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A CLASSIFICATION OF DIFFUSION PROCESSES WITH BOUNDARIES BY THEIR INVARIANT MEASURES

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Let D be a connected, compact region in R^d. If $d = 1$, then for each nice probability measure μ on D and diffusion coefficient a, there exists a unique drift such that μ is invariant for the resulting diffusion process with reflection at the boundary. For $d > 1$, there is no uniqueness. For each diffusion matrix a, reflection vector J, and nice probability measure μ on D, we classify the collection of drifts such that μ is invariant for the resulting diffusion process. We use the theory of the I-function and, in the course of things, answer a question about the I-function.

1. Introduction. Let $D \subset R^d$ be a connected, compact region defined by $\theta \leq 0$ for some $\theta \in C^2(R^d)$ with $\nabla \theta \neq 0$ on $\theta = 0$, that is, on ∂D. Consider a diffusion process on D with reflection at the boundary generated by $L = \frac{1}{2} \nabla \cdot a\nabla + b\nabla$ with boundary condition $J \cdot \nabla u(x) = 0$ for $x \in \partial D$. We will impose the following conditions on the coefficients: a is a positive matrix with entries $a_{ij} \in C^1(D)$, b, the drift is a d-vector with components $b_i \in C^1(D)$ (henceforth we will say $b \in C^1(D)$), and J is a C^1-vector field on ∂D which satisfies $J \cdot n(x) \leq \alpha < 0$ for $x \in \partial D$ and α a constant. Here $n(= \nabla\theta/|\nabla\theta|)$ is the outward unit normal on ∂D.

The above conditions on the coefficients are sufficient to guarantee the existence and uniqueness of a diffusion process with the above generator [3]. The conditions on a and J and θ allow us to write J (up to multiplication by a scalar function which is of course irrelevant in defining the process) in the form $J = -a \cdot n + T$ where T is a C^1-vector field on ∂D. Denote by $I(a, b, T)$ the unique diffusion process corresponding to a, b, and T and let $\mathscr{A}(a, T) = \{I(a, b, T), b \in C^1(D)\}$. A unique invariant measure exists for each diffusion process above. Let $P'(D)$ be the set of probability measures μ on D with strictly positive densities $\varphi \in C^2(D)$ and let $g = \varphi^{1/2}$. We consider the following question. Given $\mu \in P'(D)$, for which diffusion processes in the above class is μ invariant?

Remark. In one dimension, $T \equiv 0$ automatically and, for any a, there is a unique diffusion process for which μ is invariant, namely the one with drift given by $b = a(g'/g)$.

In two or more dimensions, there is no such uniqueness. For example, for 2-dimensional Brownian motion inside the unit circle with normal reflection at the boundary and with a drift in the θ-direction of arbitrary magnitude but depending

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only on $r = (x^2 + y^2)^{1/2}$, the invariant measure is uniform, that is, a multiple of Lebesgue measure. (The generator of the process is $L = \frac{1}{2}\Delta + f(r)y(\partial/\partial x) - f(r)x(\partial/\partial y)$ with $du/dr = 0$ on $r = 1$.) In general, if $T \equiv 0$, then one process for which μ will be invariant is $I(a, a\nabla g/g, 0)$. If $T \not\equiv 0$, then no such explicit solution exists.

To answer our question, we will fix a and T and then describe the class of drifts for which the resulting process possesses μ as its invariant measure. The method we will employ utilizes the I-function, and, in the course of things, also answers a question concerning the I-function.

We briefly describe the I-function theory. Let $\omega = x(\cdot)$ denote a sample path and define $L_t(\omega, B) = (1/t)\int_0^t \chi_{(B)}(x(s))\,ds$ for $B \subset D$. Thus, $L_t(\omega, B)$ measures the proportion of time up to t that the particular path ω spends in the set B. Hence $L_t(\omega, \cdot) \in \mathscr{P}(D)$, the space of probability measures on D. Define the I-function by

$$I(u) = -\inf_{u\in\mathscr{D}^+} \int_D \frac{Lu}{u}\,d\mu$$

where $\mathscr{D}^+ = \{u \in \mathscr{D}\colon u \geq c > 0\}$ and $\mathscr{D}$ is the domain of the generator L. Let P_x be the probability measure on $C([0, \infty), D)$, the space of continuous functions from $[0, \infty)$ to D, induced by the diffusion process starting from $x \in D$. Donsker and Varadhan [1] have shown that for open sets $G \subset \mathscr{P}(D)$, $\liminf_{t\to\infty}(1/t)\log P_x(L_t(\omega, \cdot) \in G) \geq -\inf_{\mu\in G} I(\mu)$, for all $x \in D$ and for closed sets $C \subset \mathscr{P}(D)$, $\limsup_{t\to\infty}(1/t)\log P_x(L_t(\omega, \cdot) \in C) \leq -\inf_{\mu\in C} I(\mu)$, for all $x \in D$. Thus for large t and a small neighborhood $N(\mu)$ of μ, $P_x(L_t(\omega, \cdot) \in N(\mu))$ is "roughly" $e^{-tI(\mu)}$. Furthermore $I(\mu) = 0$ if and only if μ is invariant for the process (use Lemmas 2.5 and 3.1 in [1]). It is this property of $I(\cdot)$ which we will utilize.

In [2], we gave the following representation for $I(\mu)$ which is valid for diffusion processes of the above type. For $\mu \in \mathscr{P}(D)$ with strictly positive density $\varphi \in C^1(D)$ and $g = \varphi^{1/2}$,

$$\begin{aligned} I(\mu) &= \frac{1}{2}\int_D \left(\frac{\nabla g}{g} - a^{-1}b\right)a\left(\frac{\nabla g}{g} - a^{-1}b\right)g^2\,dx \\ &\quad - \frac{1}{2}\int_{\partial D}\left(\frac{\nabla g}{g}\cdot T\right)g^2\,d\sigma \\ &\quad - \inf_{h\in C^2(D)}\left[\frac{1}{2}\int_D (\nabla h - a^{-1}b)a(\nabla h - a^{-1}b)g^2\,dx \right. \\ &\qquad\qquad \left. - \frac{1}{2}\int_{\partial D}(\nabla h \cdot T)g^2\,d\sigma\right]. \end{aligned} \tag{1.1}$$

Furthermore, there exists a unique (up to a constant) $h_{\mu,b}$ (we have suppressed the dependence on a and T) for which the infimum above is attained and, in fact, $h_{\mu,b} \in C^2$ and satisfies

$$\begin{aligned} &\nabla \cdot [g^2(b - a\nabla h_{\mu,b})] = 0 \quad \text{in} \quad D \\ &2g^2(b - a\nabla h_{\mu,b}) \cdot n = \nabla \cdot (g^2 T) \quad \text{on} \quad \partial D. \end{aligned} \tag{1.2}$$

Thus, we can recast our question in the following terms. Fix a, T and μ and solve $I(\mu) = 0$ for b.

REMARK. Note from (1.1) that $I(\mu) = 0$ if and only if $h_{\mu,b} = \nabla g/g$.

For fixed a, we establish the following equivalence classes for drifts in $C^1(D)$. We will say that 2 drifts b_1 and b_2 are a-equivalent if and only if $a^{-1}b_1$ and $a^{-1}b_2$ differ by a gradient function. That is, $b_1 \sim_a b_2$ if and only if $a^{-1}b_1 - a^{-1}b_2 = \nabla q$ for some q. We have the following simple lemma.

LEMMA 1.3. *In one dimension there is only one a-equivalence class. In two or more dimensions, there exist uncountably many equivalence classes.*

PROOF. In one dimension every drift is a gradient. For $d > 1$ dimensions, let $b_c = cav$ where $c \in \mathbb{R}$ and v is the d-vector $(x_2, -x_1, 0, \cdots, 0)$. Clearly $b_{c_1} \sim_a b_{c_2}$ if and only if $c_1 = c_2$.

From each equivalence class, pick out one drift function. Call this collection of drifts, one from each equivalence class, $\mathscr{E}_a$. Define $\mathscr{A}_\mu(a, T) = \{I(a, b, T) \in \mathscr{A}(a, T)$: μ is invariant for $I(a, b, T)\}$.

THEOREM 1.4. *We have* $b_1 - a\nabla h_{\mu,b_1} = b_2 - a\nabla h_{\mu,b_2}$ *if and only if* $b_1 \sim_a b_2$. *Also* $\mathscr{A}_\mu(a, T) = \{I(a, b, T)\colon b = \tilde{b} + a(\nabla g/g) - a\nabla h_{\mu,\tilde{b}},\ \tilde{b} \in \mathscr{E}_a\}$. *Hence there is a one-to-one correspondence between elements of* $\mathscr{E}_a$ *and elements of* $\mathscr{A}_\mu(a, T)$ *given by* $\tilde{b} \to I(a, \tilde{b} + (a\nabla g/g) - a\nabla h_{\mu,\tilde{b}}, T)$.

REMARK. In formula (1.1), the representation of the I-function, there appear two functions, g and $h_{\mu,b}$. Of course g has the probabilistic interpretation of being the square root of the density of μ. Theorem (1.4) allows us to give a probabilistic interpretation to $h_{\mu,b}$ as well, which we state as:

COROLLARY 1.5. *Consider a process* $I(a, b, T)$ *and a measure* $\mu \in \mathscr{P}'(D)$. *The I-function for the process is expressed in terms of g, the square root of the density of* μ *and* $h_{\mu,b}$ *which has the following probabilistic interpretation: Among all processes* $I(a, b, + a\nabla q, T)$ *with* $q \in C^1(D)$, *the process with* $\nabla q = (\nabla g/g) - \nabla h_{\mu,b}$ *is the unique one for which* μ *is invariant.*

Except for the fact that ∇q need not be in $C^1(D)$, this corollary follows immediately from the theorem. We will prove the corollary in Section 2 in the course of proving the theorem.

REMARK. If we let $L = ½\, \nabla \cdot a\nabla + b\nabla + (a\nabla g/g)\nabla - \nabla h\nabla$, then g^2 is an invariant density for the process generated by L if and only if $\int_D g^2 Lu\, dx = 0$ for all $u \in C^2(D) \cap (\nabla u \cdot J = 0$ on $\partial D)$. If we solve this for h, we arrive at (1.2). Hence the one-to-one correspondence between $\mathscr{E}_a$ and $\mathscr{A}_\mu(a, T)$ could be obtained this way. The advantage of our method is that one sees the probabilistic interpretation of the unique gradient which minimizes the variational part of the I-function.

2. Proof of Theorem. Suppressing the dependence on a, T and g, let $\psi(\nabla h, b) = \frac{1}{2}\int_D (\nabla h - a^{-1}b)a(\nabla h - a^{-1}b)g^2\,dx - \frac{1}{2}\int_{\partial D} (\nabla h \cdot T)g^2\,d\sigma$. Then $I(u) = \psi(\nabla g/g, b) - \inf_{h\in C^2(D)}\psi(\nabla h, b)$. To prove the first statement in the theorem, pick $b_1 \sim_a b_2$ and say $b_1 = b_2 + a\nabla q$. Then $\psi(\nabla h, b_1) = \psi(\nabla h, b_2 + a\nabla q)$, and making the substitution $\nabla\tilde{h} = \nabla h - \nabla q$, we see that $\inf_{h\in C^2(D)}\psi(\nabla h, b_1) = \inf_{\tilde{h}\in C^2(D)}\psi(\nabla\tilde{h}, b_2) - \int_{\partial D}(\nabla q \cdot T)g^2\,d\sigma$.

The infimum of the left-hand side of this equation is attained at $h = h_{\mu,b_1}$ and the infimum of the right-hand side is attained at $\tilde{h} = h_{\mu,b_2}$. Since $\nabla\tilde{h} = \nabla h - \nabla q$, we have $\nabla h_{\mu,b_2} = \nabla h_{\mu,b_1} - \nabla q$ and thus $b_1 - a\nabla h_{\mu,b_1} = (b_2 + a\nabla q) - a(\nabla h_{\mu,b_2} + \nabla q) = b_2 - a\nabla h_{\mu,b_2}$. Conversely, suppose $b_1 - a\nabla h_{\mu,b_1} = b_2 - a\nabla h_{\mu,b_2}$. Then $a^{-1}b_1 - a^{-1}b_2 = \nabla h_{\mu,b_1} - \nabla h_{\mu,b_2}$ and thus $b_1 \sim_a b_2$.

Now we show that for any $\tilde{b} \in C^1(D)$, μ is invariant for $I(a, \tilde{b} + (a\nabla g/g) - a\nabla h_{\mu,\tilde{b}}, T)$. We do this by showing that $I(\mu) = 0$ for this process. Making the substitution $\nabla\tilde{h} = \nabla h - (a\nabla g/g) + \nabla h_{\mu,\tilde{b}}$, we have

$$\begin{aligned}\inf_{h\in C^2(D)}\psi\left(\nabla h, \tilde{b} + \frac{a\nabla g}{g} - a\nabla h_{\mu,\tilde{b}}\right) &= \inf_{\tilde{h}\in C^2(D)}\psi(\nabla\tilde{h}, \tilde{b}) - \frac{1}{2}\int_{\partial D}\left(\frac{\nabla g}{g}\cdot T\right)g^2\,d\sigma \\ &\quad + \frac{1}{2}\int_{\partial D}(\nabla h_{\mu,\tilde{b}}\cdot T)g^2\,d\sigma \\ &= \psi(\nabla h_{\mu,\tilde{b}}, \tilde{b}) - \frac{1}{2}\int_{\partial D}\left(\frac{\nabla g}{g}\cdot T\right)g^2\,d\sigma + \frac{1}{2}\int_{\partial D}(\nabla h_{\mu,\tilde{b}}\cdot T)g^2\,d\sigma.\end{aligned}$$

Hence, for the process $I(a, \tilde{b} + (a\nabla g/g) - a\nabla h_{\mu,\tilde{b}}, T)$, we have

$$\begin{aligned}I(\mu) &= \psi\left(\frac{\nabla g}{g}, \tilde{b} + \frac{a\nabla g}{g} - a\nabla h_{\mu,\tilde{b}}\right) - \inf_{h\in C^2(D)}\psi\left(\nabla h, \tilde{b} + \frac{a\nabla g}{g} - a\nabla h_{\mu,\tilde{b}}\right) \\ &= \psi\left(\frac{\nabla g}{g}, \tilde{b} + \frac{a\nabla g}{g} - a\nabla h_{\mu,\tilde{b}}\right) - \psi(\nabla h_{\mu,\tilde{b}}, \tilde{b}) + \frac{1}{2}\int_{\partial D}\left(\frac{\nabla g}{g}\cdot T\right)g^2\,d\sigma \\ &\quad - \frac{1}{2}\int_{\partial D}(\nabla h_{\mu,\tilde{b}}\cdot T)g^2\,d\sigma \\ &= \frac{1}{2}\int_D(\nabla h_{\mu,\tilde{b}} - a^{-1}\tilde{b})a(\nabla h_{\mu,\tilde{b}} - a^{-1}\tilde{b})g^2\,dx \qquad (2.1) \\ &\quad - \frac{1}{2}\int_{\partial D}\left(\frac{\nabla g}{g}\cdot T\right)g^2\,d\sigma - \psi(\nabla h_{\mu,\tilde{b}}, \tilde{b}) \\ &\quad + \frac{1}{2}\int_{\partial D}\left(\frac{\nabla g}{g}\cdot T\right)g^2\,d\sigma - \frac{1}{2}\int_{\partial D}(\nabla h_{\mu,\tilde{b}}\cdot T)g^2\,d\sigma \\ &= \psi(\nabla h_{\mu,\tilde{b}}, \tilde{b}) - \psi(\nabla h_{\mu,\tilde{b}}, \tilde{b}) = 0.\end{aligned}$$

In order to complete the proof of the theorem, we must show that if μ is invariant for $I(a, b, T)$, then in fact $b = b_1 + (a\nabla g/g) - a\nabla h_{\mu,b_1}$ for some b_1.

Let $b_1 = b - (a\nabla g/g)$ and write $b = b_1 + (a\nabla g/g)$. Now consider all drifts of the form $b_1 + (a\nabla g/g) - a\nabla h$. Corollary 1.5 states that among all such drifts, the one with $\nabla h = \nabla h_{\mu,b_1}$ is the only one for which μ is invariant for $I(a, b + (a\nabla g/g) - a\nabla h, T)$. But, in particular, if $\nabla h = 0$, then $b_1 + (a\nabla g/g) - a\nabla h = b$ and μ is invariant for $I(a, b, T)$. Hence $\nabla h_{\mu,b_1} \equiv 0$ and $b = b_1 + (a\nabla g/g) = b_1 + (a\nabla g/g) - a\nabla h_{\mu,b_1}$. Thus, to complete the proof of the theorem, we will prove Corollary 1.5.

We need to show that if $h \in C^1(D)$ and $\nabla h \not\equiv \nabla h_{\mu,b}$, then μ is not invariant for $I(a, b + (a\nabla g/g) - a\nabla h, T)$. (We still have existence and uniqueness for continuous drifts—in fact, for bounded measurable drifts.) Performing the calculation as in (2.1) but with $b + (a\nabla g/g) - a\nabla h$ replacing $\tilde{b} + (a\nabla g/g) - a\nabla h_{\mu,\tilde{b}}$, we obtain $I(\mu) = \psi(\nabla h, b) - \psi(\nabla h_{\mu,b}, b) > 0$ if $\nabla h \not\equiv \nabla h_{\mu,b}$ since $\nabla h_{\mu,b}$ is the unique gradient which minimizes $\psi(\nabla h, b)$ as h varies over $C^2(D)$, or equivalently, over $C^1(D)$.

REMARK. If $b \in C(D)$, or if the density of μ is not strictly positive, then (1.1) still holds, and $h_{\mu,b}$ still exists in $W_1^2(D)$ and is unique [2]. If it can be shown that in fact $h_{\mu,b} \in C^1(D)$, then the theorem and corollary still hold with $\mathscr{E}_a$ and $\mathscr{A}_\mu(a, T)$ enlarged to include continuous drifts. Furthermore, in this case, we may consider all measures μ with densities $\varphi \in C^1(D)$.

In fact, even in the case at hand, we may consider measures μ with strictly positive densities $\varphi \in C^1(D)$. Corollary 1.5 still holds and Theorem 1.4 holds if we change the notation. The problem is that the one-to-one map $\tilde{b} \to \tilde{b} + (a\nabla g/g) - a\nabla h_{\mu,\tilde{b}}$ no longer maps $C^1(D)$ into $C^1(D)$. The proof is the same except that one must check that everything goes through at the step where we define $b_1 = b - (a\nabla g/g)$ since now $b_1 \notin C^1(D)$. The fact that for $b_1 \in C(D)$, (1.1) still holds and h_{μ,b_1} exists in $W_1^2(D)$ and is unique is all we need.

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