Zeroth-order Optimization on Riemannian Manifolds

Jiaxiang Li∗ Krishnakumar Balasubramanian† Shiqian Ma‡

March 26, 2020

Abstract

We propose and analyze zeroth-order algorithms for optimization over Riemannian manifolds, where we observe only potentially noisy evaluations of the objective function. Our approach is based on estimating the Riemannian gradient from the objective function evaluations. We consider three settings for the objective function: (i) deterministic and smooth, (ii) stochastic and smooth, and (iii) composition of smooth and non-smooth parts. For each of the setting, we characterize the oracle complexity of our algorithm to obtain appropriately defined notions of ϵ-stationary points. Notably, our complexities are independent of the ambient dimension of the Euclidean space in which the manifold is embedded in, and only depend on the intrinsic dimension of the manifold. As a proof of concept, we demonstrate the applicability of our method to the problem of black-box attacks to deep neural networks, by providing simulation and real-world image data based experimental results.

∗Department of Mathematics, University of California, Davis. Email: jxjli@ucdavis.edu
†Department of Statistics, University of California, Davis. Email: kbala@ucdavis.edu
‡Department of Mathematics, University of California, Davis. Email: sqma@ucdavis.edu. Research of this author was supported in part by NSF grant DMS-1953210
1 Introduction

In this paper, we design zeroth-order algorithms for solving the Riemannian optimization problem:

$$\min_{x \in \mathcal{M}} f(x) + h(x),$$

where $\mathcal{M}$ is a Riemannian submanifold embedded in $\mathbb{R}^n$, $f : \mathcal{M} \to \mathbb{R}$ is a smooth function but may not be convex, and $h$ is a convex and nonsmooth function. Here the convexity and smoothness are to be interpreted when the function in consideration is in the ambient Euclidean space. In the zeroth-order setting, we do not have access to the analytical forms of the function $f(x)$ or $h(x)$. Instead, we are only able to obtain potentially noisy evaluations of the functions. Such problems arise in several statistical machine learning problems such as selecting the optimal parameter for machine learning problems [SLA12], and the field of reinforcement learning [SHC+17, CRS+18, MGR18].

Our main motivation for designing zeroth-order Riemannian optimization problems arise from the design of black-box attacks to Deep Neural Networks (DNNs). DNNs have become a central technique in statistical machine learning, due to their successful performance in challenging problems arising from computer vision and image classification. However, recent studies show that DNNs are extremely vulnerable to adversarial examples: Even a well-trained DNN could completely misclassify a slightly perturbed version of the original image (which is undetectable by the human eye); see for example [SZS+13, GSS14]. As a result, many approaches have been developed to train DNNs that are robust to adversarial attacks. In [MMS+17], the authors studied the adversarial robustness of neural networks through the lens of robust optimization, which provides a unified view on attacks and defenses. In particular, the authors of [MMS+17] formulated this problem as a minimax problem: $\min_{\theta} \mathbb{E}_{(x,y) \sim \mathcal{D}} \left[ \max_{\delta \in S} \mathcal{L}(\theta, x + \delta, y) \right]$, where using the classification task as an example, $(x, y)$ denotes the pair of data drawn from distribution $\mathcal{D}$ and corresponding labels, $\theta$ is the set of model parameters, $\mathcal{L}$ is a suitable loss function, and $S$ denotes the perturbation set. Different choices of the perturbation set $S$ have been suggested in the literature. It is shown that the fast gradient sign method (FGSM) [GSS14] gives the optimal max-norm constrained perturbation: $\delta = \epsilon \text{sgn}(\nabla_x \mathcal{L}(\theta, x, y))$, where the gradient can be efficiently calculated via back-propagation. Therefore $\delta$ serves as the optimal one step perturbation to sufficiently increase the loss function and cause misclassification. A more powerful adversary is the projected gradient descent (PGD) on the negative loss function $x^{t+1} = \text{Proj}_{x+S}(x^t + \alpha \text{sgn}(\nabla_x \mathcal{L}(\theta, x, y)))$. In [GSS14, MMS+17], the perturbation set $S$ is chosen to be a box centered at the original image $x$. This is one of the typical “white-box” attack techniques [GSS14, MDFF16, PMJ+16, CW17], which assume that the DNN structure is known for attackers.

However, oftentimes in practice, the structure of the DNN is not known to the attacker. We consider such “black-box” attack problems [CZS+17, TTC+19, CLC+18]. In this setting, since the gradient information is unknown to attacker, back propagation cannot be conducted. Moreover, we consider the case where the attacker can only acquire the classification label, confidence score or loss function value. That is, only potentially noisy function value information is available. This naturally leads to the designation of zeroth-order algorithms for adversarial attacks [CZS+17]. Different from the previous zeroth-order algorithms for adversarial attacks [CZS+17], we consider the perturbation set to be a manifold, instead of a box. This is because in practice, it is believed that natural images from the class tend to lie on the same manifold [WS04]. For simplicity, we consider the manifold to be a sphere. That is, we assume that the perturbation set $S$ is given by $S(R) = \{ \delta : \|\delta\|_2 = R \}$, where $R$ is the radius of the sphere. This is consistent with the optimal $\ell_2$-norm attack studied in the literature [LHL15]. Furthermore, the sphere constraint guarantees that the perturbed image is always in a certain distance from the original image. We believe that this could guarantee the convergence toward a perturbed image with a different label more successfully, see Figure 1.
The attack image

Figure 1: Illustration of the neural network attack. $S$ is the constraint set in which we look for an image that is of different label with the original image, labeled as the attack image in the graph. For the specific image showing in the figure, $S$ is a sphere, and the portion of the ball that lies in the image class $y_0$ (in terms of volume) is larger than the portion that the sphere lies in $y_0$ (in terms of spherical area).

1.1 Related work

Riemannian Optimization. Riemannian optimization has drawn a lot of attention recently due to its wide applications in many different fields, including low rank matrix completion [BA11, Van13], phase retrieval [BEB17, SQW18], dictionary learning [CS16, SQW16], and dimensionality reduction [HS11, TFBJ18, MKJS19]. In the first-order setting, Riemannian versions of gradient descent method require $O(\epsilon^{-2})$ iterations to converge to the $\epsilon$-stationary point defined by $\|\nabla f(x)\| \leq \epsilon$; see for example [BAC18]. In the stochastic setting, existing literature study both online [Bon13, ZYYF19, WS19] and finite-sum [ZRS16, KSM18, ZYYF19, WS19] optimization. For the stochastic setting, under a stronger mean-squared assumption on the stochastic gradients, using the SPIDER variance reduction technique, [ZYYF19] established that $O(\epsilon^{-3})$ oracle calls are required to obtain a $\epsilon$-stationary point in expectation. Other variance reduction techniques have also been applied to the finite-sum case, where the Riemannian SVRG [ZRS16] technique achieves $\epsilon$-stationary solution with $O(k^{2/3}\epsilon^{-2})$ oracle calls where $k$ is number of sums. In the non-smooth setting, sub-gradient methods [BSBA14, LCD19] require $O(\epsilon^{-4})$ iterations, while the operator splitting methods such as MADMM [KGB16] lack convergence guarantee. The recently proposed manifold proximal type algorithm [CMSZ18] requires $O(\epsilon^{-2})$ number of iterations to converge to $\epsilon$-stationary solution. None of the above works consider the zeroth-order setting.

Zeroth-Order Optimization. Zeroth-order optimization in the Euclidean setting has been studied for decades in the optimization literature; we refer to [CSV09a, AH17, LMW19] for a detailed discussion. Theoretical analysis of zeroth-order methods in the nonconvex and constrained setting is still in its nascent stages except for a few works [CSV09b, BG19, SZK19, LMW19]. The authors of [CSA15, FT19] studied heuristic approaches for zeroth-order Riemannian optimization and do not provide any complexity analysis.

1.2 Main Contributions

Our main contributions for solving nonconvex optimization problems of the form in (1) are summarized below.
1. We first propose a technique for estimating the Riemannian gradient of a function \( f(x) \) based on potentially noisy function queries. This extends the classical Gaussian smoothing based gradient estimator from [NS17] to the Riemannian setting.

2. When \( h(x) \equiv 0 \) and the function evaluations of \( f(x) \) could be obtained exactly, we propose a zeroth-order Riemannian gradient descent method (ZO-RGD) and analyze its oracle complexity.

3. When \( h(x) \equiv 0 \) and when \( f(x) = \mathbb{E}_\xi [F(x, \xi)] \), due to which only noisy evaluates of \( f(x) \) could be obtained, we propose a zeroth-order Riemannian stochastic gradient descent method (ZO-RSGD) and analyze its oracle complexity.

4. When \( h(x) \) is convex but nonsmooth, we propose a zeroth-order Riemannian proximal gradient method (ZO-ManPG) and analyze its oracle complexity.

The obtained complexity results are summarized in Table 1. We emphasize that our complexities are independent of the ambient dimension \( n \) of the Euclidean space in which the manifold \( \mathcal{M} \) is embedded in, and only depend on the intrinsic dimension \( d \) of the manifold. To the best of our knowledge, these are the first such complexity results for zeroth-order Riemannian optimization.

| Algorithm   | Structure      | \text{iter} \ O(\frac{d}{\epsilon^2}) | Complexity \ O(\frac{d}{\epsilon^2}) |
|-------------|----------------|-------------------------------------|--------------------------------------|
| ZO-RGD      | Smooth         | \text{iter} \ O(\frac{d}{\epsilon^2}) | Complexity \ O(\frac{d}{\epsilon^2}) |
| ZO-RSGD     | Smooth, stochastic | \text{iter} \ O(\frac{d}{\epsilon^2}) | Complexity \ O(\frac{d}{\epsilon^2}) |
| ZO-ManPG    | Nonsmooth      | \text{iter} \ O(\frac{d}{\epsilon^2}) | Complexity \ O(\frac{d}{\epsilon^2}) |

Table 1: Summary of the convergence of our proposed methods to obtain an \( \epsilon \)-stationary solution. Here, \( d = \text{dim}(\mathcal{M}) \) is the intrinsic dimensionality of the manifold \( \mathcal{M} \). Furthermore, ITER refers to the number of iterations and COMPLEXITY refers to the number of calls to the (stochastic) zeroth-order oracle.

The rest of the paper is organized as follows: In Section 2, we review the basics of the Riemannian optimization and introduce our random gradient estimator. In Section 3, we discuss our algorithms and complexity results. In Section A, we provide more information on the Riemannian manifold and Riemannian optimization. In Section B, we give the proofs of results that characterize the quality of the proposed zeroth-order random gradient estimator and in Section C, we give proofs of the main convergence results of our zeroth-order Riemannian optimization algorithms. Finally, in Section D, we provide details of our numerical experiments for both the synthetic data and the neural network attacks.

### 2 Preliminaries

In this section, we first provide a brief review on the manifold optimization, then discuss the assumptions and zeroth-order oracle that we are going to use for our algorithms.

#### 2.1 Basics of Manifold Optimization

Let \( \mathcal{M} \subset \mathbb{R}^n \) be a differentiable manifold with dimension \( d \). For any point \( x \in \mathcal{M} \), the tangent space denoted as \( T_x \mathcal{M} \), contains all tangent vectors to \( \mathcal{M} \) at \( x \). Formally, we have:
Definition 2.1 (Tangent space). Consider a manifold \( M \) embedded in a Euclidean space. For any \( x \in M \), the tangent space \( T_x M \) at \( x \) is a linear subspace that consists of the derivatives of all smooth curves on \( M \) passing \( x \):

\[
T_x M = \{ \gamma'(0) : \gamma(0) = x, \gamma([-\delta, \delta]) \subset M \text{ for some } \delta > 0, \gamma \text{ is smooth} \}.
\] (2)

The manifold \( M \) is a Riemannian manifold if it is equipped with a metric (inner product) on the tangent space, \( \langle \cdot, \cdot \rangle_x : T_x M \times T_x M \to \mathbb{R} \), that varies smoothly on \( M \). We also introduce the concept of the dimension of a manifold.

Definition 2.2 (Dimension of a Manifold [AMS09]). The dimension of the manifold \( M \), denoted as \( \dim(M) \), is the dimension of the Euclidean space that the manifold is locally homeomorphic to. In particular, the dimension of the tangent space is always same as the dimension of the manifold.

For example, consider the Stiefel manifold \( \text{St}(n, p) \) defined by:

\[
\mathcal{M} = \text{St}(n, p) = \{ X \in \mathbb{R}^{n \times p} : X^T X = I_p \}. \] (3)

The tangent space of \( \text{St}(n, p) \) is given by \( T_x \mathcal{M} = \{ Y \in \mathbb{R}^{n \times p} : X^T Y + Y^T X = 0 \} \). Hence, the dimension of the Stiefel manifold is \( \dim(\text{St}(n, p)) = np - \frac{1}{2}p(p + 1) \). Note that the dimension of the manifold could be significantly less than the ambient dimension, \( np \), of the Euclidean space in which the Stiefel manifold is embedded in.

We now introduce the concept of a Riemannian gradient of a function \( f \).

Definition 2.3 (Riemannian gradient). Suppose \( f \) is a smooth function on \( M \). The Riemannian gradient \( \nabla f(x) \) is a vector in \( T_x M \) satisfying \( v[f] = \langle v, \nabla f(x) \rangle_x \) for any \( v \in T_x M \), and \( v[f] := \frac{d(f(\gamma(t)))}{dt} \bigg|_{t=0}, \gamma(t) \) is a function as defined in (2).

Recall the commonly used assumption of \( L \)-smooth function in Euclidean setting:

Assumption 2.4 (L-smoothness). A function \( f : \mathbb{R}^n \to \mathbb{R} \) is \( L \)-smooth, if is satisfies for all \( x, y \in \mathbb{R}^n \), \( |f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \leq \frac{L}{2} \| x - y \|^2 \).

For a given \( x \in M \), a retraction is defined as follows.

Definition 2.5 (Retraction). A retraction mapping \( R_x \) is a smooth mapping from \( T_x M \) to \( M \) such that: \( R_x(0_x) = x \), where \( 0_x \) is the zero vector in \( T_x M \), and the differential of \( R_x \) at \( 0_x \) is an identity mapping, i.e. \( \frac{dR_x(0)}{dt} \bigg|_{t=0} = \eta, \forall \eta \in T_x M \). Particularly, the exponential mapping \( \exp_x \) is a retraction which generates geodesics [AMS09]. We refer to the supplementary material for interest readers.

Now we present the Riemannian counterpart of Assumption 2.4:

Assumption 2.6 (L-retraction-smoothness). There exists \( L_g \geq 0 \) such that for all \( \eta \in T_x M \), we have

\[
|f(R_x(\eta)) - f(x) - \langle \nabla f(x), \eta \rangle_x| \leq \frac{L_g}{2} \| \eta \|^2 \] (4)

For a embedded sub-manifold of a Euclidean space, we can always use the Euclidean inner product on the tangent spaces, i.e. \( \langle \cdot, \cdot \rangle_x = \langle \cdot, \cdot \rangle, \forall x \in M \), and we always assume so for the rest of
the paper. Under this choice of Riemannian metric, we have that the Riemannian gradient of the function is simply the projection of its full gradient onto the tangent space, namely

$$\text{grad} f(x) = \text{Proj}_{T_xM} (\nabla f(x)).$$

(5)

Assumption 2.6 is also known as the restricted Lipschitz-type gradient for pullbacks. Notice that in [BAC18], they have a weaker condition in that (4) could be satisfied for only $\|\eta\|_x \leq \rho_x$, for some positive parameter $\rho_x > 0$. In our convergence analysis, we need this assumption to be held for all $\eta \in T_xM$, i.e., $\rho_x = \infty$. This assumption is satisfied when the manifold $M$ is a compact submanifold of $\mathbb{R}^n$, the retraction $R_x$ is globally defined\footnote{If the manifold is compact, then the exponential mapping $\text{Exp}_x$ is already globally defined. This is known as the HopfRinow theorem [Car92].} and function $f$ satisfies Assumption 2.4; we refer the reader to [BAC18] for more details. In the applications we are interested in, for example, optimization on Stiefel manifolds, Assumption 2.6 is satisfied naturally. We also emphasize that Assumption 2.6 is significantly weaker than the geodesic smoothness assumption defined in [ZS16]. The geodesic smoothness states that,

$$f(\text{Exp}_x(\eta)) \leq f(x) + \langle g_x, \eta \rangle_x + L_g d^2(x, \text{Exp}_x(\eta)),$$

(6)

where $g_x$ is a sub-gradient of $f$, $d(\cdot, \cdot)$ represents the geodesic distance (the shortest distance of two points on manifold). Such a condition is stronger than our Assumption 2.6 in a sense that, if the retraction is fixed to the exponential mapping\footnote{Due to lack of space, a detailed definition is given in Section A}, then geodesic smoothness implies the $L$-retraction-smoothness with the same parameter $L_g$ [BFM17].

2.2 The Zeroth-order Riemannian Gradient Estimator

In the Euclidean setting, [NS17] proposed a Gaussian smoothing technique to estimate the gradient. Our estimator for the Riemannian gradient in (5), is motivated by this approach. However, in order to use this approach, several modifications are required to make it suitable to be used in the Riemannian setting. Formally, we first define our zeroth-order Riemannian gradient estimator as below.

**Definition 2.7 (Zeroth-Order Riemannian Gradient).** Generate $u \in T_xM$, which is a standard normal distribution on the tangent space $T_xM$. Then, the zeroth-order Riemannian gradient estimator of a function $f$ at the point $x$ is given by

$$g_{\mu}(x) = \frac{f(R_x(\mu u)) - f(x)}{\mu} u.$$

(7)

Note that it’s not easy to generate a standard normal vector on the tangent space. However, if we simply sample a standard norm vector $u_0 \sim \mathcal{N}(0, I_n)$ in $\mathbb{R}^n$, and $P \in \mathbb{R}^{n \times n}$ the orthogonal projection matrix onto $T_xM$, then $Pu_0$ is naturally a standard normal distribution on the tangent plane $\mathcal{N}(0, PP^T)$, in a sense that, all the eigenvalues of the covariance matrix $PP^T$ is either 0 (eigenvectors orthogonal to the tangent plane) or 1 (eigenvectors embedded in the tangent plane). Therefore the zeroth-order Riemannian gradient estimator is alternatively given by

$$g_{\mu}(x) = \frac{f(R_x(\mu Pu_0)) - f(x)}{\mu} Pu_0.$$

(8)
The projection $P$ is easy to conduct for commonly used manifolds. For example, for the Stiefel manifold, the projection is given by $\text{Proj}_{T_X M}(Y) = (I - XX^T)Y + X \text{ skew}(X^TY)$, where $\text{skew}(A) := (A - A^T)/2$ [AMS09]. We now provide some difference between the zeroth-order gradient estimators in the Euclidean setting (proposed by [NS17]) and the Riemannian setting. In the Euclidean case, the zeroth-order gradient estimator can be viewed as estimating the gradient of the Gaussian smoothed function,

$$f_\mu(x) = \frac{1}{\kappa} \int \mathbb{R}^n f(x + \mu u) e^{-\frac{1}{2} \|u\|^2} du,$$

since we have, $\nabla f_\mu(x) = \mathbb{E}_u(g_\mu(x)) = \frac{1}{\kappa} \int \mathbb{R}^n f(x + \mu u) - f(x) \mu e^{-\frac{1}{2} \|u\|^2} du.$

This was also observed to be an instantiation of Gaussian Stein’s identity in [BG19]. However, this observation is no longer true in Riemannian setting, as we incorporate the retraction operator when evaluating $g_\mu$, and this forces us to seek for a direct evaluation of $\mathbb{E}_u(g_\mu(x))$, instead of utilizing several nice properties of the smoothed function $f_\mu$, as in the Euclidean setting.\footnote{For example, in the Euclidean setting, if $f$ is $L$-smooth, then $f_\mu$ is also $L$-smooth; see [NS17].}

We also remark that, $g_\mu(x)$ is a biased estimator of $\nabla f(x)$. Hence, the difference between them could be decomposed as $\mathbb{E}\|g_\mu(x) - \nabla f(x)\|^2 \leq 2\mathbb{E}\|g_\mu(x) - \mathbb{E}g_\mu(x)\|^2 + 2\|\mathbb{E}g_\mu(x) - \nabla f(x)\|^2$, where $\mathbb{E}\|g_\mu(x) - \mathbb{E}g_\mu(x)\|^2$ could be bounded by $\|\nabla f(x)\|^2$, and $\|\mathbb{E}g_\mu(x) - \nabla f(x)\|^2$ could be bounded by terms related to our smoothing parameter $\mu$. We thus have the following key estimates, which we leverage in our convergence analysis:

$$\mathbb{E}_{u_0}(\|g_\mu(x)\|^2) \leq \frac{\mu^2 L_g^2(d + 6)^3}{2} + 2(d + 4)\|\nabla f(x)\|^2,$$

where $d = \text{dim}(M)$ is the intrinsic dimension of the manifold $M$ under consideration. The above estimates are proved formally in Lemma [B3.3] [B3.5] and [B5] respectively.

## 3 Zeroth-order Riemannian Optimization

We now propose and analyze three zeroth-order Riemannian optimization algorithms for problems of the form in (1) by leveraging the gradient estimator in (8).

### 3.1 Zeroth-Order Riemannian Gradient Method

In this section, we focus on the smooth optimization problem with $h \equiv 0$, when $f$ satisfies two assumptions [2.4] and [2.6]. We propose ZO-RGD, the zeroth-order Riemannian gradient descent method and provide its complexity analysis. The algorithms is formally presented in Algorithm [1].

Following [BACIS18], the termination criterion is $\mathbb{E}\|\nabla f(x_k)\|^2 \leq \epsilon^2$, where the expectation is taken with respect to all of the random Gaussian vectors we draw for the first $k$ iterations. The complexity analysis is provided in Theorem [3.1].
Algorithm 1  Zeroth-Order Riemannian Gradient Descent (ZO-RGD)

1: **Input:** Initial point $x_0 \in \mathcal{M}$, smoothing parameter $\mu$, step size $\eta_k$, fixed number of iteration $N$.
2: for $k = 0$ to $N - 1$ do
3: Sample a standard Gaussian random vector $u_k$ in $T_{x_k} \mathcal{M}$ via projection.
4: Set the random oracle $g_{\mu}(x_k)$ by (7).
5: Update $x_{k+1} = R_{x_k}(-\eta_k g_{\mu}(x_k))$.
6: end for

**Theorem 3.1.** Suppose $x_k$ is the sequence generated by Algorithm 1 with the stepsize $\eta_k = \hat{\eta} = \frac{1}{2(d+4)\mu}$. Then, we have

$$
\frac{1}{N + 1} \sum_{k=0}^{N} \mathbb{E}_{\mathcal{U}_k} \|\text{grad} f(x_k)\|^2 \leq \frac{2}{\hat{\eta}} \left( \frac{f(x_0) - f(x^*)}{N + 1} + C(\mu) \right),
$$

where $\mathcal{U}_k$ denotes the set of all Gaussian random vector (or matrices) we drew for the first $k$ iterations, and $C(\mu) = \frac{\mu^2 L_0}{8 \frac{(d+3)^3}{(d+4)}^3} + \frac{\mu^2}{8 \frac{(d+6)^3}{(d+4)}^3} + \frac{\mu^2 L_0}{16 \frac{(d+6)^3}{(d+4)^2}}$. In order to have

$$
\frac{1}{N + 1} \sum_{k=0}^{N} \mathbb{E}_{\mathcal{U}_k} \|\text{grad} f(x_k)\|^2 \leq \epsilon^2,
$$

we need the smoothing parameter $\mu$ and number of iteration $N$ (which is also the number of calls to the zeroth-order oracle) to be set as

$$
\mu = \mathcal{O} \left( \frac{\epsilon}{d^{3/2}} \right), \ N = \mathcal{O} \left( \frac{d}{\epsilon^2} \right).
$$

**Remark 1.** The number of calls to the zeroth-order oracle is $O(d/\epsilon^2)$ and only depends on the intrinsic dimensionality of the manifold and is independent of the ambient dimensionality, $n$, of the Euclidean space in which the function $f$ is embedded in. Often times, the intrinsic dimensionality is much less than the ambient dimensionality and hence, we obtain a significant reduction in the number of calls to the zeroth-order oracle.

**Remark 2.** Note that in Algorithm 1 we only sample one Gaussian vector in each iteration of the algorithm. In practice, one could also sample multiple Gaussian random vector for each iteration and obtain an averaged gradient estimator. Suppose we sample $m$ i.i.d. Gaussian random vectors for each iteration and use the average $\tilde{g}_{\mu}(x) = \frac{1}{m} \sum_{i=1}^{m} g_{\mu,i}(x)$, then the bound for our zeroth-order oracle becomes

$$
\mathbb{E}((\tilde{g}_{\mu}(x) - \text{grad} f(x))^2) \leq \mu^2 L_0^2 (d + 6)^3 + \frac{2(d + 4)}{m} \|\text{grad} f(x)\|^2.
$$

Hence, the final result in Theorem 3.1 can be improved to

$$
\frac{1}{N + 1} \sum_{k=0}^{N} \mathbb{E}_{\mathcal{U}_k} \|\text{grad} f(x_k)\|^2 \leq 2L g \left( \frac{f(x_0) - f(x^*)}{N + 1} + C(\mu) \right).
$$

with $\hat{\eta} = \frac{1}{\epsilon^2}$ and $C(\mu) = \frac{\mu^2 L_0}{2 \frac{(d+6)^3}{(d+4)^2}}$. Therefore the number of iterations required is improved to $N = \mathcal{O}(1/\epsilon^2)$ when we set $\mu = \mathcal{O}(\epsilon/d^{3/2})$ and $m = \mathcal{O}(d)$. However, the zeroth-order oracle complexity is still $\mathcal{O}(d/\epsilon^2)$. In practice, a reasonable choice of $m$ results in a faster algorithm. This multi-sampling technique will play a key role in our stochastic and non-smooth case analyses.
Algorithm 2 Zeroth-order Riemannian Stochastic Gradient Descent (ZO-RSGD)

1: **Input:** Initial point \(x_0 \in \mathcal{M}\), smoothing parameter \(\mu\), multi-sample constant \(m\), step size \(\eta_k\), fixed number of iteration \(N\).

2: for \(k = 0\) to \(N - 1\) do

3: Sample the standard Gaussian random vectors \(u^k_i\) on \(T_{x_k} \mathcal{M}\) by projection, and \(\xi^k_i\), \(i = 1, \ldots, m\).

4: Set the random oracle \(\bar{g}_{\mu,\xi}(x_k)\) by (17).

5: Update \(x_{k+1} = R_{x_k}(-\eta_k \bar{g}_{\mu,\xi}(x_k))\).

6: end for

### 3.2 Zeroth-Order Riemannian Stochastic Gradient Method

In this section, we focus on the smooth optimization problem with \(h \equiv 0\), and when \(f\) takes the following form

\[f(x) := \int \xi F(x, \xi) dP(\xi),\]

where \(F\) is a function satisfying (2.4) and (2.6), w.r.t. variable \(x\), almost surely. Notice that \(f\) would also automatically satisfy Assumptions 2.4 and 2.6, since:

\[|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \leq \mathbb{E}|F(y, \xi) - F(x, \xi) - \langle \nabla F(x, \xi), y - x \rangle| \leq \frac{L}{2} \|y - x\|^2,\]

by the Jensen inequality. We have the following additional assumption on the function, which is used frequently in zeroth-order stochastic optimization [GL13, BG19]:

**Assumption 3.2.** Let \(\|\cdot\|\) be a norm in \(\mathbb{R}^n\). For all \(x \in \mathcal{M}\), we have (with \(\mathbb{E} = \mathbb{E}_\xi\))

\[\mathbb{E}[F(x, \xi)] = f(x), \quad \mathbb{E}[\nabla F(x, \xi)] = \nabla f(x)\]  \hspace{1cm} (15)

and the bound for variance:

\[\mathbb{E} \left[ \|\nabla F(x, \xi) - \nabla f(x)\|^2 \right] \leq \sigma^2\]  \hspace{1cm} (16)

**Note that these conditions then hold for the riemannian gradient, if we replace the regular gradient with Riemannian gradient, because of the non-expansiveness of the projection operation.**

In the stochastic case, sampling multiple times every iteration could improve the convergence rate. Our proposed zeroth-order Riemannian stochastic gradient estimator is given by

\[\bar{g}_{\mu,\xi}(x) = \frac{1}{m} \sum_{i=1}^{m} g_{\mu,\xi_i}(x).\]  \hspace{1cm} (17)

where

\[g_{\mu,\xi_i}(x) = \frac{F(R_x(\mu u_i), \xi_i) - F(x, \xi_i)}{\mu} u_i,\]

for \(i = 1, 2, \ldots, m\). We also immediately have that

\[\mathbb{E}_\xi g_{\mu_i,\xi_i}(x) = \frac{f(R_x(\mu u)) - f(x)}{\mu} u = g_{\mu_i}(x).\]  \hspace{1cm} (18)

The multi-sampling technique improves the estimated bound \(\mathbb{E}\|\bar{g}_{\mu,\xi}(x) - \text{grad } f(x)\|^2\), as we have

\[\mathbb{E}\|\bar{g}_{\mu,\xi}(x) - \text{grad } f(x)\|^2 \leq \mu^2 L_g^2 (d + 6)^3 + \frac{8(d + 4)}{m} \sigma^2 + \frac{8(d + 4)}{m} \|\text{grad } f(x)\|^2,\]

See Lemma C.1 for details. Now we present our convergence analysis for stochastic case.
Theorem 3.3. Suppose $x_k$ is the sequence generated by Algorithm 2 with the stepsize $\eta_k = \hat{\eta} = \frac{1}{L_g}$, we have

$$\frac{1}{N+1} \sum_{k=0}^{N} \mathbb{E}_{U_k, \Xi_k} \|\nabla f(x_k)\|^2 \leq 2L_g \left( \frac{f(x_0) - f(x^*)}{N+1} + C(\mu) \right),$$

where $C(\mu) = \frac{\mu^2 L_g}{2} (d+6)^3 + \frac{8(d+4)}{m L_g} \sigma^2$, $U_k$ denotes the set of all Gaussian random vectors and $\Xi_k$ denotes the set of all random variable $\xi_k$ we drew for the first $k$ iterations, correspondingly. In order to have

$$\frac{1}{N+1} \sum_{k=0}^{N} \mathbb{E}_{U_k, \Xi_k} \|\nabla f(x_k)\|^2 \leq \epsilon^2,$$

we need the smoothing parameter $\mu$, number of sampling at each iteration $m$ and number of iteration $N$ to be

$$\mu = \mathcal{O} \left( \frac{\epsilon}{d^{3/2}} \right), \quad m = \mathcal{O} \left( \frac{d \sigma^2}{\epsilon^2} \right), \quad N = \mathcal{O} \left( \frac{1}{\epsilon^2} \right), \quad (21)$$

therefore the number of calls to the zeroth-order oracle is given by $\mathcal{O}(d/\epsilon^4)$.

### 3.3 Zeroth-order Riemannian Proximal Gradient Method

We now consider the optimization problem of the form in (1). For the sake of notation, we use $p(x) := f(x) + h(x)$. We assume that $h$ is convex in the embedded space $\mathbb{R}^n$ and is also Lipschitz continuous with parameter $L_h$. Here, for the sake of concreteness, we restricted our discussion to the case of Stiefel manifold $\mathcal{M} = \text{St}(n,p) = \{ X \in \mathbb{R}^{n \times p} : X^T X = I_p \}$, i.e. we focus on the following optimization problem:

$$\min_{X^T X = I_p} p(X) = f(X) + h(X) \quad (22)$$

In our analysis, we only utilize the fact that Stiefel manifold is compact, and therefore the gradient is bounded. Thus the same theory would apply to other compact manifolds, or other composite optimization problems with the gradient of smooth part bounded.

The non-differentiability of $h$ prohibits Riemannian gradient methods to be applied directly. In [CMSZ18], the authors proposed a Riemannian proximal gradient type algorithm which computes the update direction as:

$$V_k := \arg\min_{V \in T_{X_k} \mathcal{M}} \langle \nabla f(X_k), V \rangle + \frac{1}{2L} \|V\|_{F}^2 + h(X_k + V),$$

and sets the update as

$$X_{k+1} = R_{X_k}(\eta_k V_k). \quad (23)$$

The algorithm is called as the Riemannian proximal gradient method. Furthermore, [CMSZ18] also provided an oracle complexity analysis in terms of converging to stationary point. Here, the following lemma from [CMSZ18] provides a notion of stationary point that could be useful for analyzing problems of the form in (22).

**Lemma 3.4.** Let $\tilde{V}_k$ be the minimizer of the problem:

$$\min_{V \in T_{X_k} \mathcal{M}} \langle \nabla f(X_k), V \rangle + \frac{1}{2L} \|V\|_{F}^2 + h(X_k + V).$$

$$\min_{V \in T_{X_k} \mathcal{M}} \langle \nabla f(X_k), V \rangle + \frac{1}{2L} \|V\|_{F}^2 + h(X_k + V). \quad (24)$$
**Algorithm 3** Zeroth-Order Riemannian Proximal Gradient Descent (ZO-ManPG)

1. **Input:** Initial point $X_0$ on $\text{St}(n,p)$, smoothing parameter $\mu$, number of multi-sample $m$, step size $\eta_k$, fixed number of iteration $N$.
2. **for** $k = 0$ to $N - 1$ **do**
3. Sample $m$ standard Gaussian random matrix $U_i$ on $T_{X_k} \mathcal{M}$ by projection, $i = 1, ..., m$.
4. Set the random oracle $\bar{g}_\mu(X_k)$ by (26).
5. Solve $V_k$ from (23).
6. Update $X_{k+1} = R_{X_k}(\eta_k V_k)$.
7. **end for**

If $\bar{V}_k = 0$, then $X_k$ is a stationary point of problem (22). We say $X_k$ is an $\epsilon$-stationary point of (22) with $t = \frac{1}{L_g}$, if $\|\bar{V}_k\|_F \leq \epsilon/L_g$.

Motivated by [CMSZ18], the zeroth-order Riemannian proximal gradient method in provided in Algorithm 3. Notice that our algorithm still used the multi-sampling technique:

$$
\bar{g}_\mu(x) = \frac{1}{m} \sum_{i=1}^{m} g_{\mu_i}(x),
$$

$$
g_{\mu_i}(x) = \frac{f(R_x(\mu u_i)) - f(x)}{\mu} u_i, \ i = 1, ..., m
$$

which will again play a key role in our convergence analysis.

**Theorem 3.5.** The sequence generated by Algorithm 3 with $\eta_k = \tilde{\eta}$ any constant smaller than $\min\{1, \tilde{\eta}\}$ and $t = \frac{1}{L_g}$, satisfies:

$$
\frac{1}{N} \sum_{k=0}^{N-1} \mathbb{E}_{\mathcal{D}_k} \|\bar{V}_k\|_F^2 \leq \frac{4t(p(X_0) - p(X^*))}{\tilde{\eta}N} + \frac{4(d + 4)}{m} t^2 M^2 + 2\mu^2 L_g^2 t^2 (d + 6)^3,
$$

where $M$ is a upper bound of the norm of $\nabla f(X)$ over the Stiefel manifold. In order to make $\min_{k=0, ..., N-1} \mathbb{E}_{\mathcal{D}_k} \|\bar{V}_k\|_F^2 \leq \frac{\epsilon^2}{L_g^2}$, we need the parameters in the following setting:

$$
\mu = \mathcal{O}\left(\frac{d}{\epsilon^3/2}\right), \ m = \mathcal{O}\left(\frac{dM^2}{\epsilon^2}\right), \ N = \mathcal{O}\left(\frac{1}{\epsilon^2}\right),
$$

and the number of calls to the zeroth-order oracle is $\mathcal{O}(d/\epsilon^4)$.

**Remark 3.** The above result applies to any optimization problems of the form in (1), with the gradient of smooth part bounded.

**Remark 4.** The subproblem (23) will naturally cost most of the time in each iteration in our zeroth-order ManPG algorithm. We use the regularized semi-smooth Newton (SSN) method [XLWZ18] to solving the subproblem and achieve very fast convergence. For the purpose of brevity, we refer to [Mif77, XLWZ18, CMSZ18] for a comprehensive study of this method.
| Dimension | $\epsilon$ | Stepsize | No. iter. Z-RGD | Aver. No. iter. RGD |
|-----------|------------|----------|----------------|--------------------|
| $15 \times 5$ | $10^{-3}$ | $10^{-2}$ | 460 ± 137 | 442 |
| $25 \times 15$ | $10^{-3}$ | $10^{-2}$ | 892 ± 99 | 852 |
| $50 \times 20$ | $10^{-2}$ | $5 \times 10^{-3}$ | 255 ± 26 | 236 |

Table 2: Result of zeroth-order Riemannian gradient descent, in comparison with Riemannian gradient descent.

4 Numerical experiments

4.1 Experiments on synthetic data

We performed three numerical experiments to justify our analysis. The first experiment is conducted on the so called Procrustes problem [AMS09], which is basically the matrix linear regression on a given manifold: $\min_X \| AX - B \|^2_F$, where $X \in \mathbb{R}^{n \times p}$, $A \in \mathbb{R}^{l \times n}$ and $B \in \mathbb{R}^{l \times p}$. The manifold we used is the Stiefel manifold $M = St(n, p)$, which will reduce to the unit ball in $\mathbb{R}^n$ under the condition $p = 1$. Such a manifold enjoys closed form solution for tangent space and retraction mappings (see Appendix). In our experiment, we pick up different dimension $n \times p$ and record the time cost to achieve prescribed precision $\epsilon$. The entries of matrix $A$ are generated by standard Gaussian distribution. The result is shown in Table 4.1 (Note that the numbers are the average and standard deviation for 100 experiments, and for each experiment, we sample $m = n \times p$ Gaussian samples for each iteration), and the multi-sample zeroth-order Riemannian optimization almost resembles the convergence rate of Riemannian optimization, as shown in Figure 2. Two more synthetic experiments are discussed in Section D.

![Figure 2](image)

Figure 2: The convergence curve of Zo-RGD v.s. RGD. x-axis is the number of iterations and y-axis is the norm of Riemannian gradient at corresponding points. Note that our zeroth-order algorithm doesn’t use gradient information in updates, while the graph still shows the norm of gradient to show the effectiveness of our method. The horizontal lines are the prescribed precisions.

4.2 Robust black-box attack of neural networks

We now propose our white-box and black-box attack algorithm, as stated in Algorithm 4 and 5 (in Section D), which are of the same spirit: instead of starting from the original image as in PGD [MMS+17] or ZOO [CZS+17] attacks, we start our zeroth-order attack from a perturbation and
maximize the loss function on the sphere. For the black-box method, to accelerate the convergence, we use Euclidean zeroth-order optimization to find a appropriate initial perturbation (Algorithm 6). It’s worth noticing that the zeroth-order attack in [CZS+17, TTC+19] has a non-smooth objective function, which has $O(n^3/\epsilon^3)$ complexity to guarantee convergence [NS17], whereas the complexity needed for our method is $O(d/\epsilon^2)$.

We first tested our method on the giant panda picture in the Imagenet data set [DDS+09], with the network structure the Inception v3 network structure [SVI+16]. The attack radius in our algorithm is proportional to the $\ell_2$ norm of the original image. Both white-box and black-box Riemannian attack are successful, which means that they both converge to images which lie in a different image class (i.e. with a different label), see Figure 3. We also tested our Algorithm 4 and 5 on the CIFAR10 dataset, and the network structure we used is the VGG net [SZ14]. We conduct our experiments on a desktop with Intel Core 9600K CPU and NVIDIA GeForce RTX 2070 GPU. The attacking image result is shown in Figure 7.

5 Conclusion

In this paper, we proposed a method for estimating the Riemannian gradient of a function given potentially noisy function queries. Our approach generalized the technique proposed in [NS17] to the Riemannian setting. We analyze the quality of the proposed zeroth-order Riemannian gradient estimator, propose three zeroth-order Riemannian optimization techniques, and characterize their oracle complexities. We show that the complexities depend only on the intrinsic dimensionality of the manifold and is independent of the ambient dimension of the Euclidean space in which the manifold is embedded into. The applicability of the developed technique to numerical problems and real-world problems in the form of black-box attack to DNNs is illustrated.

Our work opens up numerous possibilities for future work. It is interesting to develop accelerated versions of the proposed algorithms, to obtain improved complexities. It is also extremely interesting and challenging to obtain lower bounds for zeroth-order Riemannian optimization methods. Finally, it is extremely interesting to examine the use of the proposed zeroth-order Riemannian gradient estimator for volume computation of Riemannian bodies by sampling techniques.

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Figure 3: The attack on giant panda picture $\text{DD}_1^{+09}$. (a): the original image; (b): the PGD attack with a small diameter; (c) Riemannian attack (Algorithm 4) on the sphere with the same diameter; (d): Riemannian zeroth-order attack (Algorithm 5). 'Indri' refers to the class to which the original image is misclassified to.

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A More on Riemannian optimization basics

Here we provide additional discussions on the Riemannian optimization basics. Although we don’t specify our retraction to be the exponential mapping, the exponential mapping is still the most commonly used retraction for most of our applications. We first recall the geodesic of a manifold:

**Definition A.1.** A smooth curve $\gamma$ defined on manifold $M$ endowed with an affine connection $\nabla$, is called a geodesic if and only if $\gamma$ is a curve with zero acceleration:

$$\frac{D^2}{dt^2} \gamma(t) = 0$$

where the second order derivative $\frac{D^2}{dt^2}$ over the manifold could be locally expressed via

$$\frac{D^2}{dt^2} = \frac{d^2}{dt^2} x^k + \sum_{i,j} \Gamma_{ij}^k(\gamma) \frac{d}{dt} x^i \frac{d}{dt} x^j$$

where $\Gamma_{ij}^k(\gamma)$ is the Christoffel symbol which further depend locally on the coordinate chart of the given manifold.

Notice that if $\gamma(t)$ is a smooth curve defined on manifold $M$, $t \in I \subset \mathbb{R}$, then $\gamma'(t)$ can be regarded as a *velocity field* defined along curve $\gamma(t)$, but the second order derivatives depends locally on the structure of the manifold. A proper interpretation of geodesic for our applications, is simply the smooth curve on $M$ that has a zero acceleration.

Now we can provide the definition of the exponential mapping [AMS09]:

**Definition A.2.** For every $x \in M$ and $\eta \in T_x M$, there always exists a geodesic $\gamma(t; x, \eta)$ such that: $\gamma : I \subset \mathbb{R} \to M$ with $0 \in \mathcal{M}$ and $\gamma(0; x, \eta) = x$, $\gamma'(0; x, \eta) = \eta$. And the corresponding exponential mapping is defined as:

$$\text{Exp}_x : T_x M \to M : \eta \to \gamma(1; x, \eta).$$

Notice that $\text{Exp}_x$ is naturally a retraction by the properties of geodesics, by the homogeneous property $\gamma(t; x, a\eta) = \gamma(at; x, \eta)$.

Now we restate the optimality conditions for Riemannian optimization [YZS14], which justifies our convergence measure $\text{grad} f(x)$:

**Theorem A.3.** *(Necessary optimality conditions)* Let $x \in M$ be a local optimum for $\min_M f(x)$. If $f$ is differentiable at $x$, then $\text{grad} f(x) = 0$. If $f$ is twice differentiable at $x$, then $\text{Hess} f(x) \succeq 0$ (positive semidefinite).
Properties of Riemannian Zeroth-order Gradient Estimators

Here we state the bounds between our zeroth order oracle and the real gradient, where the function $f$ satisfies our Assumptions 2.4 and 2.6. Notice that the Gaussian smoothing $f_\mu$ is avoided in our proofs.

**Lemma B.1.** Suppose $X$ is a $d$ dimensional subspace of $\mathbb{R}^n$, with orthogonal projection matrix $P \in \mathbb{R}^{n \times n}$. $u_0 \sim \mathcal{N}(0, I_n)$ is a standard norm distribution and $u = Pu_0$ is the orthogonal projection of $u_0$ onto the subspace. Then $\forall x \in X$, we have

$$ x = \frac{1}{\kappa} \int_{\mathbb{R}^n} \langle x, u \rangle u e^{-\frac{1}{2} \| u_0 \|^2} du_0 $$

(31)

and

$$ \| x \|^2 = \frac{1}{\kappa} \int_{\mathbb{R}^n} \langle x, u \rangle^2 u e^{-\frac{1}{2} \| u_0 \|^2} du_0 $$

(32)

where $\| \cdot \|$ is the Euclidean norm on $\mathbb{R}^n$, and $\kappa$ is the constant for normal density function:

$$ \kappa := \int_{\mathbb{R}^n} e^{-\frac{1}{2} \| u \|^2} du = (2\pi)^{n/2}. $$

**Proof.** By the definition of covariance matrix, we have

$$ \frac{1}{\kappa} \int_{\mathbb{R}^n} u_0 u_0^T e^{-\frac{1}{2} \| u_0 \|^2} du_0 = I_n. $$

Therefore $\forall x \in X$,

$$ \frac{1}{\kappa} \int_{\mathbb{R}^n} \langle x, u \rangle u_0 e^{-\frac{1}{2} \| u_0 \|^2} du_0 = x. $$

(33)

since $\langle x, u \rangle = \langle x, u_0 \rangle$. Now impose projection on both side, we have

$$ \frac{1}{\kappa} \int_{\mathbb{R}^n} \langle x, u \rangle e^{-\frac{1}{2} \| u_0 \|^2} du_0 = Px = x. $$

Similarly, inner product $x$ on the both side of (33), we have

$$ \| x \|^2 = \frac{1}{\kappa} \int_{\mathbb{R}^n} \langle x, u \rangle^2 e^{-\frac{1}{2} \| u_0 \|^2} du_0. $$

\[ \square \]

It would be helpful to know the bound for the moments of normal distribution, thus we restate the following lemma without proof:

**Lemma B.2.** [NS17] Suppose $u \sim \mathcal{N}(0, I_n)$ is a standard norm distribution, then for all integers $p \geq 2$, we have

$$ M_p := \mathbb{E}_u(\| u \|^p) \leq (n + p)^{p/2} $$

(34)

**Corollary 1.** For $u_0 \sim \mathcal{N}(0, I_n)$ and $u = Pu_0$, where $P \in \mathbb{R}^{n \times n}$ is the orthogonal projection matrix onto a $d$ dimensional subspace $X$ of $\mathbb{R}^n$, we similarly have:

$$ \mathbb{E}_{u_0}(\| u \|^p) \leq (d + p)^{p/2} $$

(35)
Now we could provide the bound of our gradient estimator \(g_\mu(x)\) and the true Riemannian gradient \(\text{grad} f(x)\). Notice that we always assume the manifold \(\mathcal{M}\) is of dimension \(m\).

**Lemma B.3.** We have that, under Assumptions 2.4 and 2.6,

\[
\|\mathbb{E}_{\mu_0}(g_\mu(x)) - \text{grad} f(x)\| \leq \frac{\mu L_g}{2}(d + 3)^{3/2}
\]

**Proof.** Since

\[
\mathbb{E}(g_\mu(x)) - \text{grad} f(x) = \frac{1}{\kappa} \int_{\mathbb{R}^n} \left( \frac{f(R_x(\mu u)) - f(x)}{\mu} - \langle \text{grad} f(x), u \rangle \right) u e^{-\frac{1}{2}\|u_0\|^2} du_0
\]

We have

\[
\|\mathbb{E}(g_\mu(x)) - \text{grad} f(x)\| = \|\frac{1}{\mu \kappa} \int_{\mathbb{R}^n} (f(R_x(\mu u)) - f(x) - \langle \text{grad} f(x), \mu u \rangle) u e^{-\frac{1}{2}\|u_0\|^2} du_0\|
\]

\[
\leq \frac{1}{\mu \kappa} \int_{\mathbb{R}^n} L_g \|\mu u\|^2 \|u\| e^{-\frac{1}{2}\|u_0\|^2} du_0
\]

\[
= \frac{\mu L_g}{2\kappa} \int_{\mathbb{R}^n} \|u\|^3 e^{-\frac{1}{2}\|u_0\|^2} du_0
\]

\[
\leq \frac{\mu L_g}{2}(d + 3)^{3/2}
\]

where the first inequality is by L-retraction-smoothness, and the last inequality is by the corollary above. □

**Lemma B.4.** We have that, under Assumptions 2.4 and 2.6,

\[
\|\text{grad} f(x)\|^2 \leq 2\|\mathbb{E}_{\mu_0}(g_\mu(x))\|^2 + \frac{\mu^2}{2} L_g(d + 6)^3
\]

**Proof.** Since

\[
\|\text{grad} f(x)\|^2 = \|\frac{1}{\kappa} \int_{\mathbb{R}^n} \langle \text{grad} f(x), u \rangle u e^{-\frac{1}{2}\|u_0\|^2} du_0\|^2
\]

\[
= \|\frac{1}{\mu \kappa} \int_{\mathbb{R}^n} ([f(R_x(\mu u)) - f(x)] - [f(R_x(\mu u)) - f(x) - \langle \text{grad} f(x), \mu u \rangle]) u e^{-\frac{1}{2}\|u_0\|^2} du_0\|^2
\]

\[
\leq 2\|\mathbb{E}(g_\mu(x))\|^2 + \frac{2}{\mu^2} \int_{\mathbb{R}^n} (f(R_x(\mu u)) - f(x) - \langle \text{grad} f(x), \mu u \rangle) u e^{-\frac{1}{2}\|u_0\|^2} du_0\|^2
\]

\[
\leq 2\|\mathbb{E}(g_\mu(x))\|^2 + \frac{2}{\mu^2} \int_{\mathbb{R}^n} (f(R_x(\mu u)) - f(x) - \langle \text{grad} f(x), \mu u \rangle)^2 \|u\|^2 e^{-\frac{1}{2}\|u_0\|^2} du_0
\]

\[
\leq 2\|\mathbb{E}(g_\mu(x))\|^2 + \frac{\mu^2}{2} L_g(d + 6)^3
\]

where the last inequality is by applying the same trick as the previous lemma. □

**Lemma B.5.** We have that, under Assumptions 2.4 and 2.6,

\[
\mathbb{E}_{\mu_0}(\|g_\mu(x)\|^2) \leq \frac{\mu^2}{2} L_g^2(d + 6)^3 + 2(d + 4)\|\text{grad} f(x)\|^2
\]
Proof. Since
\[ \mathbb{E}(\|g_\mu(x)\|^2) = \frac{1}{\mu^2} \mathbb{E}_{\omega_0} [(f(R_x(\mu u)) - f(x))^2\|u\|^2] \]
and
\[
(f(R_x(\mu u)) - f(x))^2 = (f(R_x(\mu u)) - f(x) - \mu \langle \nabla f(x), u \rangle + \mu \langle \nabla f(x), u \rangle)^2 \\
\leq 2\left(\frac{L_g}{2} \mu^2 \|u\|^2\right)^2 + 2\mu^2 \langle \nabla f(x), u \rangle^2
\]
therefore
\[
\mathbb{E}(\|g_\mu(x)\|^2) \leq \frac{\mu^2}{2} L_g^2 \mathbb{E}(\|u\|^6) + 2\mathbb{E}(\|\langle \nabla f(x), u \rangle u\|^2) \\
\leq \frac{\mu^2}{2} L_g^2 (d + 6)^3 + 2\mathbb{E}(\|\langle \nabla f(x), u \rangle u\|^2)
\]

Now we bound the term \(\mathbb{E}(\|\langle \nabla f(x), u \rangle u\|^2)\) using the same trick as in [NS17]. WLOG, suppose \(\mathcal{X}\) is the \(d\)-dimensional subspace generated by the first \(d\) coordinates, i.e. \(\forall x \in \mathcal{X}\), the last \(n - d\) elements of \(x\) are zeros. Also for brevity, denote \(g = \nabla f(x)\). We have that
\[
\mathbb{E}(\|\langle \nabla f(x), u \rangle u\|^2) = \frac{1}{\kappa} \int_{\mathbb{R}^d} \langle \nabla f(x), u \rangle^2 \|u\|^2 e^{-\frac{1}{2} \|u\|_2^2} du_0 \\
= \frac{1}{\kappa(d)} \int_{\mathbb{R}^d} (\sum_{i=1}^{d} \sum_{i=1}^{d} g_i x_i)^2 (\sum_{i=1}^{d} x_i^2) e^{-\frac{1}{2} \sum_{i=1}^{d} x_i^2} dx_1 \cdots dx_d
\]
where \(x_i\) denotes the \(i\)-th coordinate of \(u_0\), the last \(n - d\) dimensions are integrated to be one, and \(\kappa(d)\) is the normalization constant for \(d\)-dimensional Gaussian distribution. For simplicity, denote \(x = (x_1, \ldots, x_d)\), then
\[
\mathbb{E}(\|\langle \nabla f(x), u \rangle u\|^2) = \frac{1}{\kappa(d)} \int_{\mathbb{R}^d} \langle g, x \rangle^2 \|x\|^2 e^{-\frac{1}{2} \|x\|_2^2} dx \\
\leq \frac{1}{\kappa(d)} \int_{\mathbb{R}^d} \|x\|^2 e^{-\frac{1}{2} \|x\|_2^2} \langle g, x \rangle^2 e^{-\frac{1}{2} \|x\|_2^2} dx \\
\leq \frac{2}{\kappa(d) \tau e} \int_{\mathbb{R}^d} \langle g, x \rangle^2 e^{-\frac{1}{2} \|x\|_2^2} dx \\
= \frac{2}{\kappa(d) \tau (1 - \tau)^{1+d/2} e} \int_{\mathbb{R}^d} \langle g, x \rangle^2 e^{-\frac{1}{2} \|x\|_2^2} dx \\
= \frac{2}{\tau (1 - \tau)^{1+d/2} e} \|g\|^2
\]
where the second inequality is due to the following fact: \(x^p e^{-\frac{1}{2} x^2} \leq \left(\frac{2}{\tau e}\right)^{p/2}\). Taking \(\tau = \frac{2}{(d+1)}\) will give the final result. \(\square\)

C Proofs in Section 3

C.1 Zeroth-Order Riemannian Gradient Method (ZO-RGD)

Proof of Theorem 3.1 By \(L_g\)-retraction-smooth
\[
f(x_{k+1}) \leq f(x_k) - \eta_k \langle g_\mu(x_k), \nabla f(x_k) \rangle + \frac{\eta_k^2 L_g}{2} \|g_\mu(x_k)\|^2
\]
Taking the expectation w.r.t. $u_k$ on both side, we have
\[
\mathbb{E}_{u_k} \left[ f(x_{k+1}) \right] \leq f(x_k) - \eta_k \langle \mathbb{E}_{u_k}(g_\mu(x_k)) \rangle, \nabla f(x_k) + \frac{\eta_k^2 L_g}{2} \mathbb{E}_{u_k}(\|g_\mu(x_k)\|^2) \\
\leq f(x_k) - \eta_k \langle \mathbb{E}_{u_k}(g_\mu(x_k)) \rangle, \nabla f(x_k) + \frac{\eta_k^2 L_g}{2} \left( \frac{\mu^2}{2} L_g^2 (d+6)^3 + 2(d+4) \|\nabla f(x_k)\|^2 \right)
\]
where the last inequality is by Lemma B.5. Now, take $\eta_k = \frac{1}{2(d+4) L_g}$, we have
\[
\mathbb{E}_{u_k} \left[ f(x_{k+1}) \right] \leq f(x_k) + \frac{\eta_k}{2} \|\nabla f(x_k)\|^2 - 2 \langle \mathbb{E}_{u_k}(g_\mu(x_k)) \rangle, \nabla f(x_k) \rangle + \frac{\mu^2 L_g}{16} (d+6)^3 \\
= f(x_k) + \frac{\eta_k}{2} \|\nabla f(x_k)\|^2 - \mathbb{E}_{u_k}(g_\mu(x_k)) \|\nabla f(x_k)\|^2 - \frac{\mu^2}{16} L_g (d+6)^3 \\
\leq f(x_k) + \frac{\eta_k}{2} \|\nabla f(x_k)\|^2 + \frac{\mu^2}{4} L_g (d+6)^3 \\
= f(x_k) - \frac{\eta_k}{2} \|\nabla f(x_k)\|^2 + C(\mu),
\]
where the second inequality is by Lemma B.3 and B.4 and $C(\mu) = \frac{\mu^2}{8} \frac{(d+3)^3}{(d+4)} + \frac{\mu^2}{8} \frac{(d+6)^3}{(d+4)} + \frac{\mu^2}{16} \frac{(d+6)^3}{(d+4)^2}$. Now take the expectation w.r.t $\mathcal{U}_k = \{u_0, u_1, \ldots, u_{k-1}\}$ we have
\[
\phi_{k+1} \leq \phi_k - \frac{\eta_k}{2} \mathbb{E}_{\mathcal{U}_k} \|\nabla f(x_k)\|^2 + C(\mu).
\]
Summing up $k = 0, \ldots, N$ we have
\[
\frac{1}{N+1} \sum_{k=0}^{N} \mathbb{E}_{\mathcal{U}_k} \|\nabla f(x_k)\|^2 \leq \frac{2}{\eta_k} \left( \frac{f(x_0) - f(x^*)}{N+1} + C(\mu) \right).
\]
Therefore with $\mu = O\left( \frac{c^2}{d^4} \right)$ s.t. $C(\mu) \leq \frac{c^2}{2}$, and take $N \geq 4(d+4) L_g \frac{f(x_0) - f(x^*)}{\epsilon^2}$, we have that
\[
\frac{1}{N+1} \sum_{k=0}^{N} \mathbb{E}_{\mathcal{U}_k} \|\nabla f(x_k)\|^2 \leq c^2. \text{ In brief, the steps we need is } O\left( \frac{d^4}{c^2} \right) \text{ to have an } \epsilon \text{-approximate solution, and the total zero-order oracle complexity is also } O\left( \frac{d^4}{c^2} \right). \]

Proof of the improved bound {13}. Since $\tilde{g}_\mu(x) = \frac{1}{m} \sum_{i=1}^{m} g_{\mu,i}(x)$, we have (denote $U = \{u_1, \ldots, u_m\}$):
\[
\mathbb{E}_U \|\tilde{g}_\mu(x) - \nabla f(x)\|^2 \leq 2 \mathbb{E}_U \|\tilde{g}_\mu(x) - \nabla U g_\mu(x)\|^2 + 2 \|\nabla U g_\mu(x) - \nabla f(x)\|^2 \\
= 2 \mathbb{E}_U \|\frac{1}{m} \sum_{i=1}^{m} [g_{\mu,i}(x) - \nabla U g_{\mu,i}(x)]\|^2 + 2 \|\frac{1}{m} \sum_{i=1}^{m} \nabla U g_{\mu,i}(x) - \nabla f(x)\|^2 \\
= \frac{2}{m^2} \mathbb{E}_U \sum_{i=1}^{m} \|g_{\mu,i}(x) - \nabla U g_{\mu,i}(x)\|^2 + \frac{2}{m^2} \|\sum_{i=1}^{m} \nabla U g_{\mu,i}(x) - \nabla f(x)\|^2 \\
\leq \frac{2}{m} \mathbb{E}_{u_1} \|g_{\mu,1}(x) - \nabla U g_{\mu,1}(x)\|^2 + 2 \|\mathbb{E}_{u_1} g_{\mu,1}(x) - \nabla f(x)\|^2 \\
\leq \frac{\mu^2}{m} \|g_{\mu,1}(x)\|^2 + \frac{\mu^2 L_g^2}{2} (d+3)^3 \\
\leq \frac{\mu^2}{m} L_g^2 (d+6)^3 + \frac{2}{m} \|\nabla f(x)\|^2 + \frac{\mu^2 L_g^2}{2} (n+3)^3 \\
\leq \mu^2 L_g^2 (d+6)^3 + \frac{2}{m} \|\nabla f(x)\|^2,
\]
where the second equality is from the fact that $u_i$ and $u_j$ are independent as long as $i \neq j$. \qed
proof of the remark 3. Following the $L_g$-retraction-smooth, we have:

$$f(x_{k+1}) \leq f(x_k) - \eta_k \langle \bar{g}_\mu(x), \nabla f(x_k) \rangle + \frac{\eta_k^2 L_g}{2} \|\bar{g}_\mu(x)\|^2$$

Take $\eta_k = \hat{\eta} = \frac{1}{L_g}$, we have

$$f(x_{k+1}) \leq f(x_k) - \eta_k \langle \bar{g}_\mu(x), \nabla f(x_k) \rangle + \frac{\eta_k^2 L_g}{2} \|\bar{g}_\mu(x)\|^2$$

$$= f(x_k) + \frac{1}{2L_g} (\|\bar{g}_\mu(x) - \nabla f(x)\|^2 - \|\nabla f(x)\|^2).$$

Now take the expectation for the random variables at the iteration $k$ on both side, we have

$$E_k f(x_{k+1}) \leq f(x_k) + \frac{1}{2L_g} (E_k \|\bar{g}_\mu(x) - \nabla f(x)\|^2 - \|\nabla f(x)\|^2)$$

$$\leq f(x_k) + \frac{1}{2L_g} \left( \mu^2 L_g^2 (d + 6)^3 + \frac{2(n + 4)}{m} - L_g \|\nabla f(x)\|^2 \right)$$

Summing up $k = 0, \ldots, N$ we have (assume that $m \geq 4(n + 4)$)

$$\frac{1}{N + 1} \sum_{k=0}^{N} E_{U_k} \|\nabla f(x_k)\|^2 \leq 2L_g \left( \frac{f(x_0) - f(x^*)}{N + 1} + C(\mu) \right),$$

where $C(\mu) = \frac{\mu^2 L_g^2}{2} (d + 6)^3$. \qed

C.2 Zeroth-Order Riemannian Stochastic Gradient Method (ZO-RSGD)

Lemma C.1. We have that (the expectation $E$ is taken for both Gaussian vectors $U = \{u_1, \ldots, u_m\}$ and $\xi$), if we sample $m(\geq 2)$ Gaussian random vectors for each iteration, we have an improved bound:

$$E \|\bar{g}_{\mu, \xi}(x) - \nabla f(x)\|^2 \leq \mu^2 L_g^2 (d + 6)^3 + \frac{8(d + 4)}{m} \sigma^2 + \frac{8(d + 4)}{m} \|\nabla f(x)\|^2 \quad (39)$$

Proof. Since

$$E_{U, \xi} \|\bar{g}_{\mu, \xi}(x) - \nabla f(x)\|^2 \leq 2E_{U, \xi} \|\bar{g}_{\mu, \xi}(x) - E_{U, \xi} \nabla g_{\mu}(x)\|^2 + 2E_{U, \xi} \nabla g_{\mu}(x) - \nabla f(x)\|^2$$

$$\leq \frac{2}{m} E_{U_1, \xi} \|g_{1, \mu, \xi}(x) - E_{U_1} g_{\mu}(x)\|^2 + \frac{\mu^2 L_g^2}{2} (d + 3)^3$$

$$\leq \frac{2}{m} E_{U_1, \xi} \|g_{1, \mu, \xi}(x)\|^2 + \frac{\mu^2 L_g^2}{2} (d + 3)^3$$

$$\leq \frac{2}{m} \left( \frac{\mu^2 L_g^2}{2} (d + 6)^3 + 4(d + 4) \|\nabla f(x)\|^2 + \sigma^2 \right) + \frac{\mu^2 L_g^2}{2} (d + 3)^3$$

$$\leq \mu^2 L_g^2 (d + 6)^3 + \frac{8(d + 4)}{m} \sigma^2 + \frac{8(d + 4)}{m} \|\nabla f(x)\|^2,$$

where the third inequality is by applying Lemma B.5 for the stochastic function $F(x, \xi)$. \qed
Proof of Theorem 3.3. Following the $L_g$-retraction-smooth, we have:

$$f(x_{k+1}) \leq f(x_k) - \eta_k \langle \tilde{g}_{\mu, \xi}(x), \nabla f(x_k) \rangle + \frac{\eta_k^2 L_g}{2} \|\tilde{g}_{\mu, \xi}(x)\|^2$$

Take $\eta_k = \hat{\eta} = \frac{1}{L_g}$, we have

$$f(x_{k+1}) \leq f(x_k) - \eta_k \langle \tilde{g}_{\mu, \xi}(x), \nabla f(x_k) \rangle + \frac{\eta_k^2 L_g}{2} \|\tilde{g}_{\mu, \xi}(x)\|^2 = f(x_k) + \frac{1}{2L_g} \left( \|\tilde{g}_{\mu, \xi}(x) - \nabla f(x)\|^2 - \|\nabla f(x)\|^2 \right).$$

Now take the expectation for the random variables at the iteration $k$ on both side, we have

$$\mathbb{E}_k f(x_{k+1}) \leq f(x_k) + \frac{1}{2L_g} \left( \mathbb{E}_k \|\tilde{g}_{\mu, \xi}(x) - \nabla f(x)\|^2 - \|\nabla f(x)\|^2 \right)$$

$$\leq f(x_k) + \frac{1}{2L_g} \left( \mu^2 L_g^2 (d+6)^3 + \frac{8(d+4)}{m} \sigma^2 + \left( \frac{8(d+4)}{m} - 1 \right) \|\nabla f(x)\|^2 \right)$$

Summing up $k = 0, ..., N$ we have (assume that $m \geq 16(d+4)$)

$$\frac{1}{N+1} \sum_{k=0}^{N} \mathbb{E}_k \|\nabla f(x_k)\|^2 \leq 2L_g \left( \frac{f(x_0) - f(x^*)}{N+1} + C(\mu) \right),$$

where $C(\mu) = \frac{\mu^2 L_g}{2} (d+6)^3 + \frac{8(d+4)}{m} \sigma^2$. We could bound $\frac{1}{N+1} \sum_{k=0}^{N} \mathbb{E}_k \|\nabla f(x_k)\|^2$ by $O(\epsilon^2)$, by taking $\mu = O(\frac{\sqrt{d}}{\epsilon^2})$ and $m = O(\frac{\mu^2 L_g^2}{\epsilon^2})$. In brief, the steps we need is $O(\frac{\epsilon}{\epsilon^2})$ to have an $\epsilon$-approximate solution, meanwhile the zeroth-order oracle complexity is $O(\frac{\mu}{\epsilon^2})$.

C.3 Non-smooth zeroth-order Riemannian gradient method

The subproblem (23) is the key toward achieving a stationary point, as stated in the following lemma:

Lemma C.2 ([CMSZ18], Lemma 5.3). $\tilde{V}_k$ is the minimizer of the problem:

$$\min_{V \in T_k \mathcal{M}} \langle \nabla f(X_k), V \rangle + \frac{1}{2t} \|V\|_F^2 + h(X_k + V). \quad (40)$$

If $\tilde{V}_k = 0$, then $X_k$ is a stationary point of problem (22). We say $X_k$ is an $\epsilon$-stationary point of (22) with $t = \frac{1}{L_g}$ if $\|\tilde{V}_k\|_F \leq \frac{\epsilon}{L_g}$.

However our algorithm cannot compute $\tilde{V}_k$ directly, since $\nabla f(X_k)$ is not available. The following lemma bound the distance of the computable $V_k$ and the unavailable $\tilde{V}_k$:

Lemma C.3. (Non-expansiveness) Suppose

$$V := \arg \min_{V \in T_k \mathcal{M}} \langle G_1, V \rangle + \frac{1}{2t} \|V\|_F^2 + h(X + V) \quad (41)$$

and

$$W := \arg \min_{W \in T_k \mathcal{M}} \langle G_2, W \rangle + \frac{1}{2t} \|W\|_F^2 + h(X + W) \quad (42)$$

We have

$$\|V - W\|_F \leq t \|G_1 - G_2\|_F \quad (43)$$
Proof. By the first order optimality condition [YZS14], we have

\[ 0 \in \frac{1}{t} V + G_1 + \text{Proj}_{T_X M} \partial h(X + V) \]

and

\[ 0 \in \frac{1}{t} W + G_2 + \text{Proj}_{T_X M} \partial h(X + W), \]

i.e. \( \exists P_1 \in \partial h(X + V) \) and \( P_2 \in \partial h(X + W) \) s.t.

\[ V = -t(G_1 + \text{Proj}_{T_X M}(P_1)) \]

and

\[ W = -t(G_2 + \text{Proj}_{T_X M}(P_2)). \]

Therefore we have

\[ \langle V, W - V \rangle = t\langle G_1 + \text{Proj}_{T_X M}(P_1), V - W \rangle \] (44)

and

\[ \langle W, V - W \rangle = t\langle G_2 + \text{Proj}_{T_X M}(P_2), W - V \rangle \] (45)

Now since \( V, W \in T_X M \), we have

\[ \langle \text{Proj}_{T_X M}(P_1), V - W \rangle = \langle P_1, V - W \rangle = \langle P_1, (V + X) - (W + X) \rangle \geq h(V + X) - h(W + X) \]

where the last inequality is by the convexity of \( h \). Therefore we could write (44) and (45) into

\[ \langle V, W - V \rangle \geq t\langle G_1, V - W \rangle + h(V + X) - h(W + X) \]

and

\[ \langle W, V - W \rangle \geq t\langle G_2, W - V \rangle + h(W + X) - h(V + X) \]

Summing the above inequalities together we have

\[ \langle V - W, V - W \rangle \leq t\langle G_1 - G_2, V - W \rangle \]

and the result (43) is just by applying the Cauchy-Schwarz inequality. \( \square \)

Corollary 2. Suppose \( V_k \) is given by our Algorithm 3 and \( \tilde{V}_k \) is given by Lemma 3.4, then we have

\[ \mathbb{E}_{U_k} \| V_k - \tilde{V}_k \|^2_F \leq t^2 \left( \frac{2(d+4)}{m} \| \text{grad} f(X_k) \|^2_F + \mu^2 L^2_g(d+6)^3 \right) \] (46)

Proof. By above lemma, we have

\[ \mathbb{E}_{U_k} \| V_k - \tilde{V}_k \|^2_F \leq t^2 \mathbb{E}_{U_k} \| \tilde{g}_u(X_k) - \text{grad} f(X_k) \|^2_F \]

and since

\[ \mathbb{E}_{U_k} \| \tilde{g}_u(X_k) - \text{grad} f(X_k) \|^2_F \leq \mu^2 L^2_g(d+6)^3 + \frac{2(d+4)}{m} \| \text{grad} f(x) \|^2 \]

by Remark 2. \( \square \)
The following lemma shows the sufficient decreasing property for one iteration:

**Lemma C.4.** ([CMSZ18], Lemma 5.2) For any $t > 0$, there exists a constant $\bar{\eta} > 0$ such that for any $0 \leq \eta_k \leq \min\{1, \bar{\eta}\}$, the $X_k$ and $X_{k+1}$ generated by Algorithm 3 satisfies

$$p(X_{k+1}) - p(X_k) \leq -\frac{\eta_k}{2t} \|V_k\|_F^2$$  \hspace{1cm} (47)

**Proof of Theorem 3.5.** From Lemma C.4 (summing up from 0 to $N-1$) and Corollary 2, we have:

$$p(X_0) - \mathbb{E}_{U_k} p(X_k) \geq \frac{\tilde{\eta}}{4t} \sum_{k=0}^{N-1} \mathbb{E}_{U_k} \|V_k\|_F^2 - t^2 \left( \frac{4(d+4)}{m} \|\nabla f(X_k)\|_F^2 + \mu^2 L_2^2 (d+6)^3 \right)$$

Since the manifold we are studying is the compact Stiefel manifold, and the function $f$ is Lipschitz smooth, we have that $\|\nabla f(X)\|_F$ is bounded by certain constant $M$. Therefore we have

$$p(X_0) - \mathbb{E}_{U_k} p(X_k) \geq \frac{\tilde{\eta}}{4t} \sum_{k=0}^{N-1} \mathbb{E}_{U_k} \|V_k\|_F^2 - \tilde{\eta} N t \left( \frac{(d+4)}{m} M^2 + \frac{\mu^2 L_2^2}{2} (d+6)^3 \right)$$

i.e.

$$\frac{1}{N} \sum_{k=0}^{N-1} \mathbb{E}_{U_k} \|V_k\|_F^2 \leq \frac{4t (p(X_0) - p(x^*))}{\tilde{\eta} N} + \frac{4(d+4)}{m} t^2 M^2 + 2\mu^2 L_2^2 t^2 (d+6)^3.$$  \hspace{1cm} (48)

[\[\Box\]

Note that our proof only utilizes the fact that Stiefel manifold is compact, and therefore the gradient is bounded. Thus the same theory would apply to other compact manifolds, or other composite optimization problems with the gradient of smooth part bounded.

**D Additional numerical results**

The second problem we discuss is kPCA [ZRS16, TFBJ18, ZYYF19]. kPCA on Grassmannian manifold is a Rayleigh quotient minimization problem:

$$\min_{X \in \text{Grass}(n,p)} \frac{1}{2} \text{Tr}(X^T H X), \ H \in \mathbb{R}^{n \times n}$$  \hspace{1cm} (49)

where $H$ is a symmetric positive definite matrix. This problem could be written into a finite sum problem:

$$\min_{X \in \text{Grass}(n,p)} \sum_{i=1}^{n} \frac{1}{2} \text{Tr}(X^T h_i h_i^T X), \ h_i \in \mathbb{R}^{n \times 1}$$  \hspace{1cm} (50)

The Grassmanian is defined as:

$$\text{Grass}(n,p) = \{\text{span}(X) : X \in \text{St}(n,p)\}.$$  \hspace{1cm} (51)
We refer readers to [AMS09] for details about the Grassmannian quotient manifold. We use our stochastic zeroth-order Riemannian optimization method on this problem, and tuning the choice of multi-sampling number \( m \) (Notice that \( m \) is also the sampling number for random variable \( \xi \), which is the index of \( h_i \) in this problem). In our experiment, \( n = 100 \) and \( p = 50 \), and the matrix \( H \) is generated by \( H = AA^T \), where \( A \in \mathbb{R}^{n \times p} \) is a normalized randomly generated data matrix. We show that multi-sample stochastic zeroth-order Riemannian optimization works almost same as the stochastic Riemannian optimization in Figure 4.

![Figure 4: The convergence curve of ZO-RSGD, ZO-RGD and RSGD (Riemannian stochastic gradient), with different choices of multi-sampling.](image)

Now we consider the sparse PCA problem, which is stated as follows:

\[
\min_{X \in \text{St}(n,p)} -\frac{1}{2}\text{Tr}(X^T A^T A X) + \lambda \|X\|_1
\] (52)

Such a problem naturally enjoys the desired structure for our ManPG framework. For a comprehensive review on this sparse PCA problem, we refer to [ZXS18]. For more problems that fits into the framework of ManPG, we refer to [CMSZ18]. In sparse PCA setting, \( A \in \mathbb{R}^{m \times n} \) is the normalized data matrix, so that \( H = A^T A \) is the covariance matrix. In our numerical experiments, we take \((m,n) = (10,100)\) s.t. \( H \in \mathbb{R}^{100 \times 100} \). We compare our method with the ordinary ManPG algorithm, as well as the Riemannian subgradient method [LCD+19]. We show the result of applying our zeroth-order ManPG to this problem in Figure 5.

### E Implementation Details of Black-Box Attacks

Here we provide our white and black-box Riemannian attack algorithm in Algorithm 4 and 5, respectively. For the black-box attack, to accelerate convergence, we introduce a pre-attack step to search for a sufficient large loss value on the prescribed sphere, still in a black-box manner (only use the function value). For further acceleration of the black-box attack, the hierarchical attack [CZS+17] and the auto-encoder technique [TTC+19] might be applicable. The attack result are shown in Figure 7. We also provide the loss function curve in Figure 6.
Figure 5: The convergence curve of Zo-ManPG and ManPG. We also compare with Riemannian subgradient method in terms of function value, since the convergence of Riemannian subgradient method in terms of norm are not well-studied.

Algorithm 4 White-box attack via Riemannian optimization
1: Input: Original image $\tilde{x}$, original label $y_0$, radius of the attack region $R$, step size $\eta_k$, some convergence criterion.
2: Randomly sample $\delta$ s.t. $\|\delta\| = R$.
3: Set the initial point $x_0 = \tilde{x} + \delta$, $k = 0$.
4: repeat
5: Update $x_{k+1} = R_{x_k}(\eta_k \text{grad}_x L(\theta, x, y))$, $k = k + 1$.
6: until Convergence criterion is met.

Algorithm 5 black-box attack via Riemannian zeroth-order optimization
1: Input: Original image $\tilde{x}$, original label $y_0$, radius of the attack region $R$, step size $\eta_k$, smoothing parameter $\mu$, number of multi-sample $m$, some convergence criterion.
2: Obtain $\delta$ (initial perturbation) by pre-training steps (Algorithm 6).
3: Set the initial point $x_0 = \tilde{x} + \delta$, $k = 0$.
4: repeat
5: Sample $m$ standard Gaussian random matrix $u_i$ on $T_{x_k}M$.
6: Set the random oracle $\bar{g}_\mu(x_k)$ by (26).
7: Update $x_{k+1} = R_{x_k}(\eta_k \bar{g}_\mu(x_k))$, $k = k + 1$.
8: until Convergence criterion is met.
Algorithm 6 Pre-training step for black-box attack

1: **Input:** Original image $\tilde{x}$, original label $y_0$, radius of the attack region $R$, step size $\eta_k$, smoothing parameter $\mu$, number of multi-sample $m$.
2: $x_0 = \tilde{x}$.
3: **repeat**
   4: Sample $m$ standard Gaussian random matrix $u_i$.
   5: Set the random oracle $\bar{g}_\mu(x_k)$ by (26), with $g_\mu(x) = \frac{f(x+\mu u_i)-f(x)}{\mu} u_i$
   6: Update $x_{k+1} = x_k + \eta_k \bar{g}_\mu(x_k)$.
   7: Update $\delta = x_{k+1} - \tilde{x}$, $k = k + 1$.
8: **until** $\|\delta\| \geq R$
9: $\delta = \frac{\delta}{\|\delta\|} R$

Figure 6: Loss function increasing curve while doing our attacks. The three figures correspond to the last three rows in Figure 7. For the failed the PGD attack, we notice that the function value stuck in the middle and then decreased, while white and black-box Riemannian attack increased loss value successfully.
Figure 7: The attack on CIFAR10 picture. From left to right columns: the original image; the PGD attack with a small diameter; white box Riemannian attack on the sphere with the same diameter; black box Riemannian attack on the sphere with the same diameter. Notice that for the figure in the fourth row, the PGD attack failed while the Riemannian attacks succeeded. The diameter is set to be 0.01 times the norm of the original images.