Towards Sharp Stochastic Zeroth Order Hessian Estimators over Riemannian Manifolds

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Abstract
We study Hessian estimators for real-valued functions defined over an \( n \)-dimensional complete Riemannian manifold. We introduce new stochastic zeroth-order Hessian estimators using \( O(1) \) function evaluations. We show that, for a smooth real-valued function \( f \) with Lipschitz Hessian (with respect to the Riemannian metric), our estimator achieves a bias bound of order \( O(L_2^2 \delta + \gamma \delta^2) \), where \( L_2 \) is the Lipschitz constant for the Hessian, \( \gamma \) depends on both the Levi-Civita connection and function \( f \), and \( \delta \) is the finite difference step size. To the best of our knowledge, our results provide the first bias bound for Hessian estimators that explicitly depends on the geometry of the underlying Riemannian manifold. Perhaps more importantly, our bias bound does not increase with dimension \( n \). This improves best previously known bias bound for \( O(1) \)-evaluation Hessian estimators, which increases quadratically with \( n \). We also study downstream computations based on our Hessian estimators. The supremacy of our method is evidenced by empirical evaluations.

1 Introduction
Hessian computation is one of the central tasks in optimization, machine learning and related fields. Understanding the landscape of the objective function is in many cases the first step towards solving a mathematical programming problem, and Hessian is one of the key quantities that depict the function landscape. Often in real-world scenarios, the objective function is a black-box, and its Hessian is not directly computable. In these cases, zeroth-order Hessian computation techniques are needed if one wants to understand the function landscape via its Hessian.

To this end, we introduce new zeroth-order methods for estimating a function’s Hessian at any given point over a complete \( n \)-dimensional Riemannian manifold \((M, g)\). For \( p \in M \) and a real-valued function \( f \) defined over \( M \), the Hessian estimator of \( f \) at \( p \) is

\[
\hat{H}f(p; v, w; \delta) := \sum_{i,j} f(Exp_p(\delta v + \delta w))v^i w^j ,
\]

where \( \text{Exp}_p \) is the exponential map, \( v, w \) are independently sampled from the unit sphere in \( T_p M \), \( v \otimes w \) denotes the tensor product of \( v \) and \( w \) (\( v, w \in T_p M \)), and \( \delta \) is the finite-difference step size. For a function \( f : M \to \mathbb{R} \) whose Hessian is \( L_2 \)-Lipschitz (with respect to the \( \infty \)-Schatten norm and the Riemannian metric \( g \)), our Hessian estimator satisfies

\[
\left\| \mathbb{E}_{v, w \sim S_p} \left[ \hat{H}f(p; v, w; \delta) \right] - \text{Hess}f(p) \right\| = O \left( L_2^2 \delta + \delta^2 \sup_{u \in S_p} \mathbb{E}_{v, w \sim S_p} \left[ \nabla_u^2 \left( \nabla_v^2 + \nabla_w^2 \right) f(p) - \left( \nabla_v^2 + \nabla_w^2 \right) \nabla_u^2 f(p) \right] \right),
\]

where \( \| \cdot \| \) is the \( \infty \)-Schatten norm, \( S_p \) is the unit sphere in \( T_p M \), \( \text{Hess}f(p) \) is the Hessian of \( f \) at \( p \), and \( \nabla \) is the Levi-Civita connection associated with the Riemannian metric.

This bias bound improves previously known results in two ways:

1. It provides, via the Levi-Civita connection, the first bias bound for Hessian estimators that explicitly depends on the local geometry of the underlying space;

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2. It does not increase with dimension $n$. This significantly improves best previously known bias bound for $O(1)$-evaluation Hessian estimators, which is of order $O(L^2 n^2 \delta)$, where $L$ is the Lipschitz constant and $\delta$ is the finite-difference step size. See Remark [7] for details.

We also study downstream computations for our Hessian estimator. More specifically, we introduce novel provably accurate methods for computing adjugate and inversion of the Hessian matrix, all using zeroth order information only. These zeroth order computation methods may be used as primers for further applications. The supremacy of our method over existing methods is evidenced by careful empirical evaluations.

Related Works

Zeroth order optimization has attracted the attention of many researchers. Under this broad umbrella, there stands the Bayesian optimization methods (See the review article by Shahriari et al. [2015] for an overview), comparison-based methods (e.g., Nelder and Mead [1965]), genetic algorithms (e.g., Goldberg and Holland [1988], best arm identification from the multi-armed bandit community (e.g., Bubeck et al. [2009] Audibert et al. [2010], and many others (See the book by Conn et al. [2009] for an overview). Among all these zeroth order optimization schemes, one classic and prosperous line of works focuses on estimating higher order derivatives using zeroth order information.

Zeroth order gradient estimators make up a large portion of derivative estimation literature. In the past few years, Flaxman et al. [2005] studied the stochastic gradient estimator using a single-point for the purpose of bandit learning. Duchi et al. [2015] studied stabilization of the stochastic gradient estimator via two-points (or multi-points) evaluations. Nesterov and Spokoiny [2017]; Li et al. [2020] studied gradient estimators using Gaussian smoothing, and investigated downstream optimization methods using the estimated gradient. Recently, Wang et al. [2021] studied stochastic gradient estimators over Riemannian manifolds, via the lens of the Greene-Wu convolution.

Zeroth order Hessian estimation is also a central topic in derivative estimation. In the control community, gradient-based Hessian estimators were introduced for iterative optimization algorithms, and asymptotic convergence was proved (Spall [2000]). Apart from this asymptotic result, no generic non-asymptotic bound for $O(1)$-evaluation Hessian estimators are known until recently. Based on the Stein’s identity (Stein [1981]), Balasubramanian and Ghadimi [2021] designed the Stein-type Hessian estimator, and combined it with cubic regularized Newton’s method (Nesterov and Polyak [2006]) for non-convex optimization. Li et al. [2020] generalizes the Stein-type Hessian estimators to Riemannian manifolds embedded in Euclidean spaces. Yet for previous Hessian estimators (Li et al., 2020; Balasubramanian and Ghadimi, 2021), the bias bound increases quadratically with dimension of the space. In the case of non-trivial curvature (Li et al., 2020), no geometry-aware bias bound has been given prior to our work.

2 Preliminaries and Conventions

For better readability, we list here some notations and conventions that will be used throughout the rest of this paper.

- For any $p \in \mathcal{M}$, let $U_p$ denote the open set near $p$ that is a diffeomorphic to a subset of $\mathbb{R}^n$ via the local normal coordinate chart $\phi$. Define the distance $d_p(q_1, q_2)$ $(q_1, q_2 \in U_p)$ such that
  \[d_p(q_1, q_2) = d_{\text{Euc}}(\phi(q_1), \phi(q_2)).\]
  where $d_{\text{Euc}}$ is the Euclidean distance in $\mathbb{R}^n$.

- The injectivity radius of $p \in \mathcal{M}$ (written $\text{inj}(p)$) is defined as the radius of the largest geodesic ball that is contained in $U_p$. (A1, Positive Injectivity Radius Assumption) Throughout the paper, we assume that, there exists a constant $\delta_0 > 0$, such that $\delta_0 \leq \frac{\text{inj}(p)}{2}$ for all $p \in \mathcal{M}$. Also, we assume all finite difference step sizes $\delta$ satisfy $\delta \leq \delta_0$.  


• All musical isomorphisms are omitted when there is no confusion.
• For any \( p \in \mathcal{M} \) and \( \alpha > 0 \), we use \( \alpha S_p \) (resp. \( \alpha B_p \)) to denote the origin-centered sphere (resp. ball) in \( T_p \mathcal{M} \) with radius \( \alpha \). For simplicity, we write \( S_p = 1S_p \) (resp. \( B_p = 1B_p \)). It is worth emphasizing that \( S_p \) and \( B_p \) are in \( T_p \mathcal{M} \). They are different from geodesic balls which reside in \( \mathcal{M} \).

• For \( p \in \mathcal{M} \) and \( q \in U_p \), we use \( T^q_p : T_p \mathcal{M} \to T_q \mathcal{M} \) to denote the parallel transport from \( T_p \mathcal{M} \) to \( T_q \mathcal{M} \) along the distance-minimizing geodesic connecting \( p \) and \( q \). For any \( p \in \mathcal{M} \), \( u \in T_p \mathcal{M} \) and \( q \in U_p \), define \( u_q = T^q_p(u) \). More generally, \( T^q_p \) denotes the parallel transport along the distance-minimizing geodesic from \( p \) to \( q \), among the fiber bundle that is compatible with the Riemannian structure.

• We will use the double exponential map notation (Gavrilov 2007). For any \( p \in \mathcal{M} \) and \( u, v \in T_p \mathcal{M} \) such that \( \text{Exp}_p(u) \in U_p \), we write \( \text{Exp}^\tau_p(u, v) = \text{Exp}^\tau_p(\text{Exp}_p(u)) \).

• (Definition of Hessian (e.g., Petersen 2006)) Over an \( n \)-dimensional complete Riemannian manifold \( \mathcal{M} \), the Hessian of a smooth function \( f : \mathcal{M} \to \mathbb{R} \) at \( p \) is a bilinear form \( \text{Hess}(f) : T_p \mathcal{M} \times T_p \mathcal{M} \to \mathbb{R} \) such that, for all \( u, v \in T_p \mathcal{M} \), \( \text{Hess}(f)(u, v) = \langle \nabla u df \mid p \rangle \). Since the Levi-Civita connection is torsion-free, the Hessian is symmetric: \( \text{Hess}(f)(u, v) = \text{Hess}(f)(v, u) \) for all \( u, v \in T_p \mathcal{M} \). For a smooth function \( f \), its Hessian satisfies (e.g., Absil et al. 2009), for any \( p \in \mathcal{M} \) and any \( v, \tau \in T_p \mathcal{M} \),
  \[
  \text{Hess}(f)(v, \tau) = \lim_{\tau \to 0} \frac{f(\text{Exp}_p(\tau v)) - 2 f(p) + f(\text{Exp}_p(-\tau v)) \rangle}{\tau^2}.
  \]

For simplicity and coherence with the notations in the Euclidean case, we write \( u^\top \text{Hess}(f)(v) := \text{Hess}(f)(u, v) \) for any \( u, v \in T_p \mathcal{M} \).

• Consider a Riemannian manifold \( (\mathcal{M}, g) \), a point \( p \in \mathcal{M} \), and any symmetric bilinear form \( A : T_p \mathcal{M} \times T_p \mathcal{M} \to \mathbb{R} \). The \( g \)-induced \( \infty \)-Schatten norm (the operator norm) of \( A \) is defined as
  \[
  \| A \| = \sup_{u \in T_p \mathcal{M}, \| u \| = 1} |u^\top A u|.
  \]

When it is clear from context, we simply use \( \infty \)-Schatten norm to refer to \( g \)-induced \( \infty \)-Schatten norm.

• Note. When applied to a tangent vector, \( \| \cdot \| \) is the standard norm induced by the Riemannian metric. When applied to a symmetric bilinear form, \( \| \cdot \| \) is the \( \infty \)-Schatten norm defined above.

• (A2, Lipschitz Hessian Assumption) Throughout the paper, we assume that, there exists a nonnegative constant \( L_2 \), such that for any \( p \in \mathcal{M} \) and \( q \in U_p \),
  \[
  \sup_{u \in T_p \mathcal{M}, \| u \| = 1} |u^\top \text{Hess}(f)(q) u_q - u^\top \text{Hess}(f)(p) u| \leq L_2 d(p, q).
  \]

## 3 Zeroth Order Hessian Estimation

For \( p \in \mathcal{M} \) and \( f : \mathcal{M} \to \mathbb{R} \), the Hessian of \( f \) at \( p \) can be estimated by
  \[
  \tilde{\text{H}} f (p; v, w; \delta) = \frac{\delta^2}{2} f(\text{Exp}_p(\delta v + \delta w)) v \otimes w,
  \]
where \( v, w \) are independently uniformly sampled from \( S_p \) and \( \delta \) is the finite difference step size. To study the bias of this estimator, we consider a function \( \tilde{f}^\delta \) defined as follows.

For \( p \in \mathcal{M} \), a smooth real-valued function \( f \) defined over \( \mathcal{M} \), and a number \( \delta \in (0, \delta_0) \), define a function \( f^\delta \) (at \( p \)) such that
  \[
  f^\delta (p) = \frac{1}{\delta^{2n} V^n} \int_{w \in \delta B_p} \int_{v \in \delta B_p} f(\text{Exp}_p(v + w)) \, dw \, dv,
  \]

(2)
where $V_n$ is the volume of the unit ball in $T_p\mathcal{M}$ (same as the volume of the unit ball in $\mathbb{R}^n$). Smoothings of this kind have been analytically investigated by Greene and Wu (Greene and Wu, 1973, 1976, 1979). We will first show that $\text{Hess} f^\delta(p) = \mathbb{E}_{v,w,\delta \sim \mathcal{S}_p} \left[ \hat{H}f(p; v, w; \delta) \right]$ in Lemma 1. Then we derive a bound on $\|\text{Hess} f^\delta(p) - \text{Hess} f(p)\|$, which gives a bound on $\|\mathbb{E}_{v,w,\delta \sim \mathcal{S}_p} \left[ \hat{H}f(p; v, w; \delta) \right] - \text{Hess} f(p)\|$. Henceforth, we will use $\mathbb{E}_{v,w}$ as a shorthand for $\mathbb{E}_{v,w,\delta \sim \mathcal{S}_p}$.

**Lemma 1.** Consider an $n$-dimensional complete Riemannian manifold $(\mathcal{M}, g)$. Consider $p \in \mathcal{M}$, a smooth function $f : \mathcal{M} \to \mathbb{R}$ and a small number $\delta \in (0, \delta_0]$. If $v$ and $w$ are independently randomly sampled from $\mathcal{S}_p$, then it holds that,

$$
\mathbb{E}_{v,w} \left[ \hat{H}f(p; v, w; \delta) \right] = \text{Hess} f^\delta(p).
$$

**Proof.** Define $\varphi_p = f \circ \text{Exp}_p$. By the fundamental theorem of geometric calculus, it holds that

$$
\int_{v \in \mathcal{S}_p} \int_{w \in \mathcal{S}_p} \partial_i \varphi_p(w + v) \, dv \, dw = \int_{v \in \mathcal{S}_p} \int_{w \in \mathcal{S}_p} \varphi_p(w + v) \frac{w}{\|w\|} \, dv \, dw
$$

$$
= \int_{v \in \mathcal{S}_p} \int_{w \in \mathcal{S}_p} \varphi_p(w + v) \frac{v \otimes w}{\|v\|\|w\|} \, dv \, dw.
$$

Since $v$ and $w$ are independently uniformly sampled from $\mathcal{S}_p$, it holds that

$$
\int_{\mathcal{S}_p} \int_{\mathcal{S}_p} \varphi_p(w + v) \frac{v \otimes w}{\|v\|\|w\|} \, dv \, dw = \delta^{2n-2} A_{n-1}^2 \mathbb{E}_{v,w} [\varphi_p(\delta v + \delta w)v \otimes w],
$$

where $A_{n-1}$ is the surface area of $\mathcal{S}_p$ in $T_p\mathcal{M}$ (same as the surface area of unit sphere in $\mathbb{R}^n$).

By the dominated convergence theorem, we have

$$
\partial_i \partial_j \int_{v \in \mathcal{S}_p} \int_{w \in \mathcal{S}_p} \varphi_p(w + v) \, dv \, dw = \delta^{2n-2} A_{n-1}^2 \mathbb{E}_{v,w} [\varphi_p(\delta v + \delta w)v \otimes w] .
$$

More specifically, the $\partial_i$ operations (or tangent vectors) can be defined in terms limits, and we can interchange the limit and the integral by the dominated convergence theorem.

Combining $(i)$, $(ii)$ and $(iii)$ gives

$$
\partial_i \partial_j \int_{v \in \mathcal{S}_p} \int_{w \in \mathcal{S}_p} \varphi_p(w + v) \, dv \, dw = \delta^{2n-2} A_{n-1}^2 \mathbb{E}_{v,w} [\varphi_p(\delta v + \delta w)v \otimes w] .
$$

Combining the above results gives

$$
\partial_i \partial_j f^\delta(p) = \partial_i \partial_j \frac{1}{\delta^{2n} V_n} \int_{v \in \mathcal{S}_p} \int_{w \in \mathcal{S}_p} \varphi_p(w + v) \, dv \, dw
$$

$$
= \frac{\delta^{2n-2} A_{n-1}^2}{\delta^{2n} V_n} \mathbb{E}_{v,w} [\varphi_p(\delta v + \delta w)v \otimes w]
$$

$$
= \frac{n^2}{\delta^2} \mathbb{E}_{v,w} [f(\text{Exp}_p(\delta v + \delta w))v \otimes w],
$$

where the second last equality uses $(iv)$, and last equality uses $A_{n-1} = nV_n$. 

As a result of Lemma 1, a bound on $\|\text{Hess} f^\delta(p) - \text{Hess} f(p)\|$ will give a bound on $\|\mathbb{E}_{v,w,\delta \sim \mathcal{S}_p} \left[ \hat{H}f(p; v, w; \delta) \right] - \text{Hess} f(p)\|$. To bound $\|\text{Hess} f^\delta(p) - \text{Hess} f(p)\|$, we need to explicitly extend the definition of $f^\delta$ from $p$ to a neighborhood of $p$ (Wang et al., 2021), so that the Hessian can be computed in a

\footnote{Here $\partial_i$ and $\partial_j$ are understood as Einstein's notations.}
Proposition 1. For any \( p \in \mathcal{M} \), a smooth function \( f : \mathcal{M} \to \mathbb{R} \), and a number \( \delta \in (0, \delta_0] \), define a function \( \tilde{f}^\delta \) (near \( p \)) such that

\[
\tilde{f}^\delta(q) = \mathbb{E}_{v \in S_p, w \in S_p} \left[ \tilde{f}^\delta_{v,w}(q) \right], \quad \forall q \in U_p, \tag{3}
\]

where

\[
\tilde{f}^\delta_{v,w}(q) := \frac{n^2}{4\delta^{2n}} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} f(\text{Exp}_q(tv + sw)) \left| t \right|^{n-1} \left| s \right|^{n-1} dt ds, \tag{4}
\]

with \( v, w \in S_p \).

The advantage of defining \( \tilde{f}^\delta \) via \( \tilde{f}^\delta_{v,w} \) is that \( \tilde{f}^\delta_{v,w} \) is explicitly defined in a neighborhood of \( p \). Thus we can carry out geometry-aware computations in a precise manner. Next, we verify that \([2]\) and \([3]\) agree with each other in the following proposition.

**Proposition 1.** For any \( p \in \mathcal{M} \) and any \( \delta \leq \delta_0 \), \([2]\) and \([3]\) coincide at any \( q \in U_p \).

**Proof.** At any \( q \in U_p \), we have

\[
\begin{align*}
[2] &= \frac{1}{\delta^{2n} V_n} \int_{w \in \delta S_n} \int_{v \in \delta S_n} f(\text{Exp}_q(v + w)) \, dv \, dw \\
&\overset{(i)}{=} \frac{n^2}{\delta^{2n} A_n^2} \int_{w \in \delta S_n} \int_{v \in \delta S_n} f(\text{Exp}_q(v + w)) \, dv \, dw \\
&\overset{(ii)}{=} \frac{n^2}{\delta^{2n} A_n^2} \int_{w \in \delta S_n} \int_{v \in \delta S_n} \frac{1}{4} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} f(\text{Exp}_q(tv + sw)) \left| t \right|^{n-1} \left| s \right|^{n-1} \, dt \, ds \, dv \, dw,
\end{align*}
\]

where (i) uses \( A_{n-1} = nV_n \), and (ii) changes from Cartesian coordinate to hyperspherical coordinate (in \( T_q \mathcal{M} \)). Since the Levi-Civita connection is compatible with the Riemannian metric, we know that the standard Lebesgue measure in \( \mathbb{R}^n \) is preserved after transporting to \( T_q \mathcal{M} \). This implies, for any continuous function \( h \) defined over \( T_q \mathcal{M} \), we have \( \int_{v \in S_n} h(v) \, dv \overset{(iii)}{=} \int_{v \in S_p} h(v) \, dv \). Thus we have, at any \( q \in \mathcal{M} \),

\[
[2] = \frac{n^2}{4\delta^{2n} A_n^2} \int_{w \in \delta S_n} \int_{v \in \delta S_n} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} f(\text{Exp}_q(tv + sw)) \left| t \right|^{n-1} \left| s \right|^{n-1} \, dt \, ds \, dv \, dw = [3],
\]

where (iv) uses (iii).

By Proposition \([1]\) it is sufficient to work with \( \tilde{f}^\delta_{v,w} \) and randomize \( v, w \) over a unit sphere. For any direction \( u \in S_p \), the Hessian of \( \tilde{f}^\delta_{v,w} \) along \( u \) can be explicitly written out in terms of \( f \) and \( u \).

**Lemma 2.** Consider an \( n \)-dimensional complete Riemannian manifold \((\mathcal{M}, g)\). Consider \( p \in \mathcal{M} \), a smooth function \( f : \mathcal{M} \to \mathbb{R} \) and a small number \( \delta \in (0, \delta_0] \). For any \( u, v, w \in S_p \), we have

\[
\begin{align*}
&u^\top \text{Hess}_{v,w}(p)u \\
&= \frac{n^2}{4\delta^{2n}} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} u^\top \text{Hess}_q(u) \left| t \right|^{n-1} \left| s \right|^{n-1} \, dt \, ds \\
&\quad + \frac{n^2}{4\delta^{2n}} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^\infty \frac{\left| t \right|^{n-1} \left| s \right|^{n-1}}{(2j)!} \nabla_u^2 (t \nabla_v + s \nabla_w)^{2j} f(p) \, dt \, ds \\
&\quad - \frac{n^2}{4\delta^{2n}} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^\infty \frac{\left| t \right|^{n-1} \left| s \right|^{n-1}}{(2j)!} (t \nabla_v + s \nabla_w)^{2j} \nabla_u^2 f(p) \, dt \, ds,
\end{align*}
\]
where \( q = \text{Exp}_p(tv + sw) \).

**Proof.** From the definition of Hessian, we have
\[
\begin{align*}
    u^\top \text{Hess} f^\delta_{v,w}(p) u &= \lim_{\tau \to 0} \frac{\tilde{f}^\delta_{v,w}(\text{Exp}_p(\tau u)) - 2 \tilde{f}^\delta_{v,w}(p) + \tilde{f}^\delta_{v,w}(\text{Exp}_p(-\tau u))}{\tau^2}.
\end{align*}
\]

Thus it is sufficient to fix any \( t, s \in [-\delta, \delta] \) and consider
\[
\lim_{\tau \to 0} \frac{f(\text{Exp}_p^2(\tau u, tv + sw)) - 2f(\text{Exp}_p^2(tv + sw)) + f(\text{Exp}_p^2(-\tau u, tv + sw))}{\tau^2}.
\]

For simplicity, define
\[
\phi(\tau, t, s) = f(\text{Exp}_p^2(\tau u, tv + sw)) + f(\text{Exp}_p^2(-\tau u, tv + sw)) - f(\text{Exp}_p^2(tv + sw, tu)) - f(\text{Exp}_p^2(tv + sw, -tu)).
\]

Let \( q = \text{Exp}_p(tv + sw) \), and we have
\[
\begin{align*}
    u^\top \text{Hess} f^\delta_{v,w}(p) u &= \frac{n^2}{4\delta^2 n^2} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} u^\top \text{Hess} f(q) u_q |t|^{n-1} |s|^{n-1} \, dt \, ds \\
    &\quad + \frac{n^2}{4\delta^2} \lim_{\tau \to 0} \frac{\int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \phi(\tau, t, s)|t|^{n-1} |s|^{n-1} \, dt \, ds}{\tau^2},
\end{align*}
\]
provided that the last term converges.

For any \( p \in M, v \in T_p M \) and \( q \in U_p \), define \( h_v^{(j)}(q) = \nabla^j_q f(q) \). We can Taylor expand \( h_v^{(j)}(\text{Exp}_p(u)) \) by
\[
\begin{align*}
    h_v^{(j)}(\text{Exp}_p(u)) &= h_v^{(j)}(\text{Exp}_p(ut))\big|_{t=1} \\
    &= \sum_{i=0}^{\infty} \frac{1}{i!} \frac{d^i}{dt^i} h_v^{(j)}(\text{Exp}_p(ut))\bigg|_{t=0} \\
    &= \sum_{i=0}^{\infty} \frac{1}{i!} \nabla^i u h_v^{(j)}(p) \\
    &\quad \overset{(a)}{=} \sum_{i=0}^{\infty} \frac{1}{i!} \nabla^i_v \nabla^i u f(p).
\end{align*}
\]
From above, we have, for any \( p, u, v \in T_p M \) of small norm,
\[
\begin{align*}
    f(\text{Exp}_p^2(u, v)) &= f\left(\text{Exp}_{\text{Exp}_p(u)}\left(v_{\text{Exp}_p(u)}\right)\right) \\
    &= \sum_{j=0}^{\infty} \frac{1}{j!} \nabla^j_{v_{\text{Exp}_p(u)}} f(\text{Exp}_p(u)) \\
    &= \sum_{j=0}^{\infty} \frac{1}{j!} h_v^{(j)}(\text{Exp}_p(u)) \\
    &= \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{i=0}^{\infty} \frac{1}{i!} \nabla^i u \nabla^i_v f(p),
\end{align*}
\]
where the second equality uses Taylor expansion at \( \text{Exp}_p(u) \) and the last equality uses \((a)\).
From the above computation, we expand \( f(\text{Exp}_p^2(tv + sw)) \) (and similar terms) into infinite series. Thus we can write \( \phi(\tau, t, s) \) as

\[
\phi(\tau, t, s) = f(\text{Exp}_p^2(\tau u, tv + sw)) + f(\text{Exp}_p^2(-\tau u, tv + sw)) \\
- f(\text{Exp}_p^2(tv + sw, -\tau u)) \\
= \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{1}{i!j!} \nabla^i_{\tau u} \nabla^j_{tv+sw} f(p) + \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{1}{i!j!} \nabla^i_{-\tau u} \nabla^j_{tv+sw} f(p) \\
- \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{1}{i!j!} \nabla^i_{tv+sw} \nabla^j_{-\tau u} f(p)
\]

\[
= \sum_{j=0}^{\infty} \frac{\tau^2}{2j!} \nabla^2_u \nabla^j_{tv+sw} f(p) + \sum_{j=0}^{\infty} \frac{\tau^2}{2j!} \nabla^j_u \nabla^2_{tv+sw} f(p) \\
- \sum_{j=0}^{\infty} \frac{\tau^2}{2j!} \nabla^j_{tv+sw} \nabla^2_u f(p) - \sum_{j=0}^{\infty} \frac{\tau^2}{2j!} \nabla^2_{tv+sw} \nabla^j_u f(p) + O(\tau^3),
\]

where the last equality uses that zeroth-order terms in \( \tau \) and first-order terms in \( \tau \) all cancel.

From (6), we have

\[
\lim_{\tau \to 0} \frac{\phi(\tau, t, s)}{\tau^2} = \sum_{j=1}^{\infty} \frac{1}{j!} \nabla^2_u \nabla^j_{tv+sw} f(p) - \sum_{j=1}^{\infty} \frac{1}{j!} \nabla^j_{tv+sw} \nabla^2_u f(p)
\]

\[
= \sum_{j=1}^{\infty} \frac{1}{j(2j)!} \nabla^2_u (t\nabla_v + s\nabla_w)^{2j} f(p) - \sum_{j=1}^{\infty} \frac{1}{j!} (t\nabla_v + s\nabla_w)^j \nabla^2_u f(p)
\]

\[
= \sum_{j=1}^{\infty} \frac{1}{(2j)!} (t\nabla_v + s\nabla_w)^{2j} \nabla^2_u f(p) + \text{Odd}(t, s),
\]

where \( \text{Odd}(t, s) \) denotes terms that are either odd in \( t \) or odd in \( s \).

Since \( \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \text{Odd}(t, s) \, dt \, ds = 0 \), we have

\[
\frac{n^2}{4\delta^2} \lim_{\tau \to 0} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \phi(\tau, t, s)|t|^{n-1}|s|^{n-1} \, dt \, ds \frac{\tau^2}{\tau^2} = \frac{n^2}{4\delta^2} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^{\infty} \frac{|t|^{n-1}|s|^{n-1}}{(2j)!} \nabla^2_u (t\nabla_v + s\nabla_w)^{2j} f(p) \, dt \, ds
\]

\[
- \frac{n^2}{4\delta^2} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^{\infty} \frac{|t|^{n-1}|s|^{n-1}}{(2j)!} (t\nabla_v + s\nabla_w)^j \nabla^2_u f(p) \, dt \, ds.
\]

Collecting terms from (5) and (7), we have

\[
u^T \text{Hess}_{u,v,u}(p) u = \frac{n^2}{4\delta^2} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} u^T q \text{Hess} f(q) u_q \, |t|^{n-1}|s|^{n-1} \, dt \, ds
\]

\[
+ \frac{n^2}{4\delta^2} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^{\infty} \frac{|t|^{n-1}|s|^{n-1}}{(2j)!} \nabla^2_u (t\nabla_v + s\nabla_w)^{2j} f(p) \, dt \, ds
\]

\[
- \frac{n^2}{4\delta^2} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^{\infty} \frac{|t|^{n-1}|s|^{n-1}}{(2j)!} (t\nabla_v + s\nabla_w)^j \nabla^2_u f(p) \, dt \, ds,
\]

where \( q = \text{Exp}_p(tv + sw) \). This concludes the proof.
Gathering the above results gives a bias bound for (1), which is summarized in the following theorem.

**Theorem 1.** Consider an $n$-dimensional complete Riemannian manifold $(\mathcal{M}, g)$. Consider $p \in \mathcal{M}$, a smooth function $f : \mathcal{M} \to \mathbb{R}$ and a small number $\delta \in (0, \delta_0]$. The estimator (1) satisfies

$$
\left\| \mathbb{E}_{v, w} \left[ \tilde{H}f(p; v, w; \delta) \right] - \text{Hess}f(p) \right\| 
\leq \frac{2L_2n\delta}{n + 1} + \sup_{u \in \mathcal{S}_p} \mathbb{E}_{v, w} \left[ \frac{n^2}{4\delta^2n} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^{\infty} \frac{|t|^{n-1}|s|^{n-1}}{(2j)!} \nabla^2_u (\nabla_v + s \nabla_w)^{2j} f(p) \, dt \, ds \right]
$$

where $v, w$ are independently sampled from $\mathcal{S}_p$.

**Proof.** Since the Hessian is $L_2$-Lipschitz, we have

$$
u^\top \text{Hess}f(p) u - \frac{n^2}{4\delta^2n} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^{\infty} \frac{|t|^{n-1}|s|^{n-1}}{(2j)!} \nabla^2_u (\nabla_v + s \nabla_w)^{2j} f(p) \, dt \, ds
\leq L_2 \|u\| \, |s|.
$$

Let $q = \text{Exp}_p(tv + sw)$ for simplicity. We have, for any $u, v, w \in T_p\mathcal{M}$,

$$
\left| \left| u^\top \text{Hess}f(p) u - \frac{n^2}{4\delta^2n} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} u_q^\top \text{Hess}f(q) u_q \, |t|^{n-1}|s|^{n-1} \, dt \, ds \right| \right|
\leq \frac{n^2}{4\delta^2n} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \left| u^\top \text{Hess}f(p) u - u_q^\top \text{Hess}f(q) u_q \right| \, |t|^{n-1}|s|^{n-1} \, dt \, ds
\leq L_2 \frac{n^2}{4\delta^2n} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \left( |t|^{n}|s|^{n-1} + |t|^{n-1}|s|^n \right) \, dt \, ds
\leq \frac{2L_2n\delta}{n + 1}.
$$

Thus we have

$$
\left\| \text{Hess}f(p) - \text{Hess}f^\delta(p) \right\|
= \sup_{u \in \mathcal{S}_p} \left| u^\top \mathbb{E}_{v, w} \left( \text{Hess}f^\delta_{v, w}(p) - \text{Hess}f(p) \right) u \right|
\leq \frac{2L_2n\delta}{n + 1} + \sup_{u \in \mathcal{S}_p} \mathbb{E}_{v, w} \left[ \frac{n^2}{4\delta^2n} \int_{-\delta}^{\delta} \int_{-\delta}^{\delta} \sum_{j=1}^{\infty} \frac{|t|^{n-1}|s|^{n-1}}{(2j)!} \nabla^2_u (\nabla_v + s \nabla_w)^{2j} f(p) \, dt \, ds \right]
$$

By dropping terms of order $O(\delta^4)$ and noting that $\int_{-\delta}^{\delta} f^{\delta}_t |t|^{n-1}t|s|^{n-1}s \, dt \, ds = 0$, we have

$$
\left\| \mathbb{E}_{v, w} \left[ \tilde{H}f(p; v, w; \delta) \right] - \text{Hess}f(p) \right\|
= O \left( L_2 \delta + \delta^2 \sup_{u \in \mathcal{S}_p} \mathbb{E}_{v, w, t \in \mathcal{S}_p} \left[ \nabla^2_u (\nabla^2_v + \nabla^2_w) f(p) - (\nabla^2_v + \nabla^2_w) \nabla^2_u f(p) \right] \right).
$$
4 The Euclidean Case

In this section, we will focus on numerical stabilization of the estimation, and algorithmic zeroth-order inversion of the estimated Hessian. For numerical and algorithmic purposes, we restrict our attention to the Euclidean case. We also review some existing Hessian estimators in Section 4.3. In the Euclidean case, we also use the notation $\nabla^2 f(x)$ to denote the Hessian of $f$ at $x$.

4.1 Stabilizing the Estimate

In the Euclidean case, the estimator in (1) simplifies to

$$\hat{H}_f(p; v, w; \delta) = \frac{n^2}{8\delta^2} f(p + \delta v + \delta w)vw^\top,$$

where $v, w$ are independently uniformly sampled from $\mathbb{S}^{n-1}$ (the unit sphere in $\mathbb{R}^n$). Its stabilized version is

$$\hat{H}_f(p; v, w; \delta) = \frac{n^2}{8\delta^2} \left[ f(p + \delta v + \delta w) - f(p - \delta v - \delta w) - f(p + \delta v - \delta w) + f(p - \delta v + \delta w) \right] (vw^\top + wv^\top).$$

(9)

To see why (9) stabilizes the estimate, we use Taylor expansion and get

$$f(p + \delta v + \delta w) - f(p - \delta v + \delta w) - f(p + \delta v - \delta w) + f(p - \delta v - \delta w) 
\approx \delta^2 (v + w)^\top \nabla^2 f(x) (v + w) - \frac{\delta^2}{2} (v - w)^\top \nabla^2 f(x) (v - w) 
- \frac{\delta^2}{2} (-v + w)^\top \nabla^2 f(x) (-v + w) 
= 4\delta^2 v^\top \nabla^2 f(x) w,$$

(10)

where $\nabla^2 f$ denotes the Hessian of $f$.

From the above derivation, we see that (9) removes the dependence on the zeroth-order and first-order information, and symmetrizes the estimation. This can significantly reduce variance and stabilize the estimation. A similar phenomenon for the gradient estimators is noted by Duchi et al. (2015).

4.1.1 A Random Projection Derivation

Similar to gradient estimators [Nesterov and Spokoiny, 2017; Li et al., 2020; Wang et al., 2021], one may also derive the Hessian estimator (9) using a random projection argument. Here we extend the spherical random projection derivation (Wang et al., 2021) from gradient estimation to Hessian estimation. To start with, we first prove an identity for random matrix projection in Lemma 3.

Lemma 3. Let $v, w$ be independently uniformly sampled from the unit sphere in $\mathbb{R}^n$. For any matrix $A \in \mathbb{R}^{n \times n}$, we have

$$\mathbb{E} \left[ (v^\top Aw) wv^\top \right] = \frac{1}{n^2} A.$$ 

Proof. It is sufficient to show $\mathbb{E} \left[ v^l A^k v^j w^k w^l \right] = \frac{1}{n^4} A^k_{ij}$ for any $k, l \in [n]$ (Einstein’s notation is used).

Since $v$ is uniformly sampled from $\mathbb{S}^{n-1}$ (the unit sphere in $\mathbb{R}^n$), for $k \neq i$, we have $\mathbb{E} \left[ v^l v^k \mid v^k = x \right] = 0$ for any $x$. This gives that

$$\mathbb{E} \left[ v^l v^k \right] = \int_{x \in [-1, 1]} \mathbb{P} \left( v^k = x \right) \mathbb{E} \left[ v^l v^k \mid v^k = x \right] \, dx = 0, \quad \forall k \neq i.$$
By symmetry of the sphere $S^{n-1}$ and that $E[v^i v_i] = 1$, we have $E[v^i v_k] \overset{(i)}{=} \frac{1}{n}$ for any $k \in [n]$. Combining (i) and (ii) gives

$$E[v^i v_k] \overset{(iii)}{=} \frac{1}{n} \delta^{ki},$$

where $\delta^{ki}$ is the Kronecker’s delta with two superscript.

Similarly, it holds that $E[w_j w_i] \overset{(iv)}{=} \frac{1}{n} \delta_{jl}$, where $\delta_{jl}$ is the Kronecker’s delta with two subscript. Since $v$ and $w$ are independent, (iii) and (iv) gives

$$E[v^i A^j_i w_j w_l] = \frac{1}{n^2} \delta^{kj} \delta_{jl} = \frac{1}{n^2} A^k_k,$$

which concludes the proof.

With Lemma 3, we can see that the estimator in (9) satisfies

$$\mathbb{E}[\hat{H} f(p; v, w; \delta)] \approx \frac{n^2}{8} \mathbb{E}[4 \delta^2 (v^\top \nabla^2 f(x) w) (w w^\top + w v^\top)] = \frac{n^2}{2} \left( \mathbb{E}[(v^\top \nabla^2 f(x) w) w v^\top] + \mathbb{E}[(w^\top \nabla^2 f(x)]^\top w v^\top) \right) \overset{(ii)}{=} \frac{1}{2} \nabla^2 f(x) + \frac{1}{2} [\nabla^2 f(x)]^\top = \nabla^2 f(x),$$

which is (11).

Corollary 1. In $\mathbb{R}^n$, the estimator (9) satisfies

$$\left\| \mathbb{E}[\hat{H} f(p; v, w; \delta)] - \text{Hess} f(p) \right\| \leq \frac{2L_2 n \delta}{n + 1}, \quad \forall p \in \mathbb{R}^n, \delta \in (0, \infty).$$

Proof. This corollary is a direct consequence of Theorem 1.

4.2 Zeroth Order Hessian Inversion

4.2.1 Hessian Adjugate Estimation by Cramer’s Rule

Cramer’s rule states that the inverse of a nonsingular matrix $A$ equals

$$A^{-1} = \frac{1}{\det(A)} \text{adj}(A),$$

where $\text{adj}(A)$ is the adjugate of matrix $A$. Recall the adjugate of matrix $A$ is

$$\text{adj}(A) = \left[ (-1)^{i+j} M_{ji} \right]_{1 \leq i, j \leq n},$$

where $M_{ji} = \det(A_{ji})$ and $A_{ji}$ is the submatrix of $A$ by removing the $j$-th row and $i$-th column. As suggested by the Cramer’s rule, one can estimate inverse of Hessian (up to scaling) by first estimating the unsigned minors of the Hessian and then gather the minors into a matrix. This estimation procedure is summarized in Algorithm 1.

Proposition 2. Let $\text{CHA}(m, \delta, x)$ be the estimator returned by Algorithm 1. If $\nabla^2 \tilde{f}_\delta(x)$ is nonsingular, it holds that

$$\mathbb{E}[\text{CHA}(m, \delta, x)] = \det \left( \nabla^2 \tilde{f}_\delta(x) \right) \nabla^{-2} \tilde{f}_\delta(x),$$

where $\nabla^{-2} \tilde{f}_\delta(x) := \left[ \nabla^2 \tilde{f}_\delta(x) \right]^{-1}$. 

10
A shortcoming of the satisfying
An approach for computing the inverse of Hessian is via Neumann series. For an invertible matrix 4.2.2 Hessian Inverse Estimation by Neumann Series
following zeroth order Hessian inversion method, for a special class of Hessian matrices.

The biggest advantage of the CHA method is its computational expense. For this reason, we introduce the following zeroth order Hessian inversion method, for a special class of Hessian matrices.

4.2.2 Hessian Inverse Estimation by Neumann Series
An approach for computing the inverse of Hessian is via Neumann series. For an invertible matrix $A$ satisfying $\lim_{p \to \infty} (I - A)^p = 0$, the Neumann series expands the inverse of $A$ by

$$A^{-1} = \sum_{p=0}^{\infty} (I - A)^{-1}.$$
Proposition 3. Suppose $f$ is twice-differentiable, $\alpha$-strongly convex and $\beta$-smooth with $\beta < 1$. Then it holds that

$$
\|E[NHI(m_1, m_2, m_3, \delta, x)] - \nabla^{-2}\tilde{f}^\delta(x)\| \leq \frac{(1 - \alpha)^{m_2 + 1}}{\alpha},
$$

where $\nabla^{-2}\tilde{f}^\delta(x) := \left[\nabla^2\tilde{f}^\delta(x)\right]^{-1}$.

Proof. Since $f$ is $\alpha$-strongly convex, it holds that, for any $x, y, v, w \in \mathbb{R}^n$,

$$
f(x + v + w) \geq f(y + v + w) + (x - y)^\top \nabla f(y + v + w) + \frac{\alpha}{2} \|x - y\|^2.
$$

Integrating both $v$ and $w$ over $\delta\mathbb{B}^n$ gives that

$$
\tilde{f}^\delta(x) \geq \tilde{f}^\delta(y) + (x - y)^\top \nabla \tilde{f}^\delta(y) + \frac{\alpha}{2} \|x - y\|^2,
$$

where we use the dominated convergence theorem to interchange the integral and the gradient operator. This shows that $\tilde{f}^\delta$ is also $\alpha$-strongly.

Since a differentiable function $f$ is $\beta$-smooth if and only if $f(x) \leq f(y) + \nabla f(y)^\top (x - y) + \frac{\beta}{2} \|x - y\|^2$ for all $x, y \in \mathbb{R}^n$, one can show that $\tilde{f}^\delta$ is $\beta$-smooth by repeating the above argument.

For $NHI(m_1, m_2, m_3, \delta, x)$, we have

$$
E[NHI(m_1, m_2, m_3, \delta, x)] = I + \prod_{j=1}^{m_2} \left(I - E \left[\tilde{H}f(x; v_{ijk}, w_{ijk}; \delta)\right]\right)
\quad = \sum_{j=0}^{m_2} \left(I - \nabla^2\tilde{f}^\delta(x)\right)^j.
$$

Since $\tilde{f}^\delta$ is $\alpha$-strongly convex, $\beta$-smooth ($\beta < 1$), and apparently twice-differentiable, we have

$$
0 \ll I - \nabla^2\tilde{f}^\delta(x) \ll (1 - \alpha) I.
$$
Thus we can bound the bias by
\[
\left\| E[NHI(m_1, m_2, m_3, \delta, x)] - \nabla^2 \mathcal{H}(x) \right\| \leq \sum_{j=m_2+1}^{\infty} (1 - \alpha)^j \frac{(1 - \alpha)^{m_2+1}}{\alpha}.
\]

4.3 Existing Methods for Hessian Estimation

4.3.1 Hessian Estimation via Collecting Single Entry Estimations

In the Euclidean case, one can fix a canonical coordinate system \(\{e_i\}_{i \in [n]}\), and the \((i, j)\)-th entry of the Hessian matrix of \(f\) at \(x\) can be estimated by
\[
\hat{H}_{ij} f(x; \delta) = \frac{1}{4\delta^2} \left( f(x + \delta e_i + \delta e_j) - f(x + \delta e_i - \delta e_j) 
- f(x - \delta e_i + \delta e_j) + f(x - \delta e_i - \delta e_j) \right).
\]

One can then gather the entries to obtain a Hessian estimator:
\[
\hat{H}_{\text{entry}} f(x; \delta) = \left[ \hat{H}_{ij} f(x; \delta) \right]_{i,j \in [n]}.
\]

The bias bound for (16) is in Proposition 4.

**Proposition 4.** Consider a smooth function \(f : \mathbb{R}^n \rightarrow \mathbb{R}\) satisfying \((A2)\). If the function evaluations are corrupted by independent zero-mean noise, the Hessian estimation defined by (16) satisfies, for any \(x \in \mathbb{R}^n\),
\[
\left\| E[\hat{H}_{\text{entry}} f(p; \delta)] - \text{Hess}(p) \right\| \leq \frac{2^{3/2} L_2 n \delta}{6},
\]
where the expectation is taken with respect to the noise.

**Proof.** For completeness, a proof is provided in Appendix B.

This estimator could perhaps date back to classic times when the finite difference principles were first used. Yet it needs at least \(\Omega(n^2)\) zeroth order samples to produce an estimator in an \(n\)-dimensional space. Previously, Balasubramanian and Ghadimi (2021) designed a Hessian estimator based on the Stein’s identity (Stein, 1981). Their estimator only needs \(O(1)\) zeroth-order function evaluations. This method is discussed in the next section.

4.3.2 Hessian Estimation via the Stein’s identity

A classic result for Hessian computation is the Stein’s identity (named after Charles Stein), as stated below.

**Theorem 2** (Stein’s identity). Consider a smooth function \(f : \mathbb{R}^n \rightarrow \mathbb{R}\). For any point \(x \in \mathbb{R}^n\), it holds that
\[
\nabla^2 f(x) = \frac{1}{2} E \left[ (uu^T - I) \ D_{uu} f(x) \right],
\]
where 1. \(u \sim \mathcal{N}(0, I)\), and 2.
\[
D_{uu} f(x) = \lim_{\tau \to 0} \frac{f(x + \tau u) - 2f(x) + f(x - \tau u)}{\tau^2}.
\]

**Proof.** For completeness, a convenient proof of Theorem 2 is provided in the Appendix.
One can estimate Hessian using the Stein’s identity (Balasubramanian and Ghadimi [2021]):
\[ \hat{H}^{\text{Stein}} f(x; u; \delta) = f(x + \delta u) - 2f(x) + f(x - \delta u) \frac{(uu^\top - I)}{2\delta^2}, \tag{17} \]
where \( u \sim N(0, I) \) is a standard Gaussian vector. A bias bound for (17) is in Theorem 3.

**Theorem 3** (Balasubramanian and Ghadimi [2021]). Let Assumption (A2) hold. The estimator in (17) satisfies
\[ \| E \left[ \hat{H}^{\text{Stein}} f(x; u; \delta) \right] - \nabla^2 f(x) \| \leq \frac{L^2 (n + 6)^2}{4} \delta, \]
for any \( x \in \mathbb{R}^n \) and any smooth function \( f : \mathbb{R}^n \to \mathbb{R} \).

The estimator (17) improves the entry-wise estimator in the sense that one only needs \( O(1) \) samples to produce an estimator. However, its error bound given by Theorem 3 is worse than that of (9) in Theorem 1 and that of (16) in Proposition 4. A more detailed discussion on the error bounds is in Remark 1.

**Remark 1.** We need to note that our estimator (9) and the estimator via Stein’s method (17) have different finite-difference step size. In particular, \( E_{v,w \sim \mathcal{N}(0, I)} [\delta \| v + w \|] = \Theta (\delta) \) for (9) and \( E_{u \sim N(0, I)} [\delta \| u \|] = \Theta (\sqrt{n} \delta) \) for (17). To compare the bias bounds for (9) and (17) using the same (expected) finite-difference step size, we need to downscale the bound in Theorem 3 by a factor of \( \sqrt{n} \). After this downscaling, the error bound for the Stein-type estimator (17) is \( O \left( \frac{L^2 n^2 \delta}{\sqrt{n}} \right) \) whereas the error bound for our estimator (9) is \( O \left( \frac{L^2 \delta}{\sqrt{n}} \right) \). In the experiments, we down scale the finite-difference step size when studying all results of Stein’s method estimator.

## 5 Empirical Studies

We test the performance of our estimator against the previous two estimators in noisy environments. Before proceeding, we re-define some notations for the estimators, so that the estimators are tested on the same ground and noise are properly taken into consideration. The estimators we will empirically study are

1. **Our new estimator:**
   \[
   \hat{H}^{\text{new}} f(p; m; \delta) = \frac{1}{\delta^2} \sum_{k=1}^{\lfloor m/4 \rfloor} n^2 [\epsilon_k + f(\text{Exp}_p(\delta v_k + \delta w_k)) - f(\text{Exp}_p(-\delta v_k + \delta w_k))
   - f(\text{Exp}_p(\delta v_k - \delta w_k)) + f(\text{Exp}_p(-\delta v_k - \delta w_k))](v_k \otimes w_k + w_k \otimes v_k),
   \tag{18} \]
   where \( v_k, w_k \overset{i.i.d.}{\sim} S_p \), and \( \epsilon_k \) is a mean-zero noise that is independent of all other randomness.

2. **The Stein’s estimator:**
   \[
   \hat{H}^{\text{Stein}} f(p; m; \delta) = \frac{1}{\sqrt{n}} \sum_{k=1}^{\lfloor m/4 \rfloor} \left[ f \left( \text{Exp}_p \left( \frac{\delta u_k}{\sqrt{n}} \right) \right) - 2f(p) + f \left( \text{Exp}_p \left( -\frac{\delta u_k}{\sqrt{n}} \right) \right) + \epsilon_k \right] \cdot (u_k \otimes u_k - I),
   \tag{19} \]
   where \( u_k \overset{i.i.d.}{\sim} N(0, I) \) (the standard Gaussian in \( T_p M \)), and \( \epsilon_k \) is a mean-zero noise that is independent of all other randomness.
3. The entry-wise estimator:
\[
\hat{H}_{\text{entry}} f(p; m; \delta) = \left[ \hat{H}_{ij} f(p; m; \delta) \right]_{i,j \in [n]},
\]
where
\[
\hat{H}_{ij} f(p; m; \delta) = \frac{1}{4\delta^2} \sum_{k=1}^{\frac{n}{4}} \left( f(\text{Exp}_p(\delta e_i + \delta e_j)) - f(\text{Exp}_p(\delta e_i - \delta e_j)) \right.
\]
\[ - f(\text{Exp}_p(-\delta e_i + \delta e_j)) + f(\text{Exp}_p(-\delta e_i - \delta e_j)) + \epsilon_k),
\]
\{e_i\}_i is the local normal coordinate for \( T_pM \), and \( \epsilon_k \) is a mean-zero noise that is independent of all other randomness.

![Figure 1: Results for the Manifold (I). Each violin plot summarizes estimation error of 100 estimations. More specifically, each estimation in this figure uses \( m = 3840 \) function evaluations, and 100 estimations are used to generate one violin plot. On the x-axis, “Our method” corresponds to our estimator (18); “Stein’s” corresponds to the Stein’s method (19); “Entry-wise” corresponds to the entry-wise estimator (20). Subfigures (a), (b), (c) corresponds to \( \delta = 0.05 \), \( \delta = 0.1 \), \( \delta = 0.2 \).]

Strictly speaking, the noises \( \epsilon_k \) corrupt all the zeroth-order function value observations. Specifically, the notation \( \epsilon_k + f(\text{Exp}_p(\delta v_k + \delta w_k)) - f(\text{Exp}_p(-\delta v_k + \delta w_k)) - f(\text{Exp}_p(\delta v_k - \delta w_k)) + f(\text{Exp}_p(-\delta v_k - \delta w_k)) \) should be understood in the following way. All four functions values \( f(\text{Exp}_p(\delta v_k + \delta w_k)), f(\text{Exp}_p(-\delta v_k + \delta w_k)), f(\text{Exp}_p(\delta v_k - \delta w_k)), \) and \( f(\text{Exp}_p(-\delta v_k - \delta w_k)) \) are
corrupted with mean-zero and independent noise and not directly observable. Note that all previously discussed bias bounds hold when the function evaluations are corrupted by independent mean-zero noise.

The above notations allow us to put all the estimators on the same ground more easily. With the new notations, all $\hat{H}^{\text{new}}(p;m;\delta)$, $\hat{H}^{\text{Stein}}(p;m;\delta)$ and $\hat{H}^{\text{entry}}(p;m;\delta)$ uses $m$ functions value observations and have an expected finite difference step size $\Theta(\delta)$. The redefining of the estimators is needed since 1. the entry-wise estimator needs more samples to output an estimate, and 2. the default Stein’s method in expectation uses a larger finite-difference step-size, as discussed in Remark 1.

All three methods are tested using the following test function, defined using the standard Cartesian coordinate system in $\mathbb{R}^{n+1}$.

\[ f(x) = \sum_{i=1}^{n+1} \cos(x_i) + \exp(x_1x_2). \]

Every function evaluation is corrupted with an independent noise sampled from $\mathcal{N}(0,0.0025)$. The estimators are tested over three manifolds in $\mathbb{R}^{n+1}$. More details about the three manifolds are in Table 1. In all settings, we set the number of total function evaluation $m = 3840$ and dimension of manifold $n = 8$. The results for manifold (I), the Euclidean case, is in Figure 1. Results for manifold (II) and manifold (III) are in Appendix C. Code for this section can be found at https://github.com/wangtanyu/zeroth-order-Riemann-Hess-code.

| Manifold | $p (p \in \mathbb{R}^{n+1})$ | $h(x)$, $x \in T_p \cong \mathbb{R}^n$ | $\text{Exp}_p(v)$ |
|----------|-----------------------------|----------------------------------|------------------|
| (I)      | $p = 0$                     | $h(x) = 0$                       | $(v, h(v))$      |
| (II)     | $p = 0$                     | $h(x) = 1 - \sqrt{1 - \sum_{i=1}^{n} x_i^2}$ | $(v, h(v))$ |
| (III)    | $p = 0$                     | $h(x) = \sum_{i=1}^{n/2} x_i^2 - \sum_{i=n/2+1}^{n} x_i^2$ | $(v, h(v))$ |

Table 1: Manifolds used for testing. The local metric near $p$ is implicitly specified by the exponential map.

6 Conclusion

In this paper, we study Hessian estimators over Riemannian manifolds. We design a new estimator, such that for smooth real-valued functions over an $n$-dimensional complete Riemannian manifold whose Hessian is $L_2$-Lipschitz, our estimator achieves an $O(L_2\delta + \gamma\delta^2)$ expected error, where $\gamma$ depends both on the Levi-Civita connection and the function $f$, and $\delta$ is the finite difference step size.

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### A Proof of Theorem 2

*Proof of Theorem 2* Consider \( \mathbb{E}[u_k u_h u_i u_j \partial_i \partial_j] \) for any \( k, h, i, j \in [n] \).

When \( (k, h) = (i, j) \), one has \( \mathbb{E}[u_k u_h u_i u_j \partial_i \partial_j] = \mathbb{E}[u_i^2 u_j^2 \partial_i \partial_j] \). In this case, it holds that

\[
\mathbb{E}[u_i^2 u_j^2 \partial_i \partial_j] = \partial_i \partial_h \quad \text{for } i \neq j \quad \text{and} \quad \mathbb{E}[u_i^4 \partial_i \partial_i] = 3 \partial_i \partial_h, \quad \text{for } i = j.
\]

When \( (k, h) \neq (i, j) \), \( i = j \) and \( k = h \), we have \( \mathbb{E}[u_i^2 u_j^2 \partial_i \partial_j] = \partial_i \partial_i \).
When \((k,h) \neq (i,j), \ i = j\) and \(k \neq h,\) we have \(E[u_k u_h u_i u_j] = 0.\)
When \((k,h) \neq (i,j), \ i \neq j\) and \(k = h,\) we have \(E[u_k u_h u_i u_j] = 0.\)
When \((k,h) \neq (i,j), \ i \neq j, \ k \neq h, \ k = j\) and \(h = i,\) we have \(E[u_k u_h u_i u_j] = E[u_i^2 u_h^2 \partial_k \partial_h] = \partial_k \partial_h.\)
When \((k,h) \neq (i,j), \ i \neq j, \ k \neq h, \ k = i\) and \(h = j,\) we have \(E[u_k u_h u_i u_j] = E[u_i^2 u_h^2 \partial_k \partial_h] = \partial_k \partial_h.\)
When \((k,h) \neq (i,j), \ i \neq j, \ k \neq h\) and \(k \neq j,\) we have \(E[u_k u_h u_i u_j] = 0.\)
When \((k,h) \neq (i,j), \ i \neq j, \ k \neq h\) and \(h \neq i,\) we have \(E[u_k u_h u_i u_j] = 0.\)

Now using Einstein’s notation and combining all above cases give
\[
E[u_k u_h u_i u_j \partial^i] = \partial^k \partial_h (1 - \delta_h^i) + \partial^k \partial_k (1 - \delta_h^i) + \delta_h^i \partial_i \partial^i + 2 \delta_h^i \partial_i \partial^j = \partial^k \partial_h + \delta_h^i \partial_i \partial^i,
\]
where \(\delta_h^i\) is the Kronecker’s delta.

Since \(D_{uu} f(p) = u^i u_j \partial_i \partial^j f(x)\) for all \(u\) and \(x,\) we can write \(uu^T D_{uu} f(x) = u^k u_h u_i u_j \partial_i \partial^j f(x).\)
Thus rearranging terms in \((i)\) gives
\[
E[uu^T D_{uu} f(x)] \overset{(i)}{=} 2 \nabla^2 f(x) + (\Delta f(x)) I,
\]
where \(\Delta = \partial_i \partial^i\) is the Laplace operator.

Since \(E[D_{uu} f(x)] = E[u^k u_h u_i u_j \partial_i \partial^j f(x)] = \delta_i^i \partial_i \partial^j f(x) = (\Delta f(x)) I,\) rearranging terms in \((ii)\) concludes the proof.

\[\square\]

### B Proof of Proposition 4

For completeness, we provide proof of Proposition 4. To start with, we review the definition of symmetric tensors and norms of symmetric tensors.

**Definition 1.** Let \(V = \mathbb{R}^n\) be a Euclidean vector space. An order \(k\) tensor \(T \in V^\otimes k\) is symmetric if \(T[v_1, v_2, \cdots, v_k] = T[v_{\sigma(1)}, v_{\sigma(2)}, \cdots, v_{\sigma(n)}]\) for any \(v_1, v_2, \cdots, v_k \in V,\) and any permutation of indices \(\sigma.\) For a real symmetric tensor \(T,\) the (operator) norm of \(T\) is

\[
||T|| = \sup_{v \in \mathbb{R}^n : ||v|| = 1} |T[v, v, \cdots, v]|.
\]

For simplicity, we write \(T[v] = T[v, v, \cdots, v]\) when the of the inputs to tensor \(T\) are identical.

If a three-times continuously differentiable function satisfies Assumption (A2), its third order derivative is bounded, as stated in the following proposition.

**Proposition 5.** Consider a function \(f : \mathbb{R}^n \to \mathbb{R}\) satisfying Assumption (A2). It holds that \(\|\nabla^3 f(x)\| \leq L_2\) for any \(x \in \mathbb{R}^n.\)

**Proof.** For any \(\tau > 0\) and \(x, v \in \mathbb{R}^n\) with \(\|v\| = 1,\) define \(x_{\tau,v} = x + \tau v.\) When \(\tau\) is small, Taylor’s theorem gives
\[
\left| \frac{v^T \left[ \nabla^2 f(x_{\tau,v}) \right] v - v^T \left[ \nabla^2 f(x) \right] v}{\tau} \right| \overset{(i)}{=} \left| \nabla^3 f(x_{\tau,v}) [v, v, v] \right|,
\]
where \(z_{\tau,v}\) depends on \(\tau\) and \(v\) and \(\lim_{\tau \to 0} z_{\tau,v} = x\) for any \(v,\)

Under Assumption (A2), for any \(v \in \mathbb{S}^{n-1}\) (the unit sphere in \(\mathbb{R}^n),\) it holds that
\[
\left| \frac{v^T \left[ \nabla^2 f(x_{\tau,v}) \right] v - v^T \left[ \nabla^2 f(x) \right] v}{\tau} \right| \overset{(ii)}{\leq} \|v\|^2 \left\| \nabla^2 f(x_{\tau,v}) - \nabla^2 f(x) \right\| / \tau \leq L_2.
\]

Combining \((i)\) and \((ii)\) gives
\[
|\nabla^3 f(z_{\tau,v}) [v, v, v]| \leq L_2.
\]
for any \( v \in S^{n-1} \) and any sufficiently small \( \tau \). Thus for any \( x \in \mathbb{R}^n \), we have
\[
L_2 \geq \sup_{v \in S^{n-1}} \lim_{\tau \to 0} |\nabla^3 f(z, v) [v, v, v]| = \|\nabla^3 f(x)\| .
\]

Proof. of Proposition 4. Recall \( e_i \) is the vector with 1 on its \( i \)-th entry and zeros on all other entries. By Taylor’s theorem, we have
\[
\text{Proof. of Proposition 4. Recall } e_i \text{ is the vector with 1 on its } i \text{-th entry and zeros on all other entries. By Taylor’s theorem, we have}
\]
\[
f(x + \delta e_i + \delta e_j) = f(x) + \delta(e_i + e_j)^\top \nabla f(x) + \frac{\delta^2}{2} (e_i + e_j)^\top \nabla^2 f(x)(e_i + e_j) + \frac{\delta^3}{6} \nabla^3 f(z_1)[e_i + e_j],
\]
for some \( z_1 \). Repeating the computing for \( f(x - \delta e_i + \delta e_j) \), \( f(x + \delta e_i - \delta e_j) \), and \( f(x - \delta e_i - \delta e_j) \), we get
\[
f(x + \delta e_i + \delta e_j) - f(x - \delta e_i + \delta e_j) - f(x + \delta e_i - \delta e_j) + f(x - \delta e_i - \delta e_j)
\]
\[
= \frac{\delta^2}{2} \left( [\nabla^2 f(x)]_{ii} + [\nabla^2 f(x)]_{jj} + 2 [\nabla^2 f(x)]_{ij} - [\nabla^2 f(x)]_{ii} - [\nabla^2 f(x)]_{jj} + 2 [\nabla^2 f(x)]_{ij} \right)
\]
\[
+ \frac{\delta^3}{6} \left( \nabla^3 f(z_1)[e_i + e_j] + \nabla^3 f(z_2)[e_i - e_j] + \nabla^3 f(z_3)[e_i - e_j] + \nabla^3 f(z_4)[-e_i + e_j] + \nabla^3 f(z_4)[-e_i - e_j] \right),
\]
for some \( z_1, z_2, z_3, z_4 \in \mathbb{R}^n \). Rearranging terms gives
\[
\left| \hat{H}^\text{entry}_i f^\delta(x) - [\nabla^2 f(x)]_{ij} \right| 
\leq \frac{\delta}{24} \left| \nabla^3 f(z_1)[e_i + e_j] + \nabla^3 f(z_2)[e_i - e_j] + \nabla^3 f(z_3)[-e_i + e_j] + \nabla^3 f(z_4)[-e_i - e_j] \right|,
\]
where \( z_1, z_2, z_3, z_4 \in \mathbb{R}^n \).

By Proposition 5, we have
\[
\|\nabla^3 f(x)\| \leq L_2, \quad \forall x \in \mathbb{R}^n.
\]

Thus (1) gives
\[
\left| \hat{H}^\text{entry}_i f^\delta(x) - [\nabla^2 f(x)]_{ij} \right| \leq \frac{2^{3/2} L^2 \delta}{6}.
\]

We can gather the entries into a matrix and get
\[
\left\| \mathbb{E} \left[ \hat{H}^\text{entry}_i f^\delta(x) \right]_{i,j \in [n]} - \nabla^2 f(x) \right\| \leq n \left\| \mathbb{E} \left[ \hat{H}^\text{entry}_i f^\delta(x) \right]_{i,j \in [n]} - \nabla^2 f(x) \right\|_{\max}
\]
\[
\leq \frac{2^{3/2} L^2 n \delta}{6}.
\]

\[ \square \]

C Additional Experimental Results

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Figure 2: Results for the Manifold (II). Each violin plot summarizes estimation error of 100 estimations. Specifically, each estimation in this figure uses $m = 3840$ function evaluations, and 100 estimations are used to generate one violin plot. On the $x$-axis, “Our method” corresponds to our estimator (18); “Stein’s” corresponds to the Stein’s method (19); “Entry-wise” corresponds to the entry-wise estimator (20). Subfigures (a), (b), (c) corresponds to $\delta = 0.05, \delta = 0.1, \delta = 0.2$.

Figure 3: Results for the Manifold (III). Each violin plot summarizes estimation error of 100 estimations, with the estimators defined in. Specifically, each estimation in this figure uses $m = 3840$ function evaluations, and 100 estimations are used to generate one violin plot. On the $x$-axis, “Our method” corresponds to our estimator (18); “Stein’s” corresponds to the Stein’s method (19); “Entry-wise” corresponds to the entry-wise estimator (20). Subfigures (a), (b), (c) corresponds to $\delta = 0.05, \delta = 0.1, \delta = 0.2$. 