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# Statistics and Probability Letters

journal homepage: www.elsevier.com/locate/stapro

## Probability bounds for reflecting diffusion processes

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#### ARTICLE INFO

Article history: Received 7 March 2023 Accepted 14 April 2023 Available online 22 April 2023

MSC: primary 60H10 60H30 secondary 49J30 93E20

*Keywords:* Reflecting diffusion Comparison theorem Probability bounds

#### 1. Introduction

### ABSTRACT

A solution to the optimal problem for determining vector fields which maximize (resp. minimize) the transition probabilities for a class of reflecting diffusion processes is obtained in this paper. The approach is based on a representation for the transition probability density functions. The optimal transition probabilities under the constraint that the drift vector field is bounded are studied in terms of the HJB equation. We demonstrate by simulations that, even in one dimension, by considering the nodal set of the solutions to the HJB equation, the optimal diffusion processes exhibit an interesting feature of phase transitions.

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(1.1)

The simple optimal control problem to determine vector fields b(t, x) bounded by a constant  $\kappa \ge 0$  which maximize (resp. minimize) the probability  $p_b(s, x; t, y)$  of diffusion processes

$$dX_t = b(t, X_t)dt + dB_t$$

started at  $X_s = x$  and ended at  $X_t = y$  (where  $B = (B_t)_{t \ge 0}$  is a Brownian motion) has been considered and solved explicitly in the previous work (Karatzas and Shreve, 1984, 1985; Qian et al., 2003; Qian and Zheng, 2002, 2004). The method utilized in Qian et al. (2003), Qian and Zheng (2002) is quite elementary and is based on the density version of the Cameron–Martin formula

$$p_{b+c}(s, x; t, y) = p_b(s, x; t, y) + \int_s^t \mathbb{E}_{s, x} \left\{ R_{s, r} c(r, X_r) \cdot \nabla_x p_b(r, X_r; t, y) \right\} dr$$
(1.2)

for  $0 \le s < t$ , where  $p_b(s, x; t, y)$  denotes the transition probability density of  $X_t$  defined by (1.1) under the condition that  $X_s = x$  with respect to the Lebesgue measure. Here b(t, x) and c(t, x) are two vector fields with at most linear growth,  $(X_t, \mathbb{P}_{s,x})$  is the weak solution to (1.1) in the sense of Stroock–Varadhan's article (Stroock and Varadhan, 1971), and  $R_{s,r}$  is the Cameron–Martin density process

$$R_{s,t} = \exp\left[\int_{s}^{t} c(r, X_{r}) dW_{r} - \frac{1}{2} \int_{0}^{t} |c|^{2}(r, X_{r}) dr\right],$$
(1.3)

https://doi.org/10.1016/j.spl.2023.109855 0167-7152/© 2023 Elsevier B.V. All rights reserved.







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where *W* is the martingale part of *X*. A simple inspection gives the optimal solutions  $b(t, x) = \pm \kappa (x - y)/|x - y|$ , to which an explicit formula, in dimension one, for  $p_b(s, x; t, y)$  is given in Karatzas and Shreve (1984), Qian and Zheng (2002).

The question becomes difficult if we consider the simple optimal control problem for diffusion processes with barriers, which arise from many stochastic optimization problems for example in pricing problems for options.

Let  $G \subseteq \mathbb{R}^n$  be a domain with a smooth boundary  $\partial G$ , and  $\overline{G}$  denote its closure. We wish to locate a vector field b(t, x)(for  $t \ge 0$  and  $x \in \overline{G}$ ) bounded by  $\kappa$ , which maximizes (resp. minimizes) the probability  $q_b(s, x; t, y)$  (where  $0 \le s < t$ ,  $x, y \in \overline{G}$ ) of reflecting diffusion processes

$$dX_t = b(t, X_t)dt + dB_t + dL_t \tag{1.4}$$

started at  $X_s = x \in \overline{G}$  and finished at  $X_t = y \in \overline{G}$ , where  $B = (B_t)$  is a Brownian motion in  $\mathbb{R}^n$ , L is the local time of X with respect to the boundary  $\partial G$ , so that  $t \to L_t$  increases only on  $\{t : X_t \in \partial G\}$ . In this paper, we are going to establish the following

**Theorem 1.** Let  $\kappa \ge 0$  be a constant. Given  $y \in \overline{G}$  and T > 0. Let  $u^{\pm}(t, x)$  (where  $t \ge 0$  and  $x \in \overline{G}$ ) be the unique solution to the terminal and boundary problem of the backward parabolic equation

$$\frac{\frac{\partial}{\partial t}u + \frac{1}{2}\Delta u \pm \kappa |\nabla u| = 0, \quad \text{for } 0 \le t < T, \ x \in G \\ \lim_{t \uparrow T} u(t, x) = \delta_y(x), \quad \text{for } x \in \overline{G} \\ \frac{\partial}{\partial v}u(t, \cdot)|_{\partial G} = 0, \quad \text{for } 0 \le t \le T.$$

$$(1.5)$$

Define

$$b_{\kappa}^{\pm}(t,x) = \pm \kappa \frac{\nabla u^{\pm}(t \wedge T, x)}{|\nabla u^{\pm}(t \wedge T, x)|}$$

for  $t \ge 0$  and  $x \in \overline{G}$ . Let  $q_b(s, x; t, y)$  be the transition probability density of the diffusion defined by (1.4), where b(t, x), defined on  $[0, \infty) \times \overline{G}$ , is a bounded, Borel measurable vector field such that  $|b(t, x)| \le \kappa$  for  $t \ge 0$  and  $x \in \overline{G}$ . Then

$$q_{b_{\nu}^{-}}(t,x;T,y) \le q_{b}(t,x;T,y) \le q_{b_{\nu}^{+}}(t,x;T,y)$$
(1.6)

for all  $0 \le t < T$  and  $x \in \overline{G}$ .

Obviously, given *T* and *y*, the bounds in (1.6) for  $q_b(t, x; T, y)$  are optimal, and (1.5) can be considered as the Hamilton–Jacobi–Bellman (HJB) equation for the optimization problem for  $q_b(t, x; T, y)$ .

The semi-linear parabolic equations such as (1.5) have been studied in PDE literature (see e.g. Ladyženskaja et al. (1968)). In order to carry out explicit computations, one needs to consider the nodal set of the space-derivative  $\nabla u(t, x)$ , which also solves a non-linear parabolic equation. The study of nodal sets of solutions to semi-linear parabolic equations is however a difficult subject, and is far from complete. Interesting results may be found in the papers (Han and Lin, 1994; Lin, 1991) and etc.

In the case that  $G = \mathbb{R}^n$ , given T > 0 and  $y \in \mathbb{R}^n$  then  $b^{\pm}(t, x) = \mp \kappa (x - y)/|x - y|$ , the radial direction vector fields, which have been determined in Qian et al. (2003), Qian and Zheng (2004). Here we propose a new method for determining the HJB equations for this optimization problem based on a representation for the perturbations of reflecting diffusion processes, which extends the approach in Qian et al. (2003) to reflecting diffusion processes.

The paper is organized as following. In Section 2, we establish a representation formula for the transition probability density of the reflecting diffusion process. Then, we present the proof of Theorem 1 by the study of the representation and the HJB equation. In order to gain further knowledge about the optimal transition probabilities  $q_{b_{x}^{\pm}}(t, x; T, y)$  for the general case, we demonstrate, in Section 3, by numerical simulations that the optimal diffusion processes exhibit an interesting feature of phase transitions. Hence, the HJB equation may be equivalent to a free boundary problem.

#### 2. Optimal bounds for reflecting diffusion processes

This section is devoted to the proof of Theorem 1.

The main ingredient in the proof of Theorem 1 is a density version of the Cameron–Martin formula for reflecting diffusion processes. Let  $G \subseteq \mathbb{R}^n$  be an open subset with a smooth boundary  $\partial G$ , and  $\nu$  denotes the outer unit normal vector fields along  $\partial G$ . Suppose b(t, x) and c(t, x) are two bounded (time-dependent) vector fields for  $t \ge 0$  and  $x \in \overline{G}$ . Let  $(X_t, \mathbb{P}_{s,x})$  be the reflecting diffusion process with infinitesimal generator

$$\mathscr{L}_{t,x} = \frac{1}{2}\Delta + b(t,x) \cdot \nabla$$

with its state space  $\overline{G}$ , that is,  $\mathbb{P}_{s,x}$  (for every  $s \ge 0$  and  $x \in \overline{G}$ ) is the solution to the martingale problem (see e.g. Stroock and Varadhan (1971)):

$$M_t^{[f]} = f(t, X_t) - f(s, X_s) - \int_s^t \mathscr{L}_{r, X_r} f(r, X_r) dr$$

is a local martingale (where  $t \ge s$ ) for every  $f \in C_b^{1,2}([0,\infty) \times \overline{G})$  such that  $\frac{\partial}{\partial v} f(t, \cdot)|_{\partial G} = 0$  a.s. for all t > 0. Define a family of probability measures  $\mathbb{Q}_{s,x}$  by

$$\frac{d\mathbb{Q}_{s,x}}{d\mathbb{P}_{s,x}}\bigg|_{\mathcal{F}_t} = R_{s,t} := \exp\left\{\int_s^t c(r, X_r) \cdot dW_r - \frac{1}{2}\int_s^t |c|^2(r, X_r)dr\right\},\tag{2.1}$$

where  $s \leq t$ , and W is the martingale part of X which is a Brownian motion in  $\mathbb{R}^n$  under  $\mathbb{P}_{s,x}$ .

**Lemma 2.** Under above assumptions and notations.  $(X_t, \mathbb{Q}_{s,x})$  (for  $s \ge 0$  and  $x \in \overline{G}$ ) is a reflecting diffusion process with its infinitesimal generator

$$\tilde{\mathscr{L}}_{t,x} = \frac{1}{2}\Delta + (b(t,x) + c(t,x)) \cdot \nabla.$$

That is, for any pair  $s \ge 0$  and  $x \in \overline{G}$ ,

$$\tilde{M}_t^{[f]} = f(t, X_t) - f(s, X_s) - \int_s^t \tilde{\mathscr{L}}_{r, X_r} f(r, X_r) dr$$

is a local martingale for  $t \ge s$  under the probability  $\mathbb{Q}_{s,x}$ , for every  $f \in C_b^{1,2}([0,\infty) \times \overline{G})$  such that  $\frac{\partial}{\partial \nu} f(t,\cdot)|_{\partial G} = 0$  for all t > 0.

**Proof.** Without losing generality, we may assume that s = 0 and  $x \in \overline{G}$  is fixed. Under  $\mathbb{P}_{0,x}$ ,  $M^{[f]}$  is a local martingale for any  $f \in C^{1,2}$  such that  $\frac{\partial}{\partial v} f(t, \cdot)|_{\partial G} = 0$  for all t > 0. Hence, according to the Girsanov theorem,

$$M_t^{[f]} - \langle N, M^{[f]} \rangle_t$$

is a local martingale under the probability  $\mathbb{Q}_{0,x}$ , where  $N_t = \int_0^t c(r, X_r) \cdot dW_r$ . Since the martingale part W of X is a Brownian motion, so that

$$\langle N, M^{[f]} \rangle_t = \int_0^t \langle c, \nabla f \rangle (r, X_r) dr$$

and therefore

$$\tilde{M}_{t}^{[f]} = M_{t}^{[f]} - \int_{0}^{t} \langle c, \nabla f \rangle (r, X_{r}) dr = M_{t}^{[f]} - \langle N, M^{[f]} \rangle_{t}$$

is a local martingale under  $\mathbb{Q}_{s,x}$ , which completes the proof.  $\Box$ 

By using Lemma 2, for s < t and  $x, y \in \overline{G}$  and the fact that both  $q_b(s, x; t, y)$  and  $q_{b+c}(s, x; t, y)$  are Hölder continuous, conditional on  $X_t = y$ , we may obtain that

$$\frac{q_{b+c}(s,x;t,y)}{q_b(s,x;t,y)} = \mathbb{P}_{s,t}^{x,y} \left[ \exp\left\{ \int_s^t c(r,X_r) \cdot dW_r - \frac{1}{2} \int_s^t |c|^2(r,X_r) dr \right\} \right],$$
(2.2)

where  $\mathbb{P}_{s,t}^{x,y}$  is the conditional probability  $\mathbb{P}_{s,x}[\cdot|X_t = y]$ , which is a probability measure on  $(\Omega, \mathcal{F}_t)$  given via the density process

$$\frac{d\mathbb{P}_{s,t}^{X,y}}{d\mathbb{P}_{s,x}}\Big|_{\mathcal{F}_r} = \frac{q_{b+c}(r, X_r; t, y)}{q_b(s, x; t, y)} \quad \forall \ s < r < t.$$

$$(2.3)$$

**Lemma 3.** Let b(t, x) and c(t, x) be two bounded vector fields in  $\overline{G}$ , and assume that b is smooth. Let  $(X_t, \mathbb{P}_{s,x})$  be the reflecting diffusion process with generator  $\tilde{\mathscr{L}}_{t,x}$  as in Lemma 2. Then

$$q_{b+c}(s, x; T, y) = q_b(s, x; T, y) + \int_s^T \mathbb{P}_{s,x} \left[ R_{s,r} c(r, X_r) \cdot \nabla_x q_b(r, X_r; T, y) \right] dr$$
(2.4)

for any  $0 \le s < T$ , and any  $x, y \in \overline{G}$ , where R is given in (2.1).

**Proof.** Let s < T and  $x, y \in \overline{G}$  be fixed. Then we have two positive martingales, one is the Cameron–Martin density  $R_t = R_{s,t}$  given by (2.1), which is the exponential martingale of  $N_t = \int_s^t c(r, X_r) \cdot dW_r$ , so that

$$R_t = 1 + \int_s^t R_r c(r, X_r) \cdot dW_r$$
(2.5)

for  $s \le t \le T$ , which defines the probability  $\mathbb{Q}_{s,x}$ . The another is the conditional probability density

$$M_t = \frac{q_b(t, X_t; T, y)}{q_b(s, x; T, y)}, \quad \forall \ s < t < T$$

which determines the conditional probability  $\mathbb{P}_{s,T}^{x,y}$ , which can be written as

$$M_t = \frac{q_b(t, X_t; T, y)}{q_b(s, x; T, y)} = e^{\ln q_b(t, X_t; T, y) - \ln q_b(s, x; T, y)}.$$

Since *b* is smooth, the martingale part of  $\ln q_b(t, X_t; T, y) - \ln q_b(s, x; T, y)$  equals

$$Z_t := \int_s^t \nabla \ln q_b(r, X_r; T, y) \cdot dW_r$$

so that M must coincide with the exponential martingale of Z, hence

$$M_t = 1 + \int_s^t M_r \nabla \ln q_b(r, X_r; T, y) \cdot dW_r$$
(2.6)

for s < t < T. By ((2.5), (2.6)) we have

$$\langle M, R \rangle_t = \int_s^t M_r R_r c(r, X_r) \cdot \nabla \ln q_b(r, X_r; T, y) dr$$

and therefore

$$M_t R_t - \langle M, R \rangle_t$$

is a martingale up to *T*, with  $M_s R_s = 1$ . Since both  $q_{b+c}(s, x; T, y)$  and  $q_b(s, x; T, y)$  possess the Gaussian bounds (see e.g. Aronson (1968), Stroock (1988)), therefore

$$\begin{split} \frac{q_{b+c}(s,x;T,y)}{q_b(s,x;T,y)} &= \mathbb{P}_{s,T}^{x,y} \left[ R_T \right] = \lim_{\varepsilon \downarrow 0} \mathbb{P}_{s,T}^{x,y} \left[ R_{T-\varepsilon} \right] \\ &= \lim_{\varepsilon \downarrow 0} \mathbb{P}_{s,x} \left[ M_{T-\varepsilon} R_{T-\varepsilon} \right] \\ &= 1 + \mathbb{P}_{s,x} \left[ \int_s^T M_r R_r c(r,X_r) \cdot \nabla \ln q_b(r,X_r;T,y) dr \right] \\ &= 1 + \frac{1}{q_b(s,x;T,y)} \mathbb{P}_{s,x} \left[ \int_s^T R_r c(r,X_r) \cdot \nabla q_b(r,X_r;T,y) dr \right], \end{split}$$

which completes the proof of the lemma.  $\Box$ 

**Lemma 4.** Let  $\beta$  be a constant and  $y \in \overline{G}$ . Let w(t, x) be the unique weak solution to the following non-linear parabolic equation

$$\frac{\partial}{\partial t}w = \frac{1}{2}\Delta w + \beta |\nabla w| \text{ for } t > 0 \text{ and } x \in G$$
(2.7)

subject to the initial and boundary conditions that

$$\frac{\partial}{\partial \nu} w(t, \cdot) \bigg|_{\partial G} = 0 \quad \text{for } t > 0, \text{ and } w(0, x) = \delta_y(x).$$
(2.8)

Then both w(t, x) and its weak derivative  $\nabla w(t, x)$  are Hölder continuous for t > 0 and  $x \in \overline{G}$ , and for any given T > 0,

$$q_V(t, x; T, y) = w(T - t, x) \quad \text{for } 0 \le t < T \text{ and } x \in G,$$
(2.9)

where

$$V(t, x) = \beta \frac{\nabla w(T - t, x)}{|\nabla w(T - t, x)|}$$

and V(t, x) = 0 for  $t \ge T$ .

. .

**Proof.** According to the theory of parabolic equations (see e.g. Ladyženskaja et al. (1968)), the problem ((2.7), (2.8)) has a unique weak solution w(t, x) which is Hölder continuous for t > 0 and  $x \in \overline{G}$ . We need a bit more regularity of the solution w(t, x). To this end, for  $\varepsilon > 0$  consider the semi-linear parabolic equation

$$\frac{\partial}{\partial t}w^{\varepsilon} = \frac{1}{2}\Delta w^{\varepsilon} + \beta \sqrt{|\nabla w^{\varepsilon}|^{2} + \varepsilon^{2}} \quad \text{for } t > 0 \text{ and } x \in G$$
(2.10)

subject to the same initial and boundary conditions (2.8). Then, there is a unique strong solution  $w^{\varepsilon}(t, x)$  for every  $\varepsilon > 0$ which is smooth for t > 0 and  $x \in \overline{G}$ . Let  $w_x^{\varepsilon} = \nabla w^{\varepsilon}$  denote the space derivative. By taking derivatives in x for Eq. (2.10), we find that  $w_x^{\varepsilon}$  solves the Dirichlet boundary problem

$$\frac{\partial}{\partial t}w_{x}^{\varepsilon} = \left\lfloor \frac{1}{2}\Delta + \beta \frac{\nabla w^{\varepsilon}}{\sqrt{(\nabla w^{\varepsilon})^{2} + \varepsilon^{2}}} \cdot \nabla \right\rfloor w_{x}^{\varepsilon} \text{ for } t > 0 \text{ and } x \in G$$

subject to the Dirichlet boundary condition along  $\partial G$ . Notice that

$$\left|\beta \frac{\nabla w^{\varepsilon}}{\sqrt{\left(\nabla w^{\varepsilon}\right)^{2} + \varepsilon^{2}}}\right| \leq |\beta|$$

is uniformly bounded, so according to Nash's theory (see e.g. Nash (1958), or (Fabes and Stroock, 1986; Stroock, 1988)), there is a convergent sequence  $\{w_{\kappa}^{x_n}\}$  with  $\varepsilon_n \downarrow 0$ , which tends to the weak solution W to the parabolic equation

$$\frac{\partial}{\partial t}W = \left[\frac{1}{2}\Delta + \beta \frac{\nabla w}{|\nabla w|} \cdot \nabla\right]W$$

subject to the Dirichlet boundary condition along the boundary  $\partial G$  for t > 0. W is Hölder continuous in t > 0 and  $x \in G$ . W is a modification of the weak derivative  $\nabla w(t, x)$  for t > 0 and  $x \in G$ . We may thus conclude that  $\nabla w(t, x)$  is Hölder continuous in  $(0, \infty) \times G$ .

Given T > 0, and the unique weak solution w(t, x) to ((2.7), (2.8)), u(t, x) = w(T - t, x) solves the backward parabolic equation

$$\frac{\partial}{\partial t}u + \frac{1}{2}\Delta u + \beta \frac{\nabla w(T-t,\cdot)}{|\nabla w(T-t,\cdot)|} \cdot \nabla u = 0 \text{ for } t > 0 \text{ and } x \in G$$
(2.11)

subject to the initial and boundary conditions that

$$\frac{\partial}{\partial \nu} u(t, \cdot) \bigg|_{\partial G} = 0 \quad \text{for } t < T, \text{ and } \lim_{t \uparrow T} u(t, x) = \delta_y(x).$$
(2.12)

Since  $q_V(s, x; t, y)$  is the fundamental solution of the linear parabolic equation

$$\frac{\partial}{\partial t}u = \frac{1}{2}\Delta u + V(t, x) \cdot \nabla u$$

subject to the Neumann boundary condition at boundary  $\partial G$ , hence,  $(t, x) \rightarrow \tilde{u}(t, x) =: q_V(t, x; T, y)$  solves the backward equation

$$\frac{\partial}{\partial t}\tilde{u} + \frac{1}{2}\Delta\tilde{u} + \beta \frac{\nabla w(T-t,\cdot)}{|\nabla w(T-t,\cdot)|} \cdot \nabla\tilde{u} = 0 \quad \text{for } t > 0 \text{ and } x \ge 0$$
(2.13)

subject to the same initial-boundary conditions ((2.11), (2.12)). By the uniqueness, we must have  $\tilde{u}(t, x) = u(t, x)$  for t < T and  $x \in \bar{G}$ . Hence

$$q_V(t, x; T, y) = w(T - t, x)$$
 for  $t < T$  and  $x \in \overline{G}$ .  $\Box$ 

Proof of Theorem 1

Now we have the major ingredients to prove Theorem 1. Let us explain the ideas leading to the conclusions in Theorem 1. According to the representation formula (2.4), it is apparent that the optimal probability  $q_b(s, x; T, y)$  is achieved when

$$c(r, x) \cdot \nabla_{x}q_{b}(r, x; T, y)$$

has a definite sign for any c(t, x) such that both |b + c| and |b| are bounded by  $\kappa$ . Thus for fixed T > 0 and y, we want to find a vector field b(t, x), which may depend on T and y, such that  $|b| \le \kappa$ , and  $c(t, x) \cdot \nabla q_b(t, x; T, y)$  is non-negative (resp. negative) for all t < T and  $x \in \overline{G}$  for all c(t, x) satisfying that  $|c + b| \le \kappa$ . Clearly the best we can do is to choose b(t, x) such that

$$c(t, x) = A(t, x) \pm \kappa \frac{\nabla q_b(t, x; T, y)}{|\nabla q_b(t, x; T, y)|}$$

where A(t, x) = c(t, x) + b(t, x) so that  $|A(t, x)| \le \kappa$ . That is, the optimal vector fields should satisfy the functional equation

$$b^{\pm}(t,x) = \pm \kappa \frac{\nabla q_{b^{\pm}}(t,x;T,y)}{|\nabla q_{b^{\pm}}(t,x;T,y)|} \text{ for } t \ge 0 \text{ and } x \in \bar{G}.$$
(2.14)



**Fig. 1.** Derivative  $\nabla w(t, x)$ .

The question becomes to show the existence of such vector fields  $b^{\pm}(t, x)$ . Suppose such vector fields exist, then  $(t, x) \rightarrow u(t, x) := q_{b^{\pm}}(t, x; T, y)$  is the unique (weak) solution of the Neumann boundary problem to the backward equation

$$\frac{\partial}{\partial t}u(t,x) + \frac{1}{2}\Delta u(t,x) + b^{\pm}(t,x) \cdot \nabla u(t,x) = 0 \quad \text{for } 0 < t < T \text{ and } x \ge 0$$
(2.15)

subject to the terminal condition that  $\lim_{t\uparrow T} u(t, x) = \delta_y(x)$  and the boundary condition that  $\frac{\partial}{\partial v}u(t, \cdot)|_{\partial G} = 0$ . Together with (2.14), u(t, x) solves the initial and boundary problem to the semi-linear parabolic equation

$$\frac{\partial}{\partial t}u + \frac{1}{2}\Delta u \pm \kappa |\nabla u| = 0 \text{ for } 0 < t < T \text{ and } x \in G$$
(2.16)

subject to the initial and boundary conditions above. By the general theory of parabolic equations, the previous problem (2.16) has a unique weak solution, see e.g. Ladyženskaja et al. (1968). The proof is complete.

#### 3. The HJB equation: one dimensional case

The solution w(t, x) to the HJB equation (with reflecting boundary) ((2.7), (2.8)) plays the dominating role in our discussion, thus it is interesting to look for its properties in order to gain further knowledge about the optimal probability  $q_b(t, x; T, y)$  where  $|b| \le \kappa$ . We consider the case where  $G = [0, \infty)$  and y > 0.

Let  $\beta(=\pm\kappa)$  be a constant. Recall that, for one dimensional case with  $G = [0, \infty)$ , the HJB equation for our optimization problem is the boundary problem

$$\frac{\partial}{\partial t}w = \frac{1}{2}\Delta w + \beta |\nabla w| \text{ for } t > 0 \text{ and } x \ge 0$$
(3.1)



**Fig. 2.** Free boundary s(t) for fixed y > 0 demonstrating feature of "phase transition".

subject to the initial and boundary conditions that

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$$\lim_{x \downarrow 0} \frac{\sigma}{\partial x} w(t, x) = 0 \quad \text{for } t > 0, \text{ and } w(0, x) = \delta_y(x).$$
(3.2)

The solution w(t, x) > 0 for all t > 0 and  $x \ge 0$  by the maximal principle and  $w_x(t, x) = \frac{\partial}{\partial x}w(t, x)$  (for t > 0 and  $x \ge 0$ ) is Hölder continuous in t > 0 and  $x \ge 0$ .

To gain more explicit information about the optimal bounds in (1.6), we need to understand the space derivative  $\frac{\partial}{\partial x}w(t, x)$ . For  $t = \tau > 0$  is sufficiently small

$$w(\tau, x) \cong \frac{1}{\sqrt{2\pi\tau}} \left\{ e^{-\frac{(x-y)^2}{2\tau}} + e^{-\frac{(x+y)^2}{2\tau}} \right\}$$

and

$$w_{x}(\tau, x) \cong -\frac{1}{\sqrt{2\pi\tau^{3}}} e^{-\frac{(x-y)^{2}}{2\tau}} \left\{ x - y + (x+y)e^{-\frac{2xy}{\tau}} \right\}$$

which implies that for  $\tau > 0$  small enough,  $w_x$  has exactly one zero near y other than 0. According to the no-increasing theorem of zeros (see e.g. Angenent (1988), Matano (1982)), there are at most one zero of  $w_x(t, x)$  in  $(0, \infty)$  for every t > 0. Let  $s(t) = \max \{x \ge 0 : w_x(t, x) = 0\}$  for t > 0. Then s(t) > 0 for t > 0 but small. The simulations below demonstrate that a phase transition takes place at some  $\tau_{y,\beta}$ . For  $t < \tau_{y,\beta}$ , the non-linear parabolic Eq. (3.1) may be described by a two-phase free boundary problem

$$\frac{\partial}{\partial t}w = \frac{1}{2}\Delta w + \beta \nabla w$$
 for  $0 \le x \le s(t)$  and  $t \le \tau_{y,\beta}$ 

and

$$\frac{\partial}{\partial t}w = \frac{1}{2}\Delta w - \beta \nabla w \quad \text{for } x > s(t) \text{ and } t \leq \tau_{y,\beta}.$$

While after time  $\tau_{y,\beta}$ , the parabolic equation becomes one phase flow equation

$$\frac{\partial}{\partial t}w = \frac{1}{2}\Delta w - \beta \nabla w \quad \text{for } x > 0 \text{ and } t > \tau_{y,\beta}.$$

The numerical results of the derivative  $\nabla w(t, x)$  for fixed  $\beta = 1$  and y = 0, 1, 5, 10, respectively, and  $t \in [0, 5, 5]$  and  $x \in [0, 15]$  are shown in Fig. 1. Fig. 1 shows, as long as y > 0, there is at most one root other than 0 to the equation  $w_x(t, x) = 0$  for every t > 0. For y > 0, there exists  $\tau = \tau_{y,\beta} > 0$ , such that there is exactly one s(t) > 0 for every  $0 < t < \tau_{y,\beta}$  such that  $w_x(t, s(t)) = 0$ , and for every  $t \ge \tau_{y,\beta}$  there is no zero of  $w_x(t, \cdot)$ , i.e.  $w_x(t, x) < 0$ , for any x > 0. In Fig. 2, we have plotted the zeros s(t) for fixed y > 0 and  $\beta = 1$ . The point which s(t) crosses t-axis is the time  $\tau_{y,\beta}$ . So the initial and boundary problem ((3.1), (3.2)) may be equivalent to a free boundary problem.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

No data was used for the research described in the article.

#### Acknowledgments

The authors would like to thank Professor F. H. Lin for his helpful comments on the first version of the paper and for pointing out the Refs. Angenent (1988), Matano (1982) to our attention. X. Xu was supported by China Scholarship Council, Grant No. 201706010019.

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