BOUNDARY BEHAVIOUR OF DENSITIES FOR NON-NEGATIVE DIFFUSIONS

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Abstract. It is well-known that the transition density of a diffusion process solves the corresponding Kolmogorov forward equation. If the state space has finite boundary points, then naturally one also needs to specify appropriate boundary conditions when solving this equation. However, many processes of practical importance have degenerating diffusion coefficients, and for these processes the density may explode at the boundary. We prove a simple symmetry relation for the density that transforms the forward equation into a backward equation, the boundary conditions of which being much more straightforward to handle. This relation also allows us to derive new results on the precise asymptotic behaviour of the density at boundary points where the diffusion degenerates.

1. Introduction

In this article we study non-negative time-homogeneous diffusions X_t satisfying

$$dX_t = \beta(X_t)\,dt + \sigma(X_t)\,dB_t \tag{1}$$

where B is a standard Brownian motion, and with $X_0 = x > 0$. The non-negativity is guaranteed by the assumptions $\beta(0) \geq 0$ and $\sigma(0) = 0$. We are interested in the distribution of the process X_t at times $t > 0$. For $(x, y, t) \in (0, \infty)^2 \times [0, \infty)$ denote by

$$p(x, y, t) = P_x(X_t \in (y, y + dy))/dy \tag{2}$$

the density of the process. If this density exists and is regular enough, then it satisfies the Kolmogorov forward (Fokker-Planck) equation

$$\begin{cases} p_t(x, y, t) = (\alpha(y)p(x, y, t))_{yy} - (\beta(y)p(x, y, t))_y \\ p(x, y, 0) = \delta_x(y), \end{cases} \tag{3}$$

where $\alpha(y) = \sigma^2(y)/2$ and δ_x is the Dirac measure at x. The indices t and y denote differentiation with respect to the indicated variable. To ensure uniqueness of solutions to the system (3) within a class of functions of moderate growth one also needs to specify a boundary condition at $y = 0$. However, the density of a non-negative diffusion may explode at the boundary, and it is in many cases difficult to describe the boundary conditions needed to ensure that a given solution to (3) coincides with the density of X.

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In Section 2 we state conditions under which the density $p(x, y, t)$ exists and satisfies the symmetry relation

$$m(x)p(x, y, t) = m(y)p(y, x, t). \tag{4}$$

Here m is the density of the speed measure, i.e.

$$m(x) = \frac{1}{\alpha(x)} \exp\left\{ \int_1^x \frac{\beta(z)}{\alpha(z)}\, dz \right\}. \tag{5}$$

Note that the variable y plays the role of a *forward* variable on the left hand side of (4), whereas it is a *backward* variable on the right hand side. The function mp is thus symmetric in the spatial variables, so equation (4) can be viewed as an extension of the well-known symmetry of the heat kernel to general one-dimensional time-homogeneous processes.

The equality (4) may be employed to overcome the difficulties of specifying appropriate boundary conditions for the forward equation. Indeed, if one seeks the density p, rather than solving a forward equation in the second variable, relation (4) suggests to study the density p as a function of the *first* variable instead. The advantage of this procedure is that the density p is known to be well behaved as a function of the first variable, whereas it may explode as a function of the second variable as mentioned above. This difference in behaviour is precisely captured by the function m. In [6], the boundary behaviour and regularity for the degenerate backward equation is studied, and in [4] a numerical implementation is provided. Also note that the knowledge of the boundary regularity for the backward equation provided in [5] and [6] translates via (4) into precise asymptotics for the density.

We point out that the symmetry relation (4) seems to belong to the folklore in the area of one-dimensional diffusions, but we have not been able to find a detailed proof. This relation is formulated on page 149 in [8], see also [9]. The argument in [8] relies on spectral theory and is only outlined. It seems to us that our proof is more direct and elementary, at least for the cases covered by the analysis in the present paper.

From (4) we have a natural candidate for the density. Based on straightforward integration by parts and recent regularity results for the backward equation in [6], we are able to provide a verification procedure for the density. This verification procedure is also applicable in any situation in which the backward equation has a sufficiently regular solution, and may therefore also be of independent interest.

The disposition of the paper is as follows. In Section 2 we state in Theorem 2.2 the precise assumptions underlying equation (4). We also provide a complete description of the asymptotic behaviour of the density at the boundary in Theorem 2.3, together with a few specific examples that illustrate our results. In Section 3 we give our proofs of Theorems 2.2 and 2.3.

2. Symmetry of the density

Throughout this article we work under the following assumptions on the coefficients β and σ.

Hypothesis 2.1. *The drift $\beta : [0,\infty) \to \mathbb{R}$ is continuously differentiable with a bounded derivative, and it satisfies $\beta(0) \geq 0$. The volatility $\sigma : [0,\infty) \to [0,\infty)$ satisfies $\sigma(0) = 0$, $\sigma(x) > 0$ for $x > 0$, and the linear bound*

$$|\sigma(x)| \leq C(1+x)$$

for all $x \in (0,\infty)$, where C is a positive constant. Moreover, $\alpha := \sigma^2/2$ is continuously differentiable on $[0,\infty)$.

Hypothesis 2.1 ensures the existence and uniqueness of a strong solution to (1), compare Section IX.3 in [11]. Note that the imposed conditions $\sigma(0) = 0$ and $\beta(0) \geq 0$ forces the solution to stay non-negative. In fact, it follows from standard comparison results (see Theorem IX.3.7 in [11]) that if X reaches the state zero at some time t_0, then X either remains at zero for all times after t_0 if $\beta(0) = 0$, or is pushed back into the domain $(0,\infty)$ again by the drift if $\beta(0) > 0$. In some cases, however, zero is an unattainable boundary point for the diffusion X.

Theorem 2.2. *Assume Hypothesis 2.1 holds, and let m be defined as in (5). Then the corresponding density $p(x,y,t) : (0,\infty)^3 \to [0,\infty)$ exists and is continuous, and it satisfies*

$$m(x)p(x,y,t) = m(y)p(y,x,t). \tag{6}$$

As pointed out in the introduction, this result appeared in [8], see also [9]. However, the proof in [8] is sketchy and relies on rather advanced functional analysis. We believe that our proof is much more elementary and direct. It relies on integration by parts for which the out-integrated terms can be handled using recent regularity results for the backward equation provided in [6]. The proof is given in Section 3.

A consequence of Theorem 2.2 is that one can circumvent the problem of boundary conditions for the forward equation. Indeed, rather than solving the forward equation, the density p may be found by first solving a backward equation, and then using relation (6). The backward equation for a fixed forward variable y is given by

$$\begin{cases} p_t(x,y,t) = \alpha(x)p_{xx}(x,y,t) + \beta(x)p_x(x,y,t) & \text{for } (x,t) \in (0,\infty)^2 \\ p(x,y,0) = \delta_y(x) \\ p_t(0,y,t) = \beta(0)p_x(0,y,t). \end{cases} \tag{7}$$

In fact, a slight extension of the arguments in [6] gives that the density p is the unique classical solution to (7) that is bounded at spatial infinity. We emphasize that by a classical solution we mean a solution that is C^1 up to and including the boundary $x = 0$, so all derivatives in (7) exist in a classical sense. Also note that the boundary condition at $x = 0$ can be obtained heuristically by formally inserting $x = 0$ into the equation upon recalling that $\alpha(0) = 0$, and that this boundary condition is easily implemented numerically, compare [4].

Another consequence of Theorem 2.2 and the regularity results for the backward equation provided in [5] and [6] is that the asymptotic behaviour of the density for small values of y can be deduced. Our results on the asymptotic behaviour are summarised in the following theorem.

Theorem 2.3. *For fixed $x > 0$, the density $p(x, y, t)$ satisfies $p(x, y, t)/m(y) \to C(t)$ as $y \to 0$ for some continuously differentiable function $C(t) := p(0, x, t)/m(x) \geq 0$.*

(i) *If $\beta(0) > 0$, then $C(t)$ is positive for $t > 0$.*
(ii) *If $\beta(0) = 0$, then the function $C(t) \equiv 0$. In this case, define*

$$D(t) = \lim_{y \downarrow 0} \frac{p(x, y, t)}{ym(y)}.$$

(iia) *If there exists a constant $\epsilon > 0$ such that $\sigma(x) \geq \epsilon x^{1-\epsilon}$ for $0 < x < \epsilon$, then $D(t)$ is positive for $t > 0$.*
(iib) *If there exists $\epsilon > 0$ such that $\sigma(x) \leq \epsilon^{-1} x$ for $x \in (0, \epsilon)$, then $D \equiv 0$.*

Below we study a few examples. First we illustrate the symmetry relation (6) in the case when X is a geometric Brownian motion.

Example Let X be a geometric Brownian motion, i.e. $\beta(z) = rz$ and $\sigma(z) = \sigma z$ (with a slight abuse of notation) for some constants r and $\sigma > 0$. Then

$$X_t = x \exp\{(r - \sigma^2/2)t + \sigma B_t\}.$$

The density of the speed measure is given by

$$m(x) = \frac{2}{\sigma^2 x^2} \exp\left\{ \int_1^x \frac{2r}{\sigma^2 z}\, dz \right\} = \frac{2}{\sigma^2} x^{2r/\sigma^2 - 2},$$

and the density of X_t is

$$p(x, y, t) = \frac{1}{y\sigma\sqrt{t}} f\left(\frac{\ln(y/x) - (r - \sigma^2/2)t}{\sigma\sqrt{t}} \right),$$

where

$$f(z) = \frac{1}{\sqrt{2\pi}} \exp\{-z^2/2\}$$

is the density of a standard normal random variable. It is then straightforward to check that

$$\frac{p(x, y, t)}{p(y, x, t)} = \frac{m(y)}{m(x)}.$$

Moreover,

$$\frac{p(x, y, t)}{ym(y)} \to 0$$

as $y \to 0$ in accordance with (iib) of Theorem 2.3.

Next we show how Theorem 2.2 can be used to determine the density and its asymptotics by solving the backward equation.

Example Let X be the CIR-process, i.e.

$$dX_t = (b - aX_t)\, dt + \sigma\sqrt{X_t}\, dB_t,$$

where b, a and σ are positive constants. The distribution of the CIR-process can be found for example on page 57 in [2], but is rather involved and the asymptotics close to zero are far from apparent. However, according to classical results by Feller [7], the density explodes if $b < \sigma^2/2$, it tends to zero if $b > \sigma^2/2$, and it tends to a positive number if $b = \sigma^2/2$.

In line with Theorem 2.2, the density $y \mapsto p(x,y,t)$ can be found by first solving the *backward* equation

$$\begin{cases} p_t(x,y,t) = \frac{\sigma^2 x}{2} p_{xx}(x,y,t) + (b-ax)p_x(x,y,t) & \text{for } t > 0 \\ p(x,y,0) = \delta_y(x) \\ p_t(0,y,t) = bp_x(0,y,t) \end{cases}$$

to determine the function $x \mapsto p(x,y,t)$. Since the lateral boundary condition $p_t = bp_x$ for the backward equation is easily implemented, it is straightforward to solve this equation numerically, compare [4]. Next, to determine the function $y \mapsto p(x,y,t)$, one uses the fact that

$$m(x) = \frac{2}{\sigma^2} x^{\frac{2b}{\sigma^2}-1} \exp\left\{\frac{2a}{\sigma^2}(1-x)\right\}$$

and employs the relation

$$p(x,y,t) = m(y)p(y,x,t)/m(x) = (y/x)^{2b/\sigma^2-1} \exp\left\{\frac{2a}{\sigma^2}(x-y)\right\} p(y,x,t).$$

By (i) of Theorem 2.3 we find that for fixed x and t, the density $p(x,y,t)$ behaves like a positive multiple of y^{2b/σ^2-1} for small y. Thus our method refines the results of Feller refered to above (these precise asymptotics are also hinted at in [10], but no formal proof is provided).

Example The Constant Elasticity of Variance (CEV) process is given by

$$dX_t = \sigma X_t^\gamma \, dB_t,$$

where $\sigma > 0$ and $\gamma \in [1/2, 1]$ are constants. Clearly, geometric Brownian motion is contained as the special case $\gamma = 1$. In order to determine the transition density $p(t,x,y)$ as a function of y, one may first solve the backward equation

$$\begin{cases} p_t(x,y,t) = \frac{\sigma^2 x^{2\gamma}}{2} p_{xx}(x,y,t) & \text{for } t > 0 \\ p(x,y,0) = \delta_y(x) \\ p(0,y,t) = 0, \end{cases}$$

and then the density is easily found using the relation $p(x,y,t) = (x/y)^{2\gamma} p(y,x,t)$. By (iia) of Theorem 2.3 we have $p(x,y,t) \sim y^{1-2\gamma}$ for small y if $\gamma < 1$.

3. Proofs of Theorems 2.2 and 2.3

3.1. **Proof of Theorem 2.2.** Let $p_0 : (0,\infty) \to [0,\infty)$ be a smooth and non-negative function with compact support. Below p_0 is the density of an initial distribution, so we also assume that it integrates to unity. Our candidate for the density of X_t, where X_0 is independent of the Brownian motion B and has density p_0, is

$$q(y,t) := F(y,t)m(y), \tag{8}$$

where F is defined by

$$F(y,t) = E_y\left[p_0(X_t)/m(X_t)\right].$$

It follows from [6] that F is the unique bounded classical solution to the corresponding backward equation

$$(9)\qquad \begin{cases} F_t(y,t) = \alpha F_{yy}(y,t) + \beta F_y(y,t) & \text{for } (y,t) \in (0,\infty)^2 \\ F(y,0) = p_0(y)/m(y) \\ F_t(0,t) = \beta(0) F_y(0,t). \end{cases}$$

Also note that $q(y,0) = p_0(y)$, so q certainly has the correct initial value.

Lemma 3.1. *The function q satisfies the forward equation*

$$(10)\qquad q_t = (\alpha q)_{yy} - (\beta q)_y$$

for $(y,t) \in (0,\infty)^2$.

Proof. This follows from straightforward differentiation of q defined in (8) together with (9). □

Lemma 3.2. *Let T be a positive constant. Then there exists an integrable function $H : (0,\infty) \to (0,\infty)$ such that $q(x,t) \le H(x)$ for $(x,t) \in (0,\infty) \times [0,T]$.*

Proof. Since p_0/m has compact support, it satisfies

$$p_0(x)/m(x) \le h(x) := \begin{cases} 0 & \text{if } x \notin [a,b] \\ C & \text{if } x \in [a,b] \end{cases}$$

for some positive constants a, b and C. The ordinary differential equation

$$(11)\qquad \alpha\varphi_{xx} + \beta\varphi_x - \varphi = 0$$

has a decreasing solution φ and an increasing solution ψ. These are unique up to multiplication with positive constants if one in addition requires that $e^{-t}\varphi(X_t)$ and $e^{-t}\psi(X_t)$ are local martingales. (More explicitly, if 0 is a non-singular boundary point for X, then an appropriate boundary condition for ψ is needed at 0.) It follows that the function φ satisfies

$$E_x e^{-\tau_b} = \varphi(x)/\varphi(b)$$

for $x > b$, and ψ satisfies

$$E_x e^{-\tau_a} = \psi(x)/\psi(a)$$

for $x < a$, where $\tau_b = \inf\{t : X_t = b\}$ and $\tau_a = \inf\{t : X_t = a\}$ are the first hitting times of b and a, respectively. For further properties of the functions φ and ψ, see Chapter 4.6 in [8] or pages 18-19 in [1]. For $t \in [0,T]$ we then have

$$(12)\qquad \begin{aligned} F(x,t) &= E_x p_0(X_t)/m(X_t) \le E_x h(X_t) \le e^t E_x e^{-(\tau_b \wedge t)} h(X_{\tau_b \wedge t}) \\ &\le e^t E_x e^{-\tau_b} h(X_{\tau_b}) = C e^t \frac{\varphi(x)}{\varphi(b)} \le D\varphi(x) \end{aligned}$$

for some constant D. Consequently, the candidate function q satisfies

$$\begin{aligned} q(x,t) \le D\varphi(x)m(x) &= D(\varphi_{xx}(x) + \frac{\beta}{\alpha}\varphi_x(x)) \exp\{\int_1^x \frac{\beta}{\alpha}\,dy\} \\ &= D(\varphi_x(x) \exp\{\int_1^x \frac{\beta}{\alpha}\,dy\})_x, \end{aligned}$$

where we used (11). Since $\varphi_x(x)\exp\{\int_1^x \frac{\beta}{\alpha}\,dy\} \to 0$ as $x \to \infty$ (see page 130 in [8]), the function H can be defined by $H(x) = D\varphi(x)m(x)$ for $x > b$.

Similarly, for $x < a$ and $t \in [0,T]$ we have $F(x,t) \le D\psi(x)$ where D is a constant possibly different from above. It follows that

$$q(x,t) \le D\psi(x)m(x) = D(\psi_x(x)\exp\{\int_1^x \frac{\beta}{\alpha}\,dy\})_x.$$

Since $\psi_x(x)\exp\{\int_1^x \frac{\beta}{\alpha}\,dy\}$ has a finite limit at $x=0$, see page 130 in [8], we may define $H(x) = D\psi(x)m(x)$ for $x < a$. Since q is bounded on $[a,b]$, the lemma follows. □

Remark A similar bound is also valid for the time derivative of the candidate density. More precisely, the function H in Lemma 3.2 can be chosen so that $|q_t(x,t)| \le H(x)$ for $(x,t) \in (0,\infty)\times[0,T]$. To see this, note that $q_t = F_t m$, and that F_t has the stochastic representation

$$F_t(y,t) = E_y\left[f(X_t)\right],$$

where $f(x) = \alpha(x)F_{xx}(x,0) + \beta(x)F_x(x,0)$.

Let g be a C^∞ function on $(0,\infty)$ with compact support, and define

$$u(y,t) := E_{y,t}g(X_T)$$

for some fixed time $T > 0$. By the results in [6], the function u is the unique bounded classical solution of

$$\left\{\begin{array}{ll} u_t + \alpha u_{yy} + \beta u_y = 0 & \text{for } (y,t)\in(0,\infty)\times(0,T) \\ u(y,T) = g(y) & \\ u_t(0,t) + \beta(0)u_y(0,t) = 0. & \end{array}\right. \tag{13}$$

Proposition 3.3. *For any $t \in [0,T]$ we have*

$$\int_0^\infty u(y,t)q(y,t)\,dy = \int_0^\infty u(y,0)q(y,0)\,dy. \tag{14}$$

Proof. Integration by parts gives

$$\begin{aligned}\int_0^\infty\int_0^t u_s(y,s)q(y,s)\,dsdy &= \int_0^\infty u(y,t)q(y,t) - u(y,0)q(y,0)\,dy \\ &\quad - \int_0^\infty\int_0^t u(y,s)q_s(y,s)\,dsdy.\end{aligned} \tag{15}$$

These integrals are all finite by Lemma 3.2 and the remark after its proof (note here that $u_s q = u_s F m$ and $uq_s = uF_s m$, so the first integral is of the same type as the last one since the roles of u and F are interchangeable).

On the other hand, we also have

$$\begin{aligned}-\int_0^\infty u_s(y,s)q(y,s)\,dy &= \int_0^\infty (\alpha u_{yy}(y,s) + \beta u_y(y,s))\,q(y,s)\,dy \\ &= \int_0^\infty u(y,s)((\alpha q)_y - \beta q)_y(y,s)\,dy \\ &\quad + \left[u_y(y,s)(\alpha q)(y,s) - u(y,s)((\alpha q)_y - \beta q)(y,s)\right]_{y=0}^\infty.\end{aligned} \tag{16}$$

Now note that $(\alpha q)_y - \beta q$ is an anti-derivative with respect to y of the integrable function q_s. Thus it has finite limits both at zero and infinity. The function u tends to zero at infinity since $u \le D'\varphi$ by a similar argument as in (12), so we have $u(\infty,s)((\alpha q)_y - \beta q)(\infty,s) = 0$. Furthermore, if $\beta(0) = 0$, then $u(0,s)=0$ and the term $u((\alpha q)_y-\beta q)$ vanishes at zero. On the other hand, if $\beta(0)>0$, then

$$(\alpha q)_y-\beta q=F_y\exp\{\int_1^y\frac{\beta}{\alpha}dz\}\to 0 \tag{17}$$

as $y\to 0$ since F_y is bounded and $\alpha(y)\leq Cy$ for $y\in(0,C^{-1})$, where $C>0$ is some constant. Consequently, the out-integrated term

$$[u(y,s)((\alpha q)_y-\beta q)(y,s)]_{y=0}^{\infty}$$

equals zero. Also note that since

$$u((\alpha q)_y-\beta q)=uF_y\exp\{\int_1^y\frac{\beta}{\alpha}dz\},$$

the two terms $u((\alpha q)_y-\beta q)$ and $u_y\alpha q=u_yF\exp\{\int_1^y\frac{\beta}{\alpha}dz\}$ are of the same type. More precisely, u and F are both solutions to the same backward equation, so their roles are interchangeable in the arguments above. Consequently, all out-integrated terms in (16) vanish, which implies that

$$\begin{aligned} -\int_0^\infty u_s(y,s)q(y,s)\,dy &= \int_0^\infty u(y,s)((\alpha q)_y-\beta q)_y(y,s)\,dy \\ &= \int_0^\infty u(y,s)q_s(y,s)\,dy. \end{aligned} \tag{18}$$

Integrating (18) and combining with (15), it follows that

$$\int_0^\infty u(y,0)q(y,0)\,dy=\int_0^\infty u(y,t)q(y,t)\,dy,$$

which finishes the proof. □

Now let Z be a random variable independent of the Brownian motion B and with density p_0. Denote by X^Z the solution of (1) with initial condition $X_0=Z$. By the law of total probability and choosing $t=T$ in (14) we find that

$$\begin{aligned} Eg(X_T^Z) &= \int_0^\infty u(y,0)q(y,0)\,dy \\ &= \int_0^\infty u(y,T)q(y,T)\,dy=\int_0^\infty g(y)q(y,T)\,dy. \end{aligned}$$

Since this holds for any smooth function g with bounded support, the function $q(y,T)$ is indeed the density of X_T^Z. Now replace the starting distribution p_0 by a sequence of distributions p_0^n that approximates a point mass at a point x and denote the corresponding q by q^n. Letting $n\to\infty$ we find that

$$E_xg(X_T)=\int_0^\infty g(y)q(y,T)\,dy,$$

where the standard notation is used, i.e. the subindex x means that $X_0=x$, and q is the pointwise limit of q^n. Since this holds for any smooth function g with compact support, $q(y,T)$ is the density at y of X_T started at x, i.e. $q(y,T)=p(x,y,T)$.

On the other hand, by the definition of q^n we have that

$$q^n(y,T) = m(y)E_y\left[\frac{p_0^n(X_T)}{m(X_T)}\right].$$

The expression on the right-hand side tends to $\frac{m(y)}{m(x)}p(y,x,T)$ as n tends to infinity, compare (2). This finishes the proof of Theorem 2.2.

Remark The fact that $(\alpha q)_y - \beta q = 0$ at $y = 0$ if $\beta(0) > 0$, compare (17), is for us a consequence of the construction of q. In contrast, in [10], based on [7], it appears as a boundary condition imposed to ensure that the solution to the forward equation has total mass one. Note, however, that this condition is difficult to implement numerically since $\alpha(0) = 0$. Also note that our approach works just as well in the case where the total mass on the strictly positive real axis is less than one.

3.2. **Proof of Theorem 2.3.** The existence and differentiability of C follow from Theorem 2.2 and the C^1 regularity of $(x,t) \mapsto p(x,y,t)$ provided in [6].

Now assume that $\beta(0) > 0$. Then the diffusion X can reach any non-empty interval $(a,b) \subseteq (0,\infty)$ with positive probability if started from 0. It follows using the maximum principle that $p(0,y,t) > 0$, which proves (i).

Next assume that $\beta(0) = 0$. Then the boundary condition for the backward equation is $p_t(0,y,t) = \beta(0)p_x(0,y,t) = 0$. Since $p(0,y,0) = 0$, this integrates to $p(0,y,t) = 0$. By (6),

$$\frac{p(x,y,t)}{m(y)} = \frac{p(y,x,t)}{m(x)} \to 0$$

as $y \to 0$, which proves that $C(t) = 0$. Now, under the assumption in (iia), the derivative $p_x(0,y,t)$ is strictly positive by Theorem 2 in [5], so $D(t) > 0$. Similarly, under the assumption in (iib), the derivative $p_x(0,y,t)$ is 0 (see Theorem 3 in [5]), so $D(t) = 0$. This finishes the proof of Theorem 2.3.

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