MULTIVARIATE APPROXIMATIONS IN WASSERSTEIN DISTANCE BY STEIN’S METHOD AND BISMUT’S FORMULA

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ABSTRACT. Stein’s method has been widely used for probability approximations. However, in the multi-dimensional setting, most of the results are for multivariate normal approximation or for test functions with bounded second- or higher-order derivatives. For a class of multivariate limiting distributions, we use Bismut’s formula in Malliavin calculus to control the derivatives of the Stein equation solutions by the first derivative of the test function. Combined with Stein’s exchangeable pair approach, we obtain a general theorem for multivariate approximations with near optimal error bounds on the Wasserstein distance. We apply the theorem to the unadjusted Langevin algorithm.

AMS 2010 subject classification: 60F05, 60H07.

Keywords and phrases: Bismut’s formula, Langevin algorithm, Malliavin calculus, multivariate approximation, rate of convergence, Stein’s method, Wasserstein distance.

1. INTRODUCTION

Let $W$ and $Z$ be $d$-dimensional random vectors, $d \geq 1$, where $Z$ has the density

$$Ke^{-U(x)} , \quad x \in \mathbb{R}^d$$

for a given function $U : \mathbb{R}^d \to \mathbb{R}$ and a possibly unknown normalizing constant $K$. We are concerned with bounding their Wasserstein distance, defined as follows:

$$d_W(\mathcal{L}(W), \mathcal{L}(Z)) : = \sup_{h \in \text{Lip}(\mathbb{R}^d, 1)} |E[h(W)] - E[h(Z)]|,$$

where Lip$(\mathbb{R}^d, 1)$ denotes the set of Lipschitz functions $h : \mathbb{R}^d \to \mathbb{R}$ with Lipschitz constant 1, that is, $|h(x) - h(y)| \leq |x - y|$ for any $x, y \in \mathbb{R}^d$, and $| \cdot |$ denotes the Euclidean metric.

Our main tool is Stein’s method for probability approximations [37]. Since it was first introduced, there have been many developments in multivariate probability approximations. However, most of the results are for multivariate normal approximation or for test functions $h$ with bounded second- or higher-order derivatives. See, for example, [16, 7, 30, 24]. Although these results may be used to deduce error bounds for the Wasserstein distance, such error bounds are far from optimal. The literature on (near) optimal error bounds for the Wasserstein distance are limited to a few special cases, including multivariate normal approximation for sums of independent random vectors [39] and multivariate approximation for the stationary distribution of certain Markov chains with bounded jump sizes [19, 5].

The main difficulty in obtaining an optimal error bound for the Wasserstein distance is controlling the derivatives of the Stein equation solutions using the first derivative of the test function $h$. For multivariate non-normal approximations, the Stein equation solution is typically expressed in terms of a stochastic process (cf. (6.3)). This unexplicity means that we cannot use the usual integration by parts formula when studying its derivatives. This is in contrast to multivariate normal approximation, where we have an explicit expression of the Stein equation solution (cf. (B.4)). We use Bismut’s formula (cf. (5.11)) in Malliavin calculus to overcome this difficulty and obtain estimates for the derivatives of the Stein equation solutions for a large
class of limiting distributions. We note that Nourdin and Peccati [26, 27] first combined Malliavin calculus and Stein’s method to study normal approximation in a fixed Wiener chaos of a general Gaussian process. See [28] and [21] for generalizations to multivariate normal approximation and one-dimensional diffusion approximations, respectively.

The exchangeable pair is a powerful tool in Stein’s method to exploit the dependence structure within the random vector \( W \). It was elaborated in [38] and works for both independent and many dependent random vectors. In particular, we use a generalized version in [34] and assume that we can construct a suitable random vector \( W' \) on the same probability space and with the same distribution as \( W \). We then follow the idea of [8] and [36], by studying the conditional expectations \( \mathbb{E}[W' - W | W] \) and \( \mathbb{E}[(W' - W)(W' - W)^T | W] \) where \( T \) is the transpose operator, to identify the limiting distribution of \( W \) and obtain an error bound for the Wasserstein distance in the approximation. Our main result can be regarded as an extension of the result in [8] to the multi-dimensional setting. An additional logarithmic factor appears in our error bound due to the multi-dimensionality. We illustrate some of the techniques for removing it in the special case of multivariate normal approximation for standardized sums of independent and bounded random vectors.

Our main theorem can be used in justifying the so-called unadjusted Langevin algorithm [33], which is widely used in Bayesian inference and statistical physics to sample from a distribution that is known up to a normalizing constant. In particular, we provide an error bound for the Wasserstein distance between the sampling distribution and the target distribution in terms of the step size in the algorithm. Our result complements those in the literature by relaxing the conditions on the increment distribution.

We would like to mention two other distances between distributions that have also been widely studied. One is for comparing probabilities on convex sets in \( \mathbb{R}^d \). See, for example, [18, 2] for multivariate normal approximation for sums of independent random vectors, and [32] for sums of bounded random vectors with a certain dependency structure. Proving optimal error bounds in this case requires special techniques involving smoothing of the test functions and induction or recursion. The other distance is the so-called Wasserstein-2 distance which is stronger than the Wasserstein distance considered in this paper. See, for example, [22, 4] and the references therein for related results. The techniques used therein, which involves transportation inequalities and/or Stein kernels, are very different from ours.

The paper is organized as follows. In Section 2, we present our main result. In Section 3, we state the new properties of the Stein equation solutions and use them to prove our main result. The application to the unadjusted Langevin algorithm is discussed in Section 4. We develop Bismut’s approach to Malliavin calculus to prove the properties of the Stein equation solutions in Sections 5–7. Some of the details are deferred to Section 8 and Appendix A. In Appendix B, we illustrate some of the techniques for removing the logarithmic term in our main result for the special case of multivariate normal approximation for sums of independent and bounded random vectors.

## 2. Notation, Assumptions and the Main Result

### 2.1. Notation

The inner product of \( x, y \in \mathbb{R}^d \) is denoted by \( \langle x, y \rangle \). The Euclidean metric is denoted by \( |x| \). Each time we speak about Lipschitz functions on \( \mathbb{R}^d \), we use the Euclidean norm. \( C(\mathbb{R}^d, \mathbb{R}) \) denotes the collection of all continuous functions \( f : \mathbb{R}^d \to \mathbb{R} \) and \( C^k(\mathbb{R}^d, \mathbb{R}) \) with \( k \geq 1 \) denotes the collection of all \( k \)-th order continuously differentiable functions. \( C_0^\infty(\mathbb{R}^d, \mathbb{R}) \) denotes the set of smooth functions whose every order derivative decays to zero at infinity. For \( f \in C^2(\mathbb{R}^d, \mathbb{R}) \) and \( u, u_1, u_2, x \in \mathbb{R}^d \), the directional derivative \( \nabla_u f(x) \) and
\[ \nabla_{u_2} \nabla_{u_1} f(x) \text{ are defined by} \]
\[ \nabla_{u_2} f(x) = \lim_{\varepsilon \to 0} \frac{f(x + \varepsilon u) - f(x)}{\varepsilon}, \]
\[ \nabla_{u_2} \nabla_{u_1} f(x) = \lim_{\varepsilon \to 0} \frac{\nabla_{u_2} f(x + \varepsilon u_2) - \nabla_{u_2} f(x)}{\varepsilon}, \]
respectively. Let \( \nabla f(x) \in \mathbb{R}^d \), \( \nabla^2 f(x) \in \mathbb{R}^{d \times d} \) and \( \Delta f(x) \in \mathbb{R} \) denote the gradient, the Hessian, and the Laplacian of \( f \), respectively. It is known that \( \nabla_{u_2} f(x) = (\nabla f(x), \mathbf{u}) \) and \( \nabla_{u_2} \nabla_{u_1} f(x) = (\nabla^2 f(x), u_1 u_2^T)_{\text{HS}} \), where \( T \) is the transpose operator and \( \langle A, B \rangle_{\text{HS}} := \sum_{i,j=1}^{d} A_{ij} B_{ij} \) for \( A, B \in \mathbb{R}^{d \times d} \). Given a matrix \( A \in \mathbb{R}^{d \times d} \), its Hilbert-Schmidt norm is \( ||A||_{\text{HS}} = \sqrt{\sum_{i,j=1}^{d} A_{ij}^2} = \sqrt{\text{Tr}(A^T A)} \) and its operator norm is \( ||A||_{\text{op}} = \sup_{||u||=1} |Au| \). We have the following relations:
\[ (2.1) \quad ||A||_{\text{op}} = \sup_{||u||=1} |\langle A, u_1 u_2^T \rangle_{\text{HS}}|, \quad ||A||_{\text{op}} \leq ||A||_{\text{HS}} \leq \sqrt{d} ||A||_{\text{op}}. \]

We can also define \( \nabla_{u_2} f(x) \) and \( \nabla_{u_1} \nabla_{u_2} f(x) \) for a second-order differentiable function \( f = (f_1, \ldots, f_d)^T : \mathbb{R}^d \to \mathbb{R}^d \) in the same way as above. Define \( \nabla f(x) = (\nabla f_1(x), \ldots, \nabla f_d(x)) \in \mathbb{R}^{d \times d} \) and \( \nabla^2 f(x) = \{\nabla^2 f_i(x)\}_{i=1}^{d} \in \mathbb{R}^{d \times d \times d} \). In this case, we have \( \nabla_{u_2} f(x) = (\nabla f(x))^T u \) and \( \nabla_{u_2} \nabla_{u_1} f(x) = ((\nabla^2 f_1(x), u_1 u_2^T)_{\text{HS}}, \ldots, (\nabla^2 f_d(x), u_1 u_2^T)_{\text{HS}})^T. \)

Moreover, \( C_b(\mathbb{R}^{d_1}, \mathbb{R}^{d_2}) \) denotes the set of all bounded measurable functions from \( \mathbb{R}^{d_1} \) to \( \mathbb{R}^{d_2} \) with the supremum norm defined by
\[ ||f|| = \sup_{x \in \mathbb{R}^{d_1}} |f(x)|. \]
Denote by \( C_{p_1, \ldots, p_k} \) some positive number depending on \( k \) parameters, \( p_1, \ldots, p_k \), whose exact values can vary from line to line.

2.2. Assumptions. We aim to approximate \( W \), a \( d \)-dimensional random vector of interest, by a non-degenerate probability measure \( \mu \) on \( \mathbb{R}^d \), which is the ergodic measure (cf. Remark 2.3) of the following stochastic differential equation (SDE):
\[ (2.2) \quad dX_t = g(X_t)dt + \sqrt{2}dB_t, \quad X_0 = x, \]
where \( B_t \) is a standard \( d \)-dimensional Brownian motion and

**Assumption 2.1.** \( g \in C^2(\mathbb{R}^d, \mathbb{R}^d) \) and there exist \( \theta_0 > 0 \) and \( \theta_1, \theta_2, \theta_3 \geq 0 \) such that
\[ (2.3) \quad \langle u, \nabla_u g(x) \rangle \leq -\theta_0 \left( 1 + \theta_1 |x|^\theta_2 \right) |u|^2, \quad \forall u, x \in \mathbb{R}^d, \]
\[ (2.4) \quad |\nabla_{u_1} \nabla_{u_2} g(x)| \leq \theta_3 (1 + \theta_1 |x|)\theta_2^{-1} |u_1||u_2|, \quad \forall u_1, u_2, x \in \mathbb{R}^d. \]

Remark 2.2. By integration, (2.3) implies
\[ (2.5) \quad \langle x, g(x) - g(0) \rangle \leq -\theta_0 (|x|^2 + \frac{\theta_1 |x|^{2+\theta_2}}{1+\theta_2}), \quad \forall x \in \mathbb{R}^d, \]
and (2.4) implies
\[ (2.6) \quad |g(x)| \leq \theta_4 (1 + |x|^{1+\theta_2}), \quad \forall x \in \mathbb{R}^d, \]
where \( \theta_4 > 0 \) is a constant depending on \( \theta_1, \theta_2, \theta_3, g(0) \) and \( \nabla g(0) \).
Remark 2.3. The SDE (2.2) is known as the Langevin SDE. The conditions \( g \in C^1(\mathbb{R}^d, \mathbb{R}^d) \) and (2.3) ensure that SDE (2.2) has a unique strong solution, which hereafter is denoted by \( X^x_t \). This follows by Theorem 2.2 in [11]. In fact, (i) and (ii) of Hypothesis 2.1 in [11] automatically hold, and (iii) is verified by

\[
\langle g(x) - g(y), x - y \rangle = \int_0^1 \langle \nabla_{x-y} g(\theta x + (1-\theta)y), x - y \rangle d\theta \leq 0.
\]

Moreover, these two conditions also imply that the SDE admits a unique ergodic measure \( \mu \) such that

\[
\lim_{t \to \infty} \mathbb{E} f(X^x_t) = \mu(f)
\]

for all bounded continuous functions \( f : \mathbb{R}^d \to \mathbb{R} \). We leave the details to Appendix A.

Remark 2.4. In the literature on multivariate probability approximations by \( \mu \), it is often assumed that \( \mu \) is strongly log-concave. See, for example, Eq. (1) in [10], Assumption H2 in [13] and Theorem 2.1 in [24]. This corresponds to condition (2.3) with \( \theta_0 > 0 \) and \( \theta_1 = 0 \). We use this condition to ensure the existence of the Stein equation solution (cf. (6.3)). Moreover, because we will use integration by parts (under Malliavin calculus), we need to impose conditions on the higher-order derivatives of \( g \), such as (2.4).

Below, we give two examples of \( \mu \) that satisfy Assumption 2.1 and one counterexample.

**Example 1**: \( g(x) = -Ax \) and \( A \in \mathbb{R}^{d \times d} \) is a symmetric positive definite matrix with eigenvalues \( \lambda_1 \geq \cdots \geq \lambda_d > 0 \). The corresponding measure \( \mu \) is a Gaussian measure with the density

\[
\varphi(x) = \left( \frac{\det(A)}{2\pi} \right)^{d/2} \exp\left( -\frac{\langle x, Ax \rangle}{2} \right).
\]

It can be verified that Assumption 2.1 is satisfied with \( \theta_0 = \lambda_d, \theta_1 = 0, \theta_2 = 1, \theta_3 = 1 \), and (2.6) holds with \( \theta_4 = \lambda_1 \).

**Example 2**: \( g(x) = -c(1 + |x|^2)^{p/2}x \) with \( p \geq 0 \) and \( c > 0 \). The corresponding measure \( \mu \) has the density function

\[
K e^{-\frac{c}{p+2}(1+|x|^2)^{p/2+1}} \quad \text{with} \quad K = \left( \int_{\mathbb{R}^d} e^{-\frac{c}{p+2}(1+|x|^2)^{p/2+1}} dx \right)^{-1}.
\]

In this case, we have

\[
\langle u, \nabla_u g(x) \rangle = -c(1 + |x|^2)^{p/2} |u|^2 - cp(1 + |x|^2)^{p-2} |\langle x, u \rangle|^2,
\]

\[
\nabla^2_{u_1} \nabla_{u_2} g(x) = -cp(1 + |x|^2)^{p-1} \left( \langle x, u_1 \rangle u_2 + \langle x, u_2 \rangle u_1 + \langle u_1, u_2 \rangle x \right)
\]

\[
- cp(p-2)(1 + |x|^2)^{p-2} \langle x, u_1 \rangle \langle x, u_2 \rangle.
\]

It is then straightforward to determine \( \theta_0, \ldots, \theta_4 \) which depend on \( c \) and \( p \). We omit the details.

**Counterexample**: \( g(x) = -c|x|^p x \) with \( p \geq 1 \) and \( c > 0 \). We have

\[
\langle u, \nabla_u g(x) \rangle = -c \left( |x|^p |u|^2 + p|x|^{p-2} |\langle x, u \rangle|^2 \right),
\]

which does not satisfy (2.3) with any positive \( \theta_0 \).
2.3. Main result. We use a version of Stein’s exchangeable pair approach by Röllin [34] to exploit the dependence structure of the random vector \( W \) of interest with \( \mathbb{E}[W] < \infty \). Suppose we can construct a suitable random vector \( W' \) on the same probability space and with the same distribution as \( W \). Denote \( \delta = W' - W \) and assume that

\[
\mathbb{E}[\delta|W] = \lambda(g(W) + R_1),
\]

where \( R_1 \) is an \( \mathbb{R}^d \)-valued random vector. Further assume that

\[
\mathbb{E}[\delta \delta^T|W] = 2\lambda(I_d + R_2)
\]

where \( I_d \) denotes the \( d \times d \) identity matrix. In some applications, \( R_2 \) has the form

\[
R_2 = r_1 r_2^T + ... + r_{2p-1} r_{2p}^T,
\]

where \( p \in \mathbb{N} \) and \( r_1, ..., r_{2p} \in \mathbb{R}^d \). In the application to the unadjusted Langevin algorithm in Section 4, \( p = 1 \).

Our main result is the following theorem on multi-dimensional non-normal (including normal) approximations.

**Theorem 2.5.** Let Assumption 2.1, (2.7) and (2.8) hold. Then we have

\[
d_W(\mathcal{L}(W), \mu) \leq C_\theta \left\{ \frac{1}{\lambda} \mathbb{E} \left[ |\delta|^3 (|\delta| \vee 1) \right] + \mathbb{E}[R_1] + \sqrt{\mathbb{E}[\|R_2\|_{\text{HS}}]} \right\},
\]

where \( \mu \) is the ergodic measure of SDE (2.2) and hereafter \( C_\theta \) is short hand for \( C_{\theta_0, ..., \theta_4} \). If \( R_2 \)

has the form (2.9), then

\[
d_W(\mathcal{L}(W), \mu) \leq C_\theta \left\{ \frac{1}{\lambda} \mathbb{E} \left[ |\delta|^3 (|\delta| \vee 1) \right] + \mathbb{E}[R_1] + \sum_{i=1}^{p} \mathbb{E}[\|r_{2i-1}\| r_{2i}] \right\}.
\]

**Remark 2.6.** Note that when \( \theta_0, ..., \theta_3 \) in Assumption 2.1 and \( \theta_4 \) in (2.6) are independent of the dimension \( d \) as in the two examples above, the constant \( C_\theta \) in (2.10) and (2.11) is dimension-free.

**Remark 2.7.** Theorem 2.5 can be regarded as an extension of [38, Lecture 3, Theorem 1] and [8, Theorem 1.1] to the multi-dimensional and non-normal approximations, with a minor cost of an additional logarithmic factor.

**Remark 2.8.** If, instead of \( \mathbb{E}[\delta \delta^T|W] \approx 2\lambda I_d \) in (2.8), we have \( \mathbb{E}[\delta \delta^T|W] \approx 2\lambda \Lambda \) for an invertible, positive definite matrix \( \Lambda \), then we may approximate it by the ergodic measure of the following SDE with non-identity diffusion coefficient

\[
dX_t = g(X_t)dt + \sqrt{2}\Lambda^{1/2}dB_t, \quad X_0 = x.
\]

Our approach is still applicable to this case, although details need to be work out with greater effort, especially if we are interested in the dependence of the bound on \( \Lambda \). We may as well reduce the problem to the setting of Theorem 2.5 by considering approximating \( \Lambda^{-1/2}W \) by the ergodic measure of the SDE with identity diffusion coefficient and drift coefficient as

\[
\tilde{g}(\cdot) = \Lambda^{-1/2}g(\Lambda^{1/2} \cdot),
\]

although then the problem becomes obtaining an explicit expression of \( C_\theta \) in Theorem 2.5 in terms of the parameters appearing in Assumption 2.1.
Remark 2.9. In the case of multivariate normal approximation for sums of independent, bounded random variables \( W = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} X_i \) with \( \mathbb{E} X_i = 0, |X_i| \leq \beta \) and \( \mathbb{E} W W^T = I_d \), the bound in (2.10) reduces to, with details deferred to Appendix B,
\[
\frac{C d \beta}{\sqrt{n}} (1 + \log n),
\]
where \( C \) is an absolute constant. This is of the same order as in Theorem 2 of [39]. In this case, we may remove the additional logarithmic factor and obtain the error bound (see Appendix B)
\[
\frac{C d^2 \beta}{\sqrt{n}}.
\]

The additional logarithmic term may also be removed for \( W \) to be a sum of independent and unbounded random vectors and for \( W \) to exhibit an exchangeable pair. However, we would need certain moment assumptions and increase the dependence of the bound on the dimension.

Also in this case, under the additional assumption that \( \mathbb{E} X_i X_i^T = I_d \) for each \( i = 1, \ldots, n \), Bonis [4] obtained the optimal rate \( O(\sqrt{d \beta / \sqrt{n}}) \) in the stronger Wasserstein-2 distance, which seems better than the previous results of [9] and [41]. Moreover, his general result [4, Theorem 1] extended those in [35, 3], and improved the multidimensional bound in [41] by removing some boundedness assumption and an additional \( \log n \) factor therein. We do not know how to obtain their results using our approach.

3. STEIN’S METHOD AND THE PROOF OF THEOREM 2.5

Let \( g \) satisfy Assumption 2.1, and let \( \mu \) be the ergodic measure of of SDE (2.2). Then \( \mu \) is invariant in the sense that
\[
\int_{\mathbb{R}^d} \mathbb{E} f(X^x_t) \mu(dx) = \int_{\mathbb{R}^d} f(x) \mu(dx), \quad f \in C_0^\infty(\mathbb{R}^d, \mathbb{R}).
\]

It is well known that \( \mu \) satisfies the following equation
\[
\int_{\mathbb{R}^d} [\Delta f(x) + \langle g(x), \nabla f(x) \rangle] \mu(dx) = 0, \quad f \in C_0^\infty(\mathbb{R}^d, \mathbb{R}).
\]

See [1, p. 326] for more details.

For a Lipschitz function \( h : \mathbb{R}^d \rightarrow \mathbb{R} \), consider the Stein equation
\[
(3.1) \quad \Delta f + \langle g(x), \nabla f(x) \rangle = h(x) - \mu(h),
\]
where \( \mu(h) := \int_{\mathbb{R}^d} h(x) \mu(dx) \) which exists (cf. (5.5)). The solution \( f := f_h \) exists and we drop the subscript for ease of notation. The following theorem on the regularity of \( f \) is crucial for the proof of our main result.

Theorem 3.1. Let \( h : \mathbb{R}^d \rightarrow \mathbb{R} \) be a Lipschitz function and let \( \varepsilon \in \mathbb{R} \). For any \( u_1, u_2 \in \mathbb{R}^d \), we have
\[
(3.2) \quad \|\nabla f\| \leq C_\theta \|
abla h\|,
\]
\[
(3.3) \quad \sup_{x \in \mathbb{R}^d} |\langle \nabla^2 f(x), u_1 u_2^T \rangle_{\text{HS}}| \leq C_\theta \|\nabla h\| \|u_1\| \|u_2\|,
\]
\[
(3.4) \quad \sup_{x, u \in \mathbb{R}^d, |u| \leq 1} |\langle \nabla^2 f(x + \varepsilon u) - \nabla^2 f(x), u_1 u_2^T \rangle_{\text{HS}}| \leq C_\theta \|\nabla h\| |\varepsilon| (|\log |\varepsilon|| \vee 1) \|u_1\| \|u_2\|.
\]
Remark 3.2. Gorham et. al. [17] recently put forward a method to measure sample quality with diffusions by a Stein discrepancy, in which the same Stein equation as (3.1) has to be considered. Under the assumption that $g$ is $3$rd order differentiable, they used the Bismut-Elworthy-Li formula [15], together with smooth convolution and interpolation techniques, to prove a bound on the first, second and $(3 - \epsilon)$th derivative of $f$ for $\epsilon > 0$. They can also obtain the bound (3.4) by their approach (personal communication [23]), albeit due to the interpolation argument therein, the assumption of 3rd order differentiability of $g$ can not be removed.

We defer the proof of Theorem 3.1 to Sections 6 and 7 by deriving stochastic representations of $f$ and its derivatives as follows:

$$f(x) = \int_0^\infty e^{-t}E[f(X_t^x) + \mu(h) - h(X_t^x)]dt,$$

$$\nabla_u f(x) = \int_0^\infty e^{-t}E\left\{[f(X_t^x) - h(X_t^x) + \mu(h)]T^u_t(t)\right\}dt,$$

where $X_t^x$ is the stochastic process determined by SDE (2.2) and $T^u_t(t)$ is a stochastic integral. The representation of $\nabla^2 f(x)$ is more complicated and can be found in (6.13).

With the regularity result in Theorem 3.1, we are in a position to prove our main result.

Proof of Theorem 2.5. From the fact that $W$ and $W'$ have the same distribution and using Taylor’s expansion, we have

$$0 = \mathbb{E}[f(W') - f(W)]$$

$$= \mathbb{E}[\langle \delta, \nabla f(W) \rangle] + \frac{1}{2} \int_0^1 \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W + t\delta) \rangle]_{HS} dt.$$

By (2.7) and (2.8), we have

$$\mathbb{E}[\langle \delta, \nabla f(W) \rangle] = \mathbb{E}[\langle \mathbb{E} [\delta | W], \nabla f(W) \rangle]$$

$$= \lambda \mathbb{E}[\langle g(W), \nabla f(W) \rangle] + \lambda \mathbb{E}[\langle R_1, \nabla f(W) \rangle]$$

and

$$\int_0^1 \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W + t\delta) \rangle]_{HS} dt$$

$$= \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W) \rangle]_{HS} + \int_0^1 \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W + t\delta) - \nabla^2 f(W) \rangle]_{HS} dt$$

$$= \mathbb{E}[\mathbb{E} [\langle \delta \delta^T | W \rangle, \nabla^2 f(W) \rangle]_{HS} + \int_0^1 \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W + t\delta) - \nabla^2 f(W) \rangle]_{HS} dt$$

$$= 2\lambda \mathbb{E}[\Delta f(W)] + 2\lambda \mathbb{E}[\langle R_2, \nabla^2 f(W) \rangle]_{HS} + \int_0^1 \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W + t\delta) - \nabla^2 f(W) \rangle]_{HS} dt.$$

Combining the previous three equations, we obtain

$$\mathbb{E}[\Delta f(W) + \langle g(W), \nabla f(W) \rangle] = -\mathbb{E}[\langle R_1, \nabla f(W) \rangle] - \mathbb{E}[\langle R_2, \nabla^2 f(W) \rangle]_{HS}$$

$$- \frac{1}{2\lambda} \int_0^1 \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W + t\delta) - \nabla^2 f(W) \rangle]_{HS} dt.$$

By (3.1), we have

$$|\mathbb{E}[h(W)] - \mu(h)| \leq \mathbb{E}[|\langle R_1, \nabla f(W) \rangle| + |\mathbb{E}[\langle R_2, \nabla^2 f(W) \rangle]_{HS}|]$$

$$+ \frac{1}{2\lambda} \int_0^1 \mathbb{E}[|\langle \delta \delta^T, \nabla^2 f(W + t\delta) - \nabla^2 f(W) \rangle]_{HS}| dt.$$
By \((3.2)\), we have
\[
|\mathbb{E}[(R_1, \nabla f(W))]| \leq C_0 \|\nabla h\| |\mathbb{E}[|R_1|]|
\]
By \((3.3)\) and \((2.1)\), we have
\[
|\mathbb{E}[(R_2, \nabla^2 f(W))_{HS}]| \leq \sup_{x \in \mathbb{R}^d} |\nabla^2 f(x)||_{HS}\mathbb{E}[|R_2|]_{HS} \leq C_0 \sqrt{d} \|\nabla h\| |\mathbb{E}[|R_2|]_{HS}|
\]
If \(R_2\) has the form \((2.9)\), by \((3.3)\) we have
\[
|\mathbb{E}[(R_2, \nabla^2 f(W))_{HS}]| = \mathbb{E} \left[ \sum_{i=1}^{p} \langle r_{2i-1} r_{2i}^T, \nabla^2 f(W) \rangle_{HS} \right] \leq C_0 \|\nabla h\| \sum_{i=1}^{p} \mathbb{E}[|r_{2i-1}| |r_{2i}|].
\]
Moreover, by \((3.4)\) we have
\[
\int_0^1 |\mathbb{E}[(\delta \delta^T, \nabla^2 f(W + t\delta) - \nabla^2 f(W))_{HS}]| \, dt
\]
\[
= \int_0^1 \mathbb{E} \left[ \left\langle \delta \delta^T, \nabla^2 f \left( W + |\delta| \frac{t\delta}{|\delta|} \right) - \nabla^2 f(W) \right\rangle_{HS} \right] \, dt
\]
\[
\leq C_0 \|\nabla h\| \mathbb{E} \left[ |\delta|^3 (|\log |\delta|| \vee 1) \right].
\]
Combining the inequalities above, we obtain \((2.10)\) and \((2.11)\).

\[\square\]

4. AN APPLICATION: UNADJUSTED LANGEVIN ALGORITHM

We consider the problem of sampling a probability distribution \(\mu\) that has the density
\[
Ke^{-U(x)},
\]
where \(U(x)\) is a given function, but the normalizing constant \(K\) is unknown. This problem is encountered in Bayesian inference, where \(\mu\) is a posterior distribution, and in statistical physics, where \(\mu\) is the distribution of particle configurations. As \(K\) is unknown, we cannot sample from \(\mu\) directly. The so-called unadjusted Langevin algorithm (ULA) with fixed step size is as follows. We refer to [33, 10] and the references therein for more details. Regard \(\mu\) as the stationary distribution of the Langevin stochastic differential equation
\[
dX_t = g(X_t)dt + \sqrt{2}dB_t,
\]
where \(g(\cdot) = -\nabla U(\cdot)\) and \(B_t\) is a standard \(d\)-dimensional Brownian motion. The Euler-Maruyama discretization of \(X_t\) with step size \(s\) is
\[
Y_{k+1} = Y_k + sg(Y_k) + \sqrt{2s}Z_{k+1},
\]
where \(Y_0\) is an arbitrary initial value and \(Z_1, Z_2, \ldots\) are independent and identically distributed standard \(d\)-dimensional Gaussian random vectors. See Remark 4.2 below for other possible choices of \(\{Z_i\}\). We assume that \(\{Y_k\}\) has an invariant measure \(\mu_s\). The existence of \(\mu_s\) has been extensively studied in the literature. See, for example, [12, 33, 10]. In particular, Dalalyan [10] showed that \(\mu_s\) exists for sufficiently small \(s\), provided that \(\mu\) is strongly log-concave, and \(g\) is Lipschitz. The so-called ULA with fixed step size uses the Markov chain Monte Carlo method to sample from \(\mu_s\), then claims that \(\mu_s\) is close enough to \(\mu\) for a small \(s\).

There is a tradeoff in the choice of step size \(s\). When \(s\) becomes smaller, \(\mu_s\) is closer to \(\mu\), but it takes longer for the Markov chain to reach stationarity, and vice versa. Therefore, it is of interest to quantify the distance between \(\mu_s\) and \(\mu\) for a given \(s\).

Using our general theorem, we obtain the following result. The step size \(s\) is typically small, and for ease of presentation, we assume that \(s < 1/e\).
Theorem 4.1. Under the above setting, suppose $g(\cdot)$ satisfies Assumption 2.1. For $s < 1/e$, we have

\begin{equation}
\frac{1}{\lambda} \mathbb{E}[|\delta|^3(\log|\delta| + 1)] \leq \sqrt{s} \mathbb{E} \left[ |\tilde{\delta}|^3 (\log s + |\log|\tilde{\delta}|) \right] \leq \sqrt{s} \log s \mathbb{E} |\tilde{\delta}|^3 + \sqrt{s} \mathbb{E} \left[ |\tilde{\delta}|^3 \log|\tilde{\delta}| \right].
\end{equation}

Remark 4.2. As $s \to 0$, the leading-order term in the upper bound of (4.2) decays as $d^{3/2} s^{1/2}$ up to a logarithmic factor. Upper bounds between $\mu_s$ and $\mu$ for the stronger Wasserstein-2 distance have been obtained in the literature. See, for example, [10, 13, 4]. In particular, [13, Corollary 9] obtained a bound of the order $O(ds)$ under a slightly different set of conditions on $g$, which does not cover, say, Example 2 below Assumption 2.1. Their bound shows a lower computational complexity to achieve certain precision of the ULA. A possible way to improve our bound, which holds as long as $\{Z_i\}$ has mean 0 and covariance matrix $I_d$, is to do another Taylor's expansion in (3.7) and make use of the symmetry condition of the Gaussian (or Rademacher as in [4]) vector $Z_1$, that is, $\mathbb{E}Z_1Z_1Z_{1k} = 0$ for any $i, j, k \in \{1, \ldots, d\}$.

Proof. Suppose $Y_0 \sim \mu_s$ in (4.1). Let $W = Y_0$ and $W' = Y_1$. Because $\mu_s$ is the stationary distribution of the Markov chain (4.1), $W$ and $W'$ have the same distribution. With

$$\delta = W' - W = s g(W) + \sqrt{2s} Z_1,$$

we have

$$\mathbb{E}(\delta|W) = s g(W)$$

and

$$\mathbb{E}(\delta \delta^T|W) = 2s I_d + s^2 g(W) g^T(W).$$

In applying Theorem 2.5,

$$\lambda = s, \quad R_1 = 0, \quad R_2 = \frac{s}{2} g(W) g^T(W),$$

thus, $p = 1, r_1 = g(W)$ and $r_2 = \frac{s}{2} g^T(W)$. We have

$$\mathbb{E}[|r_1||r_2|] \leq \frac{s}{2} \mathbb{E}|g(W)|^2.$$

Recall $\tilde{\delta} = \frac{\delta}{\sqrt{s}}$ and write $g := g(W)$. We have

$$\frac{1}{\lambda} \mathbb{E}[|\tilde{\delta}|^3(\log|\tilde{\delta}| + 1)] \leq \sqrt{s} \mathbb{E} \left[ |\tilde{\delta}|^3 (\log s + |\log|\tilde{\delta}|) \right] \leq \sqrt{s} \log s \mathbb{E} |\tilde{\delta}|^3 + \sqrt{s} \mathbb{E} \left[ |\tilde{\delta}|^3 \log|\tilde{\delta}| \right].$$

Moreover,

$$\mathbb{E}|\tilde{\delta}|^3 = \mathbb{E}|\sqrt{s} g + Z_1|^3 \leq 4s^{3/2} \mathbb{E}|g|^3 + 4 \mathbb{E}|Z_1|^3,$$

hence,

$$\frac{1}{\lambda} \mathbb{E}[|\tilde{\delta}|^3(\log|\tilde{\delta}| + 1)] \leq \sqrt{s} \mathbb{E} \left[ |\tilde{\delta}|^3 (\log s + |\log|\tilde{\delta}|) \right] \leq 4 \sqrt{s} \left\{ s^{3/2} \log s \mathbb{E}|g|^3 + \log s \mathbb{E}|Z_1|^3 + \mathbb{E} \left[ |\tilde{\delta}|^3 \log|\tilde{\delta}| \right] \right\}.$$
5. PRELIMINARY: MALLIAVIN CALCULUS OF SDE (2.2)

From this section, we start our journey toward proving the crucial Theorem 3.1. We use Bismut’s approach to Malliavin calculus. To this end, we first provide a brief review of Malliavin calculus in this section; the proofs of the related lemmas are deferred to Section 8. Throughout the remaining sections, let $X_t^x$ be the solution to SDE (2.2), where $g$ satisfies Assumption 2.1.

5.1. Jacobi flow associated with SDE (2.2) ([6]). We consider the derivative of $X_t^x$ with respect to initial value $x$, which is called the Jacobian flow. Let $u \in \mathbb{R}^d$, the Jacobian flow $\nabla_u X_t^x$ along the direction $u$ is defined by

$$\nabla_u X_t^x \equiv \lim_{\varepsilon \to 0} \frac{X_t^{x+\varepsilon u} - X_t^x}{\varepsilon}, \quad t \geq 0.$$  

The above limit exists and satisfies

$$\frac{d}{dt} \nabla_u X_t^x = \nabla g(X_t^x) \nabla_u X_t^x, \quad \nabla_u X_0^x = u,$$

which is solved by

$$\nabla_u X_t^x = \exp \left\{ \int_0^t \nabla g(X_r^x) dr \right\} u.$$  

For further use, we denote

$$J_{s,t}^x = \exp \left\{ \int_s^t \nabla g(X_r^x) dr \right\}, \quad 0 \leq s \leq t < \infty.$$  

It is easy to see that $J_{s,t}^x J_{0,s}^x = J_{0,t}^x$ for all $0 \leq s \leq t < \infty$ and

$$\nabla_u X_t^x = J_{0,t}^x u.$$  

For $u_1, u_2 \in \mathbb{R}^d$, we can similarly define $\nabla_{u_2} \nabla_{u_1} X_t^x$, which satisfies

$$\frac{d}{dt} \nabla_{u_2} \nabla_{u_1} X_t^x = \nabla g(X_t^x) \nabla_{u_2} \nabla_{u_1} X_t^x + \nabla^2 g(X_t^x) \nabla_{u_2} X_t^x \nabla_{u_1} X_t^x$$  

with $\nabla_{u_2} \nabla_{u_1} X_0^x = 0$.

The following lemmas give estimates of $X_t^x$, $\nabla_{u_1} X_t^x$ and $\nabla_{u_2} \nabla_{u_1} X_t^x$ and the proofs are given in Section 8.

**Lemma 5.1.** We have

$$\mathbb{E} |X_t^x|^2 \leq e^{-\theta_0 t} |x|^2 + \frac{2d + |g(0)|^2}{\theta_0}.$$  

This further implies that the ergodic measure $\mu$ has finite 2nd moment and

$$\int_{\mathbb{R}^d} |x|^2 \mu(dx) \leq \frac{2d + |g(0)|^2}{\theta_0}.$$  

**Lemma 5.2.** For all $u_1, u_2 \in \mathbb{R}^d$ and $x \in \mathbb{R}^d$, we have the following (deterministic) estimates:

$$|\nabla_{u_1} X_t^x| \leq e^{-\theta_0 t} |u_1|,$$

$$|\nabla_{u_2} \nabla_{u_1} X_t^x| \leq C_\theta |u_1| |u_2|.$$
5.2. Bismut’s approach to Malliavin calculus for SDE (2.2) ([25]). Let \( v \in L^2_{loc}([0, \infty) \times (\Omega, \mathcal{F}, \mathbb{P}); \mathbb{R}^d) \), i.e., \( \mathbb{E} \int_0^t |v(s)|^2 ds < \infty \) for all \( t > 0 \). Further assume that \( v \) is adapted to the filtration \( (\mathcal{F}_t)_{t \geq 0} \) with \( \mathcal{F}_t := \sigma(B_s : 0 \leq s \leq t) \); i.e., \( v(t) \) is \( \mathcal{F}_t \) measurable for \( t \geq 0 \). Define

\[
V_t = \int_0^t v(s) ds, \quad t \geq 0.
\]

For a \( t > 0 \), let \( F_t : C([0, t], \mathbb{R}^d) \to \mathbb{R} \) be a \( \mathcal{F}_t \) measurable map. If the following limit exists

\[
DVF_t(B) = \lim_{\varepsilon \to 0} \frac{F_t(B + \varepsilon V) - F_t(B)}{\varepsilon}
\]

in \( L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}) \), then \( F_t(B) \) is said to be Malliavin differentiable and \( DVF_t(B) \) is called the Malliavin derivative of \( F_t(B) \) in the direction \( v \); see [20, p. 1011].

Let \( F_t(B) \) and \( G_t(B) \) both be Malliavin differentiable, then the following product rule holds:

\[
DVF_t(B)G_t(B) = DVF_t(B)DVG_t(B) + DVF_t(B)DG_t(B).
\]

When

\[
F_t(B) = \int_0^t \langle a(s), dB_s \rangle,
\]

where \( a(s) = (a_1(s), ..., a_d(s)) \) is a deterministic function such that \( \int_0^t |a(s)|^2 ds < \infty \) for all \( t > 0 \), it is easy to check that

\[
DVF_t(B) = \int_0^t \langle a(s), v(s) \rangle ds.
\]

If \( a(s) = (a_1(s), ..., a_d(s)) \) is a \( d \)-dimensional stochastic process adapted to the filtration \( \mathcal{F}_s \) such that \( \mathbb{E} \int_0^t |a(s)|^2 ds < \infty \) for all \( t > 0 \), then

\[
DVF_t(B) = \int_0^t \langle a(s), v(s) \rangle ds + \int_0^t \langle DVa(s), dB_s \rangle.
\]

The following integration by parts formula, called Bismut’s formula, is probably the most important property in Bismut’s approach to Malliavin calculus.

**Bismut’s formula.** For Malliavin differentiable \( F_t(B) \) such that \( F_t(B), DVF_t(B) \in L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}) \), we have

\[
\mathbb{E} [DVF_t(B)] = \mathbb{E} \left[ F_t(B) \int_0^t \langle v(s), dB_s \rangle \right].
\]

Let \( \phi : \mathbb{R}^d \to \mathbb{R} \) be Lipschitz and let \( F_t(B) = (F_1^t(B), ..., F_d^t(B)) \) be a \( d \)-dimensional Malliavian differentiable functional. The following chain rule holds:

\[
DVF_t(B) = \langle \nabla \phi(F_t(B)), DVF_t(B) \rangle = \sum_{i=1}^d \partial_i \phi(F_t(B)) DVF_i^t(B).
\]

Now we come back to SDE (2.2). Fixing \( t \geq 0 \) and \( x \in \mathbb{R}^d \), the solution \( X_t^x \) is a \( d \)-dimensional functional of Brownian motion \( (B_s)_{0 \leq s \leq t} \). The following Malliavin derivative of \( X_t^x \) along the direction \( V \) exists in \( L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}^d) \) and is defined by

\[
DVF X_t^x(B) = \lim_{\varepsilon \to 0} \frac{X_t^x(B + \varepsilon V) - X_t^x(B)}{\varepsilon}.
\]
We drop the $B$ in $D_V X_t^x(B)$ and write $D_V X_t^x = D_V X_t^x(B)$ for simplicity. It satisfies the equation
\[
dD_V X_t^x = \nabla g(X_s^x) D_V X_s^x dt + \sqrt{2} v(t) dt, \quad D_V X_0^x = 0,
\]
and the equation has a unique solution:
\[
(5.12) \quad D_V X_t^x = \sqrt{2} \int_0^t J_{r,t}^s v(r) dr,
\]
where $J_{r,t}^s$ is defined by (5.3). Comparing (5.2) and (5.12), if we take
\[
(5.13) \quad v(s) = \frac{1}{\sqrt{2t}} \nabla_u X_s^x, \quad 0 \leq s \leq t,
\]
(recall (5.6) and $V_i = \int_0^t v(s) ds$), because $\nabla_u X_r^x = J_{0,r}^0 u$ and $J_{r,t}^s J_{0,r}^0 = J_{0,t}^s$ for all $0 \leq r \leq t$, we have
\[
(5.14) \quad D_V X_t^x = \nabla_u X_t^x
\]
and
\[
(5.15) \quad D_V X_s^x = \frac{s}{t} \nabla_u X_s^x, \quad 0 \leq s \leq t.
\]
Let $u_1, u_2 \in \mathbb{R}^d$, and define $v_i$ and $V_i$ as (5.13) and (5.8), respectively, for $i = 1, 2$. We can similarly define $D_{V_2} \nabla_{u_1} X_s^x$, which satisfies the following equation: for $s \in [0, t]$,
\[
\frac{d}{ds} D_{V_2} \nabla_{u_1} X_s^x = \nabla g(X_s^x) D_{V_2} \nabla_{u_1} X_s^x + \nabla^2 g(X_s^x) D_{V_2} X_s^x \nabla_{u_1} X_s^x
\]
\[
= \nabla g(X_s^x) D_{V_2} \nabla_{u_1} X_s^x + \frac{s}{t} \nabla^2 g(X_s^x) \nabla_{u_2} X_s^x \nabla_{u_1} X_s^x
\]
with $D_{V_2} \nabla_{u_1} X_0^x = 0$, where the second equality is by (5.15). For further use, we define
\[
\mathcal{T}_{u_1}^x(t) := \frac{1}{\sqrt{2t}} \int_0^t \langle \nabla_{u_1} X_s^x, dB_s \rangle,
\]
\[
\mathcal{T}_{u_1,u_2}^x(t) := \mathcal{T}_{u_1}^x(t) \mathcal{T}_{u_2}^x(t) - D_{V_2} \mathcal{T}_{u_1}^x(t).
\]
The following upper bounds on Malliavin derivatives are proven in Section 8.

**Lemma 5.3.** Let $u_i \in \mathbb{R}^d$ for $i = 1, 2$, and let
\[
V_{i,s} = \int_0^s v_i(r) dr \quad \text{for} \quad 0 \leq s \leq t,
\]
where $v_i(r) = \frac{1}{\sqrt{2t}} \nabla_u X_r^x$ for $0 \leq r \leq t$. We have
\[
(5.17) \quad |D_{V_2} \nabla_{u_1} X_s^x| \leq C_0 |u_1| |u_2|.
\]

**Lemma 5.4.** Let $u_1, u_2 \in \mathbb{R}^d$ and $x \in \mathbb{R}^d$. For all $p \geq 1$, $x \in \mathbb{R}^d$, we have
\[
(5.18) \quad \mathbb{E} |\mathcal{T}_{u_1}^x(t)|^p \leq \frac{C_{0,p} |u_1|^p}{t^{p/2}},
\]
\[
(5.19) \quad \mathbb{E} |\nabla_{u_2} \mathcal{T}_{u_1}^x(t)|^p \leq \frac{C_{0,p} |u_1|^p |u_2|^p}{t^{p/2}},
\]
\[
(5.20) \quad \mathbb{E} |D_{V_2} \mathcal{T}_{u_1}^x(t)|^p \leq \frac{C_{0,p} |u_2|^p |u_1|^p}{t^p},
\]
\[
(5.21) \quad \mathbb{E} |\mathcal{T}_{u_1,u_2}^x(t)|^p \leq \frac{C_{0,p} |u_1|^p |u_2|^p}{t^p}.
\]
6. The representations of \( f, \nabla f \) and \( \nabla^2 f \)

It is well known that SDE (2.2) has the following infinitesimal generator \( \mathcal{A} \) [31, Chapter VII] defined by

\[
\mathcal{A}f(x) = \Delta f + \langle g(x), \nabla f(x) \rangle, \quad f \in \mathcal{D}(\mathcal{A}),
\]

where \( \mathcal{D}(\mathcal{A}) \) is the domain of \( \mathcal{A} \), whose exact definition depends on the underlying function space that we consider. \( \mathcal{A} \) generates a Markov semigroup \( (P_t)_{t \geq 0} \) defined by

\[
P_t f(x) = \mathbb{E}[f(X_t^x)], \quad f \in C_b(\mathbb{R}^d, \mathbb{R}).
\]

Note that \( P_t : C_b(\mathbb{R}^d, \mathbb{R}) \to C_b(\mathbb{R}^d, \mathbb{R}) \) is a linear operator. It is well known that \( P_t \) can be extended to an operator \( P_t : L^p_\mu(\mathbb{R}^d, \mathbb{R}) \to L^p_\mu(\mathbb{R}^d, \mathbb{R}) \) with \( p \geq 1 \), where \( L^p_\mu(\mathbb{R}^d, \mathbb{R}) \) is the collection of all measurable functions \( f : \mathbb{R}^d \to \mathbb{R} \) such that \( \int_{\mathbb{R}^d} |f(x)|^p \mu(dx) < \infty \). Moreover, we have

\[
P_t f(x) = \mathbb{E}[f(X_t^x)], \quad f \in L^p_\mu(\mathbb{R}^d, \mathbb{R}).
\]

The Stein equation (3.1) can be written as

\[
\mathcal{A}f(x) = h(x) - \mu(h),
\]

which is called the Poisson equation associated with \( \mathcal{A} \). The solution is given as follows.

**Proposition 6.1.** For any Lipschitz function \( h : \mathbb{R}^d \to \mathbb{R} \) with \( \|\nabla h\| < \infty \), we have the following two statements:

1. A solution to (3.1) is given by

\[
f(x) = - \int_0^\infty \mathbb{E}[h(X_t^x) - \mu(h)] dt.
\]

Moreover, we have

\[
|f(x)| \leq C_{\theta_0, \theta_1, \theta_2, d}(1 + |x|)\|\nabla h\|.
\]

2. We have

\[
f(x) = \int_0^\infty e^{-t}\mathbb{E}[f(X_t^x) + \mu(h) - h(X_t^x)] dt.
\]

**Remark 6.2.** The representation of \( f \) in (6.5) plays a crucial role in estimating \( \nabla u_1 \nabla u_2 f \). We roughly explain it as follows. By a similar argument to that used to prove (6.13) below, we can show formally that

\[
\nabla u_1 \nabla u_2 f(x) = \int_0^\infty \mathbb{E} \left[ \nabla u_1 h(X_t^x) \mathcal{L}_{u_2}(t) \right] dt.
\]

However, it is not known whether this integral is well defined. Instead, we borrow the idea from [11, Section 4] to introduce a new term \( e^{-t} \), and the corresponding new representation (6.13) will produce an integrability.

**Proof.** (1). Recall (6.1) and denote \( \hat{h} = \mu(h) - h \). Let us first show that \( \int_0^\infty P_t \hat{h}(x) ds \) is well defined. By (A.1) in Appendix A, we have

\[
\sup_{\|\nabla h\| \leq 1} |P_t h(x) - \mu(h)| = \sup_{\|\nabla h\| \leq 1} |\mathbb{E}[h(X_t^x)] - \mu(h)| \leq 2e^{-ct} \sup_{\|\nabla h\| \leq 1} |h(x) - \mu(h)|,
\]

where \( c \) depends on \( \theta_0, \theta_1, \theta_2 \). Because

\[
\sup_{\|\nabla h\| \leq 1} |h(x) - \mu(h)| \leq \int_{\mathbb{R}^d} |y - x| \mu(dy) \leq (m_1(\mu) + |x|),
\]

for some \( m_1(\mu) \).
where \( m_1(\mu) \) denotes the first absolute moment of \( \mu \), we have

\[
(6.6) \quad |P_t \hat{h}(x)| = |P_t h(x) - \mu(h)| \leq 2e^{-ct}(m_1(\mu) + |x|)||\nabla h||, \quad \forall t > 0.
\]

By (5.5), \( m_1(\mu) \) is finite; hence, \( \left| \int_0^\infty P_t \hat{h}(x)dt \right| < \infty \).

For any \( \varepsilon > 0 \), it is well known that \( \varepsilon - \mathcal{A} \) is invertible, and

\[
(\varepsilon - \mathcal{A})^{-1} \hat{h} = \int_0^\infty e^{-\varepsilon t} P_t \hat{h} dt;
\]

that is,

\[
\varepsilon \int_0^\infty e^{-\varepsilon t} P_t \hat{h} \, dt - \hat{h} = \mathcal{A} \left( \int_0^\infty e^{-\varepsilon t} P_t \hat{h} \, dt \right).
\]

As \( \varepsilon \to 0+ \),

\[
\varepsilon \int_0^\infty e^{-\varepsilon t} P_t \hat{h} \, dt - \hat{h} \to -\hat{h}, \quad \int_0^\infty e^{-\varepsilon t} P_t \hat{h} \, dt \to \int_0^\infty P_t \hat{h} \, dt.
\]

As \( \mathcal{A} \) is a closed operator, \( \int_0^\infty P_t \hat{h} \, dt \) is in the domain of \( \mathcal{A} \) and

\[
-\hat{h}(x) = \mathcal{A} \left( \int_0^\infty P_t \hat{h}(x)ds \right).
\]

Therefore, (6.3) is a solution to Eq. (3.1).

By (6.6),

\[
|f(x)| \leq \left| \int_0^\infty P_t \hat{h}(x)dt \right| \leq C_{b_0, a_1, a_2, d}(1 + |x|)||\nabla h||.
\]

Hence, (6.4) is proven.

Now we prove (2). Note that

\[
(1 - \mathcal{A})f(x) = f(x) + \hat{h}(x).
\]

By the integral representation of \( (1 - \mathcal{A})^{-1} \), we have

\[
f(x) = (1 - \mathcal{A})^{-1}[f + \hat{h}](x) = \int_0^\infty e^{-t}P_t(f + \hat{h})(x)dt,
\]

which is (6.5). \( \square \)

**Lemma 6.3.** Let \( \phi \in C^1(\mathbb{R}^d, \mathbb{R}) \) be such that \( ||\nabla \phi|| < \infty \), and let \( u, u_1, u_2 \in \mathbb{R}^d \). For every \( t > 0 \) and \( x \in \mathbb{R}^d \), we have

\[
(6.7) \quad |\nabla_u \mathbb{E} [\phi(X_t^x)]| \leq ||\nabla \phi|| |u|,
\]

and

\[
(6.8) \quad \nabla_u \mathbb{E} [\phi(X_t^x)] = \mathbb{E} [\phi(X_t^x)\mathcal{I}_u^x(t)].
\]

If, in addition, \( \phi \in C^2(\mathbb{R}^d, \mathbb{R}) \), then we have

\[
(6.9) \quad \nabla_{u_1} \nabla_{u_2} \mathbb{E} [\phi(X_t^x)] = \mathbb{E} [\nabla_{u_1} \phi(X_t^x)\mathcal{I}_{u_2}^x(t)],
\]

\[
(6.10) \quad \mathbb{E}[\nabla_{u_2} \phi(X_t^x)\mathcal{I}_{u_1}^x(t)] = \mathbb{E} [\phi(X_t^x)\mathcal{I}_{u_2, u_1}^x(t)].
\]
Lemma 6.5.\footnote{We have used the assumption (14), the first term on the right-hand side of (14) is not integrable at times, we obtain (6.13).} The idea in our proof has appeared in \cite{Elworthy-Li}. This proves (6.8). From (6.8), we have \[ \nabla_u \nabla_{u_1} \mathbb{E} [\phi(X_t^x)] = \nabla_u \mathbb{E} [\nabla_{u_1} \phi(X_t^x)] = \mathbb{E} \left[ \nabla_{u_1} \phi(X_t^x) \mathcal{I}_{u_1}(t) \right], \] where we used the assumption \( \phi \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}) \). This proves (6.9). From (5.13), (5.14), (5.9), (5.11) and a similar calculation, we have \[ \mathbb{E} \left[ \nabla_{u_2} \phi(X_t^x) \mathcal{I}_{u_1}(t) \right] = \mathbb{E} \left[ \nabla_{u_2} \nabla_{u_1} \phi(X_t^x) \right] = \mathbb{E} \left[ \nabla_{u_1} \phi(X_t^x) \mathcal{I}_{u_2}(t) \right], \] where we used the assumption \( \phi \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}) \). This proves (6.9). From (6.10), we have

\[ \nabla_{u_2} \nabla_{u_1} \mathbb{E} [\phi(X_t^x)] = \nabla_{u_2} \mathbb{E} [\nabla_{u_1} \phi(X_t^x)] = \mathbb{E} \left[ \nabla_{u_1} \phi(X_t^x) \mathcal{I}_{u_2}(t) \right], \]

where we used the assumption \( \phi \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}) \). This proves (6.9). From (5.13), (5.14), (5.9), (5.11) and a similar calculation, we have \[ \mathbb{E} \left[ \nabla_{u_2} \phi(X_t^x) \mathcal{I}_{u_1}(t) \right] = \mathbb{E} \left[ \nabla_{u_2} \nabla_{u_1} \phi(X_t^x) \right] = \mathbb{E} \left[ \nabla_{u_1} \phi(X_t^x) \mathcal{I}_{u_2}(t) \right], \] where we used the assumption \( \phi \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}) \). This proves (6.9). From (6.10) is proven.

Remark 6.4. Write \( P_t \phi(x) = \mathbb{E}[\phi(X_t^x)] \), we can see that (6.8) is the well known Bismut-Elworthy-Li formula \cite{Elworthy-Li, Seeber}. The original proof of this formula is by Itô’s formula and isometry \cite[p.254]{Elworthy-Li}, while our approach is by (5.14) and Bismut’s integration by parts formula (5.11). The idea in our proof has appeared in \cite{Seeber}, and been applied to study other problems such as the derivative formula of stochastic systems \cite{Xiong, Watanabe}. Using Bismut’s formula two times, we obtain (6.10), which is crucial in proving (3.4). Although \cite{Elworthy-Li, Seeber} also gives a second order Bismut-Elworthy-Li formula, it is not directly applicable in our analysis because the first term on the right-hand side of (14) is not integrable at 0.

Lemma 6.5.\footnote{Using the assumption \( \phi \in \mathcal{C}^1(\mathbb{R}^d, \mathbb{R}) \), we have
\[ \nabla_u f(x) = \int_0^\infty \mathbb{E} \left[ \nabla h(X_t^x) \nabla u X_t^x \mathcal{I}_t \right] dt, \] if in addition \( h \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}) \), then
\[ \nabla_u f(x) = \int_0^\infty \mathbb{E} \left[ \nabla h(X_t^x) \mathcal{I}_t \right] dt. \]}

Let \( h \in \mathcal{C}^1(\mathbb{R}^d, \mathbb{R}) \) be such that \( \| \nabla h \| < \infty \). For any \( u, u_1, u_2 \in \mathbb{R}^d \) and \( x \in \mathbb{R}^d \), we have
\begin{equation}
\nabla_u f(x) = \int_0^\infty \mathbb{E} \left[ \nabla h(X_t^x) \nabla u X_t^x \mathcal{I}_t \right] dt,
\end{equation}

\begin{equation}
\nabla_u f(x) = \int_0^\infty e^{-t} \mathbb{E} \left\{ \left[ f(X_t^x) - h(X_t^x) + \mu(h) \right] \mathcal{I}_t \right\} dt.
\end{equation}

If in addition \( h \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}) \), then
\begin{equation}
\nabla_{u_2} \nabla_{u_1} f(x) = \int_0^\infty e^{-t} \mathbb{E} \left\{ \left[ \nabla_{u_1} f(X_t^x) - \nabla_{u_1} h(X_t^x) \right] \mathcal{I}_{u_2}(t) \right\} dt.
\end{equation}
Proof. By (5.6), we have
\[
|\nabla_u \mathbb{E}[h(X^x_t) - \mu(h)]| \leq \mathbb{E}|\nabla h(X^x_t)||\nabla u X^x_t|
\]
\[
\leq \|\nabla h\| \mathbb{E}|\nabla u X^x_t| \leq \|\nabla h\| |u| e^{-\theta_0 t}, \quad t > 0.
\]
Therefore, by the dominated convergence theorem, we have
\[
\nabla_u f(x) = \int_0^\infty \nabla_u \mathbb{E}[h(X^x_t) - \mu(h)]dt
\]
\[
= \int_0^\infty \mathbb{E}[\nabla h(X^x_t)\nabla u X^x_t]dt.
\]
The previous two relations also imply
(6.14) \[\|\nabla_u f\| \leq C_0\|\nabla h\||u|\] 

By (6.7) and (6.14), we have
\[\|\nabla_u P_t[f + \mu(h) - h]\| \leq (\|\nabla f\| + \|\nabla h\|)|u| \leq C_0\|\nabla h\||u|\.
\]
By (6.5), the dominated convergence theorem and (6.8), we have
\[
\nabla_u f(x) = \int_0^\infty e^{-t}\nabla_u \mathbb{E}\left[f(X^x_t) - h(X^x_t) + \mu(h)\right]dt
\]
\[
= \int_0^\infty e^{-t}\mathbb{E}\left\{\left[f(X^x_t) - h(X^x_t) + \mu(h)\right]\mathcal{I}^x_u(t)\right\}dt.
\]
This proves (6.12). When \(h \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})\), it can be checked that \(f \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})\) and
\[
\nabla_{u_1} f(x) = \int_0^\infty e^{-t}\mathbb{E}\left[\nabla_{u_1} f(X^x_t) - \nabla_{u_1} h(X^x_t)\right]dt.
\]
By the dominated convergence theorem with (5.18) and (6.14), and by (6.8) with \(\phi = \nabla_{u_1} f\) and \(\phi = \nabla_{u_1} h\), we have
\[
\nabla_{u_2} \nabla_{u_1} f(x) = \int_0^\infty e^{-t}\mathbb{E}\left\{\left[\nabla_{u_1} f(X^x_t) - \nabla_{u_1} h(X^x_t)\right]\mathcal{I}^x_{u_2}(t)\right\}dt.
\]
\[\square\]

7. The Proof of Theorem 3.1

Now let us use the representations of \(f, \nabla f\) and \(\nabla^2 f\) developed in the previous section to prove Theorem 3.1.

Lemma 7.1. Let \(h \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})\) be such that \(\|\nabla h\| < \infty\). Then we have
(7.1) \[|\nabla_{u_2} \nabla_{u_1} f(x)| \leq C_0\|\nabla h\||u_1||u_2|,
\]
(7.2) \[|\nabla_{u_2} \nabla_{u_1} f(x + \varepsilon u) - \nabla_{u_2} \nabla_{u_1} f(x)| \leq C_0\|\nabla h\||\varepsilon| (\log|\varepsilon| + 1)|u_1||u_2|,
\]
for all \(\varepsilon \in \mathbb{R}, x, u_1, u_2 \in \mathbb{R}^d\) and \(u \in \mathbb{R}^d\) with \(|u| \leq 1\).
Proof. From (6.13), (6.14) and (5.18), we have
\[
|\nabla u_2 \nabla u_1 f(x)| \leq \int_0^\infty e^{-t} \left| \mathbb{E} \left\{ \left[ \nabla u_1 f(X^x_t) - \nabla u_1 h(X^x_t) \right] I^{x+\epsilon u}_2(t) \right\} \right| dt
\]
\[
\leq (\|\nabla f\| + \|\nabla h\|) |u_1| \int_0^\infty e^{-t} \mathbb{E} \left[ \left| I^{x+\epsilon u}_2(t) \right| \right] dt
\]
\[
\leq C_0 |\nabla h| |u_1| \int_0^\infty e^{-t-1/2} dt
\]
\[
\leq C_0 |\nabla h| |u_1| |u_2|.
\]
This proves (7.1). To prove (7.2), without loss of generality, we assume \( \epsilon > 0 \). By (6.13), we have
\[
\nabla u_2 \nabla u_1 f(x + \epsilon u) - \nabla u_2 \nabla u_1 f(x) = \int_0^{\epsilon^2} e^{-t} \Psi dt + \int_{\epsilon^2}^\infty e^{-t} \Psi dt,
\]
where
\[
\Psi = \mathbb{E} \left\{ \left[ \nabla u_1 f(X^{x+\epsilon u}_t) - \nabla u_1 h(X^{x+\epsilon u}_t) \right] I^{x+\epsilon u}_2(t) \right\}
- \mathbb{E} \left\{ \left[ \nabla u_1 f(X^x_t) - \nabla u_1 h(X^x_t) \right] I^x_2(t) \right\}.
\]
We shall prove that
\[
\left| \int_0^{\epsilon^2} e^{-t} \Psi dt \right| \leq C_0 |\nabla h| |u_1| |u_2| \epsilon, \quad \left| \int_{\epsilon^2}^\infty e^{-t} \Psi dt \right| \leq C_0 (|\log \epsilon| \vee 1) |\nabla h| |u_1| |u_2|.
\]
From these two inequalities, we immediately obtain (7.2), as desired.

By (6.14) and (5.18), we have
\[
|\Psi| \leq 2 (\|\nabla f\| + \|\nabla h\|) |u_1| \mathbb{E} \left[ \left| I^{x+\epsilon u}_2(t) \right| + \left| I^x_2(t) \right| \right] \leq C_0 \epsilon^{-1/2} |\nabla h| |u_1| |u_2|,
\]
from which we obtain the first inequality in (7.3).

We still need to prove the second inequality in (7.3). Note that
\[
\Psi = \Psi_1 + \Psi_2
\]
where
\[
\Psi_1 = \mathbb{E} \left\{ \left[ \nabla u_1 f(X^{x+\epsilon u}_t) - \nabla u_1 h(X^{x+\epsilon u}_t) \right] [I^{x+\epsilon u}_2(t) - I^x_2(t)] \right\},
\]
\[
\Psi_2 = \mathbb{E} \left\{ \left[ \nabla u_1 f(X^{x+\epsilon u}_t) - \nabla u_1 h(X^{x+\epsilon u}_t) - \nabla u_1 f(X^x_t) + \nabla u_1 h(X^x_t) \right] I^x_2(t) \right\}.
\]
For \( \Psi_1 \), we have
\[
|\Psi_1| \leq (\|\nabla f\| + \|\nabla h\|) |u_1| \mathbb{E} \left[ \left| I^{x+\epsilon u}_2(t) - I^x_2(t) \right| \right]
\]
\[
\leq C_0 |\nabla h| |u_1| \mathbb{E} \left| \int_0^\epsilon \left[ \nabla u I^{x+\epsilon u}_2(t) \right] dt \right|
\]
\[
\leq C_0 |\nabla h| |u_1| \epsilon \mathbb{E} \left| \nabla u I^{x+\epsilon u}_2(t) \right| dt
\]
\[
\leq C_0 \epsilon |\nabla h| |u_1| |u_2| t^{-1/2},
\]
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where the last inequality is by (5.19) and \(|u| \leq 1\). For \(\Psi_2\), by (6.10), we have
\[
|\Psi_2| = \left| \int_0^\varepsilon E \{ \nabla_u [\nabla u_1 f(X_t^{x+ru}) - \nabla u_1 h(X_t^{x+ru})] T_{u_2}^x(t) \} \, dr \right|
\]
\[
= \left| \int_0^\varepsilon E \{ [\nabla u_1 f(X_t^{x+ru}) - \nabla u_1 h(X_t^{x+ru})] T_{u_2}^x(t) \} \, dr \right|
\]
\[
\leq (||\nabla f|| + ||\nabla h||)|u_1| \int_0^\varepsilon E|T_{u_2}^x(t)| \, dr
\]
\[
\leq C \varepsilon ||\nabla h|| |u_1| |u_2| t^{-1},
\]
where the last inequality is by (5.21) and \(|u| \leq 1\).

Combining the estimates of \(\Psi_1\) and \(\Psi_2\), we obtain the second inequality in (7.3).

\[\square\]

**Proof of Theorem 3.1.** Note that (6.14) holds for any Lipschitz \(h\), which immediately implies (3.2).

To prove the other two inequalities, it suffices to show that (7.1) and (7.2) hold for Lipschitz \(h\). We now do so by a standard approximation.

Define
\[
h_\delta(x) = \int_{\mathbb{R}^d} \phi_\delta(y) h(x - y) \, dy \quad \text{with} \quad \delta > 0,
\]
where \(\phi_\delta\) is the density function of the normal distribution \(N(0, \delta^2 I_d)\). It is easy to see that \(h_\delta\) is smooth, \(\lim_{\delta \to 0} h_\delta(x) = h(x)\), \(\lim_{\delta \to 0} \nabla h_\delta(x) = \nabla h(x)\) and \(|h_\delta(x)| \leq C(1 + |x|)\) for all \(x \in \mathbb{R}^d\) and some \(C > 0\). Moreover, \(\|\nabla h_\delta\| \leq \|\nabla h\|.\) The solution to the Stein equation (3.1), with \(h\) replaced by \(h_\delta\), is
\[
f_\delta(x) = \int_0^\infty E[h_\delta(X_t^x) - \mu(h_\delta)] \, dt.
\]
Recall (6.6). By the dominated convergence theorem,
\[
\lim_{\delta \to 0} f_\delta(x) = \int_0^\infty E[h(X_t^x) - \mu(h)] \, dt = f(x).
\]
By (6.11) and the dominated convergence theorem,
\[
\lim_{\delta \to 0} \nabla_{u_1} f_\delta(x) = \lim_{\delta \to 0} \int_0^\infty E [\nabla h_\delta(X_t^x) \nabla_{u_1} X_t^x] \, dt = \int_0^\infty E [\nabla h(X_t^x) \nabla_{u_1} X_t^x] \, dt.
\]
As the differential operator \(\nabla\) is closed [29, Theorem 2.2.6], by the well known property of closed operators [29, Proposition 2.1.4], we know that \(f\) is differentiable and
\[
\nabla_{u_1} f(x) = \lim_{\delta \to 0} \nabla_{u_1} f_\delta(x).
\]
By (6.13), we have
\[
\nabla_{u_2} \nabla_{u_1} f_\delta(x) = \int_0^\infty e^{-t} E \left\{ \left[ \nabla_{u_1} f_\delta(X_t^x) + \nabla_{u_1} h_\delta(X_t^x) \right] T_{u_2}^x(t) \right\} \, dt,
\]
and by the dominated convergence theorem and the fact that \(\nabla^2\) is closed, we have
(7.4)
\[
\lim_{\delta \to 0} \nabla_{u_2} \nabla_{u_1} f_\delta(x) = \int_0^\infty e^{-t} E \left\{ \left[ \nabla_{u_1} f(X_t^x) + \nabla_{u_1} h(X_t^x) \right] T_{u_2}^x(t) \right\} \, dt = \nabla_{u_2} \nabla_{u_1} f(x).
\]
By (7.1), we have
\[
|\nabla_{u_2} \nabla_{u_1} f_\delta(x)| \leq C_0 \|\nabla h_\delta\| |u_1| |u_2|.
\]
Letting \( \delta \to 0 \), and by (7.4) and the fact that \( \| \nabla h_\delta \| \leq \| \nabla h \| \), we obtain (7.1) for Lipschitz \( h \). Similarly we can prove (7.2) for Lipschitz \( h \). \( \square \)

### 8. Proofs of the Lemmas in Section 5

**Proof of Lemma 5.1.** By Itô’s formula, (2.5) and Cauchy’s inequality, we have

\[
\frac{d}{ds} \mathbb{E} |X_s^x|^2 = 2 \mathbb{E} \langle \dot{X_s^x}, g(X_s^x) \rangle + 2d
\]

\[
= 2 \mathbb{E} \langle X_s^x, g(X_s^x) - g(0) \rangle + 2 \mathbb{E} \langle X_s^x, g(0) \rangle + 2d
\]

\[
\leq -2\theta_0 \mathbb{E} |X_s^x|^2 + \theta_0 \mathbb{E} |X_s^x|^2 + \frac{|g(0)|^2}{\theta_0} + 2d
\]

\[
= -\theta_0 \mathbb{E} |X_s^x|^2 + \frac{|g(0)|^2}{\theta_0} + 2d.
\]

This inequality, together with \( X_0^x = x \), implies

\[
\mathbb{E} |X_t^x|^2 \leq e^{-\theta_0 t} |x|^2 + (2d + \frac{|g(0)|^2}{\theta_0}) \int_0^t e^{-\theta_0 (t-s)} ds \leq e^{-\theta_0 t} |x|^2 + \frac{2d + |g(0)|^2/\theta_0}{\theta_0}.
\]

Let \( \chi : [0, \infty) \to [0, 1] \) be a continuous function such that \( \chi(r) = 1 \) for \( 0 \leq r \leq 1 \) and \( \chi(r) = 0 \) for \( r \geq 2 \). Let \( R > 0 \) be a large number. The previous inequality implies

\[
\mathbb{E} \left[ |X_t^x|^2 \chi (|X_t^x|/R) \right] \leq e^{-\theta_0 t} |x|^2 + \frac{2d + |g(0)|^2/\theta_0}{\theta_0}.
\]

Let \( t \to \infty \). By the ergodicity of \( X_t \) under weak topology (see Appendix A), we have

\[
\int_{\mathbb{R}^d} |x|^2 \chi (|x|/R) \mu(dx) \leq \frac{2d + |g(0)|^2/\theta_0}{\theta_0}.
\]

Letting \( R \to \infty \), we obtain

\[
\int_{\mathbb{R}^d} |x|^2 \mu(dx) \leq \frac{2d + |g(0)|^2/\theta_0}{\theta_0}.
\]

\( \square \)

**Proof of Lemma 5.2.** Recall \( \theta_0 > 0 \). By (5.1) and (2.3), we have

\[
\frac{d}{dt} |\nabla_u X_t^x|^2 = 2 \langle \nabla_u X_t^x, \nabla g(X_t^x) \nabla u X_t^x \rangle \\
\leq -2\theta_0 \left( 1 + \theta_1 |X_t^x|^{\theta_2} \right) |\nabla_u X_t^x|^2,
\]

which implies

\[
|\nabla_u X_t^x|^2 \leq \exp \left[ -2\theta_0 \int_0^t \left( 1 + \theta_1 |X_s^x|^{\theta_2} \right) ds \right] |u|^2 \leq e^{-2\theta_0 t} |u|^2.
\]

Writing \( \zeta(t) = \nabla u \nabla u X_t^x \), by (5.4), (2.3), (2.4) and (5.6), we have

\[
\frac{d}{dt} |\zeta(t)|^2 = 2 \langle \zeta(t), \nabla g(X_t^x) \zeta(t) \rangle + 2 \langle \zeta(t), \nabla^2 g(X_t^x) \nabla u X_t^x \nabla u X_t^x \rangle \\
\leq -2\theta_0 \left( 1 + \theta_1 |X_t^x|^{\theta_2} \right) |\zeta(t)|^2 + 2\theta_0 \left( 1 + \theta_1 |X_t^x|^{\theta_2-1} |\zeta(t)||u_1||u_2| \right) \\
\leq -2\theta_0 \left( 1 + \theta_1 |X_t^x|^{\theta_2} \right) |\zeta(t)|^2 + C_\theta \left( 1 + \theta_1 |X_t^x|^{\theta_2} \right) |\zeta(t)||u_1||u_2| \\
\leq -\theta_0 \left( 1 + \theta_1 |X_t^x|^{\theta_2} \right) |\zeta(t)|^2 + C_\theta \left( 1 + \theta_1 |X_t^x|^{\theta_2} \right) |u_1|^2 |u_2|^2,
\]
where the third inequality is by Cauchy’s inequality. Recall that \( \zeta(0) = 0 \). The above inequality implies

\[
|\zeta(t)|^2 \leq C_0 \int_0^t \exp \left[ -\theta_0 \int_s^t \left( 1 + \theta_1 |X_r^x|^{\theta_2} \right) dr \right] \left( 1 + \theta_1 |X_s^x|^{\theta_2} \right) ds |u_1|^2 |u_2|^2
\]

\[
\leq C_0 |u_1|^2 |u_2|^2,
\]

where the last inequality is by the following observation: for a nonnegative function \( a : [0, t] \to \mathbb{R} \),

\[
\int_0^t e^{-\int_0^r a(s)ds} a(s) ds = 1 - e^{-\int_0^t a(r)dr} \leq 1.
\]

Hence, (5.7) is proven. \( \square \)

**Proof of Lemma 5.3.** From (5.16) and the same argument as in the proof of Lemma 5.2, we obtain the estimate in the lemma, as desired. \( \square \)

**Proof of Lemma 5.4.** Thanks to Hölder’s inequality, it suffices to prove the inequalities for \( p \geq 2 \) in the lemma. By the Burkholder-Davis-Gundy inequality [31, p. 160] and (5.6), we have

\[
\mathbb{E}|\mathcal{I}_{u_1}^x(t)|^p \leq C_p \mathbb{E} \left( \int_0^t |\nabla u_1 X_s^x|^2 ds \right)^{p/2} \leq C_p |u_1|^p.
\]

By the Burkholder-Davis-Gundy inequality and (5.7), we have

\[
\mathbb{E}|\nabla u_2 \mathcal{I}_{u_1}^x(t)|^p \leq C_p \mathbb{E} \left( \int_0^t |\nabla u_1 \nabla u_2 X_s^x|^2 ds \right)^{p/2} \leq C_{\theta,p} |u_1|^p |u_2|^p.
\]

It is easy to see that \( D_1 \mathcal{I}_{u_1}^x(t) \) can be computed by (5.10) as

\[
D_1 \mathcal{I}_{u_1}^x(t) = \frac{1}{\sqrt{2t}} \int_0^t \langle D_1 \nabla u_1 X_s^x, dB_s \rangle + \frac{1}{2t^2} \int_0^t \langle \nabla u_1 X_s^x, \nabla u_2 X_s^x \rangle ds.
\]

By (5.17), Burkholder’s and Hölder’s inequalities, we have

\[
\mathbb{E} \left| \frac{1}{\sqrt{2t}} \int_0^t \langle D_1 \nabla u_1 X_s^x, dB_s \rangle \right|^p \leq C_p \mathbb{E} \left( \int_0^t |D_1 \nabla u_1 X_s^x|^2 ds \right)^{p/2} \leq C_p \mathbb{E} \left( \int_0^t |D_1 \nabla u_1 X_s^x|^p ds \right) t^{p-2} \leq C_{\theta,p} |u_2|^p |u_1|^p.
\]

By Hölder’s inequality and (5.6), we have

\[
\mathbb{E} \left| \frac{1}{2t^2} \int_0^t \langle \nabla u_1 X_s^x, \nabla u_2 X_s^x \rangle ds \right|^p \leq \frac{1}{2^p} \left( \int_0^t |\nabla u_1 X_s^x|^p |\nabla u_2 X_s^x|^p ds \right)^{p-1} \leq \frac{|u_1|^p |u_2|^p}{t^p}.
\]

Combining the previous three relations, we immediately obtain (5.20).

By the definition of \( \mathcal{I}_{u_1,u_2}^x(t) \), we have

\[
\mathbb{E}|\mathcal{I}_{u_1,u_2}^x(t)|^p \leq 2^{p-1} \mathbb{E}|\mathcal{I}_{u_1}^x(t)\mathcal{I}_{u_2}^x(t)|^p + 2^{p-1} \mathbb{E}|D_1 \mathcal{I}_{u_1}^x(t)|^p.
\]
By (5.18), we have
\[
\mathbb{E}|I_{u_1}^x(t)I_{u_2}^x(t)|^p \leq \sqrt{\mathbb{E}|I_{u_1}^x(t)|^{2p}\mathbb{E}|I_{u_2}^x(t)|^{2p}}
\leq \sqrt{\mathbb{E}|I_{u_1}^x(t)|^{2p}\mathbb{E}|I_{u_2}^x(t)|^{2p}}
\leq \sqrt{\mathbb{E}|I_{u_1}^x(t)|^{2p}\mathbb{E}|I_{u_2}^x(t)|^{2p}} \leq C_{\theta,p}t^{-p}|u_1|^p|u_2|^p,
\]
which, together with (5.20), immediately gives (5.21).

**APPENDIX A. ON THE ERGODICITY OF SDE (2.2)**

This section provides the details of the verification of the ergodicity of SDE (2.2). There are several ways to prove the ergodicity of SDE (2.2); here, we follow the approach used by Eberle [14, Theorem 1 and Corollary 2] because it gives exponential convergence in Wasserstein distance. We verify the conditions in the theorem, adopting the notations in [14]. For any \( r > 0 \), define
\[
\kappa(r) = \inf \left\{ -2\left< x - y, g(x) - g(y) \right> : x, y \in \mathbb{R}^d \text{ s.t. } |x - y| = \sqrt{2}r \right\}.
\]
Compared with the conditions in [14], SDE (2.2) has \( \sigma = \sqrt{2}I_d \) and \( G = \frac{1}{2}I_d \) and the associated intrinsic metric is \( \frac{1}{\sqrt{2}}|\cdot| \) with \(|\cdot|\) being the Euclidean distance. By (2.3), we have
\[
\langle x - y, g(x) - g(y) \rangle = \int_0^1 \langle x - y, \nabla_{x-y}g(sx + (1-s)y) \rangle ds
\leq -\theta_0 \int_0^1 (1 + \theta_1 |sx + (1-s)y|^{\theta_2}) |x - y|^2 ds,
\]
which implies that
\[
\kappa(r) \geq \inf \left\{ 2\theta_0 \int_0^1 (1 + \theta_1 |sx + (1-s)y|^{\theta_2}) ds : x, y \in \mathbb{R}^d \text{ s.t. } |x - y| = \sqrt{2}r \right\}.
\]
Therefore, we have \( \kappa(r) > 0 \) for \( r > 0 \) and thus \( \int_0^1 r\kappa(r)^{-1} dr = 0 \). Define
\[
R_0 = \inf \{ R \geq 0 : \kappa(r) \geq 0 \forall r \geq R \},
\]
\[
R_1 = \inf \{ R \geq R_0 : \kappa(r)R(R-R_0) > 8 \forall r \geq R \}.
\]
It is easy to check that \( R_0 = 0 \) and \( R_1 \in (0, \infty) \).

As \( \kappa(r) > 0 \) for all \( r > 0 \), we have \( \varphi(r) = \exp \left( -\frac{1}{4} \int_0^r s\kappa(s)^{-1} ds \right) = 1 \) and thus \( \Phi(r) = \int_0^r \varphi(s) ds = r \). Moreover, we have \( \alpha = 1 \) and
\[
c = \left( \alpha \int_0^{R_1} \Phi(s)\varphi(s)^{-1} ds \right)^{-1} = \frac{2}{R_1^2}.
\]
Applying Corollary 2 in [14], we have
\[
d_W(\mathcal{L}(X_t^x), \mu) \leq 2e^{-ct}d_W(\delta_x, \mu), \quad \forall t > 0,
\]
where \( \mathcal{L}(X_t^x) \) denotes the probability distribution of \( X_t^x \). Note that the convergence rate \( c > 0 \) only depends on \( \theta_0, \theta_1 \) and \( \theta_2 \).

From (A.1), we say that \( \mathcal{L}(X_t^x) \to \mu \) weakly, in the sense that for any bounded continuous function \( f : \mathbb{R}^d \to \mathbb{R} \), we have
\[
\lim_{t \to \infty} \mathbb{E}f(X_t^x) = \mu(f),
\]
which immediately implies
\[
\lim_{t \to \infty} \frac{1}{t} \int_0^t \mathbb{E} f(X^s) ds = \mu(f).
\]

**APPENDIX B. MULTIVARIATE NORMAL APPROXIMATION**

In this appendix, we prove the results stated in Remark 2.9 with regard to multivariate normal approximation for sums of independent, bounded random vectors.

**Theorem B.1.** Let \( W = \frac{1}{\sqrt{n}} \sum_{i=1}^n X_i \) where \( X_1, \ldots, X_n \) are independent \( d \)-dimensional random vectors such that \( \mathbb{E} X_i = 0, |X_i| \leq \beta \) and \( \mathbb{E} W W^T = I_d \). Then we have

(B.1) \( d_W(\mathcal{L}(W), \mathcal{L}(Z)) \leq C d \beta \sqrt{1 + \log n} \)

and

(B.2) \( d_W(\mathcal{L}(W), \mathcal{L}(Z)) \leq C d^2 \beta \sqrt{n} \),

where \( C \) is an absolute constant and \( Z \) has the standard \( d \)-dimensional normal distribution.

**Proof.** Note that by the same smoothing and limiting arguments as in the proof of Theorem 2.5, we only need to consider test functions \( h \in \text{Lip}(\mathbb{R}^d, 1) \), which are smooth and have bounded derivatives of all orders. This is assumed throughout the proof so that the integration, differentiation, and their interchange are legitimate.

For multivariate normal approximation, the Stein equation (3.1) simplifies to

(B.3) \( \Delta f(w) - \langle w, \nabla f(w) \rangle = h(w) - \mathbb{E} h(Z) \).

An appropriate solution to (B.3) is known to be

(B.4) \( f_h(x) = -\int_0^\infty \{ h * \phi_{r \sqrt{e^{-s}}}(e^{-s}x) - \mathbb{E} h(Z) \} ds, \)

where \(*\) denotes the convolution and \( \phi_r(x) = (2\pi r^2)^{-d/2} e^{-|x|^2/2r^2} \). From (B.3), we have

\[
d_W(\mathcal{L}(W), \mathcal{L}(Z)) = \sup_{h \in \text{Lip}(\mathbb{R}^d, 1)} |\mathbb{E} W \cdot \nabla f(W) - \mathbb{E} \Delta f(W)|
\]

with \( f := f_h \) in (B.4) (we omit the dependence of \( f \) on \( h \) for notational convenience).

Let \( C \) be a constant that may differ in different expressions. Denote

(B.5) \( \eta : = d_W(\mathcal{L}(W), \mathcal{L}(Z)) \).

Let \( \{X'_1, \ldots, X'_n\} \) be an independent copy of \( \{X_1, \ldots, X_n\} \). Let \( I \) be uniformly chosen from \( \{1, \ldots, n\} \) and be independent of \( \{X_1, \ldots, X_n, X'_1, \ldots, X'_n\} \). Define

\[ W' = W - \frac{X_I}{\sqrt{n}} + \frac{X'_I}{\sqrt{n}}. \]

Then \( W \) and \( W' \) have the same distribution. Let

\[ \delta = W' - W = \frac{X'_I}{\sqrt{n}} - \frac{X_I}{\sqrt{n}}. \]

We have, by the independence assumption and the facts that \( \mathbb{E} X_i = 0 \) and \( \mathbb{E} W W^T = I_d \),

\[
\mathbb{E}[\delta|W] = \frac{1}{n} \sum_{i=1}^n \mathbb{E} \left[ \frac{X'_i}{\sqrt{n}} - \frac{X_i}{\sqrt{n}} | W \right] = -\frac{1}{n} W.
\]
and

\[ \mathbb{E}[\delta \delta^T | W] = \frac{2}{n} I_d + \frac{1}{n} \{ \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} X_i X_i^T | W \right] - I_d \}. \]

Therefore, (2.7) and (2.8) are satisfied with

\[ \lambda = \frac{1}{n}, \quad g(W) = -W, \quad R_1 = 0, \quad R_2 = \frac{1}{2} \{ \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} X_i X_i^T | W \right] - I_d \} \]

Note that this is Example 1 below Assumption 2.1 with \( \lambda_1 = \cdots = \lambda_d = 1 \). By the boundedness condition,

\[ |\delta| \leq \frac{2\beta}{\sqrt{n}}. \]

We also have

\[ \mathbb{E}[|\delta|^2] = \frac{2}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \left| \frac{X_i}{n} \right|^2 \right] = \frac{2d}{n}. \]

As \( \beta^2 \geq \sum_{i=1}^{n} \mathbb{E} \left[ \left| \frac{X_i}{n} \right|^2 \right] = d \), we have \( \beta \geq \sqrt{d} \). Using these facts and assuming that \( \beta \leq \sqrt{n} \) (otherwise (B.1) is trivial), in applying (2.10), we have

\[ \mathbb{E} |R_1| = 0, \]

\[ \sqrt{d} \mathbb{E}[||R_2||_{HS}] \leq C\sqrt{d} \left\{ \sum_{j,k=1}^{d} \text{Var} \left[ \frac{1}{n} \sum_{i=1}^{n} X_{ij} X_{ik} \right] \right\} \]

(B.6)

\[ = C\sqrt{d} \left\{ \frac{1}{n^2} \sum_{i=1}^{n} \text{Var} \left[ X_{ij} X_{ik} \right] \right\} \leq C\sqrt{d} \left\{ \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E} \left[ X_{ij}^2 X_{ik}^2 \right] \right\} \]

\[ = C\sqrt{d} \left\{ \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E}[|X_i|^4] \right\} \leq C\sqrt{d} \beta \left\{ \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E}[|X_i|^2] \right\} = \frac{C d \beta}{\sqrt{n}}, \]

and

\[ \frac{1}{\lambda} \mathbb{E} \left[ |\delta|^3 (|\log |\delta|| \lor 1) \right] \leq C n \frac{\beta}{\sqrt{n}} (1 + \log n) \mathbb{E}[|\delta|^2] \leq \frac{C d \beta}{\sqrt{n}} (1 + \log n). \]

This proves (B.1).

To prove (B.2), we modify the argument from (3.7) by using the explicit expression of \( f \) in (B.4). With \( \delta_i = (X_i' - X_i')/\sqrt{n} \) and \( h_s(x) := h(e^{-s}x) \), we have

\[ \frac{1}{\lambda} \int_0^1 \left| \mathbb{E}[\langle \delta \delta^T, \nabla^2 f(W + t\delta) \rangle] - \nabla^2 f(W)_{HS} \right| dt \]

\[ = \int_0^1 \left| \mathbb{E} \left[ \sum_{i=1}^{n} \int_0^\infty \int_0^1 t \nabla^3_{\delta_i} (h_s + \phi_{\sqrt{s}-1})(W + ut\delta_i) du ds \right] \right| dt, \]

where \( \nabla^3_{\delta_i} := \nabla_{\delta_i} \nabla_{\delta_i} \nabla_{\delta_i} \) (cf. Section 2.1). We separate the integration over \( s \) into \( \int_0^{e^2} \) and \( \int_{e^2}^\infty \) with an \( \epsilon \) to be chosen later. For the part \( \int_0^{e^2} \), exactly following [39, pp 18-19], we have

(B.7) \[ C \mathbb{E} \sum_{i=1}^{n} \int_0^{e^2} e^{-s} |\delta_i|^2 \frac{1}{e^{2s} - 1} ds \leq C d \epsilon, \]
where we used $\sum_{i=1}^{n} \mathbb{E}|\delta_i|^2 = 2d$. The part $\int_{\mathbb{R}^d}^\infty$ is treated differently. Using the interchangeability of convolution and differentiation, we have

$$\left| \mathbb{E} \sum_{i=1}^{n} \int_{\mathbb{R}^d}^\infty \int_{0}^{1} \nabla_{\delta_i}^3 (h_s * \phi_{\sqrt{2s-1}})(W + ut\delta_i) duds \right|$$

(B.8)

$$= \left| \mathbb{E} \sum_{i=1}^{n} \int_{\mathbb{R}^d}^\infty \int_{0}^{1} h_s(W + ut\delta_i - x) \nabla_{\delta_i}^3 \phi_{\sqrt{2s-1}}(x) dx duds \right| .$$

Let $\{\hat{X}_1, \ldots, \hat{X}_n\}$ be another independent copy of $\{X_1, \ldots, X_n\}$ and be independent of $\{X'_1, \ldots, X'_n\}$, and let $\hat{W}_i = W - \frac{X_i}{\sqrt{n}} + \frac{\hat{X}_i}{\sqrt{n}}$. From this construct, for each $i$, $\hat{W}_i$ has the same distribution as $W$ and is independent of $\{X_i, X'_i\}$. Let $\hat{Z}$ be an independent standard Gaussian vector. Rewriting

$$h_s(W + ut\delta_i - x) = [h_s(W + ut\delta_i - x) - h_s(\hat{W}_i - x)]$$

$$+ [h_s(\hat{W}_i - x) - h_s(Z - x)]$$

$$+ [h_s(Z - x)],$$

the term inside the absolute value in (B.8) is separated into three terms as follows:

$$R_{31} = \mathbb{E} \sum_{i=1}^{n} \int_{\mathbb{R}^d}^\infty \int_{0}^{1} \int_{0}^{1} \left[ h_s(W + ut\delta_i - x) - h_s(\hat{W}_i - x) \right] \nabla_{\delta_i}^3 \phi_{\sqrt{2s-1}}(x) dx duds,$$

$$R_{32} = \mathbb{E} \sum_{i=1}^{n} \int_{\mathbb{R}^d}^\infty \int_{0}^{1} \int_{0}^{1} \left[ h_s(\hat{W}_i - x) - h_s(Z - x) \right] \nabla_{\delta_i}^3 \phi_{\sqrt{2s-1}}(x) dx duds,$$

$$R_{33} = \mathbb{E} \sum_{i=1}^{n} \int_{\mathbb{R}^d}^\infty \int_{0}^{1} \int_{0}^{1} \left[ h_s(Z - x) \right] \nabla_{\delta_i}^3 \phi_{\sqrt{2s-1}}(x) dx duds.$$ 

We bound their absolute values separately. From $h \in \text{Lip}(\mathbb{R}^d, 1)$, $h_s(x) = h(e^{-s}x)$ and $|X_i| \leq \beta$, we have

$$[h_s(W + ut\delta_i - x) - h_s(\hat{W}_i - x)] \leq \frac{Ce^{-s\beta}}{\sqrt{n}}.$$ 

Moreover,

$$\int_{\mathbb{R}^d} |\nabla_{\delta_i}^3 \phi_{\sqrt{2s-1}}(x)| dx \leq C|\delta_i|^3 \frac{1}{(e^{2s} - 1)^{3/2}}.$$

Therefore,

$$|R_{31}| \leq C \sum_{i=1}^{n} \mathbb{E} \int_{\mathbb{R}^d}^\infty e^{-s\beta|\delta_i|^3} \frac{1}{n^2 (e^{2s} - 1)^{3/2}} ds \leq \frac{C d \beta^2}{\epsilon n},$$

where we used $|\delta_i| \leq 2\beta/\sqrt{n}$ and $\sum_{i=1}^{n} \mathbb{E}|\delta_i|^2 = 2d$.

From the definition of $\eta$ in (B.5) and the fact that $\hat{W}_i$ has the same distribution as $W$, we have

$$|\mathbb{E}[h_s(\hat{W}_i - x) - h_s(Z - x)]| \leq e^{-s}\eta.$$ 

Using independence and the same argument as for $R_{31}$, we have

$$|R_{32}| \leq \frac{C d \beta \eta}{\epsilon \sqrt{n}}.$$
Now we bound $R_{33}$. Using integration by parts, and combining two independent Gaussians into one, we have

$$|R_{33}| = \left| \mathbb{E} \sum_{i=1}^{n} \int_{c^2}^{\infty} \int_{\mathbb{R}^d} h_s(\tilde{Z} - x) \nabla_{\delta_i} \phi_{\sqrt{e^{2s} - 1}}(x) dx dt ds \right|$$

$$= \left| \mathbb{E} \sum_{i=1}^{n} \int_{c^2}^{\infty} \int_{\mathbb{R}^d} \nabla_{\delta_i} h_s(\tilde{Z} - x) \phi_{\sqrt{e^{2s} - 1}}(x) dx ds \right|$$

$$= \left| \mathbb{E} \sum_{i=1}^{n} \int_{c^2}^{\infty} \int_{\mathbb{R}^d} \nabla_{\delta_i} h_s(x) \phi_{\sqrt{e^{2s} - 1}}(x) dx ds \right|$$

$$= \left| \mathbb{E} \sum_{i=1}^{n} \int_{c^2}^{\infty} \int_{\mathbb{R}^d} \nabla_{\delta_i} h_s(x) D^2_{\delta_i} \phi_{\sqrt{e^{2s} - 1}}(x) dx ds \right|$$

$$\leq \left| \mathbb{E} \sum_{i=1}^{n} \int_{c^2}^{\infty} \delta_i e^{-s} |\delta_i|^2 \frac{C}{e^{2s}} ds \right| \leq \frac{Cd\beta}{\sqrt{n}}.$$  

From (B.6), (B.7) and the bounds on $R_{31}$, $R_{32}$ and $R_{33}$, we have

$$\eta \leq C \left( \frac{d\beta}{\sqrt{n}} + \epsilon + \frac{d\beta^2}{en} + \frac{d\beta\eta}{\epsilon\sqrt{n}} + \frac{d\beta}{\sqrt{n}} \right).$$

The theorem is proved by choosing $\epsilon$ to be a large multiple of $d\beta/\sqrt{n}$ and solving the recursive inequality for $\eta$.

\[ \square \]

Acknowledgements

We thank Michel Ledoux for very helpful discussions. We also thank two anonymous referees for their valuable comments which have improved the manuscript considerably. Fang X. was partially supported by Hong Kong RGC ECS 24301617, a CUHK direct grant and a CUHK start-up grant. Shao Q. M. was partially supported by Hong Kong RGC GRF 14302515 and 14304917. Xu L. was partially supported by Macao S.A.R. (FDCT 038/2017/A1, FDCT 030/2016/A1, FDCT 025/2016/A1), NNSFC 11571390, University of Macau (MYRG 2016-00025-FST, MYRG 2018-00133-FST).

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