

AN INTEGRAL EQUATION FOR ROOT'S BARRIER AND THE GENERATION OF BROWNIAN INCREMENTS

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We derive a nonlinear integral equation to calculate Root's solution of the Skorokhod embedding problem for atom-free target measures. We then use this to efficiently generate bounded time–space increments of Brownian motion and give a parabolic version of Muller's classic “Random walk over spheres” algorithm.

1. Introduction. Let μ be a zero-mean probability measure on the real line and $B = (B_t)_{t \geq 0}$ denote a one-dimensional Brownian motion. The Skorokhod embedding problem given by μ consists of constructing a stopping time τ such that $(\text{SEP}_\mu) \quad B_\tau \sim \mu$ and $B^\tau = (B_{t \wedge \tau})_{t \geq 0}$ is uniformly integrable.

More than 50 years after Skorokhod [33], we can now choose from a wide range of different stopping times which solve this problem [14, 29]. In general such a stopping time may depend in a very complex way on the Brownian trajectory. This can make it computationally expensive (or even intractable) in applications to determine the actual realisation of the stopping time τ for a given Brownian trajectory. From this point of view, one of the earliest solutions of (SEP_μ) , the so-called *Root solution*, is one that stands out: in 1969 Root [31] showed that if μ has zero-mean and a second moment, then there exists a closed subset of time–space, the so-called *Root barrier*,

$$R \subset [0, \infty] \times [-\infty, \infty],$$

such that the hitting time

$$\tau = \inf\{t > 0 : (t, B_t) \in R\} \quad (\inf \emptyset = \infty)$$

solves (SEP_μ) given by μ . The Root barrier R can be described by a lower semi-continuous barrier function r ,

$$R = \{(t, x) : t \geq r(x)\},$$

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and, among all solutions $\tilde{\tau}$ of (SEP $_{\mu}$), it has the key property of minimising $\mathbb{E}[\tilde{\tau}^2]$; see Rost [32] and Loynes [21]. Unfortunately, Root’s existence proof is not constructive, and until recently it was not known how to characterise or compute R (or, equivalently, r) in terms of the measure μ . A seminal paper by Hobson [15] on applications to model independent hedging of exotic options led to a revived interest in (SEP $_{\mu}$) (the Root solution gives a lower bound on options on variance), and motivated by such applications, the Root barrier was more recently identified as the free boundary of a parabolic obstacle problem (work of Dupire, Cox and Wang, Oberhauser and Reis, [7, 8, 10, 28]). This allows one to compute R in two steps: firstly, solve numerically the nonlinear PDE (using finite difference or BSDE methods), and secondly, numerically calculate the associated free boundary of this PDE.

The first and main contribution of this paper consists of characterising the barrier function r directly via a nonlinear integral equation. More precisely, if μ is atom-free, then r solves the following equation:

$$(1.1) \quad u_{\delta_0}(x) - u_{\mu}(x) = g(r(x), x) - \int_{\{y: r(y) < r(x)\}} g(r(x) - r(y), x - y)\mu(dy) \quad \forall x \in (-\infty, \infty).$$

Here $g(t, x) = \sqrt{\frac{2t}{\pi}} e^{-x^2/(2t)} - |x| \operatorname{Erfc}(\frac{|x|}{\sqrt{2t}}) = \mathbb{E}L_t^x$ where $(L_t^x)_{t,x}$ is the Brownian local time, and u_{μ} and u_{δ_0} are the potential functions⁴ of the measures μ and the Dirac delta δ_0 , respectively. The derivation of this integral equation is short, intuitive, and entirely probabilistic as it relies solely on the Itô–Tanaka formula and the fact that the local time is an additive functional of the path of Brownian motion.

It is well known (see, e.g., [30]) that the question of uniqueness of solutions of such nonlinear integral equations is delicate in general. In this case we give a short proof of the uniqueness of the solution of (1.1) that applies to the class of measures with a continuous barrier function via the uniqueness of the viscosity solution of a nonlinear PDE characterising the Root solution of (SEP $_{\mu}$) given in [28].

In the rest of the article we then specialise to the case of barriers that have a barrier function that is symmetric around 0, continuous, and monotone. In this case it becomes numerically much easier to solve (1.1) since r does not appear anymore in the domain of the integral, and (1.1) becomes a Volterra type integral equation of the first kind. Furthermore, we again use the viscosity approach of [28] to establish sufficient and easy to verify conditions on the probability measure μ which guarantee that its barrier has these properties. These results give a theoretical justification for the application of a simple numerical scheme to this integral equation,

⁴That is, $u_{\mu}(x) = -\int |y - x|\mu(dy)$ is the formal density of the occupation measure $\mu U = \int_0^{\infty} \mu P_t dt$ where P_t denotes the semigroup of Brownian motion.

yielding a much faster and more accurate numerical method for directly computing r , for a class of symmetric probability measures μ with compact support, than the nonlinear PDE approach described above.

The second contribution of this paper is to show that (SEP_μ) , and in particular the Root solution described by the equation (1.1), can be very useful in sampling Brownian increments, an essential task in Monte Carlo schemes. Recall the arguably simplest algorithm $(\tau_0^{sim}, X_0^{sim}) = (0, 0)$ and

$$\begin{cases} X_{n+1}^{sim} = X_n^{sim} + N_n, & \text{with i.i.d. } N_n \sim \mathcal{N}(0, 1), \\ \tau_{n+1}^{sim} = \tau_n^{sim} + 1. \end{cases}$$

Then the equality holds $(\tau_n^{sim}, X_n^{sim})_{n \in \mathbb{N}} \stackrel{\text{Law}}{=} (\tau_n, B_{\tau_n})_{n \in \mathbb{N}}$ where $\tau_n = n$. We would like to stress here that this algorithm works because τ_1 solves (SEP_μ) : $B_{\tau_1} \sim \mathcal{N}(0, 1)$. In fact, setting $r \equiv 1$, that is,

$$R = \{(t, x) : t \geq 1, x \in [-\infty, \infty]\},$$

it follows $\tau_1 \equiv 1 = \inf\{t > 0 : (t, B_t) \in R\}$, and we see that Root's solution for $\mu = \mathcal{N}(0, 1)$ yields the classical Euler scheme. Note, however, that at least in principle, Root's result allows us to choose μ to be any probability measure on real numbers. The canonical choice, as pointed out by Dupire, in terms of speed of simulation on a standard computer, which is very efficient in drawing quasi-random numbers from the uniform distribution, is to take $\mu = \mathcal{U}[-1, 1]$. In this case the barrier function r can be computed (once!) arbitrarily accurately via (1.1), yielding a simulation algorithm

$$\begin{cases} X_{n+1}^{sim} = X_n^{sim} + U_n, & \text{with i.i.d. } U_n \sim \mathcal{U}[-1, 1], \\ \tau_{n+1}^{sim} = \tau_n^{sim} + r(U_n). \end{cases}$$

Again we have $(\tau_n^{sim}, X_n^{sim})_{n \in \mathbb{N}} \stackrel{\text{Law}}{=} (\tau_n, B_{\tau_n})_{n \in \mathbb{N}}$ where $(\tau_n)_n$ denote the first hitting times of $t \mapsto (t, B_t)$ of the Root barrier R , that is, $\tau_1 = \inf\{t > 0 : (t, B_t) \in R\}$, $\tau_2 = \inf\{t > \tau_1 : (t - \tau_1, B_t - B_{\tau_1}) \in R\}$, etc. What makes this algorithm particularly interesting, besides its computational efficiency, is the fact that the time-space process $(t, B_t)_{t \geq 0}$, and in particular the Brownian motion itself, is uniformly bounded between consecutive sampling times τ_n and τ_{n+1} for all $n \in \mathbb{N}$,

$$\sup_{t \in [\tau_n, \tau_{n+1}]} |B_t - B_{\tau_n}| < 2 \quad \text{and} \quad \tau_{n+1} - \tau_n < \frac{2}{\pi}$$

(the first inequality is sharp but the second is not; see Corollary 4). Such a property is particularly useful in Monte Carlo schemes for computing solutions of PDEs with time-dependent boundaries; similar observations have been made by many different authors before, for example, Milstein and Tretyakov, Deaconu and Hermann, Deaconu, Lejay, and Zein [9, 25, 34], by using different shapes (e.g., parallelepipeds) than R ; however, the above approach via the (SEP_μ) is extremal among these solutions in the sense that it allows one to sample from the arguably simplest

distribution for computational purposes $\mathcal{U}[-1, 1]$. It is also clear that Brownian scaling can be used to modify the above algorithm, which is described in detail in Section 4, to sample increments during which the uniform bound is arbitrarily small (i.e., $\mu = \mathcal{U}[-\epsilon, \epsilon]$, $\epsilon > 0$). In Section 5 we show how this sampling algorithm allows us to extend a classic Monte Carlo scheme of Muller [27], the so-called “random walks over spheres” from the elliptic to the parabolic setting.

The key idea in this paper is to relate the solution of the obstacle problem describing the Root barrier with the solution of a nonlinear integral equation. This general approach dates back to the work of McKean [23], who showed that the value function in the pricing problem for a discounted American call option can be represented in terms of the free boundary function, which itself satisfies a system of nonlinear integral equations. The question of the uniqueness of the solution of the integral equation in the context of American options was resolved by Peskir [30]; see also the work of Chadam and Chen [5].

Let us finish by mentioning that there have been a number of exciting recent developments relevant to topics treated in this paper: the work of Beiglböck and Huesmann [3] deriving the existence of such barriers via optimal transport, the paper of Galichon, Henry-Labordère, and Touzi who study (SEP_μ) as an optimal stopping problem [13], and the work of Ankirchner, Hobson, and Strack on finite embeddings [1, 2].

2. The Root barrier as the unique solution of an integral equation. We begin by recalling classic results on the existence of such barriers.

DEFINITION 1. A closed subset R of $[0, \infty] \times [-\infty, \infty]$ is a *Root barrier* R if:

- (1) $(t, x) \in R$ implies $(t + h, x) \in R \ \forall h \geq 0$,
- (2) $(+\infty, x) \in R \ \forall x \in [-\infty, \infty]$,
- (3) $(t, \pm\infty) \in R \ \forall t \in [0, +\infty]$.

Given a Root barrier R , its *barrier function* $r : [-\infty, \infty] \rightarrow [0, \infty]$ is defined as

$$r(x) := \inf\{t \geq 0 : (t, x) \in R\}, \quad x \in [-\infty, \infty].$$

Note that different barriers can embed the same law. This was resolved by Loynes by the introduction of regular barriers.

DEFINITION 2. We say that a barrier R , respectively, its barrier function r , is *regular* if r vanishes outside

$$[x_-, x_+],$$

where x_+ and x_- are the first positive, respectively, negative, zeros⁵ of r .

⁵The first positive zero of some lower-semicontinuous function $\bar{F} : [-\infty, \infty] \rightarrow [0, \infty]$ is at x_+ if $x_+ \in [0, \infty]$, $\bar{F}(x_+) = 0$ and $\bar{F}(x) > 0$ for $x \in [0, x_+)$. Similarly for the first negative zero $x_- \in [-\infty, 0]$; see [21], Section 3.

THEOREM 1 (Root [31], Loynes [21], and Rost [32]). *Let μ be a probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ that has zero mean. Then:*

- (1) *there exists exactly one regular Root barrier R such that $\tau = \inf\{t : (t, B_t) \in R\}$ solves (SEP $_{\mu}$);*
- (2) *its barrier function $r(x) = \inf\{t : (t, x) \in R\}$ is a lower semicontinuous function $r : [-\infty, \infty] \rightarrow [0, \infty]$ with $r(\pm\infty) = 0$;*
- (3) $R = \{(t, x) \in [0, \infty] \times [-\infty, \infty] : t \geq r(x)\}$.

Moreover, τ minimises for every $t \geq 0$ the residual expectation $\mathbb{E}[(\tilde{\tau} - t)^+] = \int_t^\infty \mathbb{P}(\tilde{\tau} > s) ds$ among all $\tilde{\tau}$ that are solutions of (SEP $_{\mu}$).

REMARK 1. In [21, 31] the above properties (1)–(3) are only proved under the additional assumption that μ is of finite variance. However, with the help of the PDE representation from [7, 28] one sees that the finite variance assumption is unnecessary. The details may be found in [28].

REMARK 2. Since the Root barrier R is a closed set, and the process $(t, B_t)_{t \geq 0}$ has continuous trajectories, the representation of R as in point (3) of Theorem 1 above yields

$$(2.1) \quad \tau \geq r(B_\tau).$$

For example, for $\mu = \frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_1$ this is a strict inequality a.s., but in Lemma 1 below we show that for every atom-free measure, (2.1) becomes an equality. This is intuitive but not completely trivial since it, for example, also covers the case of singular measures (i.e., not absolutely continuous with respect to Lebesgue measure but still atom-free) like Cantor’s distribution (devil’s staircase).

REMARK 3. A stopping time τ minimises the residual expectation if and only if it minimises for every convex function [wlog $f(0) = f'(0+) = 0$]

$$\mathbb{E}[f(\tau)] = \int_0^\infty (\tau - t)_+ f''(dt).$$

Denote the semigroup operator of standard Brownian motion with (P_t^B) . The potential kernel is defined as $U^B = \int_0^\infty P_t^B dt$; that is, U^B can be seen as a linear operator on the space of measures on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ by setting $\mu U^B = \int_0^\infty \mu P_t^B dt$ which is of course nothing else than the occupation measure along Brownian trajectories started with $B_0 \sim \mu$. If μ is a signed measure with $\mu(\mathbb{R}) = 0$ and finite first moment, then the Radon–Nikodym density with respect to the Lebesgue measure is given as

$$\frac{d\mu U^B}{dx} = - \int |x - y| \mu(dy).$$

Since (in dimension one) Brownian motion is recurrent, μU^B is infinite if μ is positive. However, the right-hand side $-\int_{\mathbb{R}} |x - y| \mu(dy)$ is still well defined for every μ that has a finite moment, and Chacon [4] demonstrated that this is indeed a very useful quantity to study hitting times. It plays an essential role for understanding the dynamics of the Root solution.

DEFINITION 3 (Potential function). Let μ be a probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ that has a first moment. We define $u_\mu \in C(\mathbb{R}, (-\infty, 0])$ as

$$u_\mu(x) := - \int_{\mathbb{R}} |x - y| \mu(dy)$$

and call u_μ the *potential function* of the probability measure μ .

2.1. *The barrier function solves an integral equation.*

THEOREM 2. Denote

$$g(t, x) = \sqrt{\frac{2t}{\pi}} e^{-x^2/(2t)} - |x| \operatorname{Erfc}\left(\frac{|x|}{\sqrt{2t}}\right) = \mathbb{E}L_t^x,$$

where $(L_t^x)_{t,x}$ is the Brownian local time, and let μ be an atom-free, zero-mean probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$. Then the regular barrier function r of the Root solution for (SEP_μ) solves the nonlinear Volterra integral equation

$$(2.2) \quad u_{\delta_0}(x) - u_\mu(x) = g(r(x), x) - \int_{\{y: r(y) < r(x)\}} g(r(x) - r(y), x - y) \mu(dy) \quad \forall x \in (-\infty, \infty).$$

We prepare the proof of Theorem 2 with a lemma:

LEMMA 1. *If μ is atom-free, then $r(B_\tau) = \tau$ almost surely.*

PROOF. Since μ is atom-free, the first positive and negative zeros cannot be 0, that is, $x_+ > 0$ and $x_- < 0$. We now claim that for all (t, x) in the Root barrier R ,

$$(2.3) \quad \forall h > 0, \forall y \neq x \quad R \cap [t, t + h) \times (x, y) \neq \emptyset$$

[here (y, x) should be understood as (x, y) if $x < y$]. Indeed, assume on the contrary that for some x there exists $h > 0, y \neq x$ s.t. $R \cap [r(x), r(x) + h) \times (x, y) = \emptyset$.

For simplicity, first assume $0 < y < x$ and $r(x) > 0$. Then note that due to lower semicontinuity and Loynes regularity of r , we can find $\underline{r} > 0$ and $\delta > 0$ such that

$r(z) \geq \underline{r} > 0$ for every $z \in (-\delta, x)$. Define $y' := \frac{3y+x}{4}$ and $x' := \frac{3x+y}{4}$, and note that $y < y' < x' < x$. We then have

$$\begin{aligned} \mathbb{P}(B_\tau = x) &\geq \mathbb{P}\left[\{B_s \in (-\delta, x), 0 \leq s \leq \underline{r}\} \cap \{B_s \in (y, x), \underline{r} \leq s \leq r(x)\}\right. \\ &\quad \left. \cap \left\{y < \inf_{r(x) \leq s \leq r(x)+h} B_s \leq x \leq \sup_{r(x) \leq s \leq r(x)+h} B_s\right\}\right] \\ &\geq \mathbb{P}[B_s \in (-\delta, x), 0 \leq s \leq \underline{r}] \\ &\quad \times \inf_{z \in (y', x')} \mathbb{P}[B_s \in (y - z, x - z), 0 \leq s \leq r(x) - \underline{r}] \\ &\quad \times \inf_{z \in (y', x')} \mathbb{P}\left[y - z < \inf_{0 \leq s \leq h} B_s \leq x - z \leq \sup_{0 \leq s \leq h} B_s\right] \\ &> 0. \end{aligned}$$

For the case $r(x) = 0$ we have either $x = x_+, y < x$ or $x = x_-, y > x$. In this case an analogous argument works.

Now let $t \mapsto B_t \equiv B_t(\omega)$ be any continuous path, and let t be such that $r(B_t) = t - \delta < t$. We claim that this implies that for some $s < t$, $r(B_s) < s$. Indeed, if $B_{t-(\delta/2)} = B_t$ we are done; otherwise by (2.3), there exists $y \in (B_{t-(\delta/2)}, B_t)$ s.t. $r(y) < t - \frac{\delta}{2}$. But then by continuity of B , $B_s = y$ for some $s \in (t - \frac{\delta}{2}, t)$, and this s satisfies $s > r(B_s)$.

This argument, together with inequality (2.1) and the definition of τ then imply $r(B_\tau) = \tau$. \square

Using this, we can now prove Theorem 2.

PROOF OF THEOREM 2. Note that by definition of g , and since $B_\tau \sim \mu$, the theorem can be restated as

$$u_{\delta_0}(x) - u_\mu(x) = \mathbb{E}[L_{r(x)}^x] - \int_{\{y: r(y) < r(x)\}} \mathbb{E}[L_{r(x)-r(y)}^{x-y}] \mathbb{P}(B_\tau \in dy) \quad \forall x \in (-\infty, \infty).$$

Now apply the Tanaka–Itô formula to the process $(B_{\tau \wedge t} - x)_{t \geq 0}$ to get

$$\begin{aligned} \mathbb{E}[|B_{\tau \wedge t} - x|] &= |x| + \mathbb{E}[L_{t \wedge \tau}^x] \\ (2.4) \quad &= |x| + \mathbb{E}[L_t^x + (L_t^x - L_t^x)1_{t > \tau}] \\ &= |x| + g(t, x) - \mathbb{E}[(L_t^x - L_t^x)1_{t > \tau}]. \end{aligned}$$

Note that if μ is atom-free, then r does not have jumps, and it holds that $\tau = r(B_\tau)$ a.s. We use this to transform the last term into an explicit integral by conditioning⁶

⁶Without loss of generality, we realise Brownian motion on the canonical Wiener space to justify the disintegration with the conditional expectation.

on $\{B_\tau \in dy\}$ to see that for all (t, x)

$$\begin{aligned} \mathbb{E}[(L_t^x - L_\tau^x)1_{t>\tau}] &= \int_{-\infty}^\infty \mathbb{E}[(L_t^x - L_\tau^x)1_{t>\tau} | B_\tau = y] \mathbb{P}(B_\tau \in dy) \\ &= \int_{-\infty}^\infty \mathbb{E}[(L_t^x - L_{r(y)}^x)1_{t>r(y)} | B_\tau = y] \mathbb{P}(B_\tau \in dy), \end{aligned}$$

where we have used Lemma 1 for the second equality. If we restrict attention to points $(r(x), x) \in R$, then

$$\begin{aligned} \mathbb{E}[(L_{r(x)}^x - L_\tau^x)1_{r(x)>\tau}] &= \int_{-\infty}^\infty \mathbb{E}[(L_{r(x)}^x - L_{r(y)}^x)1_{r(x)>r(y)} | B_\tau = y] \mathbb{P}(B_\tau \in dy) \\ &= \int_{\{y:r(y)<r(x)\}} \mathbb{E}[L_{r(x)}^x - L_{r(y)}^x | B_\tau = y] \mathbb{P}(B_\tau \in dy) \\ &= \int_{\{y:r(y)<r(x)\}} \mathbb{E}[L_{r(x)-r(y)}^{x-y}] \mathbb{P}(B_\tau \in dy), \end{aligned}$$

where for the third equality we have used that Brownian motion is Markov and that its local time is an additive functional of Brownian trajectories. Plugging this into (2.4) we see that

$$\mathbb{E}[|B_\tau \wedge r(x) - x|] = |x| + \mathbb{E}[L_{r(x)}^x] - \int_{\{y:r(y)<r(x)\}} \mathbb{E}[L_{r(x)-r(y)}^{x-y}] \mathbb{P}(B_\tau \in dy).$$

Since $(r(x), x) \in R$, the left-hand side multiplied by (-1) equals the potential function of μ , u_μ (see [7, 28] for a proof of this), and we have derived (2.4). \square

In Section 2.2 we show that r is not only one but the unique solution of integral equation (2.2). In general it can be hard to numerically solve the integral equation due to the appearance of the unknown r as an argument in the continuous integral kernel g as well as the domain of integration. However, in special cases where more is known about the geometry of R , this can become significantly easier, and in the rest of this article we focus on measures that lead to symmetric, bounded, and monotone barrier functions.

ASSUMPTION 1. μ is a zero-mean probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ such that the regular Root barrier solving (SEP_μ) is given by a function r that is symmetric around 0, continuous, and nonincreasing on $[0, \infty]$.

The symmetry, boundedness, and especially the monotonicity allows us to write the integral as an integral with a domain that does not depend on r . This simplifies the numerics needed to solve such integral equations for the unknown function r .

COROLLARY 1. *Let μ fulfill Assumption 1. Then r solves the nonlinear Volterra integral equation of the first kind*

$$(2.5) \quad \begin{aligned} u_{\delta_0}(x) - u_\mu(x) &= g(r(x), x) \\ &\quad - \int_x^\infty (g(r(x) - r(y), x + y) + g(r(x) - r(y), x - y))\mu(dy) \end{aligned}$$

$\forall x \in (0, \infty).$

PROOF. By assumption on r ,

$$\{y : r(y) < r(x)\} = (-x, -\infty) \cup (x, \infty),$$

and by symmetry of the local time in space the statement follows. \square

Of course, Assumption 1 is not too useful in practice since in general it can be very difficult to deduce properties of the geometry of the barrier R from μ . Therefore we provide in Section 3 simple and easy to verify conditions on μ that imply Assumption 1.

REMARK 4. The solution \tilde{r} of the equation $u_\mu(x) - u_{\delta_0}(x) = g(\tilde{r}(x), x)$ will be a lower bound for the true solution r , that is, $\tilde{r}(x) \leq r(x)$. Hence a simple inverse problem (or even a simple ODE after taking $\frac{d}{dx}$ if smoothness or r is known) gives a lower bound for r which often is quite good (e.g., if $\mu = \mathcal{U}[-1, 1]$).

2.2. *The barrier function is the unique solution of the integral equation.* We want to find the Root barrier by solving integral equation (2.2). Therefore we still need to show that (2.2) has a unique solution in a reasonable class of functions. Unfortunately, there are very few general results for the uniqueness of such nonlinear integral equations (Volterra's equation of the first kind); see [20], Chapter 5. However, by using the special structure of equation (2.2) and the connections with viscosity solutions of obstacle PDEs [28], we are able to prove uniqueness in the case when r is continuous. While Theorem 2 applies to singular distributions (like the Cantor distribution) we show the uniqueness for solutions of (2.2) only for barriers that have a continuous barrier function.

THEOREM 3. *Let μ be an atom-free and zero-mean probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$. If $r : (-\infty, \infty) \rightarrow [0, \infty]$ is any continuous function⁷ that fulfills (2.2), then*

$$(2.6) \quad \begin{aligned} u^r(t, x) &:= - \int_{-\infty}^\infty |y|p(t, x - y) dy \\ &\quad + \int_0^t \int_{-\infty}^\infty 1_{\{t \geq r(y)\}} p(x - y, t - s)\mu(dy) ds \end{aligned}$$

⁷Note that r is defined as a function taking values that may include ∞ ; hence r can be continuous, and $r(x) = \infty$ for a $x \in (-\infty, \infty)$ is still possible.

is a continuous viscosity solution with linear growth in the space variable to

$$(2.7) \quad \begin{cases} \min(u - u_\mu, \partial_t u - \frac{1}{2}\partial_{xx}u) = 0, & \text{on } [0, \infty) \times \mathbb{R}, \\ u(t, x) = -|x|, & \text{on } \{0\} \times \mathbb{R}. \end{cases}$$

PROOF. u^r is continuous on $[0, \infty) \times \mathbb{R}$ and has linear growth in space by standard computations. By defining

$$Q^r := \{(t, x), t < r(x)\}$$

it is enough to prove:

- (1) $\partial_t u^r - \frac{1}{2}\partial_{xx}u^r \geq 0$ in viscosity sense,
- (2) $\partial_t u^r - \frac{1}{2}\partial_{xx}u^r = 0$ on Q^r in classical sense,
- (3) $u^r(t, x) \geq u_\mu(x)$ on $\mathbb{R}_+ \times \mathbb{R}$, and $u^r(t, x) = u_\mu(x)$ on $(\mathbb{R}_+ \times \mathbb{R}) \setminus Q^r$.

(1) and (2) are actually true for an arbitrary measurable r : indeed, since p is the fundamental solution to the heat equation, u^r solves in a weak (distribution) sense $(\partial_t - \frac{1}{2}\partial_{xx})u = 1_{\{t \geq r(x)\}}\mu(dx) \geq 0$, and the claim follows since distribution (super)solutions to $\partial_t u - \frac{1}{2}\partial_{xx}u = 0$ are actually viscosity (super)solutions [17].

It remains to prove point (3). Therefore denote with $p(t, x) = \frac{1}{\sqrt{2\pi t}}e^{-x^2/(2t)}$ the heat kernel. By using Fubini's theorem and that $g(t, x) = \int_0^t p(s, x) ds$, we immediately see that

$$\begin{aligned} & \int_0^{r(x)} \int_{-\infty}^{\infty} 1_{\{r(x) \geq r(y)\}} p(x - y, r(x) - s)\mu(dy) ds \\ &= \int_{\{y: r(y) < r(x)\}} g(r(x) - r(y), x - y)\mu(dy). \end{aligned}$$

Hence the statement that r solves (2.2) is equivalent to the statement

$$u^r(x, r(x)) = u_\mu(x).$$

Now since $\partial_{xx}u_\mu \leq 0$, it follows by (2) and comparison for the heat equation on Q^r , that $u^r \geq u_\mu$ on Q^r . To prove that $u^r = u_\mu$ on $(\mathbb{R}_+ \times \mathbb{R}) \setminus Q^r$, we again use comparison for the heat equation to get that u^r is the unique (weak) solution with linear growth to

$$(2.8) \quad \begin{cases} \partial_t u - \frac{1}{2}\partial_{xx}u = \mu(dx), & \text{on } (\mathbb{R}_+ \times \mathbb{R}) \setminus Q^r, \\ u(t, x) = u_\mu(x), & \text{on } \{t = r(x)\}. \end{cases}$$

Note that we use the continuity of r here since it guarantees that $(\mathbb{R}_+ \times \mathbb{R}) \setminus Q^r$ is open and its parabolic boundary is $\{t = r(x)\}$. \square

REMARK 5. The representation (2.6) is not surprising considering the classic literature on free boundaries and integral equations cited in the Introduction. For the Root solution it seems to have been so far only considered for a

special case of the reversed Root (“Rost barrier”) barrier and derived via pure PDE/nonprobabilistic arguments⁸ [22].

COROLLARY 2. *Let μ be an atom-free and zero-mean probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ that has a continuous barrier function. Then the barrier function r of the Root solution of (SEP $_{\mu}$) is the unique continuous function that solves the integral equation (2.2).*

PROOF. Assume \bar{r} is any other continuous function that solves (2.2). Then by Theorem 3 above we know that $u^{\bar{r}}$ and u^r both solve the obstacle PDE (2.7); hence by the uniqueness result in [28] they coincide (with $-\mathbb{E}[|B_{t \wedge \tau} - x|]$ where $\tau = \inf\{t > 0 : t \geq r(B_t)\}$). It follows [by comparing $(\partial_t - \frac{1}{2}\partial_{xx})u^{\bar{r}}$ with $(\partial_t - \frac{1}{2}\partial_{xx})u^r$] that $r(x) = \bar{r}(x)$, $\mu(dx)$ a.e., and by continuity and Loynes regularity this implies $r = \bar{r}$. \square

REMARK 6. The uniqueness result presented here applies to a smaller class of measures than the class for which integral equation (2.2) holds. While it covers some cases when the barrier function equals ∞ , it does not apply to barriers that arise from singular measures like the Cantor distribution: while the first two steps of Theorem 3 still hold, we are not aware of a uniqueness result for the heat PDE (2.8) on a complicated (fractal like) domain as $(\mathbb{R}_+ \times \mathbb{R}) \setminus Q^r$ (it may no longer be an open set in this case).

3. Measures with symmetric, continuous and monotone barrier functions.

Assumption 1, as introduced in Section 2, is usually not easy to verify for a given measure μ . It makes a statement about the shape of the barrier R , respectively, r , and in general it is very hard to derive such properties from basic principles. In this section we use the viscosity methods developed in [28] to show that simple and easy to verify conditions imply Assumption 1.

ASSUMPTION 2. μ is a symmetric probability measure around 0 with compact support $[-k, k]$ and admits a bounded density f s.t. f is nondecreasing on $[0, k]$.

REMARK 7. If μ fulfills Assumption 2, then u_{μ} is twice differentiable on $(-k, k)$ with

$$\partial_{xx}u_{\mu} = 2f(x).$$

PROPOSITION 1. *If μ fulfills Assumption 2, then the corresponding barrier function $r : [-\infty, \infty] \rightarrow [0, \infty]$ is a continuous and nonincreasing function on $[0, k]$.*

⁸We would like to thank Cox for bringing [22] to our attention.

PROOF. We first prove the monotonicity. Define $u(t, x) = -\mathbb{E}[|B_{t \wedge \tau} - x|]$. From [28] it follows that u is the unique viscosity solution of

$$(3.1) \quad \begin{cases} \min(u - u_\mu, \partial_t u - \frac{1}{2} \partial_{xx} u) = 0, & \text{on } [0, \infty) \times [-k, k], \\ u(t, x) = u_{\delta_0}(x), & \text{on } \mathbb{R}_+ \times \{-k, k\} \cup \{0\} \times [-k, k] \end{cases}$$

and that

$$(3.2) \quad r(x) = \inf\{t : u(t, x) = u_\mu(x)\}.$$

We now prove that for any $t \geq 0$,

$$x \mapsto (u - u_\mu)(t, x)$$

is nonincreasing on $[0, k]$ which then implies that r is nonincreasing. Therefore fix a sequence such that $\delta_\varepsilon \rightarrow \delta_0$ weakly, where δ_ε has density ρ^ε smooth, symmetric around 0, decreasing on $\mathbb{R}_{\geq 0}$ and support contained in $[-\varepsilon, \varepsilon]$. We will consider the functions u^ε , unique viscosity solutions to

$$(3.3) \quad \begin{cases} \min(u^\varepsilon - u_\mu, \partial_t u^\varepsilon - \frac{1}{2} \Delta u^\varepsilon) = 0, & \text{on } [0, \infty) \times [-k, k], \\ u(0, x) = u_{\delta_\varepsilon}(x), & \text{on } \mathbb{R}_+ \times \{-k, k\} \cup \{0\} \times [-k, k]. \end{cases}$$

Note that since $u_{\delta_\varepsilon}(x) \geq u_{\delta_0}(x) - \varepsilon 1_{\{|x| \leq \varepsilon\}}$, we have that $u_{\delta_\varepsilon} \geq u_\mu$ for ε small enough, and then u^ε admits the representation

$$(3.4) \quad u^\varepsilon(t, x) = -\mathbb{E}_{\delta_\varepsilon}[|B_{t \wedge \tau^\varepsilon} - x|],$$

where B_{τ^ε} has distribution μ (for initial distribution $B_0 \sim \delta_\varepsilon$). The proof now proceeds in 3 steps.

Step 1. $\partial_x u^\varepsilon$ exists and is continuous on $[0, \infty) \times [-k, k]$.

For each t , $u^\varepsilon(t, \cdot)$ has for second (weak) derivative the measure $\mu_{t \wedge \tau^\varepsilon}$, law of $B_{t \wedge \tau^\varepsilon}$. But actually $\mu_{t \wedge \tau^\varepsilon}$ has a bounded density (uniformly in $t \geq 0$) since

$$\begin{aligned} \mathbb{P}_{\delta_\varepsilon}(B_{t \wedge \tau^\varepsilon} \in A) &\leq \mathbb{P}_{\delta_\varepsilon}(B_t \in A) + P(B_{\tau^\varepsilon} \in A) \\ &\leq \sup_{t \geq 0} \mathbb{P}_{\delta_\varepsilon}(B_t \in A) + \mu(A) \\ &\leq (C_\varepsilon + \|f\|_\infty)\lambda(A). \end{aligned}$$

Here λ is the Lebesgue measure. It follows that $\partial_x u$ exists and is continuous in x , uniformly in t . Joint continuity then follows easily as in [12], Corollary 2.7.

Step 2. $\partial_x u^\varepsilon \leq \partial_x u_\mu$ on $[0, \infty) \times [0, k]$. Set

$$D^+ = \{(t, x) \in (0, T) \times (0, 1) : u^\varepsilon(t, x) > u_\mu(t, x)\}.$$

We first verify that $w := \partial_x u^\varepsilon - \partial_x u_\mu \leq 0$ on $([0, \infty) \times [0, k]) \setminus D^+$:

- For $x \in [0, k]$, a direct computation gives $w(0, x) = -2(\delta_\varepsilon - \mu)[0, x]$. Hence

$$\partial_x w(0, x) = -2(\rho^\varepsilon - f)(x)$$

is increasing; that is, $w(0, \cdot)$ is convex, and since $w(0, k) = w(0, 0) = 0$, it follows that $w(0, x) \leq 0$, for any $x \in [0, k]$.

- $w(t, 0) = 0$ since by symmetry $u^{\delta_\varepsilon}(t, x) = u^{\delta_\varepsilon}(t, -x)$ (and idem for u^μ).
- On the remaining part $u^\varepsilon \equiv u^\mu$ so that $w \equiv 0$.

Now note that w satisfies

$$\partial_t w - \frac{1}{2} \partial_{xx} w = -\partial_x f$$

(in the distributional sense) on D^+ , and since by assumption $\partial_x f$ is a positive measure, w is a subsolution to the heat equation on D^+ . Moreover, by step 1 w is continuous and $w \leq 0$ on ∂D^+ , and hence it follows by the maximum principle that $w \leq 0$ on D^+ as well.

Step 3. For any $t \geq 0, x \mapsto (u - u_\mu)(t, x)$ is nonincreasing on $[0, k]$.

This is a simple consequence of step 2 and the fact that $u^\varepsilon \rightarrow u$ by stability of viscosity solutions.

Hence we get the desired monotonicity of $(u - u_\mu)(t, \cdot)$ for all t , and monotonicity of r follows. It follows that any discontinuity of r must be of jump-type, but it is obvious that if r jumps at x , then the distribution of B_τ would have an atom at x , which is impossible since μ has a density. Hence r is continuous. \square

To show that $r(0) = \sup_x r(x)$ is finite and to provide explicit bounds, we need to make a quantitative assumption on how fast the mass near $r(0)$ changes.

ASSUMPTION 3. $\forall x > 0, \mu([-x, x]) > 0$, and $\exists \eta \in (0, 1)$ s.t.

$$\sum_{l=0}^\infty \eta^{2l} |\ln(\mu[0, \eta^{l+1}k])| < \infty.$$

REMARK 8. A simple family of measures satisfying Assumptions 2 and 3 is given by

$$\mu_{k,\alpha}([-x, x]) = \left(\frac{x}{k}\right)^\alpha, \quad 0 \leq x \leq k,$$

or any $k > 0, \alpha \geq 1$. In particular, this includes the family of uniform distributions $\mathcal{U}[-k, k]$.

PROPOSITION 2. *If μ fulfills Assumptions 2 and 3, then the corresponding barrier function r is finite on $[0, k]$.*

PROOF. Due to the monotonicity and the fact that μ charges any neighbourhood of 0, it is clear that $r(x)$ is finite for any $x > 0$. We now prove $r(0) < \infty$.

First recall that the probability for Brownian motion to stay in an interval $(-a, a)$ is given by

$$\begin{aligned} \mathbb{P}(B_s \in (-a, a), \forall 0 \leq s \leq T) &= \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} e^{-(2n+1)^2 \pi^2 T / (8a^2)} (-1)^n \\ &\leq \frac{4}{\pi} e^{-(\pi^2 T) / (8a^2)}; \end{aligned}$$

see [11], Chapter X, Section 5. For any $0 < x < y \leq k$, we have

$$\begin{aligned} \frac{\mu([-x, x])}{\mu([-y, y])} &= \mathbb{P}(|B_\tau| \leq x \mid |B_\tau| \leq y) \\ &\leq \mathbb{P}\left(\sup_{r(y) \leq s \leq r(x)} |B_s - B_{r(y)}| \leq 2y\right) \\ &\leq \frac{4}{\pi} e^{-(\pi^2(r(x)-r(y)))/(32y^2)}. \end{aligned}$$

This can be rewritten as

$$(3.5) \quad r(x) \leq r(y) + \frac{32y^2}{\pi^2} \left(\ln\left(\frac{4}{\pi}\right) + \left| \ln\left(\frac{\mu([0, x])}{\mu([0, y])}\right) \right| \right).$$

Now fix $0 < \eta < 1$ from Assumption 3. Taking successively $(x, y) = (\eta^{l+1}k, \eta^l k)$ in (3.5) and summing, we get

$$r(\eta^{r+1}k) \leq \frac{32k^2}{\pi^2} \sum_{l=0}^r \eta^{2l} \left(\ln\left(\frac{4}{\pi}\right) + \left| \ln\left(\frac{\mu([0, \eta^{l+1}k])}{\mu([0, \eta^l k])}\right) \right| \right).$$

It only remains to let $l \rightarrow \infty$, and we finally obtain $r(0^+) < \infty$. Putting the above together gives us the desired implication. \square

COROLLARY 3. *If μ fulfills Assumptions 2 and 3 then μ fulfills Assumption 1.*

The above proofs show much more about r in the sense that they can give an explicit upper and lower bound on $\sup_{x \in \mathbb{R}} r(x) = r(0)$. For example, for the special case of $\mu = \mathcal{U}[-1, 1]$ that we are interested in for our Monte Carlo application one easily derives the following statement.

COROLLARY 4. *Let μ be the uniform distribution on $[-1, 1]$. Then*

$$r(0) \in \left[\frac{\pi}{8}, \frac{32}{\pi^2} \inf_{\eta \in (0,1)} \frac{\ln(4/(\pi\eta))}{1-\eta^2} \right].$$

PROOF. Since $\tau \leq \sup_x r(x) = r(0)$ we have

$$\mathbb{E}[|B_\tau|] \leq \mathbb{E}[|B_{r(0)}|].$$

Using $B_\tau \sim \mathcal{U}[-1, 1]$ and a simple calculation this becomes

$$\frac{1}{2} \leq \sqrt{\frac{2}{\pi} r(0)}$$

which immediately gives the lower bound. The upper bound follows from the proof of Proposition 2 since in this case

$$\frac{\mu([0, \eta^{r+1}k])}{\mu([0, \eta^r k])} = \eta. \quad \square$$

REMARK 9. Numerics given in the next section and Figure 1 show that this lower bound is actually very good ($\frac{\pi}{8} = 0.392\dots$) but that the upper bound $\frac{32}{\pi^2} \inf_{\eta \in (0,1)} \frac{\ln(4/(\pi\eta))}{1-\eta^2} = 3.774\dots$ is not.

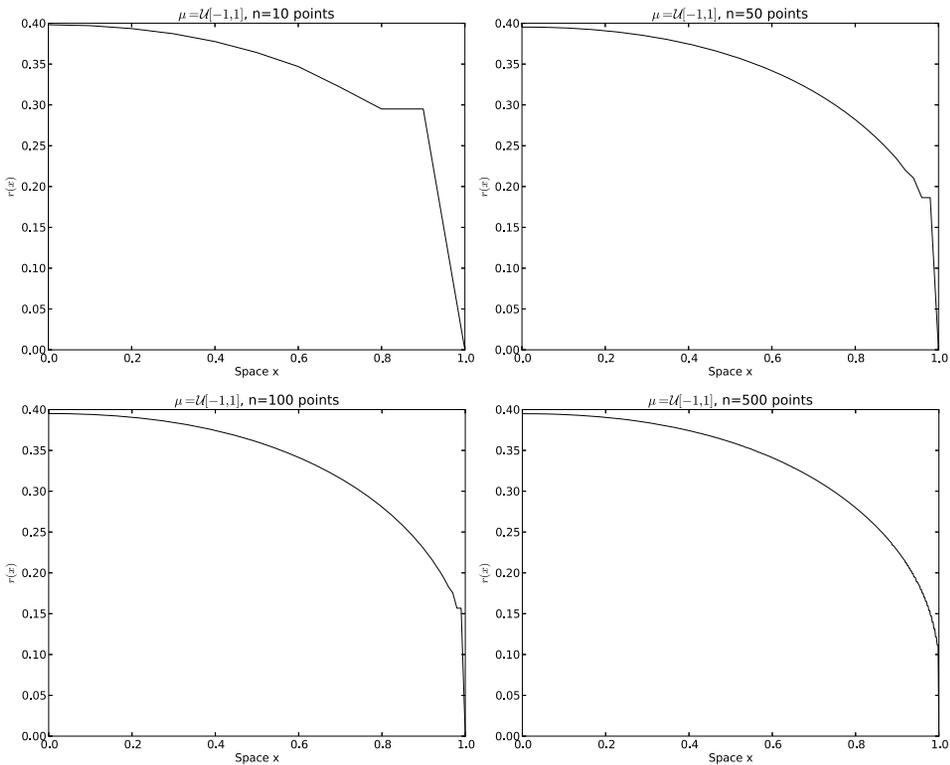


FIG. 1. The Root barrier for $\mu = \mathcal{U}[-1, 1]$. The above figures were produced with the forward Euler scheme implemented in Python (SciPy [16, 18]). The integral equation is stable in the sense that already with only 10 discretization points the approximation is fairly accurate away from $x = 1$. With $n = 500$ points the program finishes in less than 3 seconds on a standard laptop (Intel i5-3210M, 3.10 GHz, 3 MB L3, 1600 MHz FSB, 8 GB DDR3 RAM).

REMARK 10. It is interesting to compare our Proposition 2 to the results of Ankirchner and Strack [2]. On one hand, they obtain a general necessary condition for a bounded time embedding to exist, namely

$$\sup_{x \in \text{supp}(\mu)} \limsup_{\varepsilon \downarrow 0} \varepsilon^2 |\ln(\mu[x - \varepsilon, x + \varepsilon])| < \infty,$$

where we recognise the term in the series from Assumption 3. On the other hand, they also study an embedding due to Bass and obtain sufficient conditions under which the associated stopping time τ^B is bounded. Note that any almost sure bound on τ^B implies the same bound for the Root stopping time τ^R (and hence the barrier function r), since τ^R minimises $\mathbb{E}(\tau - t)_+$ for all $t \geq 0$. In fact, one can check that under Assumption 2, the sufficient conditions given in [2] all imply our Assumption 3 (of course, this does not mean that their results are a corollary of ours, since they deal with general measures while we only have to check the behaviour around the point 0). In addition, the upper bounds obtained in [2] are sometimes sharper. For instance, we could deduce from their results the upper bound $r(0) \leq \frac{2}{\pi} = 0.636\dots$ for $\mu = \mathcal{U}[-1, 1]$; that is, without running numerics we already know that $\sup_x r(x) \in [\frac{\pi}{8}, \frac{2}{\pi}]$.

3.1. *Numerics for the integral equation.* Due to the importance of such an integral equation in engineering and physics, there is an abundance of literature treating numerics; see [20] and the reference therein. We therefore do not discuss proofs of convergence, etc. Instead we give a simple example that demonstrates that already the arguably simplest scheme, a forward Euler discretisation, provides a very fast way to solve the integral equation.

To calculate r for a given μ with $\text{supp} = [-k, k]$ and density f , fix $n \in \mathbb{N}$, set $h = \frac{k}{n}$, and for every $i \in \{1, \dots, n\}$ denote with r_i the approximation to $r(ih)$. Then we know that $r_n = 0$, and (starting with $i = n - 1$) we can solve recursively the discretised nonlinear equation for r_i ,

$$\begin{aligned} &u_\mu(ih) - u_\delta(ih) \\ &= g(r_i, ih) - \sum_{j=i+1}^n (g(r_i - r_j, (i - j)h) + g(r_i - r_j, (i + j)h)) f(jh). \end{aligned}$$

4. Generating bounded Brownian time–space increments. As an application of the previous sections we now return to the approach pointed out in the **Introduction**: that an intelligent choice of μ can lead to an efficient procedure to sample from Brownian trajectories.

COROLLARY 5. *There exists a continuous bounded function*

$$r \in C_b([-1, 1], \mathbb{R}) \quad \text{with } r(x) = r(-x) \geq 0 \text{ and } r(1) = r(-1) = 0$$

which is decreasing on $[0, 1]$ such that:

(1) if B is Brownian motion carried on a probability space $(\Omega, \mathcal{F}, \mathcal{F}_t, \mathbb{P})$ satisfying the usual conditions,

(2) and the sequence of stopping times $\tau = (\tau_k)_{k \geq 0}$ is defined as

$$\tau_0 = 0 \quad \text{and} \quad \tau_{k+1} = \tau_k + \inf\{\Delta : \Delta \geq r(B_{\tau_k+\Delta} - B_{\tau_k})\}$$

[i.e., τ_1 is the exit time from $R = \{(t, x) : t \leq r(x)\}$],

then the following properties hold:

(1) if $(U_k)_{k \geq 1}$ is a sequence of i.i.d. random variables carried on a probability space $(\Omega^{\text{sim}}, \mathcal{F}^{\text{sim}}, \mathbb{P}^{\text{sim}})$, each uniformly distributed on $[-1, 1]$, $U_1 \sim \mathcal{U}[-1, 1]$, then

$$(\tau_{k+1} - \tau_k, B_{\tau_{k+1}} - B_{\tau_k})_{k \geq 0} \stackrel{\text{Law}}{=} (r(U_k), U_k)_{k \geq 0},$$

(2) $|\tau_{k+1}^\epsilon - \tau_k^\epsilon| \leq r(0) < \infty$ and $\sup_{t \in [\tau_k, \tau_{k+1}]} |B_t - B_{\tau_k}| \leq 2$ for every $k \geq 0$.

Moreover, the function r is the unique continuous solution of the integral equation

$$\begin{aligned} \frac{x^2 + 1}{2} - x &= g(r(x), x) \\ &- \frac{1}{2} \int_x^1 (g(r(x) - r(y), x - y) + g(r(x) - r(y), x + y)) dy \\ &\qquad \qquad \qquad \forall x \in [0, 1], \end{aligned}$$

where

$$g(t, x) = \mathbb{E}L_t^x = \sqrt{\frac{2t}{\pi}} e^{-x^2/(2t)} - |x| \operatorname{Erfc}\left(\frac{|x|}{\sqrt{2t}}\right).$$

PROOF. This follows directly from Theorem 2 and Markovianity of Brownian motion. \square

We refer to Figures 2 and 3 below for some examples of uniformly distributed space increments obtained by the above procedure.

Using Brownian scaling one immediately gets:

COROLLARY 6. If we fix $\epsilon > 0$ and replace in the above the sequence $\tau = (\tau_k)$ by $\tau^\epsilon = (\tau_k^\epsilon)$ defined as

$$\tau_0^\epsilon = 0 \quad \text{and} \quad \tau_{k+1}^\epsilon = \tau_k^\epsilon + \inf\left\{\Delta : \Delta \geq \epsilon^2 r\left(\frac{B_{\tau_k^\epsilon+\Delta} - B_{\tau_k^\epsilon}}{\epsilon}\right)\right\},$$

then the following properties hold:

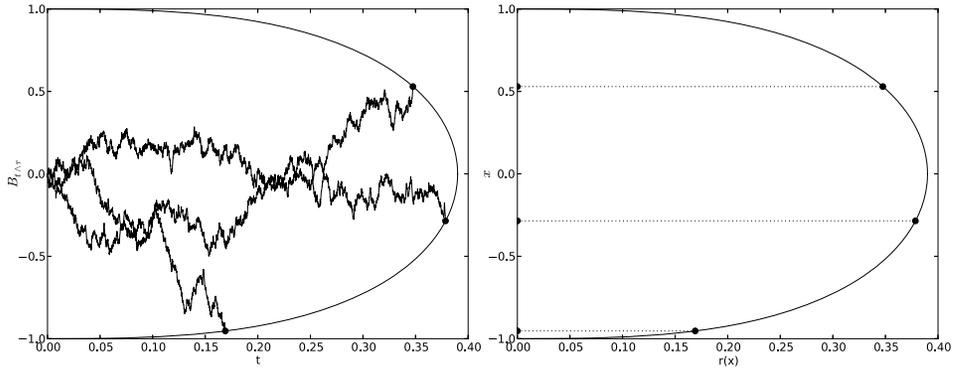


FIG. 2. The plot on the left shows three Brownian trajectories that were stopped after hitting the Root barrier for $\mu = \mathcal{U}[-1, 1]$. The plot on the right is the same but with the trajectories removed and the hitting points of the Root barrier projected back to \mathbb{R} .

(1) for a sequence $(U_k)_{k \geq 1}$ of i.i.d. random variables carried on a probability space $(\Omega^{\text{sim}}, \mathcal{F}^{\text{sim}}, \mathbb{P}^{\text{sim}})$, each uniformly distributed on $[-1, 1]$, $U_1 \sim \mathcal{U}[-1, 1]$ we have

$$(\tau_{k+1}^\epsilon - \tau_k^\epsilon, B_{\tau_{k+1}^\epsilon} - B_{\tau_k^\epsilon})_{k \geq 1} \stackrel{\text{Law}}{=} (\epsilon^2 r(U_k), \epsilon U_k)_{k \geq 1},$$

(2) $|\tau_{k+1}^\epsilon - \tau_k^\epsilon| < \epsilon^2 r(0)$ and $\sup_{t \in [\tau_k^\epsilon, \tau_{k+1}^\epsilon]} |B_t - B_{\tau_k^\epsilon}| \leq 2\epsilon$ for every $k \geq 0$.

The interest in above statement is to simulate time-space Brownian motion $t \mapsto (t, B_t)$ on a computer in an easy and efficient way: to sample one increment we only need to generate one uniformly distributed random variable U and evaluate the function r at U to match in law the increment of the time-space process $(\tau_{k+1} - \tau_k, B_{\tau_{k+1}} - B_{\tau_k})$. In pseudo code it reads Algorithm 1.

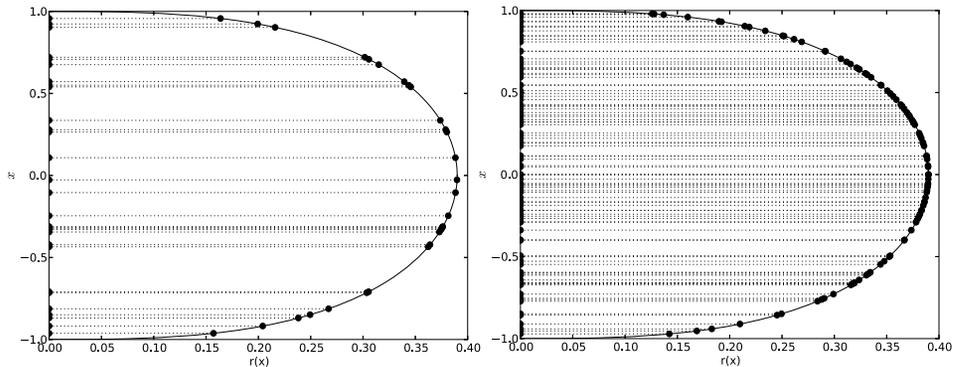


FIG. 3. Similarly to the above, both plots were drawn by using 30, respectively, 100, samples from a Brownian motion. We see can start to see that the projected points follow a $\mathcal{U}[-1, 1]$ distribution.

Algorithm 1 Generate a Brownian increment from $\mathcal{U}[-1, 1]$

```

1: function SAMPLEBMINCREMENT( $\epsilon$ )
2:    $U \leftarrow \mathcal{U}[-1, 1]$ 
3:    $\Delta B \leftarrow \epsilon * U$ 
4:    $\Delta t \leftarrow \epsilon^2 * r(U)$ 
5:   return ( $\Delta t, \Delta B$ )
6: end function

```

Contrast this with standard methods where the time step is deterministic, but a normally distributed space increment is simulated by transformations of (several) uniformly distributed random variables and table look-ups (e.g., via the Box–Muller transform, the Ziggurat algorithm, the Marsaglia polar method, etc.).

On the other hand, the function r in above statement is not given by an explicit analytic expression. However, the integral equation can be solved with great precision, and this computation needs to be done only once, then stored in a table (possibly after spline interpolation, etc.), that is, evaluating r at a point amounts to a table look-up.

The most attractive feature of the above algorithm is that one can *fix at every step a deterministic bound on the space and time increments, and both resulting increments are trivial to simulate*. In the next section we demonstrate this advantage on a short and simple but nontrivial example: a Monte Carlo simulation with adaptive step size applied to parabolic PDEs. The deterministic control over time–space increments allows us to make very big steps without leaving the time–space domain which leads to a very fast algorithm.

5. A parabolic version of Muller’s random walk over spheres. The use of exit times from a domain to simulate Brownian motion is classic and goes back to Muller in 1956 who used the uniform exit distribution of Brownian motion from a sphere to calculate elliptic PDEs (the so-called “random walk on touching spheres”) of the form

$$\begin{cases} \frac{1}{2}\Delta u = 0, & \text{on } \mathcal{D}, \\ u(x) = g(x), & \text{on } \partial\mathcal{D}, \end{cases}$$

where \mathcal{D} is a domain in \mathbb{R}^n via the Monte Carlo approximations to $u(x) = \mathbb{E}_{t,x}[g(B_{\tau_{\mathcal{D}}})]$. Here $\tau^{\mathcal{D}}$ denotes the exit time of B from \mathcal{D} . The attraction of this approach is that in every step one can choose the diameter of the sphere arbitrarily big, subject only to not intersecting $\partial\mathcal{D}$ before one samples the Brownian increment. These give big Brownian increments that lead to a very fast algorithm. To make this work for a parabolic PDE

$$(5.1) \quad \begin{cases} \partial_t u + \frac{1}{2}\Delta u = 0, & \text{on } \mathcal{D}, \\ u(t, x) = g(t, x), & \text{on } \mathcal{P}\mathcal{D} \end{cases}$$

(here we denote $\mathcal{D} = \bigcup_{t \geq 0} \{t\} \times D_t \subset [0, \infty) \times \mathbb{R}$ and the parabolic boundary $\mathcal{PD} = \partial\mathcal{D} \setminus (\{0\} \times D_0)$), it is necessary to additionally sample the distribution of the exit time from the sphere. While analytic expressions are known, it is not efficient to simulate. This has been pointed out by many authors and the work of Milstein and Tretyakov, Deaconu and Hermann, Deaconu, Lejay, and Zein [9, 25, 34], proposes the use of exit times of time–space Brownian motion from other shapes than spheres. The approach which is closest to the one presented here is the random “walk over moving spheres” (WoMS) introduced in [9]. In the short section below we show that the Root solution gives another way to construct such a random walk. It is optimal among all such approaches [9, 25, 34] in the sense that one samples simply from the uniform distribution. A (theoretical) disadvantage is that the barrier r is not known in explicit form and has to be stored as a table look-up, though the results from the previous sections show that this can be done quite easily.

5.1. *A random walk over Root barriers.* We introduce here a Monte Carlo scheme to calculate the solution of the parabolic PDE (5.1). To avoid technicalities we assume the boundary is smooth.

ASSUMPTION 4. The space–time domain is of the form

$$\mathcal{D} = \bigcup_{t \in (0, T)} \{t\} \times (a_t, b_t),$$

where $T \in (0, \infty)$ is fixed, $a, b \in C^1((0, T), \mathbb{R})$, and $a_t < b_t$ on $(0, T)$. In addition g is assumed to be regular enough so that the solution u to (5.1) satisfies

$$|u(t, x) - u(s, y)| \leq |u|_{\text{Lip}}(|t - s|^{1/2} + |x - y|) \quad \forall (t, x), (s, y) \in \mathcal{D}$$

for some constant $|u|_{\text{Lip}} < \infty$; see, for example, [19] for several standard conditions guaranteeing this.

DEFINITION 4. The parabolic distance to the boundary \mathcal{D} is defined as

$$d_{\mathcal{D}}(t, x) = \min(x - a_t, x - b_t, \sqrt{T - t}).$$

For $\delta > 0$ define \mathcal{D}_{δ} as

$$\mathcal{D}_{\delta} = \{(t, x) \in \mathcal{D} : d(t, x) \leq \delta\}.$$

REMARK 11. Since a, b are Lipschitz, one can find a function $\rho = \rho(t, x)$ such that:

- $c \cdot d_{\mathcal{D}}(t, x) \leq \rho(t, x) \leq d_{\mathcal{D}}(t, x)$ for some constant $c > 0$,
- $\forall (t, x) \in \mathcal{D}$ we have $B_{t,x}^{\rho(t,x)} \subset \overline{\mathcal{D}}$.

DEFINITION 5. Denote r the barrier function associated with $\mu = \mathcal{U}[-1, 1]$ and with $R_{t,x}^\epsilon$ its Root barrier around (t, x) after scaling with some $\epsilon > 0$, that is,

$$R_{t,x}^\epsilon = \{(t + \epsilon^2 s, x + \epsilon y) : s \geq r(y)\}.$$

We now introduce a Markov chain that is easy to generate on a computer. The motivation is the following: fix a point $(t, x) \in \mathcal{D} \setminus \mathcal{D}_\delta$, and consider the Root barrier $R_{t,x}^{\rho(t,x)}$. From the very definition of $\rho(t, x)$, it follows that a Brownian motion started at (t, x) will not have left the domain \mathcal{D} before it leaves $R_{t,x}^{\rho(t,x)}$. We now record the exit time and position of B from $R_{t,x}^{\rho(t,x)}$, and Corollary 6 tells us that the distribution of this time–space increment is $(\rho^2(t, x)r(U), \rho(t, x)U)$ for $U \sim \mathcal{U}[-1, 1]$. If this first step puts us into \mathcal{D}_δ , we stop. Otherwise we carry out the same procedure again, but now starting at $(t + \rho^2(t, x)r(U), x + \rho(t, x)U)$.

DEFINITION 6. For every $(t, x) \in \mathcal{D}$ define a Markov chain

$$M^{t,x,\delta} = (\tau_k^{t,x,\delta}, M_k^{t,x,\delta})_{k \geq 1} = (\tau_k, M_k)_{k \geq 1}$$

and a stopping time $\nu = \nu^{t,x,\delta}$ (if the context is clear, we do not write the superscripts t, x, δ) recursively as follows:

$$(\tau_0, M_0) = (t, x)$$

and

$$\begin{aligned}
 &(\tau_{k+1}, M_{k+1}) \\
 &= \begin{cases} (\rho^2(\tau_k, M_k)r(U_k), M_k + \rho(\tau_k, M_k)U_k), & \text{if } (\tau_k, M_k) \in \mathcal{D}/\mathcal{D}_\delta, \\ (\tau_k, M_{\tau_k}), & \text{if } (\tau_k, M_k) \in \mathcal{D}_\delta. \end{cases}
 \end{aligned}$$

Further denote $\nu = \inf\{k : (\tau_k, M_k) \in \mathcal{D}_\delta\}$ and

$$(\nu^{\mathcal{D}}, M_\nu^{\mathcal{D}}) = \begin{cases} (\nu, a_\nu), & \text{if } d_{\mathcal{D}}(\nu, M_\nu) = a_\nu - M_\nu, \\ (\nu, b_\nu), & \text{if } d_{\mathcal{D}}(\nu, M_\nu) = M_\nu - b_\nu, \\ (T, M_\nu), & \text{otherwise.} \end{cases}$$

Put simply, once our Markov chain enters \mathcal{D}_δ , we stop it, and $(\nu^{\mathcal{D}}, M_\nu^{\mathcal{D}})$ then records the nearest point on the boundary. This very easy to implement and spelled out in pseudocode it reads as Algorithm 2.

By construction of the Markov chain, it is clear that each sample trajectory does not contribute an error bigger than δ . The more interesting question is how many steps the chain makes on average before leaving \mathcal{D}_δ . As in Muller's elliptic version [27], the average number of steps only grows proportionally to $\log \frac{1}{\delta}$.

Algorithm 2 Random walk over Root barriers

```

1: function ROOTMONTECARLO( $t, x, samples$ )
2:    $u \leftarrow 0$ 
3:   for  $i \leftarrow 1, samples$  do
4:      $(\tau, B) \leftarrow (t, x)$ 
5:     while  $\rho(\tau, B) > \delta$  do
6:        $(\Delta\tau, \Delta B) \leftarrow SampleBMincrement(\rho(\tau, B))$ 
7:        $(\tau, B) \leftarrow (\tau + \Delta\tau, B + \Delta B)$ 
8:     end while
9:      $u \leftarrow u + g(\tau, B)$ 
10:  end for
11:   $u \leftarrow u/samples$ 
12:  return  $u$ 
13: end function

```

THEOREM 4. *If Assumption 4 holds, then there exists a unique solution u in the class $C^{1,2}(\mathcal{D}, \mathbb{R}) \cap C(\overline{\mathcal{D}}, \mathbb{R})$ that solves (5.1). Moreover, there exist constants c_1, c_2, δ_0 such that for every $\delta \in (0, \delta_0)$ one has*

$$|\mathbb{E}_{t,x}[g(\tau_v, M_v^{\mathcal{D}})] - u(t, x)| \leq c_1\delta.$$

The number of steps v is finite a.s., and for all $(t, x) \in \mathcal{D} \setminus \mathcal{D}_\delta$,

$$\mathbb{E}_{t,x}[v] \leq c_2(1 + \log(1/\delta)).$$

PROOF. Under the above assumptions on g and \mathcal{D} , the existence of a unique classical solution to (5.1) and the Feynman–Kac representation

$$u(t, x) = \mathbb{E}[g(\sigma^{t,x} \wedge T, B_{\sigma^{t,x} \wedge T}^{t,x})]$$

where $\sigma^{t,x} = \inf\{s > t : B_s^{t,x} \notin (a_s, b_s)\}$,

and $B^{t,x}$ denotes a Brownian motion started at x at time t follows from the standard results; see, for example, [19], Theorems 5.9, 5.10, 6.45, and for the Feynman–Kac verification, [6], Appendix B. Write

$$\begin{aligned} & \mathbb{E}_{t,x}[g(\tau_v, M_v^{\mathcal{D}})] - u(t, x) \\ &= \mathbb{E}_{t,x}[u(\tau_v, M_v^{\mathcal{D}})] - \mathbb{E}_{t,x}[u(\tau_v, M_v)] + \mathbb{E}_{t,x}[u(\tau_v, M_v)] - u(t, x), \end{aligned}$$

and note that the first difference on the right-hand side is bounded by $|u|_{\text{Lip}}\delta$. The second difference on the right-hand side vanishes since by construction of the Markov chain, we have $(\tau_v, M_v) \stackrel{\text{Law}}{=} (\tau_v, B_{\tau_v})$, and u is space–time harmonic on \mathcal{D} . To estimate the number of steps, we start with an idea similar to that in [24, 27] but then argue via PDE comparison. This allows us to give a short proof. For v a bounded measurable function on \mathcal{D} , define

$$Pv(t, x) = \mathbb{E}_{t,x}[v(\tau^{t,x}, B_{\tau^{t,x}})],$$

where $\tau^{t,x}$ is the first exit time from $R_{t,x}^{\rho(t,x)}$. We denote the expected number of steps with $n(t, x) = \mathbb{E}_{t,x}[v]$. It is then the unique solution to the equation

$$(5.2) \quad \begin{cases} n - Pn = 1, & \text{in } \mathcal{D} \setminus \mathcal{D}_\delta, \\ n = 0, & \text{in } \mathcal{D}_\delta. \end{cases}$$

To obtain an upper bound on n it is enough to obtain supersolutions to the above equation. Note that if v is $\mathcal{C}^{1,2}(\overline{\mathcal{D}})$, by Itô's formula we actually have

$$(5.3) \quad Pv(t, x) = v(t, x) + \mathbb{E}_{t,x} \left[\int_t^{\tau^{t,x}} \left(\partial_t + \frac{1}{2} \partial_{xx} \right) v(s, B_s) ds \right].$$

Now take

$$v^1(t, x) = \log(x - a_t + \delta) + \log(b_t - x + \delta) + \frac{1}{2} \log(T - t + \delta^2),$$

and direct computation shows that for small enough $\eta > 0$ (not depending on δ , assuming if necessary δ smaller than some suitable δ_0),

$$\begin{aligned} & \left(\partial_t + \frac{1}{2} \partial_{xx} \right) v^1(t, x) \\ &= -\frac{1}{2} \left(\frac{1}{|x - a_t + \delta|^2} + \frac{1}{|b_t - x + \delta|^2} + \frac{1}{T - t + \delta^2} \right) \\ & \quad + \left(\frac{-a'_t}{x - a_t + \delta} + \frac{b'_t}{b_t - x + \delta} \right) \\ & \leq \begin{cases} -\frac{1}{4 \delta^2 \wedge d_{\mathcal{D}}(t, x)^2}, & \text{whenever } d_{\mathcal{D}}(t, x) \leq \eta, \\ c_1, & \text{otherwise.} \end{cases} \end{aligned}$$

Now set

$$v^2(t, x) = \left(\frac{1}{\eta^2} + c_1 \right) \left(\sup_{s \in (0, T)} a_s - x \right) \left(\left(\inf_{s \in (0, T)} b_s \right) - x \right).$$

It follows that $v^2 \geq 0$ on \mathcal{D} and

$$\left(\partial_t + \frac{1}{2} \partial_{xx} \right) v^2 = - \left(\frac{1}{\eta^2} + c_1 \right).$$

Hence choosing

$$v = v^1 + v^2 + 3|\log \delta|$$

and putting the above together implies $(\partial_t + \frac{1}{2} \partial_{xx})v \leq -\frac{c_2}{d_{\mathcal{D}}^2 \wedge \delta^2}$ on \mathcal{D} . Since

$$d_{\mathcal{D}}^2(s, y) \leq c_3 d_{\mathcal{D}}^2(t, x)$$

for all $(s, y) \in R_{t,x}^{\rho(t,x)}$, we obtain from (5.3) that for all $(t, x) \in \mathcal{D} \setminus \mathcal{D}_\delta$,

$$\begin{aligned} (Pv - v)(t, x) &\leq -\frac{c_2}{c_3 d_{\overline{\mathcal{D}}}^2(t, x)} \mathbb{E}[t^{t,x} - t] \\ &= -\frac{c_2 \rho^2(t, x)}{c_3 d_{\overline{\mathcal{D}}}^2(t, x)} \\ &\leq -\frac{1}{C}. \end{aligned}$$

Since in addition $v \geq 0$ on $\overline{\mathcal{D}}$, it follows by comparison with (5.2) that the expected number of steps satisfies

$$n(t, x) \leq Cv(t, x) \leq C(1 + |\log \delta|). \quad \square$$

EXAMPLE 1. To give a numerical example, consider the function

$$u(t, x) = 4x^4 + 24(1 - t)x^2 + 12(1 - t)^2.$$

It is a simple explicit solution of the unrestricted heat equation, and by setting

$$g(t, x) = u(t, x)$$

on the parabolic boundary, it becomes the unique $C^{1,2}$ solution of (5.1). In Figure 4 are the numerics for the choice

$$T = 1, \quad a_t = 2 - t, \quad b_t = 0$$

and $\rho(t, x) = \min(\frac{2-t-x}{\sqrt{2}}, 1 - t, x)$ for $u(0, 1) = 40$.

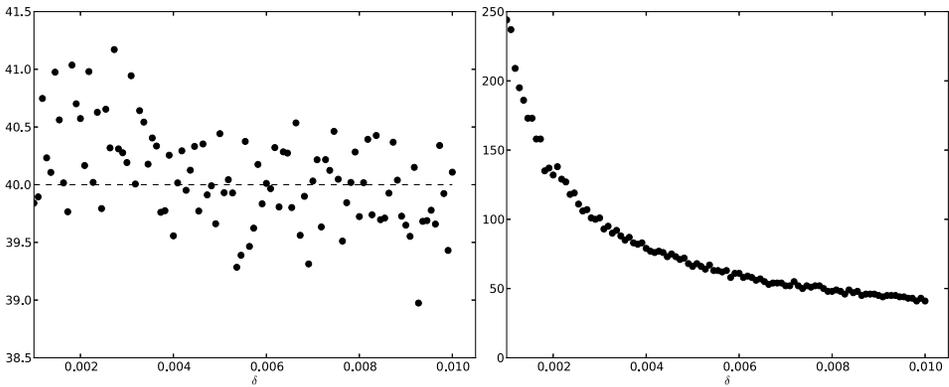


FIG. 4. The results for the Random walk over Root barriers applied to Example 1. The figure on the left shows the approximation to $u(0, 1) = 40$ and the right-hand figure the average number of steps taken before leaving the domain, both as function of $\delta \in \{0.001, \dots, 0.01\}$. Each point represents a run of the Monte Carlo scheme with 10,000 samples trajectories.

6. Conclusion and possible extensions. We have presented a new characterisation of Root's solution of the classic Skorokhod embedding problem (SEP_μ) by identifying it as the unique solution of an integral equation that has an intuitive interpretation and simple derivation. We then provided conditions on μ which imply geometric properties about the shape of the barrier. This in turn simplifies the integral equation for numerical purposes. Finally, we have shown that the Root barrier can be used to yield a new and very simple random walk over spheres algorithm. It is natural to ask for several extensions:

- The proof of Theorem 2 can be extended to other processes than Brownian motion. While existence of the Root barrier is known, the issue is to find explicit formulas for the expected local time of this process to make this actually useful for numerics (note that this is not needed for the PDE approach). Similarly, Section 2 applies (with minor modifications) to the case of one-dimensional Brownian motion started with any probability measure that is in convex order with μ .
- Not much is known about (SEP_μ) in multi dimensions.⁹ However, for radially symmetric target measures (like the uniform distribution on the unit ball) and multidimensional Brownian motion, the question is equivalent to embedding into the Bessel process; hence one can apply a simple modification of Theorem 2 in which the expected local time has still an explicit form. Unfortunately, for the general multidimensional (or even non-Brownian) case, new ideas are needed, and we hope to return to this and related Monte Carlo applications in future work.
- Section 3 provides sufficient conditions on μ such that its barrier function becomes monotone, and the integral equation (2.2) simplifies to a Volterra equation of the first kind. Numerics for nonlinear integral equations are a well-studied topic, and in principle one could hope to find fast numerics for the integral equation (2.2) such that also for the general atom-free target measures equation (2.2) becomes a competitor in numerics to the nonlinear PDE approach.

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⁹For the Root solution some existence results are known [32] but do not apply immediately; for example, one-point sets are not regular anymore which leads to issues about randomised stopping times, etc.

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