A SCALE FUNCTION APPROACH FOR STEIN'S METHOD OF ONE-DIMENSIONAL DIFFUSIONS

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ABSTRACT. For Stein's operator that can be identified as the infinitesimal generator of one-dimensional diffusion, we express the solution of the corresponding Stein's equation in terms of speed measure and scale function. This offers an unifying framework for studying Stein's equation in the classical language of diffusion processes, and yields in the particular case the Stein's density approach. We also discuss the connection with the Green function of the underlying diffusion. Examples involving common distributions are given as illustrations.

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CONTENTS

1. INTRODUCTION AND MAIN RESULTS

Consider a one-dimensional diffusion process $X = (X_t)_{t\geqslant 0}$ with transition semigroup $(P_t)_{t\geqslant 0}$ on the state space $\mathcal{X} = (l, u)$ with $-\infty \leqslant l < u \leqslant \infty$. The infinitesimal generator L of X is a second-order differential operator that acts on the space of twice differentiable functions given by

$$L = \frac{\sigma^2(x)}{2}\frac{d^2}{dx^2} + \mu(x)\frac{d}{dx},$$

where $\mu(x)$ (resp. $\sigma^2(x)$) is the drift (resp. diffusion) coefficient of X. Fix an arbitrary $x_0 \in \mathcal{X}$. Associated with the diffusion X are the two characteristics - the scale function $S(x)$ and the speed function $M(x)$. Let us recall that for $x \in \mathcal{X}$, these functions are defined by

$$S(x) := \int_{x_0}^{x} \exp\left\{-\int_{x_0}^{y}\frac{2\mu(z)}{\sigma^2(z)}\,dz\right\}dy, \quad M(x) := \int_{l}^{x}\frac{2}{\sigma^2(y)}\exp\left\{\int_{x_0}^{y}\frac{2\mu(z)}{\sigma^2(z)}\,dz\right\}dy.$$

We also denote their respective densities by writing

$$s(x) := S^{'}(x) = \exp\left\{-\int_{x_0}^{x}\frac{2\mu(z)}{\sigma^2(z)}\,dz\right\}, \quad m(x) := M^{'}(x) = \frac{2}{\sigma^2(x)s(x)}.$$

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We assume that X is positively recurrent so that there exists a unique invariant measure denoted by $\pi(dx)$. We also assume that π admits a density with respect to Lebesgue measure that we still denote by $\pi(x)$, and it can be written as a normalized speed density, that is,

$$\pi(x) = \frac{m(x)}{M(u)}.$$

A sufficient condition under which π admits a density is that the boundary points l, u are either inaccessible or reflecting, see e.g. (Bhattacharya and Waymire, 2009, Theorem 12.2(c)). We now further recall several important results on the hitting time of diffusions that will be used in our main results. Denote $\tau_y := \inf\{t \geqslant 0;\ X_t = y\}$ to be the first hitting time of $y \in \mathcal{X}$ with the usual convention that $\inf \emptyset = \infty$. For diffusions, the expected hitting time can be written in terms of the speed function and scale density, which is given by

$$\mathbb{E}_x(\tau_y) = \begin{cases} \int_x^y M(z)s(z)\,dz, & x \leqslant y, \\ \int_x^y (M(u) - M(z))s(z)\,dz, & x > y, \end{cases} \tag{1.1}$$

see for instance (Bhattacharya and Waymire, 2009, equation (10.17) and (10.19)). Denote the average hitting time of X by

$$t_{av} := \int_{\mathcal{X}}\int_{\mathcal{X}} \mathbb{E}_x(\tau_y)\pi(x)\pi(y)\,dxdy.$$

This quantity turns out to be useful in bounding the solution of the Stein's equation in our main result below. For $\alpha > 0$, we denote the fundamental increasing (resp. decreasing) solution of $L\Phi = \alpha\Phi$ by $\Phi_{\alpha,-}$ (resp. $\Phi_{\alpha,+}$), which are unique up to a multiplicative constant. Writing $\pm$ to be $+$ or $-$, the Laplace transform of the hitting time can be written in terms of $\Phi_{\alpha,\pm}$ via

$$\mathbb{E}_x(e^{-\alpha\tau_y}) = \begin{cases} \dfrac{\Phi_{\alpha,-}(x)}{\Phi_{\alpha,-}(y)}, & x \leqslant y, \\ \dfrac{\Phi_{\alpha,+}(x)}{\Phi_{\alpha,+}(y)}, & x > y. \end{cases} \tag{1.2}$$

Note that the Green function or α-resolvent, G_α, of X can be factorized into the product of $\Phi_{\alpha,\pm}$ which yields, for $x, y \in \mathcal{X}$,

$$G_\alpha(x,y) := \int_0^\infty e^{-\alpha t}P_t(x,y)\,dt = w_\alpha^{-1}\Phi_{\alpha,+}(\max\{x,y\})\Phi_{\alpha,-}(\min\{x,y\})m(y), \tag{1.3}$$

where $P_t(x,y)$ is the density of $P_t(x,dy)$ with respect to Lebesgue measure and the Wronskian is defined to be

$$w_\alpha := \frac{\Phi'_{\alpha,-}(y)\Phi_{\alpha,+}(y) - \Phi_{\alpha,-}(y)\Phi'_{\alpha,+}(y)}{s(y)} \tag{1.4}$$

that only depends on α but not on y. For further classical results on one-dimensional diffusions, we refer interested readers to Albanese and Kuznetsov (2007); Bhattacharya and Waymire (2009); Borodin and Salminen (2002); Karlin and Taylor (1981); Pitman and Yor (2003).

In this paper, we adapt a generator approach towards Stein's method. In particular, we are interested in Stein's equation associated with one-dimensional diffusions. Before we discuss our main results, let us proceed by providing a quick overview on the method itself. Stein's method is a versatile method for offering explicit error rates on various distributional approximation. This technique has been fruitful in yielding interesting and powerful results in diverse areas ranging from concentration inequalities to statistical physics, see e.g. Barbour and Chen (2005); Diaconis and Holmes (2004); Ley et al. (2017);

Reinert (2005); Ross (2011) and the references therein. The core of the method rests on the Stein's equation

$$h(x) - \mathbb{E}h(Z) = Lf_h(x)\,, \tag{1.5}$$

where $Z \sim \pi$ is the target distribution with support on $\mathcal{X}$, L is the Stein operator associated with π, h belongs to certain function class such as the class of indicator functions or Lipschitz continuous functions and f_h is the solution of the Stein's equation. In this paper, by adapting the generator approach to identify the Stein operator L, we take L to be the generator of the diffusion process X with stationary distribution π. Recall that the generator approach is first proposed by Barbour (1990); Götze (1991). Writing $\pi(f) = \int f\,d\pi$, the solution f_h can be written as

$$f_h(x) = -\int_0^\infty P_t h(x) - \pi(h)\,dt, \tag{1.6}$$

whenever the above integral exists. In the context of diffusion processes and Stein's method, we mention the work of Kusuoka and Tudor (2012, 2018) who employ Malliavin calculus technique in Stein's bound.

In Markov processes, the operator appearing on the right of (1.6)

$$D(x,y) := \int_0^\infty P_t(x,y) - \pi(y)\,dt$$

is commonly known as deviation kernel $D = (D(x,y))_{x,y\in\mathcal{X}}$ as in Coolen-Schrijner and van Doorn (2002); Mao (2004). Similar to the deviation kernel for Markov chains, we can write $D(x,y)$ in terms of the hitting time for diffusions. According to Cheng and Mao (2015); Whitt (1992), for $x, y \in \mathcal{X}$, we have

$$D(y,y) = \pi(y)\int_l^u \pi(x)\mathbb{E}_x(\tau_y)\,dx, \tag{1.7}$$

$$D(x,y) = D(y,y) - \pi(y)\mathbb{E}_x(\tau_y). \tag{1.8}$$

This operator also appears under the name of fundamental matrix Kemeny et al. (1976), ergodic potential Syski (1978) or centered resolvent Miclo (2016). Recently, this connection with the deviation kernel has been exploited by Choi (2018) in offering hitting time and mixing time bounds for Stein's factors in the context of Markov chains. We essentially follow the same spirit and provide results along the direction of one-dimensional diffusions. In the following, we denote the supremum norm of f by $||f|| := \sup_{x\in\mathcal{X}} |f(x)|$. Note that the second part of Theorem 1.1 is inspired by (Chatterjee and Shao, 2011, Lemma 4.1) in the Stein's density approach.

Theorem 1.1 (Stein's equation via scale and speed densities)**.** *Suppose that L is the infinitesimal generator of a one-dimensional diffusion on (l,u) with stationary distribution π, scale density s, speed density m, Wronskian w_α and fundamental solutions $\Phi_{\alpha,\pm}$. The solution f_h of the Stein's equation (1.5) can be expressed as*

$$f_h(x) = -Dh(x) = -\int_l^u D(y,y)h(y)\,dy + \int_l^u \pi(y)\mathbb{E}_x(\tau_y)h(y)\,dy, \tag{1.9}$$

$$f_h'(x) = s(x)\int_l^x m(z)\left(h(z) - \pi(h)\right)\,dz = -s(x)\int_x^u m(z)\left(h(z) - \pi(h)\right)\,dz. \tag{1.10}$$

In terms of $\Phi_{\alpha,\pm}$, we can write

(1.11)
$$f_h^{'}(x) = -\left(\lim_{\alpha \to 0} w_\alpha^{-1} \Phi_{\alpha,+}^{'}(x)\right) \int_l^x m(y)h(y)\,dy - \left(\lim_{\alpha \to 0} w_\alpha^{-1} \Phi_{\alpha,-}^{'}(x)\right) \int_x^u m(y)h(y)\,dy,$$

(1.12)
$$f_h^{''}(x) = s(x)m(x)h(x) - \left(\lim_{\alpha \to 0} w_\alpha^{-1} \Phi_{\alpha,+}^{''}(x)\right) \int_l^x m(y)h(y)\,dy - \left(\lim_{\alpha \to 0} w_\alpha^{-1} \Phi_{\alpha,-}^{''}(x)\right) \int_x^u m(y)h(y)\,dy.$$

In particular, if h is bounded, then

$$||f_h|| \leqslant 2t_{av}||h||. \tag{1.13}$$

If, in addition to h is bounded, that for all $x \in \mathcal{X}$, there exists constant c_1, c_2 such that

(1) $s(x)\min\{M(x), M(u) - M(x)\} \leqslant c_1$,
(2) $\frac{2|\mu(x)|}{\sigma^2(x)} s(x)\min\{M(x), M(u) - M(x)\} \leqslant c_2$,

then

$$||f_h^{'}|| \leqslant c_1||h - \pi(h)||, \tag{1.14}$$

$$||f_h^{''}|| \leqslant (1 + c_2)||h - \pi(h)||. \tag{1.15}$$

Similar to (Chatterjee and Shao, 2011, Lemma 4.2), we can state a sufficient condition on the drift $\mu(x)$ and diffusion $\sigma^2(x)$ under which (1) and (2) of Theorem 1.1 are satisfied.

Proposition 1.1. *If we have*

(i) $0 \in (l, u)$ *such that* $x_0 = 0$,
(ii) $\sigma^2(x)$ *is bounded away from zero with* $\sigma^2(x) \geqslant b > 0$ *for all* $x \in \mathcal{X}$,
(iii) $h(x) := -2\mu(x)/\sigma^2(x)$ *is non-decreasing, with* $h(x) \geqslant 0$ *for* $x > 0$ *while* $h(x) \leqslant 0$ *for* $x \leqslant 0$,

then in (1) *and* (2) *of Theorem 1.1 we can take*

$$c_1 = \max\{M(0), M(u) - M(0)\}, \quad c_2 = 2/b.$$

We will illustrate the above proposition in Example 3.1. We now provide a few remarks and establish connections of our main results to relevant papers in the literature.

Remark 1.1 (Connection with Stein's density approach). Stein's density approach is first proposed by Stein et al. (2004), and has been recently extended by Ley and Swan (2013). We now demonstrate how the Stein's density approach can actually be seen as a particular case of the form (1.10). For a given target density $\pi(x)$ which is absolutely continuous, if we take the diffusion coefficient to be $\sigma^2(x) = 2$ and the drift coefficient to be $\mu(x) = \frac{\pi^{'}(x)}{\pi(x)}$, then

$$s(x) = \exp\left\{-\ln \frac{\pi(x)}{\pi(x_0)}\right\} = \frac{\pi(x_0)}{\pi(x)}, \quad m(x) = \frac{1}{s(x)} = \frac{\pi(x)}{\pi(x_0)},$$

and so (1.10) becomes

$$f_h^{'}(x) = 1/\pi(x) \int_l^x \pi(z)\left(h(z) - \pi(h)\right)\,dz = -1/\pi(x) \int_x^u \pi(z)\left(h(z) - \pi(h)\right)\,dz,$$

which is the well-known solution of the Stein's density approach, see e.g. (Reinert, 2005, Theorem 5) or (Chatterjee and Shao, 2011, equation (4.4)).

Remark 1.2 (Connection with Kusuoka and Tudor (2012)). In this remark, we aim at recovering the form of f_h' under the setting of Kusuoka and Tudor (2012), that is, the drift function $\mu(x)$ satisfies equation (6) of Kusuoka and Tudor (2012), while we take the diffusion coefficient to be

$$\sigma^2(x) = \frac{2\int_l^x \mu(x)\pi(x)\,dx}{\pi(x)},$$

where π is a given target density. Note that under these choices

$$\frac{d}{dx}\log(\sigma^2(x)\pi(x)) = \frac{2\mu(x)}{\sigma^2(x)}, \quad s(x) = \frac{\sigma^2(x_0)\pi(x_0)}{\sigma^2(x)\pi(x)}, \quad m(x) = \frac{2\pi(x)}{\sigma^2(x_0)\pi(x_0)},$$

and so (1.10) becomes

$$f_h'(x) = \frac{2}{\sigma^2(x)\pi(x)}\int_l^x \pi(z)\left(h(z)-\pi(h)\right)\,dz = -\frac{2}{\sigma^2(x)\pi(x)}\int_x^u \pi(z)\left(h(z)-\pi(h)\right)\,dz,$$

which is equation (8) and (9) in Kusuoka and Tudor (2012).

Remark 1.3 (The form of f_h' under Kolmogorov distance). For a fixed $w \in \mathcal{X}$, we take $h = \mathbb{1}_{(l,w)}$, the indicator function of the interval (l,w). Writing $\Pi(x) = \int_l^x \pi(y)\,dy$ to be the cumulative distribution function of π, (1.10) becomes

$$f_{\mathbb{1}_{(l,w)}}'(x) = \begin{cases} s(x)M(x)(1-\Pi(w)) = M(u)s(x)\Pi(x)(1-\Pi(w)), & x \leqslant w, \\ s(x)\Pi(w)(M(u)-M(x)) = M(u)s(x)\Pi(w)(1-\Pi(x)), & x > w. \end{cases}$$

When L is the Ornstein-Uhlenbeck operator with $\sigma^2(x) = 2$ and $\mu(x) = -x$, $s(x) = \exp\{\frac{1}{2}(x^2 - x_0^2)\}$ and $M(u) = \sqrt{2\pi}\exp\{\frac{1}{2}x_0^2\}$, which is the classical result for π being the standard normal distribution, see e.g. (Ross, 2011, Lemma 2.2).

Remark 1.4 (On bounding $||f_h||$ by average hitting time for bounded h). For diffusions, L is known to be a self-adjoint operator in the weighted Hilbert space $L^2(m)$. When the essential spectrum of L is empty, (Cheng and Mao, 2015, Lemma 2.2, Theorem 1.1) prove that we can compute the average hitting time t_{av} using the non-zero eigenvalues $(-\lambda_n)_{n=1}^\infty$ of L via

$$t_{av} = \sum_{n=1}^\infty \frac{1}{\lambda_n}.$$

For example, this is the case when L is the generator of a doubly reflected Brownian motion on a finite interval $[a,b]$, see Example 3.3. We also note that in the context of finite Markov chains, Choi (2018) prove similar results in bounding Stein's factors by eigenvalues of the underlying Markov chain.

Remark 1.5 (Connection with Green function of diffusions). (1.11) and (1.12) establish interesting connection between the solution of Stein's equation with the Green function, and they perhaps open a way to compute f_h' for other processes such as Lévy processes as long as the resolvent is differentiable in the first coordinate. However, when we compare these formulae with (1.10), the computation of the derivatives of $\Phi_{\alpha,\pm}$ is in general a complicated task and involves special functions for most diffusions. As illustrations of this connection, we refer readers to Section 3 where we compute explicitly these functions for a few known examples including the Ornstein-Uhlenbeck process and the reflected Brownian motion. We also note that in (Gaunt, 2014, Lemma 3.3) similar connection has been established for the Stein's equation of Variance-Gamma distribution.

The rest of the paper is organized as follow. In Section 2, we give the proof of Theorem 1.1 and Proposition 1.1. In Section 3, we illustrate our main results by detailing a few examples that involve common diffusions and distributions.

2. Proof of Theorem 1.1 and Proposition 1.1

2.1. **Proof of Theorem 1.1.** We first prove (1.9), which is simply using (1.7) and (1.8) in (1.6). Next, we prove (1.10). The first equality of (1.10) can be shown by differentiating the right hand side and plugging the resulting expression to (1.5) together with the definition of $s(x)$ and $m(x)$, that is, let

$$g(x) := s(x) \int_l^x m(z) \left(h(z) - \pi(h)\right) \, dz,$$

and consider

$$\begin{aligned} g^{'}(x) &= s(x)m(x)(h(x) - \pi(h)) + s^{'}(x) \int_l^x m(z) \left(h(z) - \pi(h)\right) \, dz \\ &= \frac{2}{\sigma^2(x)}(h(x) - \pi(h)) - \frac{2\mu(x)}{\sigma^2(x)} s(x) \int_l^x m(z) \left(h(z) - \pi(h)\right) \, dz \\ &= \frac{2}{\sigma^2(x)}(h(x) - \pi(h)) - \frac{2\mu(x)}{\sigma^2(x)} g(x), \end{aligned}$$

and so $g(x) = f_h(x)$. To see the second equality of (1.10), we note that

$$\begin{aligned} f_h^{'}(x) &= s(x) \int_l^x m(z) \left(h(z) - \pi(h)\right) \\ &= s(x)M(u) \int_l^x \pi(z) \left(h(z) - \pi(h)\right) \\ &= -s(x)M(u) \int_x^u \pi(z) \left(h(z) - \pi(h)\right) \\ &= -s(x) \int_x^u m(z) \left(h(z) - \pi(h)\right). \end{aligned}$$

Next, we prove (1.11). Using (1.3), we observe that

$$\begin{aligned} f_h^{'}(x) &= - \lim_{\alpha \to 0} \frac{d}{dx} G_\alpha h(x) \\ &= - \lim_{\alpha \to 0} \int_l^u \frac{d}{dx} G_\alpha(x,y) h(y) \, dy \\ &= - \lim_{\alpha \to 0} \int_l^x \frac{d}{dx} w_\alpha^{-1} \Phi_{\alpha,+}(x) \Phi_{\alpha,-}(y) m(y) h(y) \, dy + \int_x^y \frac{d}{dx} w_\alpha^{-1} \Phi_{\alpha,+}(y) \Phi_{\alpha,-}(x) m(y) h(y) \, dy \\ &= - \left(\lim_{\alpha \to 0} w_\alpha^{-1} \Phi_{\alpha,+}^{'}(x)\right) \int_l^x m(y) h(y) \, dy - \left(\lim_{\alpha \to 0} w_\alpha^{-1} \Phi_{\alpha,-}^{'}(x)\right) \int_x^u m(y) h(y) \, dy, \end{aligned}$$

where we use $\Phi_{0,\pm}(x) = 1$ as X is positive recurrent in the last equality.

Moving on we now prove (1.12). By (1.3) again, consider

$$f_h^{''}(x) = - \lim_{\alpha \to 0} \frac{d^2}{dx^2} G_\alpha h(x)$$

$$
\begin{aligned}
&= -\lim_{\alpha\to 0}\frac{d}{dx}\left(\int_l^x w_\alpha^{-1}\Phi'_{\alpha,+}(x)\Phi_{\alpha,-}(y)m(y)h(y)\,dy + \int_x^y w_\alpha^{-1}\Phi_{\alpha,+}(y)\Phi'_{\alpha,-}(x)m(y)h(y)\,dy\right)\\
&= \lim_{\alpha\to 0}\left(w_\alpha^{-1}\Phi'_{\alpha,-}(x)\Phi_{\alpha,+}(x)m(x)h(x) - w_\alpha^{-1}\Phi_{\alpha,-}(x)\Phi'_{\alpha,+}(x)m(x)h(x)\right)\\
&\quad -\lim_{\alpha\to 0}\left(\int_l^x w_\alpha^{-1}\Phi''_{\alpha,+}(x)\Phi_{\alpha,-}(y)m(y)h(y)\,dy + \int_x^y w_\alpha^{-1}\Phi_{\alpha,+}(y)\Phi''_{\alpha,-}(x)m(y)h(y)\,dy\right)\\
&= s(x)m(x)h(x) - \left(\lim_{\alpha\to 0} w_\alpha^{-1}\Phi''_{\alpha,+}(x)\right)\int_l^x m(y)h(y)\,dy - \left(\lim_{\alpha\to 0} w_\alpha^{-1}\Phi''_{\alpha,-}(x)\right)\int_x^u m(y)h(y)\,dy,
\end{aligned}
$$

where we use Leibniz rule in the third equality and the definition of Wronskian (1.4) in the last equality.

Next, we prove (1.13). For bounded h, by (1.7) and the definition of t_{av}, we first bound

$$
\begin{aligned}
\left|\int_l^u D(y,y)h(y)\right| &\leqslant ||h||\int_l^u |D(y,y)|\,dy\\
&\leqslant ||h||\int_l^u \pi(y)\int_l^u \pi(x)\mathbb{E}_x(\tau_y)\,dxdy = ||h||t_{av}
\end{aligned}
$$

Also, since $D\mathbb{1}(x) = 0$ for all x, where $\mathbb{1}$ is a vector of all ones, by (1.8) we have

$$
\int_l^u D(y,y)\,dy = \int_l^u \pi(y)\mathbb{E}_x(\tau_y)\,dy.
$$

This leads to

$$
|f_h(x)| = \left|-\int_l^u D(y,y)h(y)\,dy + \int_l^u \pi(y)\mathbb{E}_x(\tau_y)h(y)\,dy\right| \leqslant ||h||2\left|\int_l^u D(y,y)\,dy\right| = 2||h||t_{av}.
$$

Finally, we prove (1.14) and (1.15). By (1.10), we have the following two inequalities:

$$
\begin{aligned}
|f'_h(x)| &\leqslant s(x)M(x)||h-\pi(h)||,\\
|f'_h(x)| &\leqslant s(x)(M(u)-M(x))||h-\pi(h)||.
\end{aligned}
$$

As a result, $|f'_h(x)| \leqslant s(x)\min\{M(x), M(u)-M(x)\}||h-\pi(h)|| \leqslant c_1||h-\pi(h)||$. As for f''_h, using the Stein's equation (1.5) we have

$$
\begin{aligned}
|f''_h(x)| &\leqslant |h(x)-\pi(h)| + \left|\frac{2\mu(x)}{\sigma^2(x)}f'_h(x)\right|\\
&\leqslant |h(x)-\pi(h)| + \left|\frac{2\mu(x)}{\sigma^2(x)}\right|s(x)\min\{M(x), M(u)-M(x)\}||h-\pi(h)||\\
&\leqslant (1+c_2)||h-\pi(h)||.
\end{aligned}
$$

2.2. **Proof of Proposition 1.1.** The proof is adapted from the proof of (Chatterjee and Shao, 2011, Lemma 4.2). We first show the expression for c_1, and it suffices for us to prove that

$$
\begin{aligned}
s(x)M(x) &\leqslant M(0), \quad l < x < 0,\\
s(x)(M(u)-M(x)) &\leqslant (M(u)-M(0)). \quad 0 < x < u.
\end{aligned}
$$

Denote $g(x) = 1/s(x)$, and note that $g'(x) = -g(x)h(x)$, where we recall $h(x) = -2\mu(x)/\sigma^2(x)$. Letting $f(x) := M(x) - M(0)g(x)$, we see that

$$
f'(x) = m(x) + M(0)g(x)h(x)
$$

$$\leqslant g(x)\left(\frac{2}{b}+M(0)h(x)\right).$$

Note that since $h(x)$ and $g(x)$ is non-decreasing for $x<0$, if $f^{'}(0)>0$, there is at most at x_0 such that $f^{'}(x_0)=0$. If $f^{'}(0)\leqslant 0$, then $f^{'}(x)\leqslant 0$. Therefore, f achieves its maximum at either $f(0)=0$ or $f(l)\leqslant M(l)=0$, that is, $f(x)\leqslant 0$, which is what we want to prove. $s(x)(M(u)-M(x))\leqslant (M(u)-M(0))$ can be proved similarly.

Next, we show that $c_2=2/b$. Consider for $x<0$,

$$\begin{aligned}
M(x) &= \int_l^x \frac{2g(z)}{\sigma^2(z)}\,dz \\
&\leqslant \int_l^x \frac{2h(z)g(z)}{bh(x)}\,dz \\
&= \frac{2}{bh(x)}\int_l^x -g^{'}(z)\,dz \\
&\leqslant \frac{2g(x)}{-bh(x)} = \frac{2g(x)}{b|h(x)|}.
\end{aligned}$$

Similarly, we have for $x\geqslant 0$,

$$M(u)-M(x)\leqslant \frac{2g(x)}{b|h(x)|}.$$

3. Examples

In this section, we illustrate our main results through various common diffusions and their respective stationary distributions. Most of the diffusions are taken from Borodin and Salminen (2002), while our primary point of comparison in the Stein's method literature are the examples in (Döbler et al., 2017, Section 3). In the following, we consider Stein's equation for standard normal distribution (Example 3.1), exponential distribution (Example 3.2), uniform distribution (Example 3.3) and gamma distribution (Example 3.4).

Example 3.1 (Ornstein-Uhlenbeck (OU) process and standard normal distribution)**.** In this example, we take $\mu(x)=-x$ and $\sigma^2(x)=2$, and L is the generator of an OU process. This leads to

$$s(x)=\exp\left\{\frac{x^2-x_0^2}{2}\right\},\quad m(x)=\exp\left\{\frac{-x^2+x_0^2}{2}\right\},$$

and the stationary distribution is well-known to be a standard normal distribution. Using these data, (1.10) becomes

$$f_h^{'}(x)=e^{x^2/2}\int_{-\infty}^x e^{-z^2/2}(h(z)-\pi(h))\,dz=-e^{x^2/2}\int_x^{\infty} e^{-z^2/2}(h(z)-\pi(h))\,dz,$$

which is (Döbler et al., 2017, equation (3.4)). We now compute $f_h^{'}$ using only information of $\Phi_{\alpha,\pm}$. Note that according to (Borodin and Salminen, 2002, Appendix 1 Example 24),

$$\Phi_{\alpha,\pm}(x)=e^{x^2/4}D_{-2\alpha}(\pm x),\quad w_\alpha=\frac{\sqrt{2\pi}}{\Gamma(2\alpha)},$$

where $D_{-v}(x)$ is the parabolic cylinder function with parameter v. As a result, we have

$$w_\alpha^{-1}\Phi'_{\alpha,\pm}(x) = \mp\frac{\Gamma(2\alpha+1)}{\sqrt{2\pi}}e^{x^2/4}D_{-2\alpha-1}(\pm x) \overset{\alpha\to 0}{\to} \mp e^{x^2/2}(1-\Phi(\pm x)),$$
$$w_\alpha^{-1}\Phi''_{\alpha,\pm}(x) = \frac{\Gamma(2\alpha+2)}{\sqrt{2\pi}}e^{x^2/4}D_{-2\alpha-2}(\pm x) \overset{\alpha\to 0}{\to} \frac{1}{\sqrt{2\pi}} \mp xe^{-x^2/2}(1-\Phi(\pm x)),$$

where we write Φ to be the cumulative distribution function of standard normal distribution. Taking $x_0 = 0$, (1.11) and (1.12) now read

$$\begin{aligned}
f_h'(x) &= e^{x^2/2}(1-\Phi(x))\int_{-\infty}^x m(z)h(z)\,dz - e^{x^2/2}\Phi(x)\int_x^\infty m(z)h(z)\,dz\\
&= e^{x^2/2}\int_{-\infty}^x e^{-z^2/2}(h(z)-\pi(h))\,dz,\\
f_h''(x) &= h(x)-\pi(h)+xe^{x^2/2}(1-\Phi(x))\int_{-\infty}^x m(z)h(z)\,dz - xe^{x^2/2}\Phi(x)\int_x^\infty m(z)h(z)\,dz\\
&= h(x)-\pi(h)+xe^{x^2/2}\int_{-\infty}^x e^{-z^2/2}(h(z)-\pi(h))\,dz,
\end{aligned}$$

as expected. Next, for Proposition 1.1 we have

$$c_1 = M(0) = M(\infty)-M(0) = \int_{-\infty}^0 e^{-x^2/2}\,dx = \sqrt{\pi/2}, \quad c_2 = 1,$$

and so by Theorem 1.1 for bounded h

$$\begin{aligned}
||f_h'|| &\leqslant \sqrt{\pi/2}||h-\pi(h)||,\\
||f_h''|| &\leqslant 2||h-\pi(h)||,
\end{aligned}$$

which are the expected results as in (Ross, 2011, Lemma 2.5).

Example 3.2 (Reflected Brownian motion at 0 and exponential distribution)**.**] In this example, we consider Brownian motion on $[0,\infty)$ with drift $\mu(x) = \mu < 0$ and diffusion $\sigma^2(x) = 1$. The scale density and speed measure are given by

$$s(x) = \exp\{-2\mu(x-x_0)\}, \quad m(x) = 2\exp\{2\mu(x-x_0)\},$$

and the stationary distribution is the exponential distribution with rate $2|\mu|$. With these information, (1.10) becomes

$$f_h'(x) = e^{-2\mu x}\int_0^x 2e^{2\mu z}(h(z)-\pi(h))\,dz = -e^{-2\mu x}\int_x^\infty 2e^{2\mu z}(h(z)-\pi(h))\,dz.$$

Next, according to (Borodin and Salminen, 2002, Appendix 1 Example 16), $\Phi_{\alpha,\pm}$ and w_α are

$$\Gamma := \sqrt{2\alpha+\mu^2}, \quad w_\alpha = \Gamma+\mu,$$
$$\Phi_{\alpha,+}(x) = e^{-(\Gamma+\mu)x}, \quad \Phi_{\alpha,-}(x) = \frac{\Gamma+\mu}{2\Gamma}e^{(\Gamma-\mu)x} + \frac{\Gamma-\mu}{2\Gamma}e^{-(\Gamma+\mu)x}.$$

The derivatives of $\Phi_{\alpha,\pm}$ are

$$\begin{aligned}
w_\alpha^{-1}\Phi'_{\alpha,+}(x) &= -e^{-(\Gamma+\mu)x} \overset{\alpha\to 0}{\to} -1,\\
w_\alpha^{-1}\Phi'_{\alpha,-}(x) &= \frac{\Gamma-\mu}{2\Gamma}e^{(\Gamma-\mu)x} - \frac{\Gamma-\mu}{2\Gamma}e^{-(\Gamma+\mu)x} \overset{\alpha\to 0}{\to} e^{-2\mu x}-1,
\end{aligned}$$

$$w_\alpha^{-1}\Phi_{\alpha,+}''(x) = (\Gamma+\mu)e^{-(\Gamma+\mu)x} \stackrel{\alpha\to 0}{\to} 0,$$
$$w_\alpha^{-1}\Phi_{\alpha,-}''(x) = \frac{(\Gamma-\mu)^2}{2\Gamma}e^{(\Gamma-\mu)x} + \frac{\Gamma^2-\mu^2}{2\Gamma}e^{-(\Gamma+\mu)x} \stackrel{\alpha\to 0}{\to} -2\mu e^{-2\mu x}.$$

(1.11) and (1.12) now read

$$\begin{aligned} f_h'(x) &= \int_0^x m(z)h(z)\,dz + (1-e^{-2\mu x})\int_x^\infty m(z)h(z)\,dz \\ &= -e^{-2\mu x}\int_x^\infty 2e^{2\mu z}(h(z)-\pi(h))\,dz, \\ f_h''(x) &= 2h(x) + 2\mu e^{-2\mu x}\int_x^\infty m(z)h(z)\,dz. \\ &= 2(h(x)-\pi(h)) + 2\mu e^{-2\mu x}\int_x^\infty 2e^{2\mu z}(h(z)-\pi(h))\,dz. \end{aligned}$$

Example 3.3 (Doubly reflected Brownian motion and uniform distribution)**.** For $a, b \in \mathbb{R}$ with $l = a < b = u$, we consider a standard Brownian motion with drift $\mu(x) = 0$ and diffusion $\sigma^2(x) = 1$ on $\mathcal{X} = [a, b]$, where a, b are the two reflecting barriers of the Brownian motion. The stationary distribution is the uniform distribution on $[a, b]$, and the scale density and speed measure are

$$s(x) = 1, \quad m(x) = 2.$$

(1.10) is now

$$f_h'(x) = \int_a^x 2(h(z)-\pi(h))\,dz.$$

Next, we recall from (Borodin and Salminen, 2002, Appendix 1 Example 5) that

$$\Phi_{\alpha,+}(x) = \cosh((b-x)\sqrt{2\alpha}), \quad \Phi_{\alpha,-}(x) = \cosh((x-a)\sqrt{2\alpha}), \quad w_\alpha = \sqrt{2\alpha}\sinh((b-a)\sqrt{2\alpha}).$$

As a result, for the derivatives of $\Phi_{\alpha,\pm}$ we have

$$\begin{aligned} w_\alpha^{-1}\Phi_{\alpha,+}'(x) &= -\frac{\sinh((b-x)\sqrt{2\alpha})}{\sinh((b-a)\sqrt{2\alpha})} \stackrel{\alpha\to 0}{\to} \frac{x-b}{b-a}, \\ w_\alpha^{-1}\Phi_{\alpha,-}'(x) &= \frac{\sinh((x-a)\sqrt{2\alpha})}{\sinh((b-a)\sqrt{2\alpha})} \stackrel{\alpha\to 0}{\to} \frac{x-a}{b-a}, \\ w_\alpha^{-1}\Phi_{\alpha,+}''(x) &= \frac{\sqrt{2\alpha}\cosh((b-x)\sqrt{2\alpha})}{\sinh((b-a)\sqrt{2\alpha})} \stackrel{\alpha\to 0}{\to} \frac{1}{b-a}, \\ w_\alpha^{-1}\Phi_{\alpha,-}''(x) &= \frac{\sqrt{2\alpha}\cosh((x-a)\sqrt{2\alpha})}{\sinh((b-a)\sqrt{2\alpha})} \stackrel{\alpha\to 0}{\to} \frac{1}{b-a}. \end{aligned}$$

(1.11) and (1.12) now read

$$\begin{aligned} f_h'(x) &= \frac{b-x}{b-a}\int_a^x 2h(z)\,dz + \frac{a-x}{b-a}\int_x^b 2h(z)\,dz \\ &= \int_a^x 2h(z)\,dz + \frac{a}{b-a}\int_a^x 2h(z)\,dz + \frac{a}{b-a}\int_x^b 2h(z)\,dz - 2x\pi(h) \\ &= \int_a^x 2(h(z)-\pi(h))\,dz, \end{aligned}$$

$$f_h''(x) = 2h(x) - \frac{1}{b-a}\int_a^x 2h(z)\,dz - \frac{1}{b-a}\int_x^b 2h(y)\,dy = 2(h(x) - \pi(h)).$$

Note that by Remark 1.4 and for bounded h,

$$t_{av} = \frac{2(b-a)^2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{(b-a)^2}{3}, \quad ||f_h|| \leqslant \frac{(b-a)^2}{3}||h||.$$

In the Stein's method literature, uniform distribution has also been studied by Kusuoka and Tudor (2012), although they used a different drift and diffusion coefficient (and hence a different Stein's equation).

Example 3.4 (CIR process and gamma distribution)**.** In this example, we look at the so-called CIR process by taking $\sigma^2(x) = 2x$ and $\mu(x) = a - bx$ with $a, b > 0$. Note that this diffusion is also known as the squared radial Ornstein-Uhlenbeck process, see e.g. (Borodin and Salminen, 2002, Appendex 1 Example 26). This leads to

$$s(x) = x^{-a}e^{bx}, \quad m(x) = x^{a-1}e^{-bx},$$

and the stationary distribution $\pi(x) \propto m(x) = x^{a-1}e^{-bx}$ is the gamma distribution with parameters a, b. (1.10) becomes

$$f_h'(x) = x^{-a}e^{bx}\int_0^x z^{a-1}e^{-bz}(h(z) - \pi(z))\,dz,$$

which is (Döbler et al., 2017, equation (3.12)). On the other hand, writing $M(x,y,z)$ (resp. $U(x,y,z)$) to be the confluent hypergeometric function of the first kind (resp. second kind), it is known from (Albanese and Kuznetsov, 2007, Section 4.4) that the fundamental solutions and the Wronskian are

$$\Phi_{\alpha,+}(x) = M(\alpha/b, a, bx), \quad \Phi_{\alpha,-}(x) = U(\alpha/b, a, bx), \quad w_\alpha = -\frac{b^{-a}}{\Gamma(\alpha/b)}.$$

Their derivatives are

$$\begin{aligned}
w_\alpha^{-1}\Phi_{\alpha,+}'(x) &= b^{a+1}\Gamma(\alpha/b+1)U(\alpha/b+1, a+1, bx) \overset{\alpha\to 0}{\to} b^{a+1}U(1, a+1, bx),\\
w_\alpha^{-1}\Phi_{\alpha,-}'(x) &= -\frac{b^{a+1}}{a}\Gamma(\alpha/b+1)M(\alpha/b+1, a+1, bx) \overset{\alpha\to 0}{\to} -\frac{b^{a+1}}{a}M(1, a+1, bx),\\
w_\alpha^{-1}\Phi_{\alpha,+}''(x) &= -b^{a+2}\Gamma(\alpha/b+2)U(\alpha/b+2, a+2, bx) \overset{\alpha\to 0}{\to} -b^{a+2}U(2, a+2, bx),\\
w_\alpha^{-1}\Phi_{\alpha,-}''(x) &= -\frac{b^{a+2}}{a(a+1)}\Gamma(\alpha/b+2)M(\alpha/b+2, a+2, bx) \overset{\alpha\to 0}{\to} -\frac{b^{a+2}}{a(a+1)}M(2, a+2, bx).
\end{aligned}$$

Substituting the above expressions to (1.11) and (1.12) give

$$f_h'(x) = -b^{a+1}U(1, a+1, bx)\int_0^x m(y)h(y)\,dy + \frac{b^{a+1}}{a}M(1, a+1, bx)\int_x^\infty m(y)h(y)\,dy,$$
$$f_h''(x) = x^{-1}h(x) + b^{a+2}U(2, a+2, bx)\int_0^x m(y)h(y)\,dy + \frac{b^{a+2}}{a(a+1)}M(2, a+2, bx)\int_x^\infty m(y)h(y)\,dy.$$

Stein's method for gamma distribution has first been studied in the Ph.D. thesis of Luk (1994), and we refer readers to Döbler et al. (2017) for an updated account on this topic.

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