Minimax Efficient Finite-Difference Stochastic Gradient Estimators Using Black-Box Function Evaluations

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Abstract

We consider stochastic gradient estimation using noisy black-box function evaluations. A standard approach is to use the finite-difference method or its variants. While natural, it is open to our knowledge whether its statistical accuracy is the best possible. This paper argues so by showing that central finite-difference is a nearly minimax optimal zeroth-order gradient estimator, among both the class of linear estimators and the much larger class of all (nonlinear) estimators.

1 Introduction

Stochastic gradient estimation is of central importance in simulation analysis and optimization. It concerns the estimation of gradients under noisy environments driven by data or Monte Carlo simulation runs. This problem arises as a key ingredient in sensitivity analysis and uncertainty quantification for simulation models, descent-based algorithms in stochastic optimization and machine learning, and other applications such as financial portfolio hedging. For an overview of stochastic gradient estimation and its applications, see, e.g., [19], [11], [13] Chapter 7 and [1] Chapter 7.

In this paper, we consider stochastic gradient estimation when only a noisy simulation oracle to evaluate the function value or model output is available. This corresponds to black-box settings in which it is costly, or even impossible, to utilize the underlying dynamics of a simulation model, or to distort the data collection mechanism in an experiment given the input. In stochastic optimization, such an oracle is also known as the zeroth-order [12, 20]. These gradient estimators are in contrast to unbiased estimators obtained from methods such as the infinitesimal perturbation analysis [15, 17], the likelihood ratio or score function method [14, 22, 21], measure-valued differentiation [16] and other variants that require structural information on model dynamics.

Under the above setting, the most natural and common approach is to use the finite-difference (FD) method [26, 9, 10]. This entails simulating the function values at two neighboring inputs and using the first principle to approximate the derivative. The resulting estimator has a bias coming from this derivative approximation, on top of the variance coming from the function evaluation noise. This leads to a subcanonical overall mean squared error (MSE) and a need to rightly tune

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the perturbation size between the two input values. It is widely known that, for twice continuously differentiable functions, the optimal attainable MSE for central finite-difference (CFD) schemes is of order $O(n^{-2/3})$, where $n$ refers to the number of differencing pairs in the simulation. On the other hand, when one uses forward or backward finite-differences, the optimal MSE deteriorates to $O(n^{-1/2})$.

Although the optimal MSEs within the classes of FD schemes are well-known, a question arises whether these classes are optimal or better compared to other, possibly much larger, classes of gradient estimators. Our goal in this paper is to give a first such study on the optimality on a class level.

Our main results show that, under a general setting, CFD is nearly optimal among any possible gradient estimation schemes. This optimality is in a minimax sense. Namely, we consider the MSE of any gradient estimator over a collection of twice differentiable functions with unknown function characteristics (e.g., function value and higher-order gradients). Subject to this uncertainty of the function, we consider the minimizer of the worst-case MSE over this function collection, giving rise to what we call the minimax risk. Among the class of linear estimators, we show that, in the one-dimensional case, CFD exactly achieves the minimax risk, whereas in the multi-dimensional case it achieves so up to a multiplicative factor that depends sublinearly on the input dimension. Furthermore, we show that, among the much larger class of all nonlinear estimators, CFD remains nearly minimax optimal up to a multiplicative factor that is polynomial in the dimension.

In terms of methodological contributions, we derive our linear minimax results by using a new elementary proof. We derive our general minimax results via Le Cam’s method \cite{24} with the imposition of an adversarially chosen hypothesis test, and the notion of modulus of continuity \cite{5} to obtain the worst-case functions derived from this test. Lastly, we also demonstrate that, without extra knowledge on the gradient, randomized schemes such as simultaneous perturbation will lead to unbounded worst-case risks in general, due to the interaction between the gradient magnitude and the additional variance coming from the random perturbation. This indicates that less conservative analyses along this line would require more information on the magnitude of the gradient of interest.

Our work is related to, and contrasted with, the derivative estimation in nonparametric regression (e.g., \cite{6, 7}), which focuses on the estimation of the conditional expectations and their derivatives given input values, a similar setting as ours. However, in these studies the data and in particular the available input values are often assumed given a priori. In contrast, in stochastic gradient estimation and optimization, one often has the capability to select the input points at which the function evaluation is conducted. This therefore endows more flexibility than nonparametric regression and, correspondingly, translates to superior minimax rates in our setting. For example, \cite{7} has established a minimax risk of order $O(n^{-4/7})$ for nonparametric derivative estimation, which is slower than our $O(n^{-2/3})$. Finally, we note that other works \cite{2, 3, 25} have studied derivative estimation uniformly well over regular or equi-spaced input design points. Moreover, these papers consider asymptotic risks as the number of input points grow, in contrast to the finite-sample results in this work.

The remainder of the paper is as follows. Section 2 focuses on linear minimax risk and the corresponding optimal or nearly optimal estimators. Section 3 focuses on general risks and estimators. Section 4 concludes the paper and discusses future directions.
2 Linear Minimax Risk and Optimal Estimators

In this section we focus on the class of linear estimators. Section 2.1 first presents the single-dimensional case. Section 2.2 generalizes it to higher-dimensional counterparts, and Section 2.3 further studies the use of simultaneous random perturbation in this setting. We will derive bounds on minimax risks and show that CFD is a nearly optimal estimator. Furthermore, these bounds are tight for any finite sample in the single-dimensional case, and also in the multi-dimensional case under additional restrictions.

2.1 Single-Dimensional Case

We first introduce our setting. Let \( f(\cdot) : \mathbb{R} \to \mathbb{R} \) be a performance measure of interest, where we have access to an unbiased estimate \( Y(x) \) for any chosen \( x \in \mathbb{R} \). In other words, \( Y(\cdot) \) is a family of random variables indexed by \( x \) such that \( E[Y(x)] = f(x) \) and \( Var(Y(x)) = \sigma^2(x) \) for any \( x \in \mathbb{R} \). Suppose \( x_0 \) is the point of interest. Our goal is to estimate the derivative \( f'(x_0) \).

Given simulation budget \( n \geq 1 \), we can simulate independently at input design points \( x_0 + \delta_j \), \( j = 1, \cdots, n \), with \( \delta_j \) of our choice, giving outputs \( Y_j(x_0 + \delta_j) \)’s. We consider the class of linear estimators in the form

\[
L_n = \sum_{j=1}^{n} w_j Y_j(x_0 + \delta_j),
\]

where \( w_j \) are the linear coefficients or weights. Note that for even budget \( n \) the CFD scheme

\[
\bar{L}_n = \frac{1}{n/2} \sum_{j=1}^{n/2} Y_{2j-1}(x_0 + \delta) - Y_{2j}(x_0 - \delta)
\]

is an example of linear estimators where \( \delta_j = (-1)^{j+1} \delta \) and \( w_j = \frac{(-1)^{j+1}}{n \delta} \), for a perturbation size \( \delta \).

We aim to study the optimality within the class of all linear estimators in the form (1), and in particular investigate the role of CFD. We use the MSE as a performance criterion, which depends on the a priori unknown function \( f \). Our premise is a minimax framework that seeks for schemes to minimize the worst-case MSE, among a suitable wide enough class of function \( f \) and simulation noise. More precisely, we consider

\[
\mathcal{A} = \{ f(\cdot) : f^{(2)}(x_0) \text{ exists}, |f^{(2)}(x_0)| \leq b \text{ and } |f(x) - f(x_0) - f'(x_0)(x-x_0) - \frac{f^{(2)}(x_0)}{2}(x-x_0)^2| \leq \frac{a}{6}|x-x_0|^3 \}
\]

and

\[
\mathcal{B} = \{ \sigma^2(\cdot) : \sigma^2(x) \leq d \},
\]

where \( a, b, d > 0 \) are assumed given. In fact, as we will see, the parameter \( b \) does not play a role in our deductions.

Roughly speaking, \( \mathcal{A} \) contains all twice differentiable functions whose second-order derivative is absolutely bounded by \( b \) and third-order derivative is absolutely bounded by \( a \). This characterization is not exact, however, since the Taylor-series type expansion in (3) applies only to the point \( x_0 \), and thus \( \mathcal{A} \) is more general than the aforementioned characterization. The reason for proposing this class, instead of other similar ones, is that \( \mathcal{A} \) allows us to obtain a very accurate minimax analysis and derivation of optimal estimators.
We define the linear minimax $L_2$-risk as

$$R(n, \mathcal{A}, \mathcal{B}) = \inf_{\delta, j=1, \ldots, n} \sup_{w_j, j=1, \ldots, n} \mathbb{E}(L_n - f'(x_0))^2,$$

which is the minimum worst-case MSE among all functions $f \in \mathcal{A}$ and noise levels in $\mathcal{B}$. The linear estimators are selected through the design points $x_0 + \delta_j$’s and linear coefficients $w_j$’s.

The following theorem gives the exact expression for the minimax risk, and shows that a suitably calibrated CFD attains this risk level. In other words, CFD is the optimal linear estimator among the problem class specified by $(\mathcal{A}, \mathcal{B})$. The proof of this result involves only elementary inequalities.

**Theorem 1.** For any $n \geq 1$,

$$R(n, \mathcal{A}, \mathcal{B}) \geq \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}.$$

Besides, if the budget $n$ is even, the CFD estimator $\bar{L}_n$ in (2) with $\delta = (\frac{18d}{a^2})^{1/6} \frac{1}{n^{1/6}}$ satisfies

$$\sup_{f(\cdot) \in \mathcal{A}, \sigma^2(\cdot) \in \mathcal{B}} \mathbb{E}((\bar{L}_n - f'(x_0))^2) = \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}.$$

Thus the estimator $\bar{L}_n$ is the best linear estimator in the class of problems defined by $(\mathcal{A}, \mathcal{B})$.

**Proof.** For any designs $\delta_j, j = 1, \ldots, n$ and linear coefficients $w_j, j = 1, \ldots, n$, supposing $f(\cdot) \in \mathcal{A}$ and $f(\cdot) \in C^3(\mathbb{R})$, we have, by Taylor’s expansion,

$$f(x_0 + \delta_j) = f(x_0) + f'(x_0)\delta_j + \frac{f^{(2)}(x_0)}{2} \delta_j^2 + \frac{f^{(3)}(x_0 + t_j\delta_j)}{6} \delta_j^3,$$

for any $j = 1, \ldots, n$, where $0 \leq t_j \leq 1$. Thus the bias of the estimator $L_n$ is

$$EL_n - f'(x_0) = f(x_0) \sum_{j=1}^n w_j + f'(x_0) \left( \sum_{j=1}^n w_j\delta_j - 1 \right) + \frac{f^{(2)}(x_0)}{2} \sum_{j=1}^n w_j\delta_j^2 + \sum_{j=1}^n \frac{f^{(3)}(x_0 + t_j\delta_j)}{6} w_j\delta_j^3.$$

On the other hand, the variance of the estimator $L_n$ is

$$Var(L_n) = \sum_{j=1}^n w_j^2 \sigma^2(x_0 + \delta_j).$$

If $\sum_{j=1}^n w_j \neq 0$, we consider the particular cases where $f'(x) = f^{(2)}(x) = f^{(3)}(x) = 0$ for all $x$, and $f(x_0)$ arbitrary, concluding that

$$\sup_{f(\cdot) \in \mathcal{A}} (EL_n - f'(x_0))^2 = \infty.$$

Therefore, for the purpose of deriving a lower bound, we can assume without loss of generality that $\sum_{j=1}^n w_j = 0$. Similarly we can assume $\sum_{j=1}^n w_j\delta_j - 1 = 0$. Furthermore, if $\delta_i = \delta_j$, we
assume w.l.o.g. \( w_i = w_j \) since it leads to smaller variance. Now consider \( f(\cdot) \in \mathcal{A} \) such that \( f(x_0 + \delta_j) = \frac{a}{6} |\delta_j|^3 \cdot \text{sign}(w_j) \), and \( f(x) = 0 \) otherwise. In such a case the MSE simplifies to

\[
\left( \sum_{j=1}^{n} \frac{a}{6} |w_j \delta_j^3| \right)^2 + \sum_{j=1}^{n} w_j^2 \sigma^2(x_0 + \delta_j).
\]

Further considering the case \( \sigma^2(x_0 + \delta_j) = d \), we get

\[
\sup_{f(\cdot) \in \mathcal{A}, \sigma^2(\cdot) \in \mathcal{B}} E(L_n - f'(x_0))^2 \geq \frac{a^2}{36} \left( \sum_{j=1}^{n} |w_j \delta_j^3| \right)^2 + d \sum_{j=1}^{n} w_j^2.
\]

Now since \( \sum_{j=1}^{n} w_j \delta_j = 1 \), by Hölder’s inequality,

\[
1 \leq \sum_{j=1}^{n} |w_j|^{1/3} |\delta_j||w_j|^{2/3} \leq \left( \sum_{j=1}^{n} |w_j \delta_j^3| \right)^{1/3} \left( \sum_{j=1}^{n} |w_j| \right)^{2/3}
\]

and so

\[
\left( \sum_{j=1}^{n} |w_j \delta_j^3| \right)^2 \geq \frac{1}{\left( \sum_{j=1}^{n} |w_j| \right)^2} \geq \frac{1}{n^2 \left( \sum_{j=1}^{n} w_j^2 \right)^2},
\]

where we used Hölder’s inequality \( \left( \sum_{j=1}^{n} |w_j| \right)^2 \leq n \left( \sum_{j=1}^{n} w_j^2 \right) \). Thus

\[
\sup_{f(\cdot) \in \mathcal{A}, \sigma^2(\cdot) \in \mathcal{B}} E(L_n - f'(x_0))^2 \geq \frac{a^2}{36} \frac{1}{n^2 \left( \sum_{j=1}^{n} w_j^2 \right)^2} + d \sum_{j=1}^{n} w_j^2 \geq \left( \frac{3a^2 d^2}{16} \right)^{1/3} n^{-2/3},
\]

where the lower bound is achieved at

\[
\sum_{j=1}^{n} w_j^2 = \left( \frac{a^2}{d} \right)^{1/3} \frac{1}{18^{1/3} n^{2/3}}.
\]

Since \( \delta_j, w_j \) are arbitrary, we conclude that

\[
\inf_{\delta_j, j=1, \ldots, n} \sup_{f(\cdot) \in \mathcal{A}, \sigma^2(\cdot) \in \mathcal{B}} E(L_n - f'(x_0))^2 \geq \left( \frac{3a^2 d^2}{16} \right)^{1/3} n^{-2/3}. \tag{4}
\]

On the other hand, supposing the budget \( n \) is even, we see that the bias of the estimator \( \tilde{L}_n \) satisfies

\[
|E\tilde{L}_n - f'(x_0)| = \left| \frac{f(x_0 + \delta) - f(x_0 - \delta)}{2\delta} - f'(x_0) \right| = \left| \frac{f(x_0 + \delta) - f(x_0 - \delta) - 2\delta f'(x_0)}{2\delta} \right|
\]

\[
= \left| \left( f(x_0 + \delta) - f(x_0) - f'(x_0) \delta - \frac{f''(x_0)}{2} \delta^2 \right) - \left( f(x_0 - \delta) - f(x_0) + f'(x_0) \delta - \frac{f''(x_0)}{2} \delta^2 \right) \right|
\]

\[
\leq \frac{\left| f(x_0 + \delta) - f(x_0) - f'(x_0) \delta - \frac{f''(x_0)}{2} \delta^2 \right|}{2\delta} + \frac{\left| f(x_0 - \delta) - f(x_0) + f'(x_0) \delta - \frac{f''(x_0)}{2} \delta^2 \right|}{2\delta} \leq \frac{a}{6} \delta^2.
\]
Theorem 2. For any $\omega_n$ estimate up to a multiplicative factor depending sublinearly on $p$, the restriction on the "third-order gradient" characterized by the $\|
abla^2 f(x_0)\|_2$ is the main distinction of the multi-dimensional setting described above, compared to the single-dimensional case, is the restriction on the "third-order gradient" characterized by the $\|
abla^2 f(x_0)\|_2$. Intuitively, the main distinction of the multi-dimensional setting described above, compared to the single-dimensional case, is the restriction on the "third-order gradient" characterized by the $\|
abla^2 f(x_0)\|_2$. We consider $R$ lower estimate of $\|f(\cdot)\|_q$ norm, where the choice of $R$ can affect the resulting risk bounds. The following theorem provides a lower estimate of $R$ and shows that applying CFD on each of the $p$ dimensions matches this lower estimate up to a multiplicative factor depending sublinearly on $p$. This implies in particular that multi-dimensional CFD is rate-optimal in the sample size $n$. Moreover, if the signs of the weights $w_j$ in $L_n^p$ are further restricted to be the same across components, then CFD achieves the exact minimax risk when $p = 1$ or 2.

**Theorem 2.** For any $n \geq 1$,

$$R_p(n, \mathcal{A}_q, \mathcal{B}) \geq p^{4/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \text{ for } q = 1, 2; \quad (6)$$

$$R_p(n, \mathcal{A}_q, \mathcal{B}) \geq p^{2/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \text{ for } q = \infty. \quad (7)$$
Besides, if the budget $n$ is a multiple of both $p$ and 2, we allocate $n/p$ budget and form the CFD estimator with $\delta = (\frac{\text{number of dimensions}}{\text{number of coefficients}})^{1/6} \frac{1}{(n/p)^{1/6}}$ on each dimension. Denote the resulting estimator as $\bar{L}_n$. Then

$$
\sup_{f(\cdot) \in A, \sigma(\cdot) \in B} E\|\bar{L}_n - \nabla f(x_0)\|_2^2 = p^{5/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}.
$$

Thus the estimator $\bar{L}_n$ is optimal in the class of problems defined by $(A, \sigma)$ up to a sublinear multiplicative factor in $p$. Moreover, if we further restrict each coefficient $w_j$ to have the same sign across components, i.e. $\text{sign}((w_j)_k) = \text{sign}((w_j)_l)$ for any $1 \leq k, l \leq p$, then we have

$$
R_p(n, A, B) \geq p^{5/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \quad \text{for } q = 1, 2;
$$

$$
R_p(n, A, B) \geq p \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \quad \text{for } q = \infty
$$

for this restricted class of linear estimators, so that $\bar{L}_n$ is exactly optimal when considering function class $A_q$ with $q = 1, 2$.

We remark that the $p^{1/3}$ gap between (6) and (8) is due to a technical challenge that the $l_\infty \to l_2$ matrix norm does not admit an explicit expression. This challenge is bypassed if one restricts the same sign across all components in each coefficient, which recovers the minimax optimality of CFD.

**Proof.** Suppose $f(\cdot) \in A_q, f(\cdot) \in C^3(\mathbb{R}^p)$. According to Taylor’s expansion

$$
f(x_0 + \delta_j) = f(x_0) + \nabla f(x_0)^T \delta_j + \frac{1}{2} \delta_j^T \nabla^2 f(x_0) \delta_j + \frac{1}{6} \sum_{k_1,k_2,k_3} (\nabla^3 f(x_0 + t_j \delta_j))_{k_1,k_2,k_3} (\delta_j)_{k_1} (\delta_j)_{k_2} (\delta_j)_{k_3},
$$

for any $j = 1, \ldots, n$, where $0 \leq t_j \leq 1$. Thus the bias of the estimator $L_n^p$ satisfies

$$
E(L_n^p)_i - (\nabla f(x_0))_i = f(x_0) \sum_{j=1}^n (w_j)_i + \nabla f(x_0)^T \left( \sum_{j=1}^n (w_j)_i \delta_j - e_i \right) + \sum_{j=1}^n \frac{1}{2} (w_j)_i \delta_j^T \nabla^2 f(x_0) \delta_j + \sum_{j=1}^n \frac{1}{6} (w_j)_i \sum_{k_1,k_2,k_3} (\nabla^3 f(x_0 + t_j \delta_j))_{k_1,k_2,k_3} (\delta_j)_{k_1} (\delta_j)_{k_2} (\delta_j)_{k_3},
$$

where $e_i$ is the ith standard basis in $\mathbb{R}^p$. On the other hand, the variance of the estimator $L_n^p$ is

$$
E\|L_n^p - EL_n^p\|_2^2 = \sum_{i=1}^p \text{Var}((L_n^p)_i) = \sum_{i=1}^p \left( \sum_{j=1}^n (w_j)_i \sigma^2(x_0 + \delta_j) \right).
$$

If $\sum_{j=1}^n (w_j)_i \neq 0$, we consider the particular cases where $(\nabla f(x))_{k_1} = 0, (\nabla^2 f(x))_{k_1,k_2} = 0, (\nabla^3 f(x))_{k_1,k_2,k_3} = 0$ for all $x$ and $k_1, k_2, k_3$, and $f(x_0)$ arbitrary, concluding that

$$
\sup_{f(\cdot) \in A_q} (E(L_n^p)_i - (\nabla f(x_0))_i)^2 = \infty.
$$

Thus, like in the proof for Theorem [1] for the purpose of deriving a lower bound, we can assume without loss of generality that $\sum_{j=1}^n w_j = 0$. Similarly we can assume $\sum_{j=1}^n (w_j)_i \delta_j - e_i = 0.$
Furthermore, if \( \delta_i = \delta_j \), we assume w.l.o.g. \( w_i = w_j \) since it leads to smaller variance. Now consider \( f(\cdot) \in \mathcal{A}_q \) such that \( f(x_0 + \delta_j) = \frac{\alpha}{6} \|\delta_j\|_q^3 \cdot \text{sign}((w_j)_{i_0}) \), and \( f(x) = 0 \) otherwise, where

\[
i_0 = \arg \max_{1 \leq i \leq p} \sum_{j=1}^{n} (w_j)_i \|\delta_j\|_q^3.
\]

In such a case the MSE is bounded from below by

\[
\left( \sum_{j=1}^{n} \frac{\alpha}{6} ((w_j)_{i_0}) \|\delta_j\|_q^3 \right)^2 + \sum_{i=1}^{p} \left( \sum_{j=1}^{n} (w_j)_i \|\delta_j\|_q^3 \right)^2.
\]

Considering the case \( \sigma^2(x_0 + \delta_j) = d \), we get

\[
\sup_{f(\cdot) \in \mathcal{A}_q, \sigma^2(\cdot) \in \mathcal{B}} E\|L^p_n - \nabla f(x_0)\|^2 \geq \frac{\alpha^2}{36} \left( \sum_{j=1}^{n} (w_j)_{i_0} \|\delta_j\|_q^3 \right)^2 + d \sum_{j=1}^{n} \|w_j\|_2^2. \tag{9}
\]

Now since \( \sum_{j=1}^{n} (w_j)_{i_0} \|\delta_j\|_q = 1 \), by Hölder’s inequality,

\[
p = \sum_{j=1}^{n} w_j^T \delta_j \leq \sum_{j=1}^{n} \|w_j\|_r^{1/3} \|\delta_j\|_q \|w_j\|_r^{2/3} \leq \left( \sum_{j=1}^{n} \|w_j\|_r \|\delta_j\|_q \right)^{1/3} \left( \sum_{j=1}^{n} \|w_j\|_r \right)^{2/3},
\]

where \( \frac{1}{q} + \frac{1}{r} = 1 \). Thus

\[
\frac{p^6}{\left( \sum_{j=1}^{n} \|w_j\|_r \right)^4} \leq \left( \sum_{j=1}^{n} \|w_j\|_r \|\delta_j\|_q \right)^2 \leq \left( \sum_{j=1}^{n} \|w_j\|_1 \|\delta_j\|_q \right)^2 \leq p^2 \left( \sum_{j=1}^{n} (w_j)_{i_0} \|\delta_j\|_q \right)^2.
\]

Since by Hölder’s inequality,

\[
\left( \sum_{j=1}^{n} \|w_j\|_r \right)^2 \leq \left( \sum_{j=1}^{n} \|w_j\|_2 \right)^2 \leq n \left( \sum_{j=1}^{n} \|w_j\|_2 \right), \quad r \geq 2
\]

\[
\left( \sum_{j=1}^{n} \|w_j\|_r \right)^2 \leq p \left( \sum_{j=1}^{n} \|w_j\|_2 \right)^2 \leq np \left( \sum_{j=1}^{n} \|w_j\|_2 \right), \quad r = 1
\]

we have

\[
\sup_{f(\cdot) \in \mathcal{A}_q, \sigma^2(\cdot) \in \mathcal{B}} E\|L^p_n - \nabla f(x_0)\|^2 \geq \frac{\alpha^2}{36} \frac{p^4}{n^2 \left( \sum_{j=1}^{n} \|w_j\|_2^2 \right)^2} + d \sum_{j=1}^{n} \|w_j\|_2^2 \geq p^{4/3} \left( \frac{3\alpha^2 d^2}{16} \right)^{1/3} n^{-2/3}, \quad q = 1, 2
\]

where the lower bound is achieved at

\[
\sum_{j=1}^{n} \|w_j\|_2^2 = \left( \frac{\alpha^2}{d} \right)^{1/3} \frac{p^{4/3}}{18^{1/3} n^{2/3}},
\]
and

\[ \sup_{f(\cdot) \in \mathcal{A}_q, \sigma^2(\cdot) \in \mathcal{B}} E\|L_n^p - \nabla f(x_0)\|_2^2 \geq \frac{a^2}{36} n^{-2/3} \leq \frac{p^2}{n^2} \left( \sum_{j=1}^n \|w_j\|_2^2 \right)^2 + d \sum_{j=1}^n \|w_j\|_2^2 \geq p^{2/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \quad q = \infty \]

where the lower bound is achieved at

\[ \sum_{j=1}^n \|w_j\|_2^2 = \left( \frac{a^2}{d} \right) \frac{p^{2/3}}{18^{1/3} n^{2/3}}. \]

Since \( \delta_j, w_j \) are arbitrary, we conclude that

\[ \inf_{\delta_j, j=1, \ldots, n} \sup_{f(\cdot) \in \mathcal{A}_q, \sigma^2(\cdot) \in \mathcal{B}} E\|L_n^p - \nabla f(x_0)\|_2^2 \geq p^{4/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \quad q = 1, 2, \]

\[ \inf_{\delta_j, j=1, \ldots, n} \sup_{f(\cdot) \in \mathcal{A}_q, \sigma^2(\cdot) \in \mathcal{B}} E\|L_n^p - \nabla f(x_0)\|_2^2 \geq p^{2/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \quad q = \infty. \]

Now supposing in addition that each \( w_j \) has the same sign across components, then instead of \( \emptyset \), we have the sharper lower bound

\[ \frac{a^2}{36} \sum_{i=1}^p \left( \sum_{j=1}^n |(w_j)_i| ||\delta_j||^3_q \right)^2 + d \sum_{j=1}^n \|w_j\|_2^2. \]

Note that by Hölder’s inequality

\[ \left( \sum_{j=1}^n \|w_j\|_1 ||\delta_j||^3_q \right) \leq p \sum_{i=1}^p \left( \sum_{j=1}^n |(w_j)_i| ||\delta_j||^3_q \right)^2. \]

Thus the \( p^{1/3} \) factor in \( \emptyset \) can be improved to \( p^{5/3} \); and the \( p^{2/3} \) factor in \( \emptyset \) can be improved to \( p \). Finally, suppose the budget \( n \) is a multiple of \( p \) and 2. We allocate \( n/p \) budget to each dimension. Then for any \( f(\cdot) \in \mathcal{A}_q \) and \( \sigma^2(\cdot) \in \mathcal{B} \), we get

\[ E \left( (L_n^p)_i - (\nabla f(x_0))_i \right)^2 \leq \left( \frac{3a^2d^2}{16} \right)^{1/3} \left( \frac{n}{p} \right)^{-2/3} = p^{2/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}. \]

Thus

\[ E\|L_n^p - \nabla f(x_0)\|_2^2 \leq p^{5/3} \left( \frac{3a^2d^2}{16} \right)^{1/3} n^{-2/3}, \]

which completes our proof. \( \square \)
2.3 Randomized Design

The discussion above has focused on deterministic designs in which the perturbation sizes \( \delta_j \) are fixed. In multi-dimensional gradient estimation, it is also common to use random perturbation in which a random vector in \( \mathbb{R}^p \) is generated and FD is taken simultaneously for all dimensions by projecting the vector onto each direction. This leads to schemes such as simultaneous perturbation [23] and Gaussian smoothing [20], and are frequently used in stochastic optimization. A question arises how these randomized schemes perform with respect to our presented risk criterion.

To proceed, let \( \delta \) be a random vector in \( \mathbb{R}^p \) where \( \delta^i, i = 1, \ldots, p \) are i.i.d. symmetrically distributed about 0 and satisfy some additional properties (described in, e.g., [23], which will not concern us as we will see), and let \( \phi(\delta) = (1/\delta^1, \ldots, 1/\delta^p)^T \). Other distributional choices of \( \delta \) and the associated \( \phi \) have also been suggested (e.g., [20, 8]), for which our subsequent argument follows similarly. Suppose the simulation budget \( n \) is even. We choose a scaling parameter \( h > 0 \), then repeatedly and independently simulate \( \delta_j \in \mathbb{R}^p \) and \( Y_j(\cdot) \)'s and output

\[
S_n = \frac{1}{n/2} \sum_{j=1}^{n/2} Y_{2j-1}(x_0 + h\delta_j) - Y_{2j}(x_0 - h\delta_j) / 2h \phi(\delta_j).
\]

The following theorem shows that, without further assumptions on the magnitude of the first-order gradient, the \( L_2 \)-risk of random perturbation can be arbitrarily large.

**Theorem 3.** For any \( n \geq 2 \) even,

\[
\sup_{f(\cdot) \in \mathcal{A}_q, \sigma^2(\cdot) \in \mathbb{R}} E\|S_n - \nabla f(x_0)\|_2^2 = \infty.
\]

**Proof.** First note that by independence,

\[
E\|S_n - ES_n\|_2^2 = \frac{2}{n} \text{tr} \left( \text{Cov} \left( \frac{Y(x_0 + h\delta) - Y(x_0 - h\delta)}{2h} \phi(\delta) \right) \right) = \frac{2}{n} \sum_{i=1}^p \text{Var} \left( \frac{Y(x_0 + h\delta) - Y(x_0 - h\delta)}{2h\delta^i} \right).
\]

Next, by conditioning on \( \delta \), we have

\[
\text{Var} \left( \frac{Y(x_0 + h\delta) - Y(x_0 - h\delta)}{2h\delta^i} \right) = \text{Var} \left( \frac{f(x_0 + h\delta) - f(x_0 - h\delta)}{2h\delta^i} \right) + E \left[ \frac{\sigma^2(x_0 + h\delta) + \sigma^2(x_0 - h\delta)}{4h^2\delta^i} \right] \geq \text{Var} \left( \frac{f(x_0 + h\delta) - f(x_0 - h\delta)}{2h\delta^i} \right).
\]

Now consider \( f(\cdot) \in \mathcal{A}_q \) and \( f(x) = f(x_0) + \rho \mathbf{1}^T(x - x_0) \), where \( \rho \in \mathbb{R} \) and \( \mathbf{1} \in \mathbb{R}^p \) denotes the vector of all ones. Thus we get

\[
\text{Var} \left( \frac{f(x_0 + h\delta) - f(x_0 - h\delta)}{2h\delta^i} \right) = \rho^2 \text{Var} \left( \frac{\mathbf{1}^T \delta}{\delta^i} \right) > 0.
\]

Sending \( \rho \to \infty \) we conclude that

\[
\sup_{f(\cdot) \in \mathcal{A}_q} \text{Var} \left( \frac{f(x_0 + h\delta) - f(x_0 - h\delta)}{2h\delta^i} \right) = \infty.
\]
Finally note the bias-variance decomposition,
\[ E\|S_n - \nabla f(x_0)\|^2_2 = \|ES_n - \nabla f(x_0)\|^2_2 + E\|S_n - ES_n\|^2_2 \geq E\|S_n - ES_n\|^2_2 \geq \frac{2}{n} \sum_{i=1}^p \text{Var}\left( \frac{f(x_0 + h\delta) - f(x_0 - h\delta)}{2h\delta} \right). \]
which completes our proof.

The unboundedness of the worst-case $L_2$-risk in Theorem 3 is due to the interaction between the gradient of interest and the variance from the random perturbation. This hints that in general, to restrain the worst-case $L_2$-risk for such schemes, extra knowledge on the magnitude of the gradient is needed.

### 3 General Minimax Risk

We now expand our analysis to consider estimators that are possibly nonlinear. Section 3.1 first presents the single-dimensional case. Section 3.2 then presents the generalization to the multi-dimensional counterpart. We derive bounds for the minimax risks and show that, in these expanded classes, the CFD estimators are still nearly optimal.

#### 3.1 Single-Dimensional Case

Adopting the notations from the previous sections, suppose the budget is $n$. We select the input design points $x_1, \cdots, x_n$ and for convenience let $Y_j = Y_j(x_j)$ be the independent unbiased noisy function evaluation of $f$ at $x_j$ with simulation variance $\sigma^2(x_j)$. We are interested in estimating $f'$ at $x_0$, which w.l.o.g. we take as the origin 0. Denote $\hat{\theta} = \hat{\theta}(Y_1, \cdots, Y_n)$ as a generic estimator. We consider the class of problems specified by

\[ \mathcal{A} = \{f : f^{(2)}(0) \text{ exists}, \quad |f(x) - f(0) - f'(0)x - \frac{f^{(2)}(0)}{2}x^2| \leq \frac{a}{6}|x|^3 \text{ and } |f^{(2)}(0)| \leq b\} \]
and

\[ \mathcal{B} = \{\sigma^2(\cdot) : \sigma^2(x) \leq d\}, \]
where $a, b, d > 0$. Like in Section 2, the parameter $b$ does not play a role subsequently. Define the minimax risk as

\[ R(n, \mathcal{A}, \mathcal{B}) = \inf_{\hat{\theta}} \sup_{f_j, j=1,\cdots,n, f(\cdot) \in \mathcal{A}, \sigma^2(\cdot) \in \mathcal{B}} E(\hat{\theta} - \hat{f}'(0))^2. \]

**Theorem 4.** For any $n \geq 1$,

\[ R(n, \mathcal{A}, \mathcal{B}) \geq \frac{1}{16} e^{-2/3} \left( \frac{3ad}{n} \right)^{2/3}. \tag{12} \]
Consequently, the CFD estimator $\hat{L}_n$ in (2) is optimal up to a constant multiplicative factor.

The last conclusion in Theorem 4 is a simple consequence from combining the risk estimate of $\hat{L}_n$ in Theorem 1 with (12). In contrast to the elementary proof for Theorem 1, here we use Le Cam’s method (e.g., [24]) and the notion of modulus of continuity [3] to estimate the minimax risk. Specifically, Le Cam’s method derives minimax lower bounds by constructing a hypothesis test and
using its error to inform a bound. The error of the hypothesis test, in turn, is analyzable by the Neyman-Pearson lemma. The lower bound provided by Le Cam’s method involves the distance between two functions, and tightening the lower bound then becomes a functional optimization problem that can be viewed as the dual or inverse of the formulation to attain the so-called modulus of continuity. Consequently, finding the extremal or worst-case functions for the inverse modulus of continuity will give the resulting lower bound.

**Proof.** Consider arbitrary functions \( f_1, f_2 \in \mathcal{F} \), we follow Le Cam’s method. Now for any estimator \( \hat{\theta} \), we have

\[
\epsilon^2 = (f'_1(0) - f'_2(0))^2 \leq 2(\hat{\theta} - f'_1(0))^2 + 2(\hat{\theta} - f'_2(0))^2.
\]

Define test statistic \( \psi \) by

\[
\psi(Y_1, \cdots, Y_n) = \begin{cases} 
1 & \text{if } |\hat{\theta} - f'_2(0)| \leq |\hat{\theta} - f'_1(0)|, \\
2 & \text{if } |\hat{\theta} - f'_2(0)| > |\hat{\theta} - f'_1(0)|.
\end{cases}
\]

Let \( E_k, k = 1, 2 \) denote the expectation (and \( P_k \) and \( p_k \) as the probability measure and density) under model

\[
Y_j \sim f_k(x_j) + \eta_j, j = 1, \cdots, n,
\]

where \( \eta_j, j = 1, \cdots, n \) i.i.d. follows normal distribution with mean zero and variance \( d \). We have

\[
E_k(\hat{\theta} - f'_k(0))^2 \geq E_k(\hat{\theta} - f'_k(0))^2 I(\psi = k) \geq \frac{\epsilon^2}{4} P_k(\psi = k).
\]

Thus

\[
\sup_{f \in \mathcal{F}, \sigma^2 \in \mathcal{B}} E(\hat{\theta} - f'(0))^2 \geq \max_{k=1,2} E_k(\hat{\theta} - f'_k(0))^2 \geq \frac{\epsilon^2}{4} P_1(\psi = 1) + P_2(\psi = 2).
\]

Taking infimum over all possible estimators, we get

\[
\inf_{\hat{\theta}} \sup_{f \in \mathcal{F}, \sigma^2 \in \mathcal{B}} E(\hat{\theta} - f'(0))^2 \geq \frac{\epsilon^2}{8} \inf_{\psi}(P_1(\psi = 1) + P_2(\psi = 2)).
\]

The right hand side is minimized by the Neyman-Pearson test, i.e.

\[
\psi_0(y_1, \cdots, y_n) = \begin{cases} 
1 & \text{if } p_2(y_1, \cdots, y_n) \geq p_1(y_1, \cdots, y_n), \\
2 & \text{if } p_2(y_1, \cdots, y_n) < p_1(y_1, \cdots, y_n).
\end{cases}
\]

Thus by a standard relation (e.g. Lemma 2.6 in [24])

\[
\inf_{\hat{\theta}} \sup_{f \in \mathcal{F}, \sigma^2 \in \mathcal{B}} E(\hat{\theta} - f'(0))^2 \geq \frac{\epsilon^2}{8} \int \min\{p_1(y_1, \cdots, y_n), p_2(y_1, \cdots, y_n)\} dy \geq \frac{\epsilon^2}{16} e^{-KL(P_1, P_2)},
\]

where \( KL(P_1, P_2) \) denote the KL divergence between the distributions \( P_1, P_2 \). Now since \( P_1 \sim \mathcal{N}(\mu_1, d\mathcal{I}_{n \times n}) \) and \( P_2 \sim \mathcal{N}(\mu_2, d\mathcal{I}_{n \times n}) \), where \( \mu_k = (f_k(x_1), \cdots, f_k(x_n)), k = 1, 2 \), by direct computation,

\[
KL(P_1, P_2) = \frac{1}{2d}(\mu_2 - \mu_1)^T(\mu_2 - \mu_1) = \frac{1}{2d}\|\mu_2 - \mu_1\|_2^2 \leq \frac{n}{2d} \sup_x |f_1(x) - f_2(x)|^2.
\]
To this end, we consider a constrained functional optimization problem for each \( \epsilon \):

\[
\omega(\epsilon) = \inf \left\{ \sup_x |f_1(x) - f_2(x)| : |f_1'(0) - f_2'(0)| = \epsilon, f_1, f_2 \in \mathcal{A} \right\}. \tag{13}
\]

Solving the optimization in (13) yields a tightest upper bound for \( KL(P_1, P_2) \), and further obtains a tightest lower bound for \( \frac{1}{n} e^{-KL(P_1, P_2)} \). The decision variables in the outer problem in (13) are a pair of functions \((f_1, f_2)\), where we would later denote \((f_1^*, f_2^*)\) as the solutions, which constitute the extremal or worst-case functions. Note that \( \omega(\epsilon) \) is the inverse function of the so-called modulus of continuity at the point \( x_0 = 0 \), which is defined by

\[
\epsilon(\omega) = \sup \left\{ |f_1'(0) - f_2'(0)| : \sup_x |f_1(x) - f_2(x)| \leq \omega, f_1, f_2 \in \mathcal{A} \right\}.
\]

By Lemma 7 of [5], the extremal pair of functions in attaining the modulus function \( \epsilon(\omega) \) can be chosen in the form \( f_1^* = f \) and \( f_2^* = -f \) for some \( f \). Thus

\[
\omega(\epsilon) = 2 \inf \left\{ \sup_x |f(x)| : |f'(0)| = \epsilon/2, f \in \mathcal{A} \right\}. \tag{14}
\]

If \( f(x) \) solves problem (14), so does \(-f(-x)\). As the absolute value is a convex function, \((f(x) - f(-x))/2\) is then also a solution. Therefore, we can restrict attention to odd functions in our search for a solution to (14).

For each odd function \( f \in \mathcal{A} \),

\[
|f(x) - f'(0)x| = |f(x) - f(0) - f'(0)x - \frac{f^{(2)}(0)}{2} x^2| \leq \frac{a}{6} |x|^3.
\]

It follows that

\[
|f(x)| \geq |f'(0)x| - |f(x) - f'(0)x| \geq \frac{e}{2} |x| - \frac{a}{6} |x|^3.
\]

Consider the function \( f^* \) which increases with a gradient \( \epsilon/2 \) at \( x_0 = 0 \) and is as close to 0 as possible:

\[
f^*(x) = \text{sign}(x) \left[ \frac{e}{2} |x| - \frac{a}{6} |x|^3 \right]_+.
\]

It is easy to verify that \( f^*(x) \) is an odd function, \( f^*(x) \in \mathcal{A} \), and \( \sup_x |f(x)| \geq \sup_x |f^*(x)| \) for any odd function \( f \in \mathcal{A} \). Therefore, \( f^*(x) \) is a solution to problem (14).

Since \( \omega(\epsilon) = \frac{2e}{3} \sqrt{\frac{e}{\pi}} \), we get

\[
\inf_{\hat{\theta}} \sup_{f \in \mathcal{A}, \sigma^2 \in \mathcal{B}} E(\hat{\theta} - f'(0))^2 \geq \frac{e^2}{16} e^{-2\frac{3\sigma^4}{16}}.
\]

Now take \( \epsilon = \left(\frac{3\sigma^4}{n}\right)^{1/3} \), we get

\[
\inf_{\hat{\theta}} \sup_{f \in \mathcal{A}, \sigma^2 \in \mathcal{B}} E(\hat{\theta} - f'(0))^2 \geq \frac{1}{16} e^{-2/3} \left(\frac{3\sigma^4}{n}\right)^{2/3}.
\]

We complete our proof by noting that the above bound holds for any design points \( x_1, \cdots, x_n \). \( \square \)
Figure 1 visualizes the above worst-case function

\[ f^*(x) = \text{sign}(x) \left[ \frac{\epsilon}{2} |x| - \frac{a}{6} |x|^3 \right] \]

in function class \( \mathcal{A} \). Intuitively, when function evaluations of \( f_1 \) and \( f_2 \) are close but their gradients at \( x_0 = 0 \) are quite different, we cannot easily find an estimator to minimize the errors in gradient estimation for these two functions at the same time. Such a scenario is considered as the worst case. Consider \((f_1, f_2)\) taken in the form \((f, -f)\), and the difference between \( f'_1(0) \) and \( f'_2(0) \) is \( \epsilon \). As shown in Figure 1, \( f^* \) increases with a gradient \( \epsilon/2 \) at \( x_0 = 0 \). In order to make function evaluations of \( f_1 \) and \( f_2 \) as close as possible, \( f^* \) needs to be as close to 0 as possible. Ultimately, with these worst-case functions indexed by \( \epsilon \), we take \( \epsilon = \left( \frac{3ad}{n} \right)^{1/3} \) in our lower-bound derivation to balance the maximization of gradient difference \( \epsilon \) and the minimization of function evaluation difference.

Figure 1: Worst-case function in attaining the inverse modulus of continuity

3.2 Multi-Dimensional Case

Suppose now that the input design points are \( x_1, \cdots, x_n \in \mathbb{R}^p \), and \( Y_j = Y_j(x_j) \) are independent unbiased noisy function evaluations of \( f : \mathbb{R}^p \to \mathbb{R} \) at \( x_j \) with simulation variance \( \sigma^2(x_j) \). Here we would like to estimate \( \nabla f \) at (w.l.o.g.) the origin \( x_0 = 0 \). Denote \( \hat{\theta} = \hat{\theta}(Y_1, \cdots, Y_n) \) as a generic \( \mathbb{R}^p \)-valued estimator like before. We consider the class of problems

\[ \mathcal{A}_q = \{ f(\cdot) : \nabla^2 f(0) \text{ exists}, \| \nabla^2 f(0) \|_2 \leq b \text{ and } |f(x) - f(0) - \nabla f(0)^T x - \frac{1}{2} x^T \nabla^2 f(0) x| \leq \frac{a}{6} \| x \|_q^3 \} \]

and

\[ \mathcal{B} = \{ \sigma^2(\cdot) : \sigma^2(x) \leq d \}, \]

where \( a, b, d > 0 \), and \( \| \cdot \|_q \) denotes the \( \ell_q \)-norm, \( q \in \{1, 2, \infty\} \). Define the minimax risk as

\[ R_p(n, \mathcal{A}_q, \mathcal{B}) = \inf_{\hat{\theta}} \sup_{f(\cdot) \in \mathcal{A}_q, \sigma^2(\cdot) \in \mathcal{B}} E \left\| \hat{\theta} - \nabla f(0) \right\|_2^2. \]
Theorem 5. For any \( n \geq 1 \),
\[
R_p(n, \mathcal{A}_q, \mathcal{B}) \geq \frac{1}{16} e^{-2/3} \left( \frac{3d p^{3/2}}{n} \right)^{2/3}, \text{ for } q = 1,
\]
\[
R_p(n, \mathcal{A}_q, \mathcal{B}) \geq \frac{1}{16} e^{-2/3} \left( \frac{3d}{n} \right)^{2/3}, \text{ for } q = 2, \infty.
\]

Consequently, the CFD estimator that divides budget equally among all dimensions, \( \bar{\epsilon} \), described in Theorem 2, is optimal up to a multiplicative factor polynomial in \( p \) for \( q = 1, 2, \infty \).

Similar to the proof for Theorem 4, Le Cam’s method and the modulus of continuity are used to obtain the worst-case hypothesized functions for the general minimax risk. However, here the choice of \( q \) in function class \( \mathcal{A}_q \) affects the modulus function, and thus the resulting worst-case functions and risk bounds.

Proof. Following Le Cam’s method in the proof for Theorem 4 and replacing \( \epsilon^2 = (f_1'(0) - f_2'(0))^2 \) by \( \epsilon^2 = \| \nabla f_1(0) - \nabla f_2(0) \|^2_2 \) for the multi-dimensional setting, we have, for any \( f_1, f_2 \in \mathcal{A}_q \),
\[
R_p(n, \mathcal{A}_q, \mathcal{B}) \geq \frac{\| \nabla f_1(0) - \nabla f_2(0) \|^2_2}{16} \epsilon^2 \frac{\| \mu_2 - \mu_1 \|^2_2}{2d},
\]
where \( \mu_k = (f_k(x_1), \ldots, f_k(x_n)), k = 1, 2 \).

In order to maximize the lower bound, let us define the modulus function \( \epsilon_{\mathcal{A}_q} \) for function class \( \mathcal{A}_q \):
\[
\epsilon_{\mathcal{A}_q}(\omega) = \sup \left\{ \| \nabla f_1(0) - \nabla f_2(0) \|^2_2 : \sup_x |f_1(x) - f_2(x)| \leq \omega, f_1, f_2 \in \mathcal{A}_q \right\},
\]
which is not only a function of \( \omega \) (like that in Theorem 4) but also affected by the choice of \( q \). Here the extremal pair \((f_1, f_2)\) attaining the modulus function will be different for different \( q \). First, by Lemma 7 of [5], the extremal pair can be chosen of the form: \( f_1 = f \) and \( f_2 = -f \). Thus
\[
\epsilon_{\mathcal{A}_q}(\omega) = 2 \sup \left\{ \| \nabla f(0) \|^2_2 : \sup_x |f(x)| \leq \omega/2, f \in \mathcal{A}_q \right\}.
\]

It follows that \( \epsilon_{\mathcal{A}_q} \) is the inverse function of
\[
\omega_{\mathcal{A}_q}(\epsilon) = 2 \inf \left\{ \sup_x |f| : \| \nabla f(0) \|^2_2 = \epsilon/2, f \in \mathcal{A}_q \right\}.
\]

If \( f(x) \) solves the problem (12), so does \(-f(-x)\). As the norm is a convex function, \((f(x) - f(-x))/2\) is then also a solution. Therefore, we can restrict attention to odd functions in our search for a solution to (13).

For each odd function \( f \in \mathcal{A}_q \),
\[
|f(x) - \nabla f(0)^T x| = |f(x) - f(0) - \nabla f(0)^T x - \frac{1}{2} x^T \nabla^2 f(0) x| \leq \frac{a}{6} \| x \|_q^3.
\]

It follows that
\[
|f(x)| \geq |\nabla f(0)^T x| - |f(x) - \nabla f(0)^T x| \geq |\nabla f(0)^T x| - \frac{a}{6} \| x \|_q^3.
\]
Therefore
\[
\sup_x |f(x)| \geq \sup_x \left[ |\nabla f(0)^T x| - \frac{a}{6} \|x\|_q^3 \right]_+.
\]
Denote \( X_+ = \{ x : \nabla f(0)^T x \geq 0 \} \) and \( X_- = \{ x : \nabla f(0)^T x < 0 \} \). Note that the odd function
\[
g(x) = \left[ \nabla f(0)^T x - \frac{a}{6} \|x\|_q^3 \right]_+ \cdot 1_{x \in X_+} + \left[ \nabla f(0)^T x + \frac{a}{6} \|x\|_q^3 \right]_+ \cdot 1_{x \in X_-}
\]
belongs to \( \mathcal{A}_q \), \( \sup_x |f(x)| \geq \sup_x |g(x)| \), and also that \( \nabla g(0) = \nabla f(0) \). Therefore, we consider functions of the form
\[
f(x) = \left[ \nabla f(0)^T x - \frac{a}{6} \|x\|_q^3 \right]_+ \cdot 1_{x \in X_+} + \left[ \nabla f(0)^T x + \frac{a}{6} \|x\|_q^3 \right]_+ \cdot 1_{x \in X_-}
\]
with \( \|\nabla f(0)\|_2 = \epsilon/2 \) in searching for a solution to (15). Moreover, denote \( \xi^* \) as a solution to the following problem
\[
\min_{\|\xi\|_2 = \epsilon/2} \max_{\|x\|_q = 1, \xi^T x \geq 0} \xi^T x. \tag{16}
\]
We see that
\[
f^*(x) = \left[ (\xi^*)^T x - \frac{a}{6} \|x\|_q^3 \right]_+ \cdot 1_{(\xi^*)^T x \geq 0} + \left[ (\xi^*)^T x + \frac{a}{6} \|x\|_q^3 \right]_+ \cdot 1_{(\xi^*)^T x < 0}
\]
is a solution to (15).

For \( q = 1 \) and \( 2 \), it is easy to verify that
\[
\xi^* = \left( \frac{\epsilon}{2 \sqrt{p}}, \ldots, \frac{\epsilon}{2 \sqrt{p}} \right)
\]
is a solution to (16). Therefore,
\[
f^*(x) = \text{sign} \left( \sum_{i=1}^{p} (x)_i \right) \left[ \frac{\epsilon}{2 \sqrt{p}} \sum_{i=1}^{p} (x)_i \right]_+ - \frac{a}{6} \|x\|_q^3 .
\]
Moreover, we have
\[
\sup_x |f^*(x)| = \sup_{t \geq 0} \left[ \frac{\epsilon}{2} \sqrt{pt} - \frac{a}{6} p^{3/2} t^3 \right]_+ = \frac{\epsilon}{3} \sqrt{\frac{\epsilon}{a}} p^{-3/4}, \text{ for } q = 1,
\]
\[
\sup_x |f^*(x)| = \sup_{t \geq 0} \left[ \frac{\epsilon}{2} \sqrt{pt} - \frac{a}{6} p^{3/2} t^3 \right]_+ = \frac{\epsilon}{3} \sqrt{\frac{\epsilon}{a}}, \text{ for } q = 2.
\]

For \( q = \infty \), it is easy to verify that
\[
\xi^* = \left( \frac{\epsilon}{2}, 0, \ldots, 0 \right)
\]
is a solution to (16). Therefore,
\[
f^*(x) = \text{sign} \left( (x)_1 \right) \left[ \frac{\epsilon}{2} |(x)_1| - \frac{a}{6} \|x\|_q^3 \right]_+ .
\]
Moreover, we have
\[
\sup_x |f^*(x)| = \sup_{t \geq 0} \left[ \frac{\epsilon}{2} t - \frac{a}{6} t^3 \right]_+ = \frac{\epsilon}{3} \sqrt{\frac{\epsilon}{a}}.
\]
Thus
\[ \omega_{\mathcal{A}_q}(\epsilon) = \frac{2\epsilon}{3} \sqrt[3]{\frac{e}{a} \rho^{-3/4}}, \text{ for } q = 1, \]
\[ \omega_{\mathcal{A}_q}(\epsilon) = \frac{2\epsilon}{3} \sqrt[3]{\frac{e}{a}}, \text{ for } q = 2, \infty. \]

Therefore, we have
\[ R_p(n, \mathcal{A}_q, \mathcal{B}) \geq \frac{e^2}{16} - \frac{n \omega_{\mathcal{A}_q}(\epsilon)}{2d} = \frac{e^2}{16} \left( 1 - \frac{2ne^3}{9ad} \right), \text{ for } q = 1, \]
\[ R_p(n, \mathcal{A}_q, \mathcal{B}) \geq \frac{e^2}{16} - \frac{n \omega_{\mathcal{A}_q}(\epsilon)}{2d} = \frac{e^2}{16} \left( 1 - \frac{2ne^3}{9ad} \right), \text{ for } q = 2, \infty. \]

Further by choosing
\[ \epsilon = \left( \frac{3ad}{n} \right)^{1/3}, \text{ for } q = 1, \]
\[ \epsilon = \left( \frac{3ad}{n} \right)^{1/3}, \text{ for } q = 2, \infty, \]
we get
\[ R_p(n, \mathcal{A}_q, \mathcal{B}) \geq \frac{1}{16} e^{-2/3} \left( \frac{3ad}{n} \right)^{2/3} \approx 0.0667 \left( \frac{ad}{n} \right)^{2/3}, \text{ for } q = 1, \]
\[ R_p(n, \mathcal{A}_q, \mathcal{B}) \geq \frac{1}{16} e^{-2/3} \left( \frac{3ad}{n} \right)^{2/3} \approx 0.0667 \left( \frac{ad}{n} \right)^{2/3}, \text{ for } q = 2, \infty. \]

Figure 2 visualizes the above worst-case function \( f^* \) for a two-dimensional case in function class \( \mathcal{A}_q \) with different \( q \). Similar to the discussion for Figure 1, worst-case functions serve to balance the maximization of the gradient difference and the minimization of the function evaluation difference. Since \( \ell_1 \)-norm is the largest among the three considered norms, the worst-case function for \( q = 1 \) descends to 0 most rapidly. The worst-case function for \( q = 2 \) takes a round shape, and the boundary of its zeros is circular. The worst-case function for \( q = \infty \) decreases only when the value in the maximal dimension increases and therefore appears the sharpest. In addition, each dimension of the worst-case function for \( q = 1 \) or \( q = 2 \) has the same derivative at point \( x_0 = 0 \). However, the worst-case function for \( q = \infty \) has a non-zero derivative at point \( x_0 = 0 \) only along one of its dimensions.

4 Conclusion

In this paper we studied the minimax optimality of stochastic gradient estimators when only noisy function evaluations are available, with respect to the worst-case MSE among unknown twice differentiable functions. We derived the exact minimax risk for the class of linear estimators, and showed that CFD is optimal within this class, in the single-dimensional case. We extended the
analysis to the multi-dimensional case, by showing the optimality of CFD up to a multiplicative factor sublinear in the dimension, and exactly if the signs of weights in the linear estimator are restricted to be the same across components. We also showed that, without further assumptions on the gradient magnitude, the worst-case risk of random perturbation schemes can be unbounded. Next we approximated the minimax risk over the general class of (nonlinear) estimators and showed that CFD is still nearly optimal over this much larger estimator class. These approximations were shown up to a constant factor in the single-dimensional case and an additional factor depending polynomially on the dimension in the multi-dimensional case. We used elementary techniques in the linear minimax analyses and Le Cam’s method and the modulus of continuity in the general minimax analyses. In future work, we will investigate the use of additional a priori information on the considered function class, and tighten our minimax estimates using potential alternate approaches.

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