The second approach (Section 5) is based on the classic idea due to Volterra (around 1896) on how to approximate an integral equation (of the first kind) by a system of n equations in n unknowns. Since the integral equation for b is nonlinear, the resulting system is also nonlinear. We propose a numerical method for approximating b at finitely many points.

Both methods produce an approximation of the boundary value. Hence it is necessary to evaluate the respective errors, that is, the difference between the exact unknown value and the computed approximation. We limit the study of the error at the discretization time knots obtained with constant discretization step h . The error of the first method is discussed in Section 4. It is due to multiple causes but it is dominated by the error due to the substitution of the continuous boundary b with a piecewise-linear boundary c and it is $O(h^2)$. Furthermore, due to the use of the Monte Carlo method to evaluate some involved integrals, the resulting boundary is estimated with a fixed confidence level α . The error of the second approach

is evaluated in Section 6 and it is $O(h)$ or $O(h^2)$ depending upon the numerical method used to evaluate the involved integral. In Section 7 we illustrate the goodness of the proposed methods by means of a set of examples. Finally, in Section 8 we consider the boundary corresponding to the exponential FPT distribution and we give a numerical answer to the 1976 Shiryayev question.

2. First passage time: the direct and inverse problem. Given a standard Wiener process $W = (W_t)_{t \geq 0}$ started at zero, and a sufficiently regular function $b: (0, \infty) \rightarrow \mathbb{R}$ satisfying $b(0+) \geq 0$, denote

$$(2.1) \quad \tau_b = \inf\{t > 0 | W_t \geq b(t)\}$$

the FPT of W over b , and set

$$(2.2) \quad f_b(t) = \frac{d}{dt} \mathbb{P}(\tau_b \leq t)$$

to denote its density function for $t > 0$. In the sequel we also need to consider the Wiener process starting in x_0 at time t_0 ; in this case we write $f_b(t|x_0, t_0)$ in spite of $f_b(t)$. Throughout we assume that all regularity assumptions ensuring the existence of the objects introduced and properties imposed are fulfilled.

By $p_{a,b}(t, x|s, y)$, we denote the transition probability density function of W at t constrained by the *absorbing* boundary b over $[s, t]$ given that $W_s = y$, that is,

$$(2.3) \quad p_{a,b}(t, x|s, y) = \frac{\partial}{\partial x} \mathbb{P}(W_t \leq x, \tau_b > t | W_s = y)$$

for $x \leq b(t)$ with $t > s \geq 0$ and $y < b(s)$ given and fixed.

Under the hypothesis that the stochastic process (in this case the Wiener process) is assigned, the *direct first-passage time problem* seeks to determine F_b when b is given. The *inverse first-passage time problem* seeks to determine b when F_b is given. It is interesting to note that the IFPT problem looks for the boundary $b(t)$ that is a deterministic time dependent function. Furthermore, as proved by Strassen (1967), if the boundary $b \in C^1(\mathbb{R}^+)$, then the probability distribution of the FPT is absolutely continuous with continuous density.

In the literature there exist some equations that relate quantities (2.2) and (2.3), allowing, in a limited number of cases, to solve the direct FPT problem [cf. Ricciardi and Sato (1990)]. In Section 2.1 we list some existing closed form results for the Wiener process. These results will be used in Sections 3 and 7 to numerically validate the reliability of the two algorithms proposed. In absence of the analytical solution, the direct problem can be solved numerically, making use of one of the algorithms proposed in the literature [Buonocore, Nobile and Ricciardi (1987) and Zucca (2002)]. In Section 7 we use the algorithm introduced in Buonocore, Nobile and Ricciardi (1987) to estimate the FPT p.d.f. for a set of assigned boundaries. These numerical evaluations make it possible to enlarge the test set for the validation of the IFPT algorithms proposed in this paper. Finally, we briefly recall in

Section 2.2 some results that will be useful later on [cf. Peskir (2002)], since one of the two algorithms proposed for the IFPT method requires the knowledge of $b(0)$.

In the sequel we will assume that $t_0 = x_0 = 0$ when this gives no loss of generality.

2.1. *Known boundaries.* The first-passage time density f_b for a Wiener process is known explicitly in a few cases. The following three will be of interest in the sequel:

1. *Linear boundary.* If the boundary is given by

$$(2.4) \quad c(t) = \alpha + \beta t$$

with $\alpha > x_0$ and $\beta \in \mathbb{R}$, then [cf. Doob (1949), page 397, and Malmquist (1954), page 526]

$$(2.5) \quad \begin{aligned} f_c(t|t_0, x_0) &= \frac{\alpha - x_0}{\sqrt{2\pi(t-t_0)^3}} e^{-(\alpha + \beta(t-t_0) - x_0)^2 / (2(t-t_0))} \\ &= \frac{\alpha - x_0}{(t-t_0)^{3/2}} \varphi\left(\frac{\alpha + \beta(t-t_0) - x_0}{\sqrt{t-t_0}}\right) \end{aligned}$$

for $t > 0$, where $\varphi(x) = (1/\sqrt{2\pi})e^{-x^2/2}$ is the standard normal probability density function. Note that (2.5) is known as the Bachelier–Lévy formula.

2. *Daniels boundary.* If the boundary is given by

$$(2.6) \quad d(t) = \frac{\alpha}{2} - \frac{t}{\alpha} \log\left(\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} + \gamma e^{-\alpha^2/t}}\right),$$

where $\alpha > 0$, $\beta \geq 0$ and $\gamma > -\beta^2/4$, then [cf. Daniels (1969)]

$$(2.7) \quad \begin{aligned} f_d(t) &= \frac{1}{\sqrt{2\pi t^3}} \left(e^{-d(t)^2/(2t)} - \frac{\beta}{2} e^{-(d(t)-\alpha)^2/(2t)} \right) \\ &= \frac{1}{t^{3/2}} \left(\varphi\left(\frac{d(t)}{\sqrt{t}}\right) - \frac{\beta}{2} \varphi\left(\frac{d(t)-\alpha}{\sqrt{t}}\right) \right) \end{aligned}$$

for $t > 0$.

3. *Piecewise-linear boundary.* If the boundary is given by

$$(2.8) \quad c(t) = \alpha_i + \beta_i t \quad \text{for } t \in [t_{i-1}, t_i] \text{ and } i \geq 1,$$

where $t_i = t_0 + ih$, $h > 0$ and $\alpha_i, \beta_i \in \mathbb{R}$ with $t_0 \geq 0$. Setting $\alpha_{i+1} = \alpha_i + \beta_i t_i$, we get that $t \mapsto c(t)$ is continuous on $[t_0, \infty)$. Let us denote by $c_i = c(t_i)$ the knots of c for $i \geq 0$.

The transition density function of W in x_1, x_2, \dots, x_n at t_1, t_2, \dots, t_n constrained by the *absorbing* piecewise-linear boundary c over $[t_0, t_n]$ given that $W_{t_0} = x_0 < \alpha_1$ is [recall (2.3) above]

$$\begin{aligned}
 & p_{a,c}(t_1, x_1; t_2, x_2; \dots; t_n, x_n | t_0, x_0) \\
 &= \prod_{i=1}^n p_{a,c}(t_i, x_i | t_{i-1}, x_{i-1}) \\
 (2.9) \quad &= \prod_{i=1}^n \left(1 - e^{-2(c_i - x_i)(c_{i-1} - x_{i-1}) / (t_i - t_{i-1})} \right) \\
 &\quad \times \frac{1}{\sqrt{2\pi(t_i - t_{i-1})}} \exp\left(-\frac{(x_i - x_{i-1})^2}{2(t_i - t_{i-1})}\right)
 \end{aligned}$$

for $(x_1, x_2, \dots, x_n) \in \mathbb{R}^n$ with $x_i \leq c_i$ for $1 \leq i \leq n$ and $x_0 < c_0$ where $t_0 < t_1 < t_2 < \dots < t_n$ are given and fixed. This implies

$$\begin{aligned}
 (2.10) \quad & \mathbb{P}(W_{t_1} \in C_1, \dots, W_{t_n} \in C_n, \tau_c > t_n | W_{t_0} = x_0) \\
 &= \int_{C_1} \dots \int_{C_n} p_{a,c}(t_1, x_1; \dots; t_n, x_n | t_0, x_0) dx_1 \dots dx_n
 \end{aligned}$$

for any Borel set $C_i \subseteq \langle -\infty, c_i]$ with $1 \leq i \leq n$.

The identity (2.9) is a well-known fact in the case $n = 1$ [cf. Doob (1949), equation (4.2) and Section 5, or Durbin (1971), Lemma 1]. The case of general $n \geq 2$ [cf. Wang and Pötzelberger (1997)] follows readily by induction arguments using that W has stationary independent increments.

Since there are only a few cases where the FPT density function is known in closed form, there has been a big effort in the past to find numerical approximation for it. One of the most used algorithms has been presented in Buonocore, Nobile and Ricciardi (1987). This method solves a Volterra integral equation of the second kind derived from the Fortet equation but characterized by a nonsingular kernel. In Section 7 we apply this method to determine numerically the FPT density function in the case of a time periodic oscillating boundary.

2.2. Limits at zero. One of the key issues in the numerical treatment of the inverse first-passage problem is to know $b(0+)$ in terms of $f_b(0+)$ and vice versa. In this section we display some known results on this relation. We will make use of these facts in Sections 7 and 8 below.

In the notation of Section 2, let $W = (W_t)_{t \geq 0}$ be a standard Wiener process started at zero, let $b : \langle 0, \infty \rangle \rightarrow \mathbb{R}$ be a continuous function satisfying $b(0+) \geq 0$, and let us assume that the first-passage time τ_b from (2.1) has a continuous density function f_b having a limit $f_b(0+)$ in $[0, \infty]$. Then the following facts are known to hold [cf. Peskir (2002)].

If there are $\varepsilon > 0$ and $\delta > 0$ such that

$$(2.11) \quad b(t) \geq \sqrt{(2 + \varepsilon)t \log(1/t)}$$

for all $t \in \langle 0, \delta \rangle$, then $f_b(0+) = 0$. If there is $\delta > 0$ such that

$$(2.12) \quad b(t) \leq \sqrt{2t \log(1/t)}$$

for all $t \in \langle 0, \delta \rangle$, then $f_b(0+) = +\infty$. Moreover, if we define a boundary g by setting

$$(2.13) \quad g(t) = \sqrt{2t \log(1/t) + t \log \log(1/t) + ct}$$

for $t \in \langle 0, \delta_c \rangle$ with $c \in \mathbb{R}$ given and fixed, then the limit $f_g(0+)$ exists and is given by

$$(2.14) \quad f_g(0+) = \frac{e^{-c/2}}{\sqrt{4\pi}}.$$

Observe that g from (2.13) locally at zero lies between the two functions appearing on the l.h.s. of (2.11) and (2.12) respectively (where $\varepsilon > 0$ may be as small as one likes).

3. First approach: a piecewise linear approximation via Monte Carlo simulation. In this section we face the IFPT problem by looking for a piecewise-linear approximation of the unknown boundary b with an approach that can be considered analogous to the method used by Durbin (1971) for the direct FPT problem. Thus, we determine the piecewise-linear boundary c (2.8) that approximates the exact boundary b corresponding to the given first-passage density f_b .

First we consider the inverse problem when $f_b(0+) = 0$ and we assume that $b(0+) > 0$ is known. Then, using the notation of Section 2 (with $t_0 = 0$), we set $c_0 = b(0+)$ and, thus, $\alpha_1 = b(0+)$ as well. When $b(0+)$ is unknown we can guess its value, but in this case the error at the initial knot can dominate the final one. Since the resulting algorithm uses the Monte Carlo approach to estimate involved integrals, henceforth we call it the PLMC (Piecewise Linear Monte Carlo) method. In the following we consider a time discretization $t_i = t_0 + ih$, $i = 1, 2, \dots$, where h is a positive constant. The choice h constant is made to simplify our notation, but the method can be easily extended to a nonconstant h .

The driving idea of our algorithmic approach is to equate the probability of the FPT of W through c in $\langle t_{i-1}, t_i \rangle$ and the analogous probability determined by the given first-passage density f_b in the same interval. The resulting equations allow to determine the coefficients α_i and β_i in (2.8) successively on the intervals $\langle t_{i-1}, t_i \rangle$ for $i \geq 1$. The algorithm can be divided in two successive steps.

STEP 1. We determine the value of β_1 in (2.8) such that the probability of the first-passage of W through c in $(0, t_1]$ equals the probability of the first-passage of W through b in $(0, t_1]$, that is, we look for the value of β such that

$$(3.1) \quad \int_0^{t_1} f_c(t) dt = \int_0^{t_1} f_b(t) dt,$$

where $f_c(t)$ is given by (2.5).

STEP 2. Given $\alpha_1, \dots, \alpha_n$ and β_1, \dots, β_n with $n \geq 1$, we set $\alpha_{n+1} = \alpha_n + \beta_n t_n$ and we determine the value of β_{n+1} such that the probability of the first-passage time of W through c in $(t_n, t_{n+1}]$ equals the probability of the first-passage time of W through b in $(t_n, t_{n+1}]$, that is, we look for the value of β such that

$$(3.2) \quad \int_{t_n}^{t_{n+1}} \int_{-\infty}^{c_n} \cdots \int_{-\infty}^{c_1} \left(f_c(t|t_n, x_n) \prod_{i=1}^n p_{a,c}(t_i, x_i|t_{i-1}, x_{i-1}) \right) dx_1 \cdots dx_n dt = \int_{t_n}^{t_{n+1}} f_b(t) dt,$$

where $f_c(t|t_n, x_n)$ is the density function of the first-passage time of W over $\alpha_{n+1} + \beta_{n+1}t$ for $t > t_n$ given that $W_{t_n} = x_n$, that is, it is given by (2.5) with $\alpha := c_n$ and $\beta = \beta_{n+1}$, while $p_{a,c}(t_i, x_i; t_{i-1}, x_{i-1})$ is given by (2.9) for $1 \leq i \leq n$ (where $t_0 = x_0 = 0$).

REMARK 3.1. The product appearing on the l.h.s. of (3.2) involves the known functions (2.9) depending upon $\alpha_1, \dots, \alpha_n$ and β_1, \dots, β_n determined in the preceding step. The unknown α_{n+1} and β_{n+1} appear in (3.2) only within the function $f_c(t|t_n, x_n)$. Furthermore, α_{n+1} can (by continuity of c at t_n) be expressed in terms of β_{n+1} and the known α_n and β_n as follows:

$$(3.3) \quad \alpha_{n+1} = \alpha_n + (\beta_n - \beta_{n+1})t_n$$

so that we only need to determine β_{n+1} from the equation (3.2).

Let us now detail the two steps of the algorithm. In order to solve the equation (3.1) and (3.2) for the unknown β_1 and β_n respectively, it is necessary to compute the integrals involved.

Discretizing the integral of the l.h.s. in (3.1) by a rectangular method [cf. Atkinson (1989)], we obtain a nonlinear function of the unknown β_1 while the r.h.s. of (3.1) is easily computable by standard means. Various approximate methods can then be used to solve the resulting equation. Here we use the middle point method.

In the successive steps, mainly when n becomes large, the multiple integrals of the l.h.s. of (3.2) cannot be handled by standard numerical methods. To handle the problem, we adapt the Monte Carlo method proposed by Wang and Pötzelberger (1997) to our case.

For this, note that, using expression (2.5) for $f_c(t|t_n, x_n)$ and (3.3), we get

$$\begin{aligned}
 H(\beta_{n+1}; x_n) &:= \int_{t_n}^{t_{n+1}} f_c(t|t_n, x_n) dt \\
 &= \int_{t_n}^{t_{n+1}} \frac{c_n - x_n}{(t - t_n)^{3/2}} \varphi\left(\frac{c_n - x_n + \beta_{n+1}(t - t_n)}{\sqrt{t - t_n}}\right) dt \\
 &= 1 - \Phi\left(\frac{\beta_{n+1}(t_{n+1} - t_n) + (c_n - x_n)}{\sqrt{t_{n+1} - t_n}}\right) \\
 (3.4) \quad &+ e^{-2\beta_{n+1}(c_n - x_n)} \Phi\left(\frac{\beta_{n+1}(t_{n+1} - t_n) - (c_n - x_n)}{\sqrt{t_{n+1} - t_n}}\right) \\
 &= 1 - \Phi\left(\frac{\beta_{n+1}(t_{n+1} - t_n) + \alpha_n + \beta_n t_n - x_n}{\sqrt{t_{n+1} - t_n}}\right) \\
 &+ e^{-2\beta_{n+1}(\alpha_n + \beta_n t_n - x_n)} \\
 &\quad \times \Phi\left(\frac{\beta_{n+1}(t_{n+1} - t_n) - \alpha_n - \beta_n t_n + x_n}{\sqrt{t_{n+1} - t_n}}\right)
 \end{aligned}$$

for each $n \geq 1$. Here $\Phi(x) = \int_{-\infty}^x \varphi(z) dz$ is the integral of the standard normal density. It follows by (2.9) and (3.4) that the equation (3.2) can be rewritten as follows:

$$\begin{aligned}
 (3.5) \quad &E\left(H(\beta_{n+1}; X_n) \prod_{i=1}^n I(X_i \leq c_i) e^{-2(c_i - X_i)(c_{i-1} - X_{i-1})/(t_i - t_{i-1})}\right) \\
 &= \int_{t_n}^{t_{n+1}} f_b(t) dt,
 \end{aligned}$$

where $X_i \sim N(0, t_i - t_{i-1})$, $i = 1, \dots, n$, are independent random variables (and $X_0 \equiv 0$). A Monte Carlo method can now be used to estimate the l.h.s. of (3.5).

In order to find an approximation of β_{n+1} , we can use, as in the Step 1 above, the iterative middle point procedure. Using then (3.3), one obtains α_{n+1} and thus determines c on $(t_n, t_{n+1}]$.

REMARK 3.2. For each $n \geq 1$ given and fixed, the equation (3.5) defines a nonlinear function of the unknown parameter β_{n+1} depending on it only through H from (3.4). Since the l.h.s. of (3.5) is monotone in β_{n+1} , equation (3.5) admits a unique solution $\beta_{n+1} \in \mathbb{R}$.

REMARK 3.3. Finally, we modify the algorithm to include the case $f_b(0+) > 0$. In this case the equation (3.1) cannot be used on $(0, t_1]$ since the piecewise-linear boundary c must satisfy $c(0+) > 0$, while the condition $f_b(0+) > 0$ implies $c(0+) = 0$ (cf. Section 2.2). However, we can use (2.14) to estimate the boundary in a neighborhood of zero. The use of this expression on

the first discretization interval allows then the iteration of the previous algorithm on the successive intervals if we disregard the possible crossing happened in the neighborhood of zero.

4. PLMC method error estimation. The errors involved in the approximation of the boundary values via the PLMC method can be classified in three types according to the causes generating them. The first one is due to the piecewise linear approximation of the boundary, the second one is due to the Monte Carlo approximation of the integrals on the l.h.s. of (3.2) and the third one is due to the root method used to compute the zeros of (3.2). The last error can be disregarded since it depends on a tolerance that can be fixed in advance to make it negligible with respect to the other errors. In the following subsections we successively focus the study on the other two errors involved in the method. We explicitly underline how these two errors have different mathematical natures. Indeed, the first one, as the root error, is purely numerical, being determined by our approximation of the unknown function via a piecewise linear one. On the contrary, the second error has a statistical nature since it is related with the evaluation of an integral via a Monte Carlo method.

4.1. *Error due to the piecewise linear approximation.* The PLMC method estimates the boundary values through a piecewise linear approximation, but we limit the study of the error at the knots $t_n, n = 1, 2, \dots$. Furthermore, at this step we assume the absence of other causes of error and we define *error of the method at the n th knot* the distance between the boundary b and its approximated value c on the n th knot $|\epsilon_n^{\text{PLMC}}| = |b(t_n) - c(t_n)|, n = 1, 2, \dots$. In order to gain an estimate of such error, we first consider in Lemma 4.1 the error due to the boundary linearization on a single step. In doing this analysis we hypothesize to know the true value of the boundary on the previous intervals. A second step considered in Lemma 4.2 studies the propagation of the error, that is, we admit an error δ in the estimation of the boundary value at node $n - 1$ and we evaluate its consequences on the next node n . Finally, in Theorem 4.3 we determine the global error of the PLMC Method.

LEMMA 4.1. *Let $(W_t)_{t \geq 0}$ be a Wiener process bounded by a monotone concave (or convex) boundary $b \in \mathcal{C}^2([0, \infty))$. If we approximate in $(0, t_n]$ the boundary $b(t)$ with the boundary $\hat{c}_n(t)$, for $n = 1, 2, \dots$, defined by*

$$(4.1) \quad \hat{c}_n(t) = \begin{cases} b(t), & t \in (0, t_{n-1}], \\ b(t_{n-1}) + \hat{\beta}_n(t - t_{n-1}), & t \in [t_{n-1}, t_n], \end{cases}$$

the resulting error at the knot t_n , as $h \rightarrow 0$, is

$$|b(t_n) - \hat{c}(t_n)| \sim O(h^2).$$

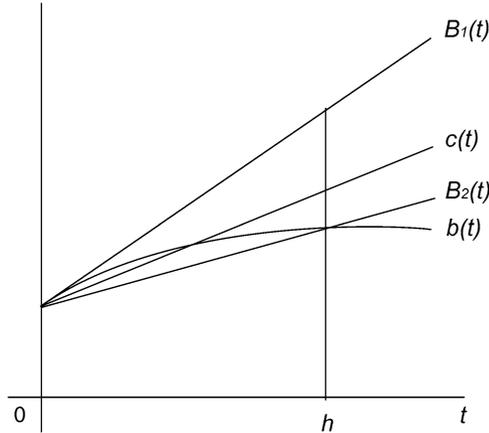


FIG. 1. Boundary $b(t)$, its tangent $B_1(t)$ in $t = 0$, the linear boundary $c(t)$ determined by the PLMC method and the secant $B_2(t)$ in $t = h$.

PROOF. We limit ourself to the case of a concave boundary since the convex case can be dealt in a similar way. Moreover, we split the proof in two parts, first taking into account the first discretization step and later a generic step.

STEP 1. Let us consider the following three straight lines (cf. Figure 1) on $(0, h]$:

1. $B_1(t)$: the tangent to $b(t)$ in $t = 0$,

$$y = \alpha_1 + b'(0)t.$$

2. $c(t)$: the linear boundary determined via the PLMC method in the first discretization interval $(0, h]$,

$$y = \alpha_1 + \beta_1 t.$$

3. $B_2(t)$: the secant through $(0, \alpha_1)$ and $(h, b(h))$,

$$y = \alpha_1 + \frac{b(h) - \alpha_1}{h}t.$$

Due to the concavity and monotonicity hypotheses on the boundary $b(t)$, it holds for all $t \in (0, h]$

$$B_2(t) \leq b(t) \leq B_1(t),$$

that implies [cf. Sacerdote and Smith (2004)]

$$\mathbb{P}(\tau_{B_1} \in (0, h]) \leq \mathbb{P}(\tau_c \in (0, h]) = \mathbb{P}(\tau_b \in (0, h]) \leq \mathbb{P}(\tau_{B_2} \in (0, h]).$$

Hence, we get

$$B_2(t) \leq c(t) \leq B_1(t),$$

that implies the ordering of the slopes

$$(4.2) \quad \frac{b(h) - \alpha_1}{h} \leq \beta_1 \leq b'(0).$$

Note that β_1 is a function of h : $\beta_1(h)$. When $h \rightarrow 0$, due to the hypothesis $\alpha_1 = b(0)$, the inequality (4.2) implies

$$(4.3) \quad \beta_1 = \beta_1(h) \xrightarrow{h \rightarrow 0} b'(0).$$

On the first knot the distance between $b(t)$ and the linear boundary of the PLMC method results in

$$\begin{aligned} |(\alpha_1 + \beta_1(h)h) - b(h)| &= \left| (b(0) + \beta_1(h)h) - \left(b(0) + b'(0)h + \frac{b''(\xi)}{2!}h^2 \right) \right| \\ &= \left| (\beta_1(h) - b'(0))h - \frac{b''(\xi)}{2!}h^2 \right| \\ &\leq |(\beta_1(h) - b'(0))h| + \left| \frac{b''(\xi)}{2!}h^2 \right| \\ &\leq |\beta_1'(h)h^2| + \left| \frac{b''(\xi)}{2!}h^2 \right| \\ &= O(h^2) + O(h^2) = O(h^2), \end{aligned}$$

where we made use of (4.3), of the mean value theorem, of the triangular inequality and of the McLaurin expansion of $b(t)$ and $\beta_1(t)$. Here $\xi \in (0, h]$ and $\eta \in (0, h]$.

STEP n . The boundary (4.1) coincides with the boundary $b(t)$ on $(0, t_{n-1})$ and it is determined solving

$$(4.4) \quad \mathbb{P}(\tau_b \in [t_{n-1}, t_n]) = \mathbb{P}(\tau_{\hat{c}} \in [t_{n-1}, t_n])$$

on $[t_{n-1}, t_n]$. Equation (4.4) implies

$$(4.5) \quad \begin{aligned} &\mathbb{P}\{\tau_b \in [t_{n-1}, t_n] | X_t < b(t), t \leq t_{n-1}\} \mathbb{P}\{X_t < b(t), t \leq t_{n-1}\} \\ &= \mathbb{P}\{\tau_{\hat{c}} \in [t_{n-1}, t_n] | X_t < \hat{c}_n(t), t \leq t_{n-1}\} \mathbb{P}\{X_t < \hat{c}_n(t), t \leq t_{n-1}\} \end{aligned}$$

and, using (4.1), one has

$$(4.6) \quad \begin{aligned} &\mathbb{P}(\tau_b \in [t_{n-1}, t_n] | X_t < b(t), t \leq t_{n-1}) \\ &= \mathbb{P}(\tau_{b(t_{n-1}) + \hat{\beta}_n(t-t_{n-1})} \in [t_{n-1}, t_n] | X_t < b(t), t \leq t_{n-1}). \end{aligned}$$

The proof of Step 1 can now be repeated to the conditional probabilities in (4.6) in order to complete the proof. \square

Let us denote $\hat{\alpha}_n$ the estimate of α_n and let $\hat{\beta}_n(\hat{\alpha}_n)$ be the corresponding estimate of the slope $\beta_n(\alpha_n)$ obtained with the PLMC method on the interval $[t_{n-1}, t_n]$.

LEMMA 4.2. An error $|\delta| = |\widehat{\alpha}_n - \alpha_n|$ propagates on the estimate $\widehat{\beta}_n(\widehat{\alpha}_n)$:

$$|\Delta\beta_n| = |\beta_n(\alpha_n) - \widehat{\beta}_n(\widehat{\alpha}_n)| \sim O(\delta).$$

PROOF. We separate the proof in two parts; the first one concerning the case of the first interval and the second one concerning the generic n th interval.

STEP 1. Let us first prove that $\beta_1 = \beta_1(\alpha_1)$ is a continuous and differentiable function. When $\alpha_1 = b(0)$ define

$$F_1(\alpha_1, \beta_1) := 1 - \int_{-\infty}^{\alpha_1 + \beta_1 t_1} (1 - e^{-2\alpha_1/t_1(\alpha_1 + \beta_1 t_1 - x)}) \frac{1}{\sqrt{2\pi t_1}} e^{-x^2/(2t_1)} dx - k_1,$$

where k_1 is the r.h.s. of (3.1). Recognizing the first two terms as the l.h.s. of (3.1), equation (3.1) becomes $F_1(\alpha_1, \beta_1) = 0$. This is an implicit equation in β_1 and α_1 that admits a continuous and differentiable solution $\beta_1 = \beta_1(t)$ if Dini's theorem holds. The hypothesis of Dini's theorem is verified since

$$\frac{\partial F_1(\alpha_1, \beta_1)}{\partial \beta_1} = - \int_{-\infty}^{\alpha_1 + \beta_1 t_1} \frac{2\alpha_1}{\sqrt{2\pi t_1}} e^{-2\alpha_1/t_1(\alpha_1 + \beta_1 t_1 - x) - x^2/(2t_1)} dx$$

is nonzero for all α_1, β_1 , having for the hypothesis $\alpha_1 \neq 0$. Hence, we get that $\beta_1 = \beta_1(\alpha_1)$ is a continuous and differentiable function and the error connected with the use of $\widehat{\alpha}_1$ in spite of α_1 is propagated on β_1 . Hence, β_1 becomes $\widehat{\beta}_1 = \beta_1 + \Delta\beta_1$ with

$$\Delta\beta_1 = \beta_1(\alpha_1 + \delta) - \beta_1(\alpha_1) \sim O(\delta)$$

since $\beta_1(\alpha_1)$ is continuous and differentiable.

STEP n . For $n = 2, 3, \dots$, we proceed in analogy with step one showing that $\beta_n = \beta_n(\alpha_n)$ is a continuous and differentiable function. Let us consider the approximated stepwise linear boundary $c(t)$ in the time interval $[0, t_n]$. Let us define

$$\begin{aligned} &F_n(\alpha_n, \beta_n) \\ &:= \int_0^{c_1} \cdots \int_0^{c_{n-1}} dx_1 \cdots dx_{n-1} \prod_{i=0}^{n-1} f_a(x_i, t_i | x_{i-1}, t_{i-1}) \\ &\quad \times \left[1 - \int_{-\infty}^{\alpha_n + \beta_n t_n} (1 - \exp\{-2(c_{n-1} - x_{n-1}) \right. \\ &\quad \quad \quad \times (\alpha_n + \beta_n t_n - x_n) \\ &\quad \quad \quad \left. / (t_n - t_{n-1})\}) \right. \\ &\quad \quad \left. \times \exp\left\{-\frac{(x_n - x_{n-1})^2}{(2(t_n - t_{n-1}))}\right\} / (\sqrt{2\pi(t_n - t_{n-1})}) dx_n \right] \\ &\quad - k_n, \end{aligned}$$

so that equation (3.2) reads $F_n(\alpha_n, \beta_n) = 0$. This is an implicit equation in β_n and α_n that admits a continuous and differentiable solution $\beta_n = \beta_n(t)$ if Dini's theorem holds.

Note that

$$\begin{aligned} & \frac{\partial F_n(\alpha_n, \beta_n)}{\partial \beta_n} \\ &= - \int_0^{c_1} \dots \int_0^{c_{n-1}} \prod_{i=0}^{n-1} f_a(x_i, t_i | x_{i-1}, t_{i-1}) \\ & \quad \times \int_{-\infty}^{\alpha_n + \beta_n t_n} 2t_n(c_{n-1} - x_{n-1}) \\ & \quad \times e^{-2(c_{n-1} - x_{n-1})(\alpha_n + \beta_n t_n - x_n)/(t_n - t_{n-1})} \\ & \quad \times e^{-(x_n - x_{n-1})^2/(2(t_n - t_{n-1}))} \\ & \quad / ((t_n - t_{n-1})\sqrt{2\pi(t_n - t_{n-1})}) dx_n \end{aligned}$$

is nonzero for all α_n, β_n , since $x_{n-1} < c_{n-1}$. Hence, Dini's theorem holds and we get that $\beta_n = \beta_n(\alpha_n)$ is a continuous and differentiable function. If $\widehat{\alpha}_n = \alpha_n + \delta$, the error on α_n is propagated on β_n as

$$\widehat{\beta}_n = \beta_n + \Delta\beta_n,$$

where

$$\Delta\beta_n = \beta_n(\alpha_n + \delta) - \beta_n(\alpha_n) \sim O(\delta). \quad \square$$

THEOREM 4.3. *The error of the PLMC method at the discretization knots t_n , $n = 1, 2, \dots$, is*

$$|\epsilon_n^{\text{PLMC}}| = |b(t_n) - c(t_n)| \sim O(\max(\delta, h^2))$$

when α_1 is affected by an error of the order of $\delta \geq 0$.

PROOF. When α_1 is affected by an error of the order of δ , by Lemmas 4.1 and 4.2, we get that

$$\begin{aligned} |b(t_1) - c(t_1)| &\leq |b(t_1) - \widehat{c}_1(t_1)| + |\widehat{c}_1(t_1) - c(t_1)| \\ &\sim O(h^2) + O(\delta) \\ &\sim O(\max(\delta, h^2)). \end{aligned}$$

By induction, let $|b(t_{n-1}) - c(t_{n-1})| \sim O(\max(\delta, h^2))$, then

$$\begin{aligned} |\widehat{c}_n(t_n) - c(t_n)| &= |b(t_{n-1}) + \widehat{\beta}_n(t_n - t_{n-1}) - c_{n-1} - \beta_n(t_n - t_{n-1})| \\ &= |b(t_{n-1}) - c_{n-1} + (\widehat{\beta}_n - \beta_n)h| \end{aligned}$$

$$\begin{aligned} &\leq |b(t_{n-1}) - c_{n-1}| + |(\widehat{\beta}_n - \beta_n)h| \\ &\sim O(\max(\delta, h^2)) + O(\max(\delta h, h^3)) \\ &\sim O(\max(\delta, h^2)) \end{aligned}$$

and we obtain

$$\begin{aligned} |b(t_n) - c(t_n)| &\leq |b(t_n) - \widehat{c}_n(t_n)| + |\widehat{c}_n(t_n) - c(t_n)| \\ &\sim O(h^2) + O(\max(\delta, h^2)) \\ &\sim O(\max(\delta, h^2)). \end{aligned} \quad \square$$

REMARK 4.1. If the boundary $b(t)$ is not monotone nor convex (or concave) but is sufficiently well behaved, one can proceed with a similar reasoning on each monotonicity and convexity interval. Hence, choosing h in a suitable way, the step-wise boundary has still an error $|\epsilon_n^{\text{PLMC}}| \sim O(\max(\delta, h^2))$.

4.2. *Error due to the Monte Carlo approximation.* Disregarding the error related to the numerical integration of the l.h.s. of (3.1) at the first step of the algorithm that can be well controlled with a careful use of numerical approximations, we focus on the next steps when the multiple integrals of the l.h.s. of (3.2),

$$\begin{aligned} F(\beta_{n+1}) = &\int_{t_n}^{t_{n+1}} \int_{-\infty}^{c_n} \cdots \int_{-\infty}^{c_1} \left(f_c(t|t_n, x_n) \right. \\ &\left. \times \prod_{i=1}^n p_{a,c}(t_i, x_i | t_{i-1}, x_{i-1}) \right) dx_1 \cdots dx_n dt, \end{aligned}$$

are evaluated via Monte Carlo method. Using the Law of Large Numbers, we approximate the expectation on the l.h.s. of (3.5) with its sample mean. Hence, for a fixed confidence level α , we get

$$\begin{aligned} P \left(\left| \frac{1}{M} \sum_{j=1}^M H(\beta_{n+1}; X_{n,j}) \right. \right. \\ \left. \left. \times \prod_{i=1}^n I(X_{i,j} \leq c_i) e^{-2(c_i - X_{i,j})(c_{i-1} - X_{i-1,j}) / (t_i - t_{i-1})} \right. \right. \\ \left. \left. - F(\beta_{n+1}) \right| < \delta_\alpha \right) > \alpha, \end{aligned}$$

where $X_{n,j} \sim N(0, t_i - t_{i-1}), i = 1, \dots, n, j = 1, \dots, M$, are independent random variables. Letting $x_{n,j}, i = 1, \dots, n, j = 1, \dots, M$, be a sample of $X_{n,j}$, with an

accuracy δ_α in the computation of the integral, we obtain a confidence interval for β_{n+1} at the same level α :

$$\left[F^{-1} \left(\frac{1}{M} \sum_{j=1}^M H(\beta_{n+1}; x_{n,j}) \right) \times \prod_{i=1}^n I(x_{i,j} \leq c_i) e^{-2(c_i - x_{i,j})(c_{i-1} - x_{i-1,j}) / (t_i - t_{i-1})} \pm \delta_\alpha \right].$$

REMARK 4.2. The computations necessary to get the Monte Carlo evaluations are not excessively expensive. Hence, we can choose a very large value for the size M for the number of simulations involved in the integral estimation. This allows to make this error negligible with respect to the error determined by the piecewise linear approximation of the boundary, but as a consequence of the use of the Monte Carlo method, our results are characterized by a reliability α .

5. An approximation by the nonlinear Volterra integral equation. The algorithm discussed in the previous section is reliable and easily implemented, but it is computationally expensive since the Monte Carlo method requires long times of computation. In this section we therefore consider an alternative approach of pure numerical nature which is computationally more attractive. Since this method is based on the approximation of a non linear Volterra integral equation, it will be referred to as VIE (Volterra Integral Equation) method.

Let us consider the integral equation [cf. Peskir (2002)]:

$$(5.1) \quad \Psi \left(\frac{b(t)}{\sqrt{t}} \right) = \int_0^t \Psi \left(\frac{b(t) - b(s)}{\sqrt{t-s}} \right) f_b(s) ds \quad (t > 0),$$

where $\Psi(x) = 1 - \Phi(x)$ and $\Phi(x) = \int_{-\infty}^x \varphi(z) dz$ is the standard normal distribution. Equation (5.1) is a Volterra integral equation of the first kind in f_b , but it is a *nonlinear* Volterra integral equation of the second kind in b and its kernel is non-singular in the sense that it is bounded. Moreover the nonlinear functions involved in the equation are bounded and Ψ is invertible. These features allow the development of the following numerical algorithm that approximate (5.1) in a simple and reliable way.

We numerically solve this equation to evaluate the approximate value b^* of b at the knots $t_i = ih$ for $i = 1, \dots, n$, where $h = t/n$ (and $t > 0$ is given and fixed). To this aim we follow the original idea of Volterra [see, e.g., Linz (1985), Chapter VII], that is, we approximate the integral on the l.h.s. of (5.1) with the Euler method

$$(5.2) \quad \Psi \left(\frac{b^*(t_i)}{\sqrt{t_i}} \right) = \sum_{j=1}^i \Psi \left(\frac{b^*(t_i) - b^*(t_j)}{\sqrt{t_i - t_j}} \right) f_b(t_j)h \quad (i = 1, \dots, n),$$

getting a nonlinear system of n equations in n unknowns $b^*(t_1), \dots, b^*(t_n)$. The i th equation of (5.2) for $i \geq 2$ makes use of the values $b^*(t_1), \dots, b^*(t_{i-1})$ found in the preceding steps. Hence, equations (5.2) can be solved iteratively using the iterative middle point method [cf. Atkinson (1989)], which then gives approximate values for the unknown boundary b at the points t_1, \dots, t_n .

We recall that the local consistency error for (5.1) for a generic discretization method of the integral is [cf. Linz (1985)]

$$\begin{aligned}
 \delta(h, t_i) = & \int_0^{t_i} \Psi\left(\frac{b(t_i) - b(t_s)}{\sqrt{t_i - s}}\right) f_b(s) ds \\
 (5.3) \quad & - h \sum_{j=0}^i \omega_{ij} \Psi\left(\frac{b(t_i) - b(t_j)}{\sqrt{t_i - t_j}}\right) f_b(t_j),
 \end{aligned}$$

where ω_{ij} are the integration weights of the adopted discretization schema. In (5.2) we use the Euler method for which we have $\omega_{ij} = 1$ and $\omega_{i0} = 0$, for each $j = 1, \dots, i, i = 1, \dots, n$. Since $\max_{0 < i < n} \delta(h, t_i) = O(h)$, the method is consistent of order 1.

REMARK 5.1. Note that the system (5.2) is triangular and this makes it especially efficient if one wishes to compute b^* at the next knot, when it is known in the previous ones. Moreover, unlike the PLMC method, here the knowledge of $b(0)$ is not required since we use the “forward” Euler method, also known as right-hand rectangular rule [cf. Atkinson (1989)].

REMARK 5.2. In spite of the Euler method, we could use the extended trapezoidal formula [cf. Abramowitz and Stegun (1964), page 885, formula 25.4.2] with weights $\omega_{i0} = \omega_{ii} = 1/2$ for each $i = 1, \dots, n$ and $\omega_{ij} = 1$ for each $j = 1, \dots, i - 1, i = 1, \dots, n$, to approximate the integral in (5.1). In this case (5.2) is replaced by

$$\begin{aligned}
 \Psi\left(\frac{b^*(t_i)}{\sqrt{t_i}}\right) = & \frac{1}{2} \Psi\left(\frac{b^*(t_i) - b^*(0)}{\sqrt{t_i}}\right) f_b(0)h \\
 (5.4) \quad & + \sum_{j=1}^{i-1} \Psi\left(\frac{b^*(t_i) - b^*(t_j)}{\sqrt{t_i - t_j}}\right) f_b(t_j)h \\
 & + \frac{1}{4} f_b(t_i)h \quad (i = 1, \dots, n).
 \end{aligned}$$

This approximation is consistent of order 2, but in the general case requests the knowledge of $b(0)$. However, when $f_b(0) = 0$ the first term in the r.h.s. of (5.4) vanishes and we obtain again a triangular system independent from the knowledge of $b(0)$.

REMARK 5.3. The unnecessary of the knowledge of $b(0)$ is a numerical advantage, but it hides some problems connected with the initial point t_1 . To illustrate this, note that the algorithm uses the approximation (5.2) that for $i = 1$ reads

$$(5.5) \quad \Psi\left(\frac{b(t_1)}{\sqrt{t_1}}\right) = \frac{1}{2}f_b(t_1)t_1,$$

using that $\Psi(0) = 1/2$ (when b is smooth). Recall that $t_1 = t/n$ so that $t_1 \rightarrow 0$ as $n \rightarrow \infty$. Taking then $b(t) = \sqrt{2t \log(1/t)}$, for example, it is easily verified that $\lim_{n \rightarrow \infty} 2\Psi(b(t_1)/\sqrt{t_1})/t_1 = 0$, while the result of Peskir (2002) implies that $f_b(0+) = +\infty$. Thus, the approximation (5.5) in this case fails in a neighborhood of zero. A closer look shows that it is valid if $f_b(0+) = 0$ (under certain mild regularity conditions). It follows that the more $f_b(0+)$ is away from zero, the less accurate (5.5) becomes in a neighborhood of zero.

REMARK 5.4. To improve the boundary estimation for small times, we can consider the flux equation introduced in Ricciardi, Sacerdote and Sato (1984) and its approximation as $t \rightarrow 0$ to get

$$(5.6) \quad f_b(t) \approx \frac{b(t)}{\sqrt{2\pi t^3}} \exp\left[-\frac{b(t)^2}{2t}\right], \quad t < \epsilon,$$

where ϵ is small enough to make it acceptable to approximate the r.h.s. of the flux equation with its first term. It is an implicit nonlinear equation in terms of $b(t)$ that can be numerically solved. Since this equation loses reliability as the time t increases, it is necessary to control the validity of this equation for the value of t of interest. Substituting the solution $\hat{b}(t)$ of (5.6) in the complete equation (2.8) in Ricciardi, Sacerdote and Sato (1984), we obtain an estimator $\hat{f}_b(t)$ of the FPT density function. The evaluation of the relative error between this estimator and the known value of the density function allows to guess the time interval where this approximation is reliable.

6. VIE method error estimation. Nonlinear integral equations are considered in Linz (1985), but the integral equation (5.1) differs from nonlinear integral equations studied there due to the expression on the l.h.s. Indeed, it contains the unknown function in an implicit way through a further nonlinear function. However, working in analogy with the methods used in Linz (1985), we can prove the convergence of the VIE method of Section 5. To this end, we recall a convergence theorem used by Linz (1985).

THEOREM 6.1. *Let the sequence ξ_0, ξ_1, \dots satisfy*

$$(6.1) \quad |\xi_n| \leq A \sum_{i=0}^{n-1} |\xi_i| + B_n, \quad n = r, r + 1, \dots,$$

where $A > 0, |B_n| \leq B$ and assume that it exists a constant $\eta > 0$ such that

$$(6.2) \quad \sum_{i=0}^{r-1} |\xi_i| \leq \eta.$$

Then

$$(6.3) \quad |\xi_n| \leq (1 + A)^{n-r} (B + A\eta), \quad n = r, r + 1, \dots$$

We now can prove the convergence of the proposed method.

THEOREM 6.2. *The error ϵ_n^{VIE} of the VIE method at the discretization knots $t_n, n = 1, 2, \dots, is$*

$$(6.4) \quad |\epsilon_n^{\text{VIE}}| = |b(t_n) - b^*(t_n)| \sim O(h)$$

if the integral in (5.1) is approximated via the Euler formula.

If $f_b(0) = 0$ and the extended trapezoidal formula is used for the integral in (5.1), the error becomes

$$(6.5) \quad |\epsilon_n^{\text{VIE}}| = |b(t_n) - b^*(t_n)| \sim O(h^2).$$

PROOF. We split the proof of (6.4) in two parts, the first one concerning the first discretization interval and the second one concerning a generic step n .

STEP 1. Choosing $t = t_1$ and subtracting (5.2) from (5.1), we get

$$(6.6) \quad \Psi\left(\frac{b(t_1)}{\sqrt{t_1}}\right) = \Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right) + \delta(h, t_1).$$

Using the inverse function Ψ^{-1} , we obtain

$$(6.7) \quad \frac{b(t_1)}{\sqrt{t_1}} = \Psi^{-1}\left[\Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right) + \delta(h, t_1)\right].$$

Substituting the Taylor expansion of Ψ^{-1} around $y = \Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right)$ in this last equation, we get

$$(6.8) \quad \begin{aligned} \frac{b(t_1)}{\sqrt{t_1}} &= \frac{b^*(t_1)}{\sqrt{t_1}} + \delta(h, t_1) \frac{d\Psi^{-1}(y)}{dy} \Big|_{y=\Psi(b^*(t_1)/\sqrt{t_1})+\theta\delta(h,t_1)} \\ &= \frac{b^*(t_1)}{\sqrt{t_1}} + \sqrt{2\pi} \delta(h, t_1) e^{\hat{z}^2/2}, \end{aligned}$$

where $\theta \in (0, 1)$ [cf. Abramowitz and Stegun (1964)] and

$$(6.9) \quad \hat{z} = \Psi^{-1}\left[\Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right) + \theta\delta(h, t_1)\right] < L$$

with $L < \infty$.

To prove (6.9), note that if $\delta(h, t_1) \geq 0$, one has

$$(6.10) \quad \Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right) + \theta\delta(h, t_1) \geq \Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right)$$

and, due to the decreasing monotonicity of Ψ^{-1} , one gets

$$(6.11) \quad \hat{z} \leq \frac{b^*(t_1)}{\sqrt{t_1}} < L_1.$$

Elsewhere, when $\delta(h, t_1) \leq 0$ one has

$$(6.12) \quad \Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right) + \theta\delta(h, t_1) \geq \Psi\left(\frac{b^*(t_1)}{\sqrt{t_1}}\right) + \delta(h, t_1) = \Psi\left(\frac{b(t_1)}{\sqrt{t_1}}\right),$$

hence,

$$(6.13) \quad \hat{z} \leq \frac{b(t_1)}{\sqrt{t_1}} < L_2.$$

Choosing $L = \max(L_1, L_2)$, we get (6.9). Hence from (6.8) and (6.9) we get

$$|\epsilon_1^{\text{VIE}}| = |b(t_1) - b^*(t_1)| \leq |\sqrt{2\pi t_1}\delta(h, t_1)e^{L^2/2}| < k|\delta(h, t_1)| = O(h),$$

since the Euler method is consistent of order 1.

STEP n . Choosing $t = t_n$ and subtracting (5.2) from (5.1), we get

$$(6.14) \quad \Psi\left(\frac{b(t_n)}{\sqrt{t_n}}\right) = \Psi\left(\frac{b^*(t_n)}{\sqrt{t_n}}\right) + \gamma_n, \quad n = 2, 3, \dots,$$

where

$$(6.15) \quad \begin{aligned} \gamma_n &= \gamma_n(h, t_1, \dots, t_n) \\ &= h \sum_{j=1}^n f_b(t_j) \left\{ \Psi\left(\frac{b(t_n) - b(t_j)}{\sqrt{t_n - t_j}}\right) - \Psi\left(\frac{b^*(t_n) - b^*(t_j)}{\sqrt{t_n - t_j}}\right) \right\} \\ &\quad + \delta(h, t_n), \quad n = 2, 3, \dots \end{aligned}$$

Mimicking the procedure used for case $n = 1$, we apply the inverse function Ψ^{-1} to (6.14) and we expand in Taylor series the resulting r.h.s. around $y = \Psi\left(\frac{b^*(t_n)}{\sqrt{t_n}}\right)$. Thus, we get

$$(6.16) \quad \begin{aligned} \frac{b(t_n)}{\sqrt{t_n}} &= \frac{b^*(t_n)}{\sqrt{t_n}} + \gamma_n \frac{d\Psi^{-1}(y)}{dy} \Big|_{y=\Psi(b^*(t_n)/\sqrt{t_n})+\theta\gamma_n} \\ &= \frac{b^*(t_n)}{\sqrt{t_n}} + \sqrt{2\pi}\gamma_n e^{\hat{\delta}_n^2/2}, \end{aligned}$$

where $\theta \in (0, 1)$ [cf. Abramowitz and Stegun (1964)] and

$$(6.17) \quad \hat{v}_n = \Psi^{-1} \left[\Psi \left(\frac{b^*(t_n)}{\sqrt{t_n}} \right) + \theta \gamma_n \right] < M_n$$

with $M_n < \infty$ for each $n = 1, 2, \dots$.

The last inequality can be proved analogously to (6.11) and (6.13) in Step 1. Hence, from (6.16) we get

$$(6.18) \quad |\epsilon_n^{\text{VIE}}| = |b(t_n) - b^*(t_n)| \leq |\sqrt{2\pi t_n} \gamma_n e^{M_n^2/2}| < k |\gamma_n|.$$

Let us now split the term γ_n as the sum of a contribution of the accumulated error due to the previous steps and a contribution due to the consistency of the numerical approximation of the integral in (5.1). To this goal, we bound the module of γ_n using the triangular inequality to get

$$(6.19) \quad \begin{aligned} |\gamma_n| &\leq h \sum_{j=1}^n f_b(t_j) \left| \Psi \left(\frac{b(t_n) - b(t_j)}{\sqrt{t_n - t_j}} \right) - \Psi \left(\frac{b^*(t_n) - b^*(t_j)}{\sqrt{t_n - t_j}} \right) \right| \\ &\quad + |\delta(h, t_n)| \\ &= h \sum_{j=1}^{n-1} f_b(t_j) \left| \frac{1}{\sqrt{2\pi(t_n - t_j)}} \int_{b^*(t_n) - b^*(t_j)}^{b(t_n) - b(t_j)} e^{-u^2/(2(t_n - t_j))} du \right| \\ &\quad + |\delta(h, t_n)|, \end{aligned}$$

where the last equality uses the definition of Ψ and the fact that the last term in the sum is zero. Bounding the integrand in (6.19) with 1, we get

$$(6.20) \quad |\gamma_n| < h \sum_{j=1}^{n-1} \frac{f_b(t_j)}{\sqrt{2\pi(t_n - t_j)}} (|\epsilon_n^{\text{VIE}}| - |\epsilon_j^{\text{VIE}}|) + |\delta(h, t_n)|$$

and (6.18) becomes

$$(6.21) \quad \begin{aligned} |\epsilon_n^{\text{VIE}}| &\leq \sqrt{2\pi t_n} M h \sum_{j=1}^{n-1} \frac{f_b(t_j)}{\sqrt{2\pi(t_n - t_j)}} |\epsilon_n^{\text{VIE}}| \\ &\quad + \sqrt{2\pi t_n} M h \sum_{j=1}^{n-1} \frac{f_b(t_j)}{\sqrt{2\pi(t_n - t_j)}} |\epsilon_j^{\text{VIE}}| + \sqrt{2\pi t_n} M |\delta(h, t_n)|, \end{aligned}$$

where $M = \max_n \{\exp(M_n)\}$ and, hence,

$$(6.22) \quad \begin{aligned} |\epsilon_n^{\text{VIE}}| &\left(1 - M h \sum_{j=1}^{n-1} \frac{f_b(t_j)}{\sqrt{t_n - t_j}} \right) \\ &\leq M h \sum_{j=1}^{n-1} \frac{f_b(t_j)}{\sqrt{t_n - t_j}} |\epsilon_j^{\text{VIE}}| + \sqrt{2\pi} M |\delta(h, t_n)|. \end{aligned}$$

If

$$(6.23) \quad h < \frac{1}{M \sum_{j=1}^{n-1} f_b(t_j) / \sqrt{t_n - t_j}} = \frac{1}{k},$$

we get

$$(6.24) \quad |\epsilon_n^{\text{VIE}}| \leq \frac{MhF}{1 - hk} \sum_{j=1}^{n-1} |\epsilon_j^{\text{VIE}}| + \frac{\sqrt{2\pi}M}{1 - hk} |\delta(h, t_n)|,$$

where $F = \sup_{j,n} \frac{f_b(t_j)}{\sqrt{2\pi(t_n - t_j)}}$.

Applying the convergence Theorem 6.1 with

$$(6.25) \quad A_n = \frac{MhF}{1 - hk} < A,$$

$$(6.26) \quad B_n = \frac{2\pi M}{1 - hk} |\delta(h, t_n)| < B$$

and noting that by inductive argument one has

$$(6.27) \quad \sum_{j=1}^{n-1} |\epsilon_j^{\text{VIE}}| \leq \eta,$$

we finally obtain

$$(6.28) \quad |\epsilon_n^{\text{VIE}}| \leq \left(\max |\delta(h, t_n)| 2\pi M + MhF \sum_{j=1}^{n-1} |\epsilon_j^{\text{VIE}}| \right) \frac{1}{1 - hk} e^{t_n MF / (1 - hk)}.$$

Recalling that the method is consistent of order 1, part 1 of the theorem is proved. Using equation (6.21) in the case of the extended trapezoidal scheme, one easily proves formula (6.5). \square

REMARK 6.1. Note that the error of the method is dominated by the consistency error.

REMARK 6.2. To prove Theorem 6.2, we simply use the monotonicity properties of the function Ψ . Hence, the method can be easily extended to different diffusion processes, simply substituting Ψ in (5.1) with the survival function of the considered process.

7. Examples. In this section we check the stability of the algorithms presented in Sections 3 and 5 by means of some examples where a closed form solution is available. We also show other examples where the solution is numerically evaluated. First we apply the algorithms of Sections 3 and 5 for a Daniels boundary b for two sets of parameters (Section 2). Later we apply them to the case of an

oscillating boundary with different parameters. In these later cases the FPT density function has been numerically estimated via the Buonocore, Nobile and Ricciardi algorithm (1987). We consider the mean square deviation as an index of the goodness of the two methods

$$(7.1) \quad \sigma_n^{(i)} = \frac{1}{n} \sum_{j=0}^n (b(t_j) - \hat{b}^{(i)}(t_j))^2, \quad i = 1, 2,$$

where $\hat{b}^{(1)}$ denotes the approximating boundary determined by the PLMC algorithm of Section 3 and $\hat{b}^{(2)}$ denotes the approximating boundary determined by the VIE algorithm of Section 5.

We apply the two algorithms to the following two cases:

1. Daniels boundary with parameters $\alpha = 1, \beta = 0.5, \gamma = 0.5$ and $\alpha = 1, \beta = 1, \gamma = 0.5$. We first apply the PLMC algorithm in the interval $[0, 2]$ with a discretization step $h = 0.2$ and we compute the integrals by a Monte Carlo method using 10^4 simulations. Under these conditions we estimate the mean square deviation, obtaining $\sigma_n^{(1)} = 9.4 \cdot 10^{-5}$ and $\sigma_n^{(1)} = 3.4 \cdot 10^{-5}$ respectively.

We also apply to these examples the VIE algorithm of Section 5 with discretization step $h = 0.01$ and the resulting mean square deviations are $\sigma_n^{(2)} = 4.3 \cdot 10^{-5}$ and $\sigma_n^{(2)} = 4.6 \cdot 10^{-5}$ respectively.

2. Oscillating boundary

$$(7.2) \quad b(t) = \alpha + \beta \cos(\gamma t)$$

with parameters $\alpha = 1, \beta = 0.5, \gamma = 2$ and $\alpha = 1, \beta = 1, \gamma = 2$ respectively. Repeating the PLMC algorithm under exactly the same conditions as above, we get the following mean square deviations: $\sigma_n^{(1)} = 6.6 \cdot 10^{-4}$ and $\sigma_n^{(1)} = 6.4 \cdot 10^{-3}$ respectively. The application of the VIE algorithm to the two sets of parameters gives $\sigma_n^{(2)} = 4.9 \cdot 10^{-3}$ and $\sigma_n^{(2)} = 3.4 \cdot 10^{-3}$.

These results confirm the reliability of the methods. The four cases are illustrated in Figures 2, 3, 5 and 6 where the exact boundary shape (left) is compared with the approximating ones obtained by means of the algorithms of Section 3 (center) and Section 5 (right).

REMARK 7.1. With reference to the PLMC method, we underline that the goodness of the approximation does not depend only on the discretization step h , but also on the probability mass for the boundary to be crossed in the discretization subinterval of length h . It is thus recommendable to avoid excessively small discretization steps. However, as shown in our examples, quite large values of h give small value for the mean square deviation.

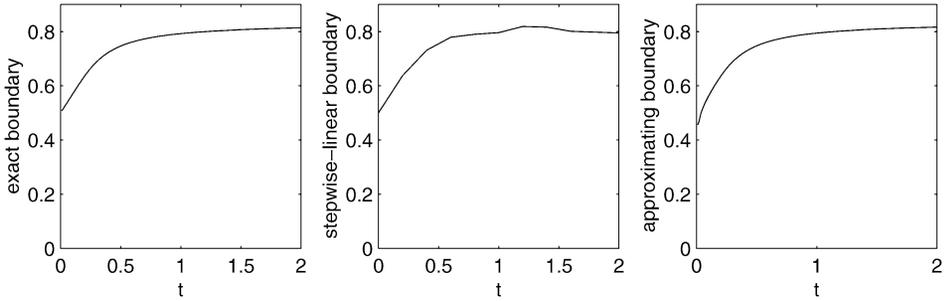


FIG. 2. Daniels boundary with parameters $\alpha = 1, \beta = 0.5, \gamma = 0.5$ (left) compared with the approximating ones obtained by means of the PLMC method (center) and the VIE method (right).

REMARK 7.2. A comparison between the exact and the approximating boundary obtained from the PLMC algorithm in Figures 2 and 3 with the first-passage density function in Figure 4 shows the rise of larger oscillations as t increases. This fact can be explained by observing that as t increases the probability of crossing the boundary on each discretized interval becomes smaller and the Monte Carlo method is subject to a larger relative error. A further improvement of the method could be to use an adaptive step built on a constant probability mass of the first-passage density function on each interval.

REMARK 7.3. In Figures 2 and 3 we observe that the approximating boundary obtained from the VIE algorithm of Section 5 has a large error for short times. This result can be explained by the rough approximation in the first steps of the present method and is related to the use of the Euler method. In Remark 5.4 we introduced an improvement of the method for small times. In Figure 7 we compare the approximation obtained via the VIE method (dash dot line) and two different corrections via (5.6) in a special case of Daniels boundary (full line). The stars indicate the values of the boundary solution of (5.6), while the two other curves

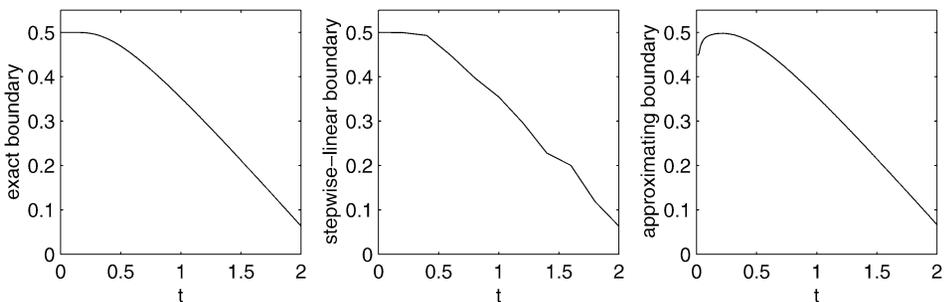


FIG. 3. Daniels boundary with parameters $\alpha = 1, \beta = 1, \gamma = 0.5$ (left) compared with the approximating ones obtained by means of the PLMC method (center) and the VIE method (right).

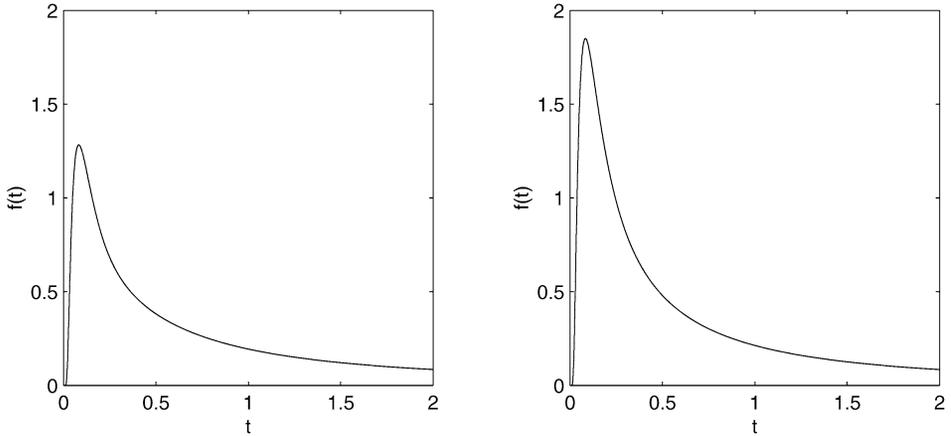


FIG. 4. The first-passage density function through a Daniels boundary with parameters $\alpha = 1, \beta = 0.5, \gamma = 0.5$ (left) and with parameters $\alpha = 1, \beta = 1, \gamma = 0.5$ (right).

substitute the first one or two values of $b(t)$ with the solution of (5.6). We observe that the new boundary estimates are more reliable.

REMARK 7.4. The evaluation of the difference between the exact boundary and the approximating one, obtained with the PLMC method, shows that the approximating boundary oscillates around the real one.

8. The exponential case. Let us apply our algorithms to numerically solve the original Shiryaev’s problem, that is, to approximate the boundary corresponding to an exponential first-passage density function.

Let us thus consider a first-passage density function $f_b(t) = e^{-t}$ for $t > 0$ corresponding to the exponential distribution with parameter $\lambda = 1$. In order to apply the PLMC method, we note that this particular choice of distribution requires to

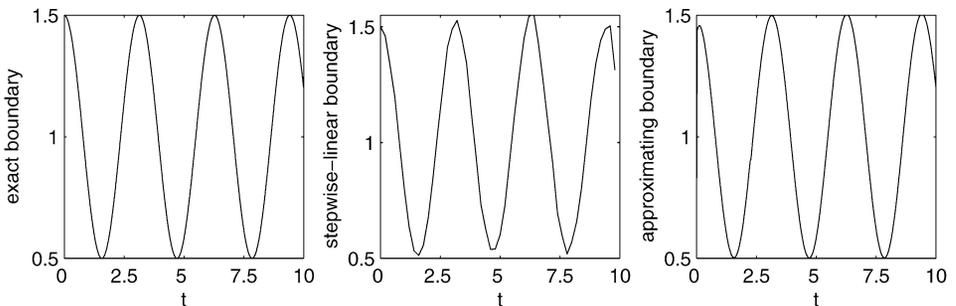


FIG. 5. Oscillating boundary with parameters $\alpha = 1, \beta = 0.5, \gamma = 2$ (left) compared with the approximating ones obtained by means of the PLMC method (center) and the VIE method (right).

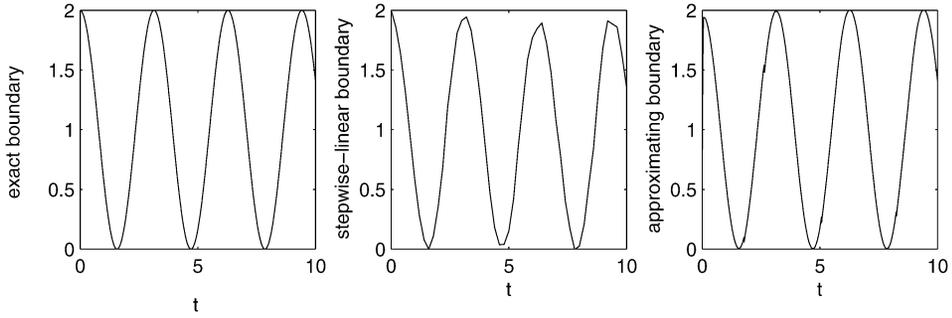


FIG. 6. Oscillating boundary with parameters $\alpha = 1, \beta = 1, \gamma = 2$ (left) compared with the approximating ones obtained by means of the PLMC method (center) and the VIE method (right).

study a first-passage time τ_b such that $f_b(0+) > 0$. As indicated in Section 2.2, this implies that the boundary b should be an upper function for W that vanishes at zero so that $b'(0+) = +\infty$.

Making use of (2.14) and introducing more generally the following notation:

$$(8.1) \quad \kappa = f_b(0+) > 0,$$

we obtain an approximation of the boundary b in the neighborhood of zero by choosing

$$(8.2) \quad c = -2 \log(\sqrt{4\pi\kappa}).$$

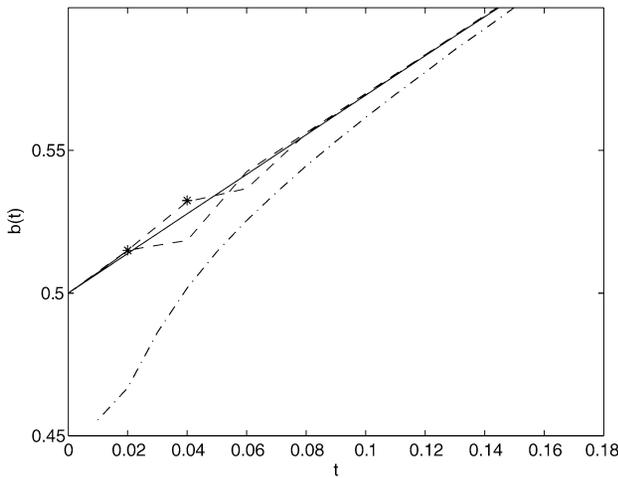


FIG. 7. Daniels boundary with parameters $\alpha = 1, \beta = 0.5, \gamma = 0.5$ (full line) compared with the approximating ones obtained by means of the VIE method (dash dot line) and by means of the VIE method modified for small times (dashed lines) substituting the first one or two values of $b(t)$ with the solution of (5.6). The stars indicate the values of the boundary obtained as a solution of (5.6).

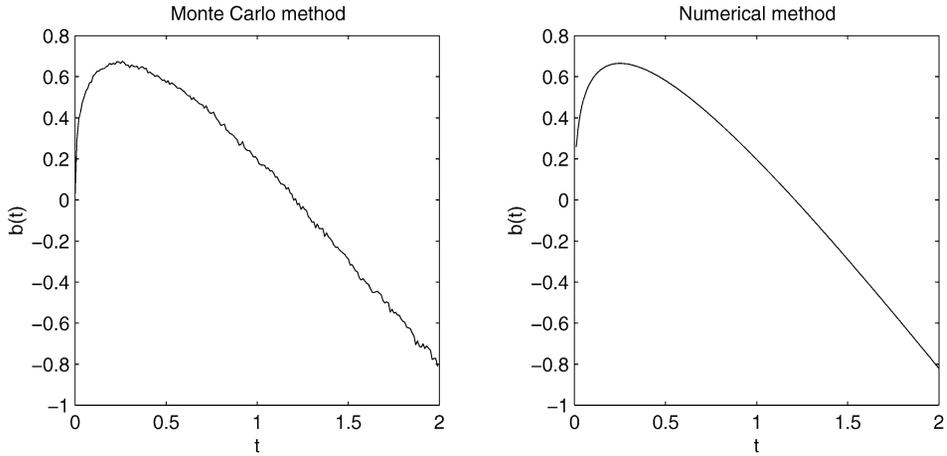


FIG. 8. Numerical evaluations of the approximating boundaries for an exponential first-passage density function with parameter $\lambda = 1$ obtained by means of the PLMC method (left) and the VIE method (right) with a discretization step $h = 0.01$.

On the first interval we approximate the boundary b by (2.13), where c is given by (8.2). On the successive intervals we simply apply the algorithm with

$$(8.3) \quad c_2 = g(t_1) = \sqrt{2t_1 \log(1/t_1) + t_1 \log \log(1/t_1) + ct_1}.$$

In Figure 8 we plot the boundaries corresponding to an exponential first-passage density function with $\lambda = 1$ obtained by the two different algorithms described in the previous sections; the plot on the r.h.s. is obtained applying the PLMC method with the step $h = 0.01$ and with a number of simulations for the Monte Carlo method equal to 10^4 , while the plot on the l.h.s. is obtained applying the VIE method with discretization step $h = 0.01$.

A heuristic confirmation of the stability of the algorithms is given by the nearness of the two curves. Furthermore, an intuitive reasoning about the shape of the boundary confirms our result. To obtain an exponential first-passage density function, a large part of the sample paths should cross the boundary very soon but, as the time goes on, other sample paths, that have not yet reached the boundary, should be able to cross it too. This makes intuitive the fact that the boundary must decrease in order to be reachable by the sample paths whose initial trend was negative.

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