Multivariate Stein Factors for a Class of Strongly Log-concave Distributions

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Abstract

We establish uniform bounds on the low-order derivatives of Stein equation solutions for a broad class of multivariate, strongly log-concave target distributions. These "Stein factor" bounds deliver control over Wasserstein and related smooth function distances and are well-suited to analyzing the computable Stein discrepancy measures of Gorham and Mackey. Our arguments of proof are probabilistic and feature the synchronous coupling of multiple overdamped Langevin diffusions.

Keywords: Stein's method; Stein factors; multivariate log-concave distribution; overdamped Langevin diffusion; generator method; synchronous coupling; Stein discrepancy.

1 Introduction

In 1972, Stein [22] introduced a powerful method for bounding the maximum expected discrepancy, $d_{\mathcal{H}}(Q,P) \triangleq \sup_{h\in\mathcal{H}} |\mathbb{E}_Q[h(X)] - \mathbb{E}_P[h(Z)]|$, between a target distribution P and an approximating distribution Q. Stein's method classically proceeds in three steps:

1. First, one identifies a linear operator $\mathcal{A}$ that generates mean-zero functions under the target distribution. A common choice for a continuous target on $\mathbb{R}^d$ is the infinitesimal generator of the overdamped Langevin diffusion[1] (also known as the Smoluchowski dynamics) [19, Secs. 6.5 and 4.5] with stationary distribution P:

$$(\mathcal{A}u)(x) = \tfrac{1}{2}\langle \nabla u(x), \nabla \log p(x)\rangle + \tfrac{1}{2}\langle \nabla, \nabla u(x)\rangle. \tag{1.1}$$

   Here, p represents the density of P with respect to Lebesgue measure.

2. Next, one shows that, for every test function h in a convergence-determining class $\mathcal{H}$, the *Stein equation*

$$h(x) - \mathbb{E}_P[h(Z)] = (\mathcal{A}u_h)(x) \tag{1.2}$$

   admits a solution u_h in a set $\mathcal{U}$ of functions with uniformly bounded low-order derivatives. These uniform derivative bounds are commonly termed *Stein factors*.

3. Finally, one uses whatever tools necessary to upper bound the *Stein discrepancy*[2]

$$\sup_{u\in\mathcal{U}} |\mathbb{E}_Q[(\mathcal{A}u)(X)]| = \sup_{u\in\mathcal{U}} |\mathbb{E}_Q[(\mathcal{A}u)(X)] - \mathbb{E}_P[(\mathcal{A}u)(Z)]|, \tag{1.3}$$

   which by construction upper bounds the reference metric $d_{\mathcal{H}}(Q,P)$.

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[1] The modifier "overdamped" is derived from the physical analogy of an oscillator damped by friction.

[2] Not to be confused with the "Stein discrepancy" of [16], which names an entirely different quantity.

To date, this recipe has been successfully used with the Langevin operator (1.1) to obtain explicit approximation error bounds for a wide variety of univariate targets P [see, e.g., 7, 6].[3] The same operator has been used to analyze multivariate Gaussian approximation [2, 14, 20, 5, 17, 18], but few other multivariate distributions have established Stein factors. To extend the reach of the multivariate literature, we derive uniform Stein factor bounds for a broad class of strongly log-concave target distributions in Theorem 2.1. The result covers common Bayesian target distributions, including Bayesian logistic regression posteriors under Gaussian priors, and explicitly relates the Stein discrepancy (1.3) and practical Monte Carlo diagnostics based thereupon [12] to standard probability metrics, like the Wasserstein distance.

Notation and terminology We let $C^k(\mathbb{R}^d)$ denote the set of real-valued functions on $\mathbb{R}^d$ with k continuous derivatives. We further let $\|\cdot\|_2$ denote the ℓ_2 norm on $\mathbb{R}^d$ and define the operator norms $\|v\|_{op} \triangleq \|v\|_2$ for vectors $v \in \mathbb{R}^d$, $\|W\|_{op} \triangleq \sup_{v\in\mathbb{R}^d:\|v\|_2=1} \|Wv\|_2$ for matrices $W \in \mathbb{R}^{d\times d}$, and $\|T\|_{op} \triangleq \sup_{v\in\mathbb{R}^d:\|v\|_2=1} \|T[v]\|_{op}$ for tensors $T \in \mathbb{R}^{d\times d\times d}$. We say a function $f \in C^2(\mathbb{R}^d)$ is *k-strongly concave* for $k > 0$ if

$$v^\top \nabla^2 f(x) v \le -k\|v\|_2^2, \quad \text{for all} \quad x, v \in \mathbb{R}^d,$$

and we term a function *k-strongly log-concave* if $\log f$ is k-strongly concave. We finally let $\nabla^0 h \triangleq h$ for all functions h and define the Lipschitz constants

$$M_k(h) \triangleq \sup_{x,y\in\mathbb{R}^d, x\neq y} \frac{\left\|\nabla^{k-1}h(x) - \nabla^{k-1}h(y)\right\|_{op}}{\|x-y\|_2} \quad \text{for all } h \in C^{k-1}(\mathbb{R}^d) \text{ and integers } k \ge 1.$$

2 Stein factors for strongly log-concave distributions

Consider a target distribution P on $\mathbb{R}^d$ with strongly log-concave density p. The following result bounds the derivatives of Stein equation solutions in terms of the smoothness of $\log p$ and the underlying test function h. The proof, found in Section 3, is probabilistic, in the spirit of the generator method of Barbour [1] and Gotze [14], and features the synchronous coupling of multiple overdamped Langevin diffusions.

Theorem 2.1 (Stein factors for strongly log-concave distributions)**.** *Suppose that* $\log p \in C^4(\mathbb{R}^d)$ *is k-strongly concave with* $M_3(\log p) \le L_3$ *and* $M_4(\log p) \le L_4$*. For each* $x \in \mathbb{R}^d$*, let* $(Z_{t,x})_{t\ge 0}$ *represent the overdamped Langevin diffusion with infinitesimal generator* (1.1) *and initial state* $Z_{0,x} = x$*. Then, for each Lipschitz* $h \in C^3(\mathbb{R}^d)$*, the function*

$$u_h(x) \triangleq \int_0^\infty \mathbb{E}_P[h(Z)] - \mathbb{E}[h(Z_{t,x})]\, dt$$

solves the the Stein equation (1.2) *and satisfies*

$$M_1(u_h) \le \frac{2}{k} M_1(h), \quad M_2(u_h) \le \frac{2L_3}{k^2} M_1(h) + \frac{1}{k} M_2(h), \text{ and}$$
$$M_3(u_h) \le \left(\frac{6L_3^2}{k^3} + \frac{L_4}{k^2}\right) M_1(h) + \frac{3L_3}{k^2} M_2(h) + \frac{2}{3k} M_3(h).$$

Theorem 2.1 implies that the Stein discrepancy (1.3) with set

$$\mathcal{U} \triangleq \left\{ u \in C^2(\mathbb{R}^d) \middle| \max\left(\frac{M_1(u)}{\frac{2}{k}}, \frac{M_2(u)}{\frac{2L_3}{k^2} + \frac{1}{k}}, \frac{M_3(u)}{(\frac{6L_3^2}{k^3} + \frac{L_4+3L_3}{k^2} + \frac{2}{3k})} \right) \le 1 \right\}$$

bounds the *smooth function distance* $d_{\mathcal{M}}(Q,P) = \sup_{h\in\mathcal{M}} |\mathbb{E}_Q[h(X)] - \mathbb{E}_P[h(Z)]|$ for

$$\mathcal{M} \triangleq \left\{ h \in C^3(\mathbb{R}^d) \;\middle|\; \max(M_1(h), M_2(h), M_3(h)) \le 1 \right\}.$$

[3] In the univariate setting, the operator (1.1) is commonly called *Stein's density operator*.

Our next result shows that control over the smooth function distance also grants control over the L_1-*Wasserstein distance* (also known as the Kantorovich-Rubenstein or earth mover's distance), $d_{\mathcal{W}}(Q,P) = \sup_{h\in\mathcal{W}} |\mathbb{E}_Q[h(X)] - \mathbb{E}_P[h(Z)]|$, and the *bounded-Lipschitz metric*, $d_{\mathrm{BL}}(Q,P) = \sup_{h\in\mathrm{BL}} |\mathbb{E}_Q[h(X)] - \mathbb{E}_P[h(Z)]|$, which exactly metrizes convergence in distribution on $\mathbb{R}^d$. These metrics govern the test function classes

$$\mathcal{W} \triangleq \{h : \mathbb{R}^d \to \mathbb{R} \mid M_1(h) \le 1\} \quad \text{and} \quad \mathrm{BL} \triangleq \mathcal{W} \cap \{h : \mathbb{R}^d \to \mathbb{R} \mid \sup_{x\in\mathbb{R}^d} |h(x)| \le 1\}.$$

Lemma 2.2 (Smooth-Wasserstein inequality)**.** *If μ and ν are probability measures on $\mathbb{R}^d$ with finite means, and $G \in \mathbb{R}^d$ is a standard normal random vector, then*

$$\max(d_{\mathrm{BL}}(\mu,\nu), d_{\mathcal{M}}(\mu,\nu)) \le d_{\mathcal{W}}(\mu,\nu) \le 3\max\left(d_{\mathcal{M}}(\mu,\nu),\ \sqrt[3]{d_{\mathcal{M}}(\mu,\nu)\sqrt{2}\,\mathbb{E}[\|G\|_2]^2}\right).$$

Proof. The first inequality follows directly from the inclusions $\mathrm{BL} \subset \mathcal{W}$ and $\mathcal{M} \subset \mathcal{W}$.

To establish the second, we fix $h \in \mathcal{W}$ and $t > 0$ and define the smoothed function

$$h_t(x) = \int_{\mathbb{R}^d} h(x+tz)\phi(z)dz \quad \text{for each} \quad x \in \mathbb{R}^d,$$

where ϕ is the density of a vector of d independent standard normal variables. We first show that h_t is a close approximation to h when t is small. Specifically, if $X \in \mathbb{R}^d$ is an integrable random vector, independent of G, then, by the Lipschitz assumption on h,

$$|\mathbb{E}[h(X) - h_t(X)]| = |\mathbb{E}[h(X) - h(X+tG)]| \le t\mathbb{E}[\|G\|_2].$$

We next show that the derivatives of h_t are bounded. Fix any $x \in \mathbb{R}^d$. Since h is Lipschitz, it admits a weak gradient, ∇h, bounded uniformly by 1 in $\|\cdot\|_2$. We alternate differentiation and integration by parts to develop the representations

$$\begin{aligned}
\nabla h_t(x) &= \int_{\mathbb{R}^d} \nabla h(x+tz)\phi(z)dz = \frac{1}{t}\int_{\mathbb{R}^d} zh(x+tz)\phi(z)dz,\\
\nabla^2 h_t(x) &= \frac{1}{t}\int_{\mathbb{R}^d} \nabla h(x+tz)z^\top\phi(z)dz = \frac{1}{t^2}\int_{\mathbb{R}^d}(zz^\top - I)h(x+tz)\phi(z)dz, \quad \text{and}\\
\nabla^3 h_t(x)[v] &= \frac{1}{t^2}\int_{\mathbb{R}^d} \nabla h(x+tz)v^\top(zz^\top - I)\phi(z)dz
\end{aligned}$$

for each $v \in \mathbb{R}^d$. The uniform bound on ∇h now yields $M_1(h_t) \le 1$,

$$\begin{aligned}
M_2(h_t) &\le \frac{1}{t}\sup_{v\in\mathbb{R}^d:\|v\|_2=1}\int_{\mathbb{R}^d}|\langle z,v\rangle|\phi(z)dz = \frac{1}{t}\sqrt{\frac{2}{\pi}}\sup_{v\in\mathbb{R}^d:\|v\|_2=1}\|v\|_2 = \frac{1}{t}\sqrt{\frac{2}{\pi}}, \quad \text{and}\\
M_3(h_t) &\le \frac{1}{t^2}\sup_{v,w\in\mathbb{R}^d:\|v\|_2=\|w\|_2=1}\int_{\mathbb{R}^d}|v^\top(zz^\top - I)w|\phi(z)dz\\
&\le \frac{1}{t^2}\sup_{v,w\in\mathbb{R}^d:\|v\|_2=\|w\|_2=1}\sqrt{\int_{\mathbb{R}^d}|v^\top(zz^\top - I)w|^2\phi(z)dz}\\
&= \frac{1}{t^2}\sup_{v,w\in\mathbb{R}^d:\|v\|_2=\|w\|_2=1}\sqrt{\langle v,w\rangle^2 + \|v\|_2^2\|w\|_2^2} \le \frac{\sqrt{2}}{t^2}.
\end{aligned}$$

In the final equality we have used the fact that $\langle v,Z\rangle$ and $\langle w,Z\rangle$ are jointly normal with zero mean and covariance $\Sigma = \begin{bmatrix}\|v\|_2^2 & \langle v,w\rangle\\ \langle v,w\rangle & \|w\|_2^2\end{bmatrix}$, so that the product $\langle v,Z\rangle\langle w,Z\rangle$ has the distribution of the off-diagonal element of the Wishart distribution [23] with scale Σ and 1 degree of freedom.

We can now develop a bound for $d_{\mathcal{W}}$ using our smoothed functions. Let

$$b_t \triangleq \max\Big(1, \tfrac{1}{t}\sqrt{\tfrac{2}{\pi}}, \tfrac{\sqrt{2}}{t^2}\Big) = \max\Big(1, \tfrac{\sqrt{2}}{t^2}\Big)$$

represent the maximum derivative bound of h_t, and select $X \sim \mu$ and $Z \sim \nu$ to satisfy $d_{\mathcal{W}}(\mu,\nu) = \mathbb{E}[\|X - Z\|_2]$. If we let $c = \sqrt[3]{d_{\mathcal{M}}(\mu,\nu)\sqrt{2}\,\mathbb{E}[\|G\|_2]^2}$, we then have

$$\begin{aligned} d_{\mathcal{W}}(\mu,\nu) &\leq \inf_{t>0} \sup_{h\in\mathcal{W}} |\mathbb{E}_\mu[h(X) - h_t(X)]| + |\mathbb{E}_\nu[h(Z) - h_t(Z)]| + |\mathbb{E}_\mu[h_t(X)] - \mathbb{E}_\nu[h_t(Z)]| \\ &\leq \inf_{t>0} 2t\mathbb{E}[\|G\|_2] + b_t d_{\mathcal{M}}(\mu,\nu) \leq 2c + \max(d_{\mathcal{M}}(\mu,\nu), c) \leq 3\max(d_{\mathcal{M}}(\mu,\nu), c), \end{aligned}$$

where we have chosen $t = \sqrt[3]{d_{\mathcal{M}}(\mu,\nu)\sqrt{2}/\mathbb{E}[\|G\|_2]}$ to achieve the third inequality. □

Remark 2.3. While Lemma 2.2 targets Lipschitz test functions, comparable results can be obtained for non-smooth functions, like the indicators of convex sets, by adapting the smoothing technique of [3, Lem. 2.1].

2.1 Example application to Bayesian logistic regression

Before turning to the proof of Theorem 2.1, we illustrate a practical application to measuring the quality of Monte Carlo or cubature sample points in Bayesian inference. Consider the Bayesian logistic regression posterior density [see, e.g., 11]

$$p(\beta) \propto \underbrace{\exp\Big(-\|\beta\|_2^2/(2\sigma^2)\Big)}_{\text{multivariate Gaussian prior}} \underbrace{\textstyle\prod_{l=1}^L e^{y_l\langle\beta,v_l\rangle}/(1+e^{\langle\beta,v_l\rangle})}_{\text{logistic regression likelihood}}$$

based on L observed datapoints (v_l, y_l) and a known prior hyperparameter $\sigma^2 > 0$. In this standard model of binary classification, $\beta \in \mathbb{R}^d$ represents our inferential target, an unknown parameter vector with a multivariate Gaussian prior; $y_l \in \{0,1\}$ is the class label of the l-th observed datapoint; and $v_l \in \mathbb{R}^d$ is an associated vector of covariates.

Since the normalizing constant of p is unknown, it is common practice to approximate expectations $\int h(\beta)p(\beta)d\beta$ under p with sample estimates, $\frac{1}{n}\sum_{i=1}^n h(\beta_i)$, based on sample points $\beta_i \in \mathbb{R}^d$ drawn from a Markov chain or a cubature rule [11]. Theorem 2.1 furnishes a way to uniformly bound the error of this approximation, $|\frac{1}{n}\sum_{i=1}^n h(\beta_i) - \int h(\beta)p(\beta)d\beta|$, for all sufficiently smooth functions h.

Concretely, we have, for all ℓ_2 unit vectors $u_1, u_2, u_3, u_4 \in \mathbb{R}^d$,

$$\begin{aligned} u_1^\top \nabla^2 \log p(\beta) u_1 &= -1/\sigma^2 - \sum_{l=1}^L \frac{e^{\langle\beta,v_l\rangle}}{(1+e^{\langle\beta,v_l\rangle})^2}\langle v_l, u_1\rangle^2 \leq -1/\sigma^2, \\ \nabla^3 \log p(\beta)[u_1,u_2,u_3] &= -\sum_{l=1}^L \frac{e^{\langle\beta,v_l\rangle}(1-e^{\langle\beta,v_l\rangle})}{(1+e^{\langle\beta,v_l\rangle})^3} \prod_{m=1}^3 \langle v_l, u_m\rangle \leq \frac{\sum_{l=1}^L \|v_l\|_2^3}{6\sqrt{3}}, \text{ and} \\ \nabla^4 \log p(\beta)[u_1,u_2,u_3,u_4] &= -\sum_{l=1}^L \frac{4e^{2\langle\beta,v_l\rangle} - e^{3\langle\beta,v_l\rangle} - e^{\langle\beta,v_l\rangle}}{(1+e^{\langle\beta,v_l\rangle})^4} \prod_{m=1}^4 \langle v_l, u_m\rangle \leq \frac{\sum_{l=1}^L \|v_l\|_2^4}{8}. \end{aligned}$$

Hence, Theorem 2.1 applies with $k = 1/\sigma^2$, $L_3 = \frac{\sum_{l=1}^L\|v_l\|_2^3}{6\sqrt{3}}$, and $L_4 = \frac{\sum_{l=1}^L\|v_l\|_2^4}{8}$. We may now plug the associated Stein factors

$$(c_1, c_2, c_3) \triangleq \Big(2\sigma^2, \tfrac{\sigma^4\sum_{l=1}^L\|v_l\|_2^3}{3\sqrt{3}} + \sigma^2, \tfrac{\sigma^6(\sum_{l=1}^L\|v_l\|_2^3)^2}{18} + \tfrac{\sigma^4\sum_{l=1}^L\|v_l\|_2^4}{8} + \tfrac{\sigma^4\sum_{l=1}^L\|v_l\|_2^3}{2\sqrt{3}} + \tfrac{2\sigma^2}{3}\Big)$$

into the non-uniform graph Stein discrepancy of [12] to obtain a computable upper bound on $d_{\mathcal{M}}(Q,P)$ or $d_{\mathcal{W}}(Q,P)$ for any discrete probability measure $Q = \frac{1}{n}\sum_{i=1}^n \delta_{\beta_i}$.

3 Proof of Theorem 2.1

Before tackling the main proof, we will establish a series of useful lemmas. We will make regular use of the following well-known Lipschitz property:

$$M_k(h) = \sup_{x\in\mathbb{R}^d} \left\|\nabla^k h(x)\right\|_{op} \quad \text{for all} \quad h \in C^k(\mathbb{R}^d) \quad \text{and} \quad \text{each integer } k \geq 1. \tag{3.1}$$

3.1 Properties of overdamped Langevin diffusions

Our first lemma enumerates several properties of the overdamped Langevin diffusion that will prove useful in the proofs to follow.

Lemma 3.1 (Overdamped Langevin properties)**.** *If $\log p \in C^2(\mathbb{R}^d)$ is strongly concave, then the overdamped Langevin diffusion $(Z_{t,x})_{t\geq 0}$ with infinitesimal generator* (1.1) *and $Z_{0,x} = x$ is well-defined for all times $t \in [0,\infty)$, has stationary distribution P, and satisfies* strong continuity *on $L = \{f \in C^0(\mathbb{R}^d) : \frac{|f(x)|}{1+\|x\|_2^2} \to 0 \text{ as } \|x\|_2 \to \infty\}$ with norm $\|f\|_L \triangleq \sup_{x\in\mathbb{R}^d} \frac{|f(x)|}{1+\|x\|_2^2}$, that is, $\|\mathbb{E}[f(Z_{t,\cdot})] - f\|_L \to 0$ as $t \to 0^+$ for all $f \in L$.*

Proof. Consider the Lyapunov function $V(x) = \|x\|_2^2 + 1$. The strong log-concavity of p, the Cauchy-Schwarz inequality, and the arithmetic-geometric mean inequality imply that

$$\begin{aligned}
(\mathcal{A}V)(x) &= \langle x, \nabla \log p(x)\rangle + d = \langle x, \nabla \log p(x) - \nabla \log p(0)\rangle + \langle x, \nabla \log p(0)\rangle + d \\
&\leq -k\|x\|_2^2 + \|x\|_2\|\nabla \log p(0)\|_2 + d \leq \left(\frac{1}{2} - k\right)\|x\|_2^2 + \frac{1}{2}\|\nabla \log p(0)\|_2^2 + d \leq k'V(x)
\end{aligned}$$

for some constants $k, k' \in \mathbb{R}$. Since $\log p$ is locally Lipschitz, [15, Thm. 3.5] implies that the diffusion $(Z_{t,x})_{t\geq 0}$ is well-defined, and [21, Thm. 2.1] guarantees that P is a stationary distribution. The argument of [13, Prop. 15] with [15, Thm. 3.5] substituted for [15, Thm. 3.4] and [10, Sec. 5, Cor. 1.2] now yields strong continuity. □

3.2 High-order weighted difference bounds

A second, technical lemma bounds the growth of weighted smooth function differences in terms of the proximity of function arguments. The result will be used to characterize the smoothness of $Z_{t,x}$ as a function of the starting point x (Lemma 3.3) and, ultimately, to establish the smoothness of u_h (Theorem 2.1).

Lemma 3.2 (High-order weighted difference bounds)**.** *Fix any weights $\lambda, \lambda' > 0$ and any vectors $x, y, z, w, x', y', z', w' \in \mathbb{R}^d$. If $h \in C^2(\mathbb{R}^d)$, then*

$$\begin{aligned}
&|\lambda(h(x) - h(y)) - \lambda'(h(x') - h(y')) - \langle\nabla h(y), \lambda(x-y) - \lambda'(x'-y')\rangle| \\
&\leq \tfrac{1}{2}M_2(h)(2\lambda'\|y-y'\|_2\|x'-y'\|_2 + \lambda\|x-y\|_2^2 + \lambda'\|x'-y'\|_2^2).
\end{aligned} \tag{3.2}$$

Moreover, if $h \in C^3(\mathbb{R}^d)$, then

$$\begin{aligned}
&|\lambda(h(x) - h(y) - (h(z) - h(w))) - \lambda'(h(x') - h(y') - (h(z') - h(w'))) \\
&- \langle\nabla h(z), \lambda(x - y - (z-w)) - \lambda'(x'-y'-(z'-w'))\rangle| \\
&\leq M_2(h)[\|y'-x'\|_2\|\lambda(z-x) - \lambda'(z'-x')\|_2 \\
&+ \lambda'\|z-z'\|_2\|x'-y'-(z'-w')\|_2 + \lambda\|z-x\|_2\|(y-x)-(y'-x')\|_2 \\
&+ \tfrac{1}{2}(\lambda\|x-y-(z-w)\|_2\|x-y+z-w\|_2 + \lambda'\|x'-y'-(z'-w')\|_2\|x'-y'+z'-w'\|_2)] \\
&+ M_3(h)\Big[\tfrac{1}{2}\|y'-x'\|_2(2\lambda'\|x-x'\|_2\|z'-x'\|_2 + \lambda\|z-x\|_2^2 + \lambda'\|z'-x'\|_2^2) \\
&+ \tfrac{1}{2}(\lambda\|z-x\|_2\|y-x\|_2^2 + \lambda'\|z'-x'\|_2\|y'-x'\|_2^2) \\
&+ \tfrac{1}{6}(\lambda\|w-z\|_2^3 + \lambda\|y-x\|_2^3 + \lambda'\|w'-z'\|_2^3 + \lambda'\|y'-x'\|_2^3)\Big].
\end{aligned} \tag{3.3}$$

Proof. To establish the second-order difference bound (3.2), we first apply Taylor's theorem with mean-value remainder to $h(x) - h(y)$ and $h(x') - h(y')$ to obtain

$$\begin{aligned}&\lambda(h(x) - h(y)) - \lambda'(h(x') - h(y')) - \langle \nabla h(y), \lambda(x-y) - \lambda'(x'-y')\rangle \\ &= \lambda'\langle \nabla h(y) - \nabla h(y'), x' - y'\rangle + (\lambda\langle \nabla^2 h(\zeta)(x-y), x-y\rangle - \lambda'\langle \nabla^2 h(\zeta')(x'-y'), x'-y'\rangle)/2\end{aligned}$$

for some $\zeta, \zeta' \in \mathbb{R}^d$. Cauchy-Schwarz, the definition of the operator norm, and the Lipschitz gradient relation (3.1) now yield the advertised conclusion (3.2).

To derive the third-order difference bound (3.3), we apply Taylor's theorem with mean-value remainder to $h(w) - h(z)$, $h(y) - h(x)$, $h(w') - h(z')$, and $h(y') - h(x')$ to write

$$\begin{aligned}&|\lambda(h(x) - h(y) - (h(z) - h(w))) - \lambda'(h(x') - h(y') - (h(z') - h(w'))) \\ &- \langle \nabla h(z), \lambda(x - y - (z - w)) - \lambda'(x' - y' - (z' - w'))\rangle| \qquad (3.4)\\ &= |\lambda'\langle \nabla h(z) - \nabla h(z'), x' - y' - (z' - w')\rangle + \lambda\langle \nabla h(z) - \nabla h(x), (y - x) - (y' - x')\rangle \\ &+ \langle \lambda(\nabla h(z) - \nabla h(x)) - \lambda'(\nabla h(z') - \nabla h(x')), y' - x'\rangle \\ &+ \lambda\langle \nabla^2 h(z)(w - z), w - z\rangle/2 - \lambda\langle \nabla^2 h(x)(y - x), y - x\rangle/2 \\ &- \lambda'\langle \nabla^2 h(z')(w' - z'), w' - z'\rangle/2 + \lambda'\langle \nabla^2 h(x')(y' - x'), y' - x'\rangle/2 \\ &+ \lambda\nabla^3 h(\zeta'')[w - z, w - z, w - z]/6 - \lambda\nabla^3 h(\zeta'''')[y - x, y - x, y - x]/6 \\ &- \lambda'\nabla^3 h(\zeta''')[w' - z', w' - z', w' - z']/6 + \lambda'\nabla^3 h(\zeta''''')[y' - x', y' - x', y' - x']/6|\end{aligned}$$

for some $\zeta'', \zeta''', \zeta'''', \zeta''''' \in \mathbb{R}^d$. We will bound each line in this expression in turn. First we see, by Cauchy-Schwarz and the Lipschitz property (3.1), that

$$\begin{aligned}&|\lambda'\langle \nabla h(z) - \nabla h(z'), x' - y' - (z' - w')\rangle + \lambda\langle \nabla h(z) - \nabla h(x), (y - x) - (y' - x')\rangle| \\ &\leq M_2(h)(\lambda'\|z - z'\|_2\|x' - y' - (z' - w')\|_2 + \lambda\|z - x\|_2\|(y - x) - (y' - x')\|_2).\end{aligned}$$

Next, we invoke our second-order difference bound (3.2) on the $C^2(\mathbb{R}^d)$ function $x \mapsto \langle \nabla h(x), y' - x'\rangle$, apply the Cauchy-Schwarz inequality, and use the definition of the operator norm to conclude that

$$\begin{aligned}&|\langle \lambda(\nabla h(z) - \nabla h(x)) - \lambda'(\nabla h(z') - \nabla h(x')), y' - x'\rangle| \\ &\leq M_2(h)\|y' - x'\|_2\|\lambda(z - x) - \lambda'(z' - x')\|_2 \\ &+ \frac{1}{2}M_3(h)\|y' - x'\|_2(2\lambda'\|x - x'\|_2\|z' - x'\|_2 + \lambda\|z - x\|_2^2 + \lambda'\|z' - x'\|_2^2).\end{aligned}$$

To bound the subsequent line, we note that Cauchy-Schwarz, the definition of the operator norm, and the Lipschitz property (3.1) imply that

$$\begin{aligned}&|\langle \nabla^2 h(z)(w - z), w - z\rangle - \langle \nabla^2 h(x)(y - x), y - x\rangle| \\ &= |\langle \nabla^2 h(z)(w - z + y - x), x - y - (z - w)\rangle + \langle (\nabla^2 h(z) - \nabla^2 h(x))(y - x), y - x\rangle| \\ &\leq M_2(h)\|x - y - (z - w)\|_2\|x - y + z - w\|_2 + M_3(h)\|z - x\|_2\|y - x\|_2^2.\end{aligned}$$

Similarly,

$$\begin{aligned}&|\langle \nabla^2 h(z')(w' - z'), w' - z'\rangle - \langle \nabla^2 h(x')(y' - x'), y' - x'\rangle| \\ &\leq M_2(h)\|x' - y' - (z' - w')\|_2\|x' - y' + z' - w'\|_2 + M_3(h)\|z' - x'\|_2\|y' - x'\|_2^2.\end{aligned}$$

Finally, Cauchy-Schwarz and the definition of the operator norm give

$$\begin{aligned}&|\lambda\nabla^3 h(\zeta'')[w - z, w - z, w - z] - \lambda\nabla^3 h(\zeta'''')[y - x, y - x, y - x] \\ &- \lambda'\nabla^3 h(\zeta''')[w' - z', w' - z', w' - z'] + \lambda'\nabla^3 h(\zeta''''')[y' - x', y' - x', y' - x']| \\ &\leq M_3(h)(\lambda\|w - z\|_2^3 + \lambda\|y - x\|_2^3 + \lambda'\|w' - z'\|_2^3 + \lambda'\|y' - x'\|_2^3).\end{aligned}$$

Bounding the third-order difference (3.4) in terms of these four estimates yields (3.3). $\square$

3.3 Synchronous coupling lemma

Our proof of Theorem 2.1 additionally rests upon a series of coupling inequalities which serve to characterize the smoothness of $Z_{t,x}$ as a function of x. The couplings espoused in the lemma to follow are termed *synchronous*, because the same Brownian motion is used to drive each process.

Lemma 3.3 (Synchronous coupling inequalities)**.** *Suppose that $\log p \in C^4(\mathbb{R}^d)$ is k-strongly concave with $M_3(\log p) \leq L_3$ and $M_4(\log p) \leq L_4$. Fix a d-dimensional Wiener process $(W_t)_{t\geq 0}$, any vectors $x, x', v, v' \in \mathbb{R}^d$ with $\|v\|_2 = \|v'\|_2 = 1$, and any weights $\epsilon, \epsilon', \epsilon'' > 0$, and define the growth factors*

$$
\begin{aligned}
f_1(x, x', \epsilon, \epsilon', \epsilon'') &\triangleq \|x - x'\|_2 + (\epsilon'' + \epsilon')/2 + \epsilon(3 + \epsilon/\epsilon'' + \epsilon/\epsilon' + \|x - x'\|_2/\epsilon')/3 \quad \textit{and} \\
f_2(x, x', \epsilon, \epsilon', \epsilon'') &\triangleq \|x - x'\|_2 + 3(\epsilon'' + \epsilon')/2 + \epsilon(3 + \epsilon/\epsilon'' + \epsilon/\epsilon')/3.
\end{aligned} \tag{3.5}
$$

For each starting point of the form $z + b'v' + bv$ with $z \in \{x, x'\}$, $b' \in \{0, \epsilon', \epsilon''\}$, and $b \in \{0, \epsilon\}$, consider an overdamped Langevin diffusion $(Z_{t,z+b'v'+bv})_{t\geq 0}$ solving the stochastic differential equation

$$
dZ_{t,z+b'v'+bv} = \frac{1}{2}\nabla \log p(Z_{t,z+b'v'+bv})dt + dW_t \quad \textit{with} \quad Z_{0,z+b'v'+bv} = z + b'v' + bv, \tag{3.6}
$$

and define the differenced processes

$$
\begin{aligned}
V_t &\triangleq (Z_{t,x'+\epsilon''v'} - Z_{t,x'})/\epsilon'' - (Z_{t,x+\epsilon'v'} - Z_{t,x})/\epsilon' \quad \textit{and} \\
U_t &\triangleq Z_{t,x'+\epsilon''v'+\epsilon v} - Z_{t,x'+\epsilon''v'} - (Z_{t,x'+\epsilon v} - Z_{t,x'})/\epsilon\epsilon'' \\
&\quad - Z_{t,x+\epsilon'v'+\epsilon v} - Z_{t,x+\epsilon'v'} - (Z_{t,x+\epsilon v} - Z_{t,x})/\epsilon\epsilon'.
\end{aligned}
$$

These coupled processes almost surely satisfy the synchronous coupling bounds,

$$
e^{kt/2}\|Z_{t,x+\epsilon v} - Z_{t,x}\|_2 \leq \epsilon, \tag{3.7}
$$

$$
e^{kt/2}\|V_t\|_2 \leq \frac{L_3}{k}(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2), \quad \textit{and} \tag{3.8}
$$

$$
e^{kt/2}\|U_t\|_2 \leq \frac{3L_3^2}{k^2} f_1(x, x', \epsilon, \epsilon', \epsilon'') + \frac{L_4}{2k} f_2(x, x', \epsilon, \epsilon', \epsilon''), \tag{3.9}
$$

the second-order differenced function bound,

$$
\begin{aligned}
&(h_2(Z_{t,x'+\epsilon''v'}) - h_2(Z_{t,x'}))/\epsilon'' - (h_2(Z_{t,x+\epsilon'v'}) - h_2(Z_{t,x}))/\epsilon' \\
&\leq \left(M_1(h_2)\frac{L_3}{k}e^{-kt/2} + M_2(h_2)e^{-kt}\right)(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2),
\end{aligned} \tag{3.10}
$$

and the third-order differenced function bound,

$$
\begin{aligned}
&(h_3(Z_{t,x'+\epsilon''v'+\epsilon v}) - h_3(Z_{t,x'+\epsilon''v'}) - (h_3(Z_{t,x'+\epsilon v}) - h_3(Z_{t,x'})))/(\epsilon\epsilon'') \\
&\quad - (h_3(Z_{t,x+\epsilon'v'+\epsilon v}) - h_3(Z_{t,x+\epsilon'v'}) - (h_3(Z_{t,x+\epsilon v}) - h_3(Z_{t,x})))/(\epsilon\epsilon') \\
&\leq \left(M_1(h_3)\frac{3L_3^2}{k^2}e^{-kt/2} + M_2(h_3)\frac{3L_3}{k}e^{-kt}\right) f_1(x, x', \epsilon, \epsilon', \epsilon'') \\
&+ \left(M_1(h_3)\frac{L_4}{2k}e^{-kt/2} + M_3(h_3)e^{-3kt/2}\right) f_2(x, x', \epsilon, \epsilon', \epsilon'')
\end{aligned} \tag{3.11}
$$

for each $t \geq 0$, $h_2 \in C^2(\mathbb{R}^d)$, and $h_3 \in C^3(\mathbb{R}^d)$.

Proof. By Lemma 3.1, each process $(Z_{t,z+b'v'+bv})_{t\geq 0}$ with $z \in \{x, x'\}$, $b' \in \{0, \epsilon', \epsilon''\}$, and $b \in \{0, \epsilon\}$ is well-defined for all times $t \in [0, \infty)$. The first-order bound (3.7) is well known, and a concise proof can be found in [4].

Second-order bounds To establish the second conclusion (3.8), we consider the Itô process of second-order differences

$$V_t = \frac{1}{2}\int_0^t \frac{\nabla \log p(Z_{s,x'+\epsilon'' v'}) - \nabla \log p(Z_{s,x'})}{\epsilon''} - \frac{\nabla \log p(Z_{s,x+\epsilon' v'}) - \nabla \log p(Z_{s,x})}{\epsilon'}\, ds$$

and apply Itô's lemma to the mapping $(t, w) \mapsto e^{kt/2}\|w\|_2$. This yields

$$\begin{aligned}
&e^{kt/2}\|V_t\|_2 = e^0\|V_0\|_2 + \int_0^t ke^{ks}\|V_s\|_2 + e^{ks}\frac{d}{ds}\|V_s\|_2\, ds \\
&= \int_0^t \frac{e^{ks/2}}{2\|V_s\|_2}(k\|V_s\|_2^2 \\
&+ \langle V_s, (\nabla \log p(Z_{s,x'+\epsilon''v'}) - \nabla \log p(Z_{s,x'}))/\epsilon'' - (\nabla \log p(Z_{s,x+\epsilon'v'}) - \nabla \log p(Z_{s,x}))/\epsilon'\rangle)ds.
\end{aligned}$$

Fix a value $s \in [0, t]$. For any $h_2 \in C^2(\mathbb{R}^d)$, the Lemma 3.2 second-order difference inequality (3.2), the first order coupling bound (3.7), Cauchy-Schwarz, and the Lipschitz identity (3.1) together give the estimates

$$\begin{aligned}
&(h_2(Z_{s,x'+\epsilon''v'}) - h_2(Z_{s,x'}))/\epsilon'' - (h_2(Z_{s,x+\epsilon'v'}) - h_2(Z_{s,x}))/\epsilon' \\
&\leq \langle \nabla h_2(Z_{s,x'}), V_s\rangle + \frac{1}{2}M_2(h_2)(2\|Z_{s,x'} - Z_{s,x}\|_2\|Z_{s,x+\epsilon'v'} - Z_{s,x}\|_2/\epsilon' \\
&\quad + \|Z_{s,x'+\epsilon''v'} - Z_{s,x'}\|_2^2/\epsilon'' + \|Z_{s,x+\epsilon'v'} - Z_{s,x}\|_2^2/\epsilon') \\
&\leq \langle \nabla h_2(Z_{s,x'}), V_s\rangle + M_2(h_2)e^{-ks}(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2) \qquad (3.12) \\
&\leq M_1(h_2)\|V_s\|_2 + M_2(h_2)e^{-ks}(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2). \qquad (3.13)
\end{aligned}$$

Applying the estimate (3.12) to the $C^2(\mathbb{R}^d)$ function $h_2(z) = \langle V_s, \nabla \log p(z)\rangle$ with $M_2(h_2) = \sup_{z\in\mathbb{R}^d}\left\|\nabla^3 \log p(z)[V_s]\right\|_{op} \leq L_3\|V_s\|_2$, yields

$$\begin{aligned}
&\langle V_s, (\nabla \log p(Z_{s,x'+\epsilon''v'}) - \nabla \log p(Z_{s,x'}))/\epsilon'' - (\nabla \log p(Z_{s,x+\epsilon'v'}) - \nabla \log p(Z_{s,x}))/\epsilon'\rangle \\
&\leq \langle V_s, \nabla^2 \log p(Z_{s,x'})V_s\rangle + L_3\|V_s\|_2 e^{-ks}(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2) \\
&\leq -k\|V_s\|_2^2 + L_3\|V_s\|_2 e^{-ks}(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2),
\end{aligned}$$

where, to achieve the second inequality, we used the k-strong log-concavity of p. Now we may derive the second-order synchronous coupling bound (3.8), since

$$e^{kt/2}\|V_t\|_2 \leq \frac{L_3}{2}(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2)\int_0^t e^{-ks/2}ds \leq \frac{L_3}{k}(\|x - x'\|_2 + (\epsilon'' + \epsilon')/2).$$

Applying the synchronous coupling bound (3.8) to the estimate (3.13) finally delivers the second-order differenced function bound (3.10).

Third-order bounds To establish the third conclusion (3.9), we consider the Itô process of third-order differences

$$\begin{aligned}
U_t = \frac{1}{2}\int_0^t &\frac{\nabla \log p(Z_{s,x'+\epsilon''v'+\epsilon v}) - \nabla \log p(Z_{s,x'+\epsilon''v'}) - (\nabla \log p(Z_{s,x'+\epsilon v}) - \nabla \log p(Z_{s,x'}))}{\epsilon\epsilon''} \\
&- \frac{\nabla \log p(Z_{s,x+\epsilon'v'+\epsilon v}) - \nabla \log p(Z_{s,x+\epsilon'v'}) - (\nabla \log p(Z_{s,x+\epsilon v}) - \nabla \log p(Z_{s,x}))}{\epsilon\epsilon'}\, ds
\end{aligned}$$

and invoke Itô's lemma once more for the mapping $(t, w) \mapsto e^{kt/2}\|w\|_2$. This produces

$$e^{kt/2}\|U_t\|_2 = e^0\|U_0\|_2 + \int_0^t ke^{ks}\|U_s\|_2 + e^{ks}\frac{d}{ds}\|U_s\|_2\, ds$$
$$= \int_0^t \frac{e^{ks/2}}{2\|U_s\|_2}\big(k\|U_s\|_2^2$$
$$+ \tfrac{1}{\epsilon\epsilon''}\langle U_s, \nabla \log p(Z_{s,x'+\epsilon''v'+\epsilon v}) - \nabla \log p(Z_{s,x'+\epsilon''v'}) - (\nabla \log p(Z_{s,x'+\epsilon v}) - \nabla \log p(Z_{s,x'}))\rangle$$
$$- \tfrac{1}{\epsilon\epsilon'}\langle U_s, \nabla \log p(Z_{s,x+\epsilon'v'+\epsilon v}) - \nabla \log p(Z_{s,x+\epsilon'v'}) - (\nabla \log p(Z_{s,x+\epsilon v}) - \nabla \log p(Z_{s,x}))\rangle\big) ds.$$

Fix a value $s \in [0, t]$, and introduce the shorthand $c_1 \triangleq f_1(x, x', \epsilon, \epsilon', \epsilon'')$ and $c_2 \triangleq f_2(x, x', \epsilon, \epsilon', \epsilon'')$. For any $h_3 \in C^3(\mathbb{R}^d)$, the Lemma 3.2 third-order difference inequality (3.3), the coupling bounds (3.7) and (3.8), Cauchy-Schwarz, and the Lipschitz identity (3.1) together imply the estimates

$$\begin{aligned}
&(h_3(Z_{s,x'+\epsilon''v'+\epsilon v}) - h_3(Z_{s,x'+\epsilon''v'}) - (h_3(Z_{s,x'+\epsilon v}) - h_3(Z_{s,x'})))/(\epsilon\epsilon'') \\
&\quad - (h_3(Z_{s,x+\epsilon'v'+\epsilon v}) - h_3(Z_{s,x+\epsilon'v'}) - (h_3(Z_{s,x+\epsilon v}) - h_3(Z_{s,x})))/(\epsilon\epsilon') \\
&\le \langle \nabla h_3(Z_{s,x'+\epsilon''v'}), U_s\rangle + M_2(h_3)\frac{L_3}{k}e^{-ks}(2\|x - x'\|_2 + \|x - x' + (\epsilon' - \epsilon'')v'\|_2) \\
&\quad + M_2(h_3)\frac{L_3}{k}e^{-ks}((\epsilon'' + \epsilon')/2 + \epsilon(3 + \epsilon/\epsilon'' + \epsilon/\epsilon' + \|x - x'\|_2/\epsilon')) \\
&\quad + M_3(h_3)e^{-3ks/2}(\|x - x' + (\epsilon' - \epsilon'')v'\|_2 + (\epsilon'' + \epsilon')/2 + \epsilon(3 + \epsilon/\epsilon'' + \epsilon/\epsilon')/3). \\
&\le \langle \nabla h_3(Z_{s,x'+\epsilon''v'}), U_s\rangle + M_2(h_3)\frac{3L_3}{k}e^{-ks}c_1 + M_3(h_3)e^{-3ks/2}c_2, && (3.14) \\
&\le M_1(h_3)\|U_s\|_2 + M_2(h_3)\frac{3L_3}{k}e^{-ks}c_1 + M_3(h_3)e^{-3ks/2}c_2, && (3.15)
\end{aligned}$$

where we have applied the triangle inequality to achieve (3.14). Applying the bound (3.14) to the thrice continuously differentiable function $h_3(z) = \langle U_s, \nabla \log p(z)\rangle$ with $M_2(h_3) = \sup_{z\in\mathbb{R}^d} \left\|\nabla^3 \log p(z)[U_s]\right\|_{op} \le L_3\|U_s\|_2$ and $M_3(h_3) \le L_4\|U_s\|_2$ gives

$$\begin{aligned}
&(h_3(Z_{s,x'+\epsilon''v'+\epsilon v}) - h_3(Z_{s,x'+\epsilon''v'}) - (h_3(Z_{s,x'+\epsilon v}) - h_3(Z_{s,x'})))/(\epsilon\epsilon'') \\
&\quad - (h_3(Z_{s,x+\epsilon'v'+\epsilon v}) - h_3(Z_{s,x+\epsilon'v'}) - (h_3(Z_{s,x+\epsilon v}) - h_3(Z_{s,x})))/(\epsilon\epsilon') \\
&\le \langle U_s, \nabla^2 \log p(Z_{s,x'+\epsilon''v'})U_s\rangle + \|U_s\|_2(\frac{3L_3^2}{k}e^{-ks}c_1 + L_4e^{-3ks/2}c_2). \\
&\le -k\|U_s\|_2^2 + \|U_s\|_2\frac{3L_3^2}{k}e^{-ks}c_1 + \|U_s\|_2L_4e^{-3ks/2}c_2.
\end{aligned}$$

In the final line, we used the k-strong log-concavity of p. Our efforts now yield (3.9) via

$$e^{kt/2}\|U_t\|_2 \le \int_0^t \frac{3L_3^2}{2k}e^{-ks/2}c_1 + \frac{L_4}{2}e^{-ks}c_2 ds \le \frac{3L_3^2}{k^2}c_1 + \frac{L_4}{2k}c_2.$$

The third-order differenced function bound (3.11) then follows by applying the third-order synchronous coupling bound (3.9) to the estimate (3.15). □

3.4 Proof of Theorem 2.1

By Lemma 3.1, for each $x \in \mathbb{R}^d$, the overdamped Langevin diffusion $(Z_{t,x})_{t\ge0}$ is well-defined with stationary distribution P. Moreover, for each $x \in \mathbb{R}^d$, the diffusion $(Z_{t,x})_{t\ge0}$, by definition, satisfies

$$dZ_{t,x} = \frac{1}{2}\nabla \log p(Z_{t,x})dt + dW_t \quad \text{with} \quad Z_{0,x} = x,$$

for $(W_t)_{t\geq 0}$ a d-dimensional Wiener process. In what follows, when considering the joint distribution of a finite collection of overdamped Langevin diffusions, we will assume that the diffusions are coupled in the manner of Lemma 3.3, so that each diffusion is driven by a shared d-dimensional Wiener process $(W_t)_{t\geq 0}$.

Fix any $x \in \mathbb{R}^d$ and any $h \in C^3(\mathbb{R}^d)$ with bounded first, second, and third derivatives. We divide the remainder of our proof into five components, establishing that u_h exists, u_h is Lipschitz, u_h has a Lipschitz gradient, u_h has a Lipschitz Hessian, and u_h solves the Stein equation (1.2).

Existence of u_h To see that the integral representation of $u_h(x)$ is well-defined, note that

$$\int_0^\infty |\mathbb{E}_P[h(Z)] - \mathbb{E}[h(Z_{t,x})]|\, dt = \int_0^\infty \left| \int_{\mathbb{R}^d} \mathbb{E}[h(Z_{t,y})] - \mathbb{E}[h(Z_{t,x})]\; p(y)dy \right| dt$$
$$\leq M_1(h) \int_0^\infty \int_{\mathbb{R}^d} \mathbb{E}\big[\|Z_{t,y} - Z_{t,x}\|_2\big]\; p(y)dy\; dt \leq M_1(h)\, \mathbb{E}_P[\|Z - x\|_2] \int_0^\infty e^{-kt/2}\; dt < \infty.$$

The first relation uses the stationarity of P, the second uses the Lipschitz relation (3.1), the third uses the first-order coupling inequality (3.7) of Lemma 3.3, and the last uses the fact that strongly log-concave distributions have subexponential tails and therefore finite moments of all orders [8, Lem. 1].

Lipschitz continuity of u_h We next show that u_h is Lipschitz. Fix any vector $v \in \mathbb{R}^d$, and consider the difference

$$|u_h(x+v) - u_h(x)| = \left| \int_0^\infty \mathbb{E}[h(Z_{t,x}) - h(Z_{t,x+v})]\; dt \right| \leq M_1(h) \int_0^\infty \mathbb{E}\big[\|Z_{t,x} - Z_{t,x+v}\|_2\big]\; dt$$
$$\leq \|v\|_2 M_1(h) \int_0^\infty e^{-kt/2}\; dt = \frac{2}{k}\|v\|_2 M_1(h). \tag{3.16}$$

The second relation is an application of the Lipschitz relation (3.1), and the third applies the first-order coupling inequality (3.7) of Lemma 3.3.

Lipschitz continuity of ∇u_h To demonstrate that u_h is differentiable with Lipschitz gradient, we first establish a weighted second-order difference inequality for u_h.

Lemma 3.4. *For any vectors $x, x', v' \in \mathbb{R}^d$ with $\|v'\|_2 = 1$ and weights $\epsilon', \epsilon'' > 0$,*

$$|(u_h(x' + \epsilon'' v') - u_h(x'))/\epsilon'' - (u_h(x + \epsilon' v') - u_h(x))/\epsilon'|$$
$$\leq (\|x - x'\|_2 + (\epsilon'' + \epsilon')/2)\left(M_1(h)\frac{2L_3}{k^2} + M_2(h)\frac{1}{k} \right). \tag{3.17}$$

Proof. We apply the Lemma 3.3 second-order function coupling inequality (3.10) to obtain

$$|(u_h(x' + \epsilon'' v') - u_h(x'))/\epsilon'' - (u_h(x + \epsilon' v') - u_h(x))/\epsilon'|$$
$$= \left| \int_0^\infty \mathbb{E}[h(Z_{t,x'+\epsilon' v}) - h(Z_{t,x'})]/\epsilon' - \mathbb{E}[h(Z_{t,x+\epsilon v}) - h(Z_{t,x})]/\epsilon\; dt \right|$$
$$\leq (\|x - x'\|_2 + (\epsilon' + \epsilon)/2) \int_0^\infty M_1(h)\frac{L_3}{k} e^{-kt/2} + M_2(h) e^{-kt}\; dt.$$

The desired bound follows by integrating the final expression. □

Now, fix any $x, v \in \mathbb{R}^d$ with $\|v\|_2 = 1$. As a first application of the Lemma 3.4 second-order difference inequality (3.17), we will demonstrate the existence of the directional derivative

$$\nabla_v u_h(x) \triangleq \lim_{\epsilon \to 0} \frac{u_h(x + \epsilon v) - u_h(x)}{\epsilon}. \tag{3.18}$$

Indeed, Lemma 3.4 implies that, for any integers $m, m' > 0$,

$$\begin{aligned}&|m'(u_h(x + v/m') - u_h(x)) - m(u_h(x + v/m) - u_h(x))| \\ \leq &\left(\frac{1}{2m} + \frac{1}{2m'}\right)\left(M_1(h)\frac{2L_3}{k^2} + M_2(h)\frac{1}{k}\right).\end{aligned}$$

Hence, the sequence $\left(\frac{u_h(x+v/m)-u_h(x)}{1/m}\right)_{m=1}^{\infty}$ is Cauchy, and the directional derivative (3.18) exists.

To see that the directional derivative (3.18) is also Lipschitz, fix any $v' \in \mathbb{R}^d$, and consider the bound

$$\begin{aligned}|\nabla_v u_h(x + v') - \nabla_v u_h(x)| &\leq \lim_{\epsilon \to 0} \left| \frac{u_h(x + \epsilon v + v') - u_h(x + v')}{\epsilon} - \frac{u_h(x + \epsilon v) - u_h(x)}{\epsilon} \right| \\ \leq \lim_{\epsilon \to 0} (\|v'\|_2 + \epsilon)\left(M_1(h)\frac{2L_3}{k^2} + M_2(h)\frac{1}{k}\right) &= \|v'\|_2 \left(M_1(h)\frac{2L_3}{k^2} + M_2(h)\frac{1}{k}\right),\end{aligned} \tag{3.19}$$

where the second inequality follows from Lemma 3.4. Since each directional derivative is Lipschitz continuous, we may conclude that u_h is continuously differentiable with Lipschitz continuous gradient ∇u_h. Our Lipschitz function deduction (3.16) and the Lipschitz relation (3.1) additionally supply the uniform bound $M_1(u_h) \leq \frac{2}{k} M_1(h)$.

Lipschitz continuity of $\nabla^2 u_h$ To demonstrate that ∇u_h is differentiable with Lipschitz gradient, we begin by establishing a weighted third-order difference inequality for u_h.

Lemma 3.5. *Fix any vectors $x, x', v, v' \in \mathbb{R}^d$ with $\|v\|_2 = \|v'\|_2 = 1$ and weights $\epsilon, \epsilon', \epsilon'' > 0$, and define $f_1(x, x', \epsilon, \epsilon', \epsilon'')$ and $f_2(x, x', \epsilon, \epsilon', \epsilon'')$ as in* (3.5) *. Then,*

$$\begin{aligned}&|(u_h(x' + \epsilon'' v' + \epsilon v) - u_h(x' + \epsilon'' v') - (u_h(x' + \epsilon v) - u_h(x')))/(\epsilon\epsilon'') \\ &- (u_h(x + \epsilon' v' + \epsilon v) - u_h(x + \epsilon' v') - (u_h(x + \epsilon v) - u_h(x)))/(\epsilon\epsilon')| \\ \leq &\left(M_1(h)\frac{6L_3^2}{k^3} + M_2(h)\frac{3L_3}{k^2}\right) f_1(x, x', \epsilon, \epsilon', \epsilon'') + \left(M_1(h)\frac{L_4}{k^2} + M_3(h)\frac{2}{3k}\right) f_2(x, x', \epsilon, \epsilon', \epsilon'').\end{aligned} \tag{3.20}$$

Proof. Introduce the shorthand $c_1 \triangleq f_1(x, x', \epsilon, \epsilon', \epsilon'')$ and $c_2 \triangleq f_2(x, x', \epsilon, \epsilon', \epsilon'')$. We apply the Lemma 3.3 third-order function coupling inequality (3.11) to the thrice continuously differentiable function h to obtain

$$\begin{aligned}&|(u_h(x' + \epsilon'' v' + \epsilon v) - u_h(x' + \epsilon'' v') - (u_h(x' + \epsilon v) - u_h(x')))/(\epsilon\epsilon'') \\ &- (u_h(x + \epsilon' v' + \epsilon v) - u_h(x + \epsilon' v') - (u_h(x + \epsilon v) - u_h(x)))/(\epsilon\epsilon')| \\ = &\left| \int_0^\infty \mathbb{E}[(h(Z_{t,x'+\epsilon''v'+\epsilon v}) - h(Z_{t,x'+\epsilon''v'}) - (h(Z_{t,x'+\epsilon v}) - h(Z_{t,x'})))]/(\epsilon\epsilon'') \right. \\ &\left. - \mathbb{E}[(h(Z_{t,x+\epsilon'v'+\epsilon v}) - h(Z_{t,x+\epsilon'v'}) - (h(Z_{t,x+\epsilon v}) - h(Z_{t,x})))]/(\epsilon\epsilon')\, dt \right| \\ \leq &\int_0^\infty \left(M_1(h)\frac{3L_3^2}{k^2} e^{-kt/2} + M_2(h)\frac{3L_3}{k} e^{-kt}\right) c_1 + \left(M_1(h)\frac{L_4}{2k} e^{-kt/2} + M_3(h) e^{-3kt/2}\right) c_2 \, dt.\end{aligned}$$

Integrating this final expression yields the advertised bound. □

Now, fix any $x, v, v' \in \mathbb{R}^d$ with $\|v\|_2 = \|v'\|_2 = 1$. As a first application of the Lemma 3.5 third-order difference inequality (3.20), we will demonstrate the existence of the second-order directional derivative

$$\begin{aligned}\nabla_{v'}\nabla_v u_h(x) &\triangleq \lim_{\epsilon'\to 0} \frac{\nabla_v u_h(x+\epsilon' v') - \nabla_v u_h(x)}{\epsilon'} \\ &= \lim_{\epsilon'\to 0}\lim_{\epsilon\to 0} \frac{u_h(x+\epsilon' v'+\epsilon v) - u_h(x+\epsilon v) - (u_h(x+\epsilon' v') - u_h(x))}{\epsilon\epsilon'}.\end{aligned} \tag{3.21}$$

Lemma 3.5 guarantees that, for any integers $m, m' > 0$,

$$\begin{aligned}&|m'(\nabla_v u_h(x+v'/m') - \nabla_v u_h(x)) - m(\nabla_v u_h(x+v'/m) - \nabla_v u_h(x))| \\ &\leq \lim_{\epsilon\to 0} |m'(u_h(x+v'/m'+v\epsilon) - u_h(x+v'/m') - (u_h(x+v\epsilon) - u_h(x)))/\epsilon \\ &\qquad - m(u_h(x+v'/m+v\epsilon) - u_h(x+v'/m) - (u_h(x+v\epsilon) - u_h(x)))/\epsilon| \\ &\leq \left(\frac{1}{m} + \frac{1}{m'}\right)\left(M_1(h)\left(\frac{3L_3^2}{k^3} + \frac{3L_4}{2k^2}\right) + M_2(h)\frac{3L_3}{2k^2} + M_3(h)\frac{1}{k}\right).\end{aligned}$$

Hence, the sequence $\left(\frac{\nabla_v u_h(x+v'/m) - \nabla_v u_h(x)}{1/m}\right)_{m=1}^{\infty}$ is Cauchy, and the directional derivative (3.21) exists.

To see that the directional derivative (3.21) is also Lipschitz, fix any $v'' \in \mathbb{R}^d$, and consider the bound

$$\begin{aligned}&|\nabla_{v'}\nabla_v u_h(x+v'') - \nabla_{v'}\nabla_v u_h(x)| \\ &\leq \lim_{\epsilon'\to 0}\left|\frac{\nabla_v u_h(x+v''+\epsilon' v') - \nabla_v u_h(x+v'')}{\epsilon'} - \frac{\nabla_v u_h(x+\epsilon' v') - \nabla_v u_h(x)}{\epsilon'}\right| \\ &\leq \lim_{\epsilon'\to 0}\lim_{\epsilon\to 0}\left|\frac{u_h(x+v''+\epsilon' v'+\epsilon v) - u_h(x+v''+\epsilon v) - (u_h(x+v''+\epsilon' v') - u_h(x+v''))}{\epsilon\epsilon'}\right. \\ &\qquad \left. - \frac{u_h(x+\epsilon' v'+\epsilon v) - u_h(x+\epsilon v) - (u_h(x+\epsilon' v') - u_h(x))}{\epsilon\epsilon'}\right| \\ &\leq \|v''\|_2\left(M_1(h)\left(\frac{6L_3^2}{k^3} + \frac{L_4}{k^2}\right) + M_2(h)\frac{3L_3}{k^2} + M_3(h)\frac{2}{3k}\right),\end{aligned}$$

where the final inequality follows from Lemma 3.5. Since each second-order directional derivative is Lipschitz continuous, we conclude that $u_h \in C^2(\mathbb{R}^d)$ with Lipschitz continuous Hessian $\nabla^2 u_h$. Our Lipschitz gradient result (3.19) and the Lipschitz relation (3.1) further furnish the uniform bound $M_2(u_h) \leq M_1(h)\frac{2L_3}{k^2} + M_2(h)\frac{1}{k}$.

Solving the Stein equation Finally, we show that u_h solves the Stein equation (1.2). Introduce the notation $(P_t h)(x) \triangleq \mathbb{E}[h(Z_{t,x})]$. Since $(P_t)_{t\geq 0}$ is strongly continuous on the Banach space L of Lemma 3.1 and $h \in L$, the generator $\mathcal{A}$, defined in (1.1), satisfies

$$h - P_t h = \mathcal{A}\int_0^t \mathbb{E}_P[h(Z)] - P_s h\, ds \quad \text{for all} \quad t \geq 0$$

by [9, Prop. 1.5]. The left-hand side limits in L to $h - \mathbb{E}_P[h(Z)]$ as $t \to \infty$, as

$$\begin{aligned}|h(x) - \mathbb{E}_P[h(Z)] - (h(x) - (P_t h)(x))| &= \left|\int_{\mathbb{R}^d} \mathbb{E}[h(Z_{t,y})] - \mathbb{E}[h(Z_{t,x})]\, p(y)dy\right| \\ &\leq M_1(h)\int_{\mathbb{R}^d} \mathbb{E}\big[\|Z_{t,y} - Z_{t,x}\|_2\big]\, p(y)dy \leq M_1(h)\,\mathbb{E}_P[\|Z - x\|_2]e^{-kt/2}\end{aligned}$$

for each $x \in \mathbb{R}^d$ and $t \geq 0$. Here we have used the stationarity of P, the Lipschitz relation (3.1), the first-order coupling inequality (3.7) of Lemma 3.3, and the integrability of Z [8, Lem. 1] in turn. Meanwhile, the right-hand side limits to $\mathcal{A}u_h$, since $\mathcal{A}$ is closed [9, Cor. 1.6]. Therefore, u_h solves the Stein equation (1.2).

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