

A Primer on Zeroth-Order Optimization in Signal Processing and Machine Learning

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Abstract—Zeroth-order (ZO) optimization is a subset of gradient-free optimization that emerges in many signal processing and machine learning applications. It is used for solving optimization problems similarly to gradient-based methods. However, it does not require the gradient, using only function evaluations. Specifically, ZO optimization iteratively performs three major steps: gradient estimation, descent direction computation, and solution update. In this paper, we provide a comprehensive review of ZO optimization, with an emphasis on showing the underlying intuition, optimization principles and recent advances in convergence analysis. Moreover, we demonstrate promising applications of ZO optimization, such as evaluating robustness and generating explanations from black-box deep learning models, and efficient online sensor management.

Index Terms—Zeroth-order (ZO) optimization, nonconvex optimization, gradient estimation, black-box adversarial attacks, machine learning, deep learning

I. INTRODUCTION

Many signal processing, machine learning (ML) and deep learning (DL) applications involve tackling complex optimization problems that are difficult to solve analytically. Often the objective function itself may not be in analytical closed form, only permitting function evaluations but not gradient evaluations. Optimization corresponding to these types of problems falls into the category of zeroth-order (ZO) optimization with respect to black-box models, where explicit expressions of the gradients are difficult to compute or infeasible to obtain. ZO optimization methods are gradient-free counterparts of first-order (FO) optimization methods. They approximate the full

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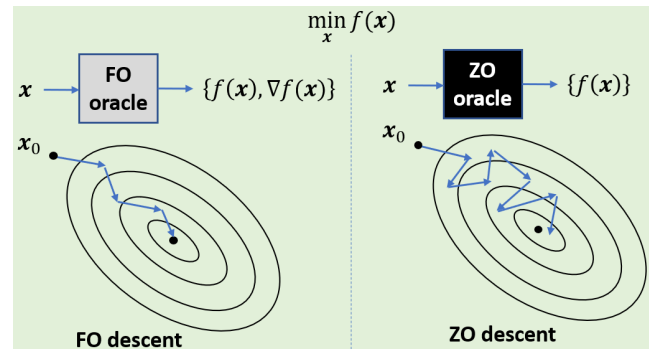


Fig. 1: An illustration of FO optimization (left plot) versus ZO optimization (right plot). Here the former solves the optimization problem $\min_{\mathbf{x}} f(\mathbf{x})$ with the white-box objective function f , and the latter solves the problem when f is a black-box function. Typically, ZO optimization has a slower convergence speed than FO optimization.

gradients or stochastic gradients through function value based gradient estimates. Interest in ZO optimization has grown rapidly in the past few years since the concept of gradient estimation by finite difference approximations was proposed in the 1950s and 1980s [1], [2].

It is worth noting that derivative-free methods for black-box optimization had been studied by the optimization community long before they had impact on signal processing and ML/DL. Traditional derivative-free optimization (DFO) methods can be classified into two categories: direct search-based methods (DSMs) and model-based methods (MBMs) [3]–[6]. DSMs include the Nelder-Mead simplex method [7], the coordinate search method [8], and the pattern search method [9], to name a few. MBMs contain model-based descent methods [10] and trust region methods [11]. Evolutionary optimization is another class of generic population-based meta heuristic DFO algorithms, and includes particle swarm optimization methods [12] and genetic algorithms [13]. Some Bayesian optimization (BO) methods [14] tackle black-box optimization problems by modelling the objective function as a Gaussian process (GP) that is learned

from the history of function evaluations. However, learning an accurate GP model is computationally intensive.

Conventional DFO methods have two main shortcomings. First, they are often difficult to scale to large-size problems. For example, the off-the-shelf DFO solver COBYLA [15] only supports problems with a maximum of 2^{16} variables (SciPy Python library [16]), which is smaller than the size of a single ImageNet image [17]. Second, DFO methods lack a convergence rate analysis and they may require a significant amount of effort to be customized to the particular applications. ZO optimization has three main advantages over DFO: a) ease of implementation with only small modification of commonly-used gradient-based algorithms, b) computationally efficient approximations to derivatives when they are difficult to compute, and c) comparable convergence rates to FO algorithms [18]–[21]. An illustrative example of ZO optimization versus FO optimization is shown in Figure 1.

ZO optimization has attracted increasing attention due to its success in solving emerging signal processing and ML/DL problems. First, ZO optimization serves as a powerful and practical tool for evaluating adversarial robustness of ML/DL systems [22]. We note that the research in adversarial robustness is receiving increased attention in recent years. ZO based methods for exploring vulnerability of DL to black-box adversarial attacks are able to reveal the most susceptible features. Such ZO methods can be as effective as state-of-the-art white-box attacks, despite only having access to the inputs and outputs of the targeted deep neural networks (DNNs) [23], [24]. Moreover, ZO optimization can generate explanations and provide interpretations of prediction results in a gradient-free and model-agnostic manner [25]. Furthermore, ZO optimization can also be used to solve automated ML problems, e.g., automated backpropagation in DL, where the gradients with respect to ML pipeline configuration parameters are intractable [26]. ZO optimization is also applicable to ML applications where the full gradient must be kept private [27]. In addition, ZO optimization provides computationally-efficient alternatives for second-order optimization such as robust training by curvature regularization [28], meta-learning [29], transfer learning [30], and online network management [27].

In this paper, we provide a comprehensive review of recent development in ZO optimization for signal processing and ML.

In Sections II and III, we review various types of ZO gradient estimators as well as ZO algorithms. Section IV presents a promising connection between ZO optimization and adversarial ML. Section V illustrates an application of ZO optimization to online sensor management. More applications are provided in Section VI. We discuss open issues and state our conclusions in Sections VII and VIII, respectively.

II. GRADIENT ESTIMATION VIA ZO ORACLE

In this section, we provide an overview of gradient estimation techniques for optimization with a black-box objective function. The resulting gradient estimate forms the basis for constructing the descent direction used in ZO optimization algorithms. We categorize the ZO gradient estimates into two types, *1-point*, and *multi-point* estimates, based on the number of queried function evaluations. As the number of function evaluations increases, a more accurate gradient estimate is expected but at the cost of increased query complexity.

A. 1-point estimate

We start by the principles of *randomized* gradient estimation in the context of 1-point estimation. Let $f(\mathbf{x})$ be a continuously differentiable objective function on a d -dimension variable $\mathbf{x} \in \mathbb{R}^d$. The 1-point gradient estimate of f has the generic form

$$\hat{\nabla} f(\mathbf{x}) := \frac{\phi(d)}{\mu} f(\mathbf{x} + \mu \mathbf{u}) \mathbf{u}, \quad (1)$$

where $\mathbf{u} \sim p$ is a random direction vector drawn from a certain distribution p , which is typically chosen as either the standard multivariate normal distribution $\mathcal{N}(\mathbf{0}, \mathbf{I})$ [19] or the multivariate uniform distribution $\mathcal{U}(\mathcal{S}(0, 1))$ on a unit sphere centered at $\mathbf{0}$ with radius 1 [20], $\mu > 0$ is a perturbation radius (also called a smoothing parameter), and $\phi(d)$ denotes a certain dimension-dependent factor related to the choice of the distribution p . If $p = \mathcal{N}(\mathbf{0}, \mathbf{I})$, then $\phi(d) = 1$; If $p = \mathcal{U}(\mathcal{S}(0, 1))$, then $\phi(d) = d$.

The *rationale* behind (1) is that it is an *unbiased* estimate of the gradient of the *smoothed* version of f over a random perturbation $\mathbf{u} \sim p'$ with smoothing parameter μ ,

$$f_\mu(\mathbf{x}) := \mathbb{E}_{\mathbf{u} \sim p'} [f(\mathbf{x} + \mu \mathbf{u})], \quad (2)$$

where p' is specified as $\mathcal{N}(\mathbf{0}, \mathbf{I})$ if $p = \mathcal{N}(\mathbf{0}, \mathbf{I})$ in (1), or the multivariate uniform distribution on a unit ball $\mathcal{U}(\mathcal{B}(0, 1))$ if

$p = \mathcal{U}(\mathcal{S}(0, 1))$ in (1). The unbiasedness of (1) with respect to $\nabla f_\mu(\mathbf{x})$ is assured by [19], [31]:

$$\mathbb{E}_{\mathbf{u} \sim p} [\hat{\nabla} f(\mathbf{x})] = \nabla f_\mu(\mathbf{x}). \quad (3)$$

The meaning of (3) can be elucidated by considering the scalar case $d = 1$. Given $p = \mathcal{U}(\mathcal{S}(0, 1))$, applying the fundamental theorem of calculus to (2) yields $\nabla f_\mu(x) = \frac{d}{dx} \int_{-\mu}^{\mu} \frac{1}{2} f(x+u) du = \frac{1}{2\mu} [f(x+\mu) - f(x-\mu)]$, which is equal to $\mathbb{E}_{u \sim p} [\hat{\nabla} f(x)]$ from (1).

Although the 1-point estimate (1) is unbiased with respect to the gradient of the smoothed function $\nabla f_\mu(\mathbf{x})$, it is a *biased* approximation of the true gradient $\nabla f(\mathbf{x})$. Furthermore, the 1-point estimate is not commonly used in practice since it suffers from high variance, defined as $\mathbb{E}[\|\hat{\nabla} f(\mathbf{x}) - \nabla f_\mu(\mathbf{x})\|_2^2]$, which slows convergence [20].

B. Multi-point ZO estimate

A natural extension of (1) is the directional derivative approximation (*2-point estimate*) [19], [21],

$$\hat{\nabla} f(\mathbf{x}) := \frac{\phi(d)}{\mu} [f(\mathbf{x} + \mu \mathbf{u}) - f(\mathbf{x})] \mathbf{u}, \quad (4)$$

which satisfies the unbiasedness condition (3) for any \mathbf{u} such that $\mathbb{E}_{\mathbf{u} \sim p} [\mathbf{u}] = \mathbf{0}$. The mean squared approximation error of the gradient estimate (4) with respect to the true gradient $\nabla f(\mathbf{x})$ obeys [31], [32],

$$\mathbb{E}[\|\hat{\nabla} f(\mathbf{x}) - \nabla f(\mathbf{x})\|_2^2] = O(d) \|\nabla f(\mathbf{x})\|_2^2 + O\left(\frac{\mu^2 d^3 + \mu^2 d}{\phi(d)}\right), \quad (5)$$

where we adopt the big O notation to highlight the dominant factors d and μ affecting gradient estimation error. It is worth noting that the (coordinate-wise) two-point ZO estimate for finding the optimum of a regression function was initially proposed in the 1950s [1]. This gradient estimation technique was further studied in the 1980s in the context of simultaneous perturbation stochastic approximation [2], [33].

The approximation error (5) of the 2-point estimate in (4) provides several insights. First, the gradient estimate gets better as the smoothing parameter μ becomes smaller. However, in a practical system, if μ is too small, then the function difference could be dominated by system noise and it may fail to represent the differential [32], [34]. Thus, careful selection of the smoothing parameter μ is important for convergence of ZO optimization methods. Second, different from the first-order stochastic gradient estimate, the ZO gradient estimate yields a dimension-dependent variance that increases as $O(d) \|\nabla f(\mathbf{x})\|_2^2$. Thus, variance cannot be reduced even if $\mu \rightarrow 0$. Thus, some

recent work has focused on the design of variance-reduced gradient estimates.

Mini-batch sampling is the most commonly-used approach to reduce the variance of ZO gradient estimates [21], [27]. Instead of using a single random direction, the average of b i.i.d. samples $\{\mathbf{u}_i\}_{i=1}^b$ drawn from p are used for gradient estimation, leading to the *multi-point estimate*

$$\hat{\nabla} f(\mathbf{x}) := \frac{\phi(d)}{\mu} \sum_{i=1}^b [(f(\mathbf{x} + \mu \mathbf{u}_i) - f(\mathbf{x})) \mathbf{u}_i], \quad (6)$$

with the approximation error [31]

$$O\left(\frac{d}{b}\right) \|\nabla f(\mathbf{x})\|_2^2 + O\left(\frac{\mu^2 d^3}{\phi(d)b}\right) + O\left(\frac{\mu^2 d}{\phi(d)}\right). \quad (7)$$

In (7), the first two terms correspond to the reduced variance of the 2-point estimate $\mathbb{E}[\|\hat{\nabla} f(\mathbf{x}) - \nabla f_\mu(\mathbf{x})\|_2^2]$ due to the drawing of b random direction vectors. And the third term, independent of b , corresponds to the approximation error due to the gradient of the smoothed function $\|\nabla f(\mathbf{x}) - \nabla f_\mu(\mathbf{x})\|_2^2$.

When the number of function evaluations reaches the problem dimension d in (6), then instead of using *randomized* directions $\{\mathbf{u}_i\}_{i=1}^d$, one can employ the *deterministic coordinate-wise* gradient estimate $\frac{1}{\mu} \sum_{i=1}^d [(f(\mathbf{x} + \mu \mathbf{e}_i) - f(\mathbf{x})) \mathbf{e}_i]$, which yields a lower approximation error, of order $O(d\mu^2)$ [1], [31], [34]. Here $\mathbf{e}_i \in \mathbb{R}^d$ denotes the i th elementary basis vector, with 1 at the i th coordinate and 0s elsewhere. In practice, the multi-point gradient estimate (6) is usually implemented with $2 \leq b \leq d$. The previously introduced multi-point estimates are computed by using *forward* differences of function values. An alternative is the *central* difference variant that uses $(f(\mathbf{x} + \mu \mathbf{u}) - f(\mathbf{x} - \mu \mathbf{u}))$, where \mathbf{u} can be either randomized or deterministic [1], [2]. These central difference estimates have similar approximation errors to the forward difference estimates [31], [34], [35].

III. ZO OPTIMIZATION ALGORITHMS

In this section, we present a unified algorithmic framework covering many commonly-used ZO optimization methods. We provide a thorough overview of existing algorithms in different problem settings and delve into the factors that influence their convergence.

A. The generic form of the ZO algorithm

Let us consider a stochastic optimization problem

$$\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}) := \mathbb{E}_\xi [f(\mathbf{x}; \xi)], \quad (8)$$

where $\mathbf{x} \in \mathbb{R}^d$ are optimization variables, \mathcal{X} is a closed convex set, f is a possibly *nonconvex* objective function, and ξ is a

certain random variable that captures stochastic data samples or noise. If ξ obeys a uniform distribution over n empirical samples $\{\xi_i\}_{i=1}^n$, then problem (8) reduces to a finite-sum formulation with objective function $f(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}; \xi_i)$. And if $\mathcal{X} = \mathbb{R}^d$, then problem (8) simplifies to the unconstrained optimization problem.

Algorithm 1 Generic form of ZO optimization

Initialize $\mathbf{x}_0 \in \mathcal{X}$, gradient estimation operation $\phi(\cdot)$, descent direction updating operation $\psi(\cdot)$, number of iterations T , and learning rate $\eta_t > 0$ at iteration t ,

for $t = 1, 2, \dots, T$ **do**

1. Gradient estimation:

$$\hat{\mathbf{g}}_t = \phi(\{f(\mathbf{x}_t; \xi_j)\}_{j \in \Omega_t}^t), \quad (9)$$

where Ω_t denotes a set of mini-batch stochastic samples used at iteration t ,

2. Descent direction computation:

$$\mathbf{m}_t = \psi(\{\hat{\mathbf{g}}_i\}_{i=1}^t), \quad (10)$$

3. Point updating:

$$\mathbf{x}_t = \Pi_{\mathcal{X}}(\mathbf{x}_{t-1}, \mathbf{m}_t, \eta_t), \quad (11)$$

where $\Pi_{\mathcal{X}}$ denotes a point updating operation subject to the constraint $\mathbf{x} \in \mathcal{X}$.

end for

Most ZO optimization methods mimic their first-order counterparts, and involve three steps, shown in Algorithm 1, *gradient estimation* (9), *descent direction computation* (10), and *point updating* (11). Without loss of generality, we specify (9) as a variant of (6) built on a mini-batch of empirical samples $\{\xi_j\}_{j \in \Omega_t}$,

$$\hat{\mathbf{g}}_t = \phi(\{f(\mathbf{x}_t; \xi_j)\}_{j \in \Omega_t}^t, \alpha) = \frac{1}{|\Omega_t|} \sum_{j \in \Omega_t} \hat{\nabla} f(\mathbf{x}_t; \xi_j), \quad (12)$$

where $\hat{\nabla} f(\mathbf{x}_t; \xi_j)$ is given by (6) as the gradient of the function $f(\cdot; \xi)$, and $|\Omega_t|$ denotes the cardinality of the set of mini-batch samples at iteration t .

Next, we elaborate on the descent direction computation and the point updating step used in many ZO algorithms.

1) *ZO algorithms for unconstrained optimization:* We consider the ZO stochastic gradient descent (ZO-SGD) method [18], the ZO sign-based SGD (ZO-signSGD) [36], the ZO stochastic variance reduced gradient (ZO-SVRG) method [32], [37]–[39], and the ZO Hessian-based (ZO-Hess) algorithm [40], [41]. These algorithms employ the same point updating rule (11),

$$\mathbf{x}_t = \mathbf{x}_{t-1} - \eta_t \mathbf{m}_t.$$

However, they adopt different strategies to form the descent direction \mathbf{m}_t in (10).

- ZO-SGD [18]: The descent direction \mathbf{m}_t is set as the current gradient estimate $\mathbf{m}_t = \hat{\mathbf{g}}_t$. Note that ZO-SGD becomes the ZO stochastic coordinate descent (ZO-SCD) method [34] as the coordinate-wise gradient estimate is used. Moreover, if the full batch of stochastic samples are used, then ZO-SGD becomes ZO gradient descent (ZO-GD) [19].

- ZO-signSGD [36]: The descent direction \mathbf{m}_t is given by the sign of the current gradient estimate $\mathbf{m}_t = \text{sign}(\hat{\mathbf{g}}_t)$, where $\text{sign}(\cdot)$ denotes the element-wise sign operation. Using the sign operation scales down the (coordinate-wise) estimation errors [36], [42].

- ZO-SVRG [32], [37]–[39]: The descent direction \mathbf{m}_t is formed by combining $\hat{\mathbf{g}}_t$ with a control variate of reduced variance, $\mathbf{m}_t = \hat{\mathbf{g}}_t - \mathbf{c}_t + \mathbb{E}_{\xi}[\mathbf{c}_t]$, where \mathbf{c}_t denotes a control variate, which is commonly given by a gradient estimate evaluated at \mathbf{x}_{t-1} but the entire dataset of n empirical samples.

- ZO-Hess [40]: The descent direction \mathbf{m}_t incorporates the approximate Hessian $\hat{\mathbf{H}}_t$ [40], $\mathbf{m}_t = \hat{\mathbf{H}}_t^{-1/2} \hat{\mathbf{g}}_t$, where $\hat{\mathbf{H}}_t$ is constructed either by the second-order Gaussian Stein’s identity [41] or the diagonalization-based Hessian approximation [40]. The former approach was used in [41] to develop the ZO stochastic cubic regularized Newton (ZO-SCRN) method.

2) *ZO algorithms for constrained optimization:* We next present the ZO projected SGD (ZO-PSGD) [43], the ZO stochastic mirror descent (ZO-SMD) [21], the ZO stochastic conditional gradient (ZO-SCG) algorithm [41], [44], and the ZO adaptive momentum method (ZO-AdaMM) [45] for constrained optimization. The aforementioned algorithms, with the exception of the ZO-AdaMM, specify the descent direction (10) as the current gradient estimate $\mathbf{m}_t = \hat{\mathbf{g}}_t$. Their key difference lies in how they implement the point updating step (11).

- ZO-PSGD [43]: By letting $\Pi_{\mathcal{X}}$ be the Euclidean distance based projection operation, the point updating step (11) is given by $\mathbf{x}_t = \arg \min_{\mathbf{x} \in \mathcal{X}} \|\mathbf{x} - (\mathbf{x}_{t-1} - \eta_t \mathbf{m}_t)\|_2^2$.

- ZO-SMD [21]: Upon defining a Bregman divergence $D_h(\mathbf{x}, \mathbf{y})$ with respect to a strongly convex and differentiable function h , $D_h(\mathbf{x}, \mathbf{y}) = h(\mathbf{x}) - h(\mathbf{y}) - (\mathbf{x} - \mathbf{y})^T \nabla h(\mathbf{y})$, the point updating step (11) is given by $\mathbf{x}_t = \arg \min_{\mathbf{x} \in \mathcal{X}} \mathbf{m}_t^T \mathbf{x} + \frac{1}{\eta_t} D_h(\mathbf{x}, \mathbf{x}_t)$. For example, if $h(\mathbf{x}) = \frac{1}{2} \|\mathbf{x}\|_2^2$, then $D_h(\mathbf{x}, \mathbf{y}) = \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2$, and $\mathbf{x}_t = \arg \min_{\mathbf{x} \in \mathcal{X}} \|\mathbf{x} - (\mathbf{x}_{t-1} - \eta_t \mathbf{m}_t)\|_2^2$, which reduces to ZO-PSGD.

- ZO-SCG [41], [44]: The point updating step (11) calls for

a linear minimization oracle [41], $\mathbf{z}_t = \arg \min_{\mathbf{x} \in \mathcal{X}} \mathbf{m}_t^T \mathbf{x}$, and forms a feasible point update through the linear combination $\mathbf{x}_t = (1 - \eta_t)\mathbf{x}_{t-1} + \eta_t\mathbf{z}_t$. Similar algorithms, known as ZO Frank-Wolfe, were also developed in [46], [47].

- ZO-AdaMM [45]: Different from ZO-PSGD, ZO-SMD and ZO-SCG, ZO-AdaMM adopts a momentum-type descent direction (rather than the current estimate $\hat{\mathbf{g}}_t$), an adaptive learning rate (rather than the constant rate η_t), and a projection operation under Mahalanobis distance (rather than Euclidean distance). ZO-AdaMM can strike a balance between the convergence speed and accuracy. However, it requires tuning extra algorithmic hyperparameters in addition to the learning rate and smoothing parameters [45], [48].

B. ZO optimization in complex settings

Here we review ZO algorithms for composite optimization, min-max optimization, distributed optimization, and structured high-dimensional optimization.

1) *ZO composite optimization*: Consider the following problem, with a smooth+nonsmooth composite objective function,

$$\underset{\mathbf{x} \in \mathbb{R}^d}{\text{minimize}} \quad f(\mathbf{x}) + g(\mathbf{x}), \quad (13)$$

where f is a black-box smooth function (possibly nonconvex), and g is a white-box non-smooth regularization function. The form of problem (13) arises in many sparsity-promoted applications, e.g., adversarial attack generation [49] and online sensor management [27]. The ZO proximal SGD (ZO-ProxSGD) algorithm [43] and ZO (stochastic) alternating direction method of multipliers (ZO-ADMM) [27], [50], [51] were developed to solve problem (13). We remark that problem (8) can also be cast as (13) by introducing the indicator function of the constraint $\mathbf{x} \in \mathcal{X}$ in the objective of (8) by letting $g(\mathbf{x}) = 0$ if $\mathbf{x} \in \mathcal{X}$ and ∞ if $\mathbf{x} \notin \mathcal{X}$.

2) *ZO min-max optimization*: By *min-max*, we mean that the problem is a composition of inner maximization and outer minimization of the objective function,

$$\min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \quad f(\mathbf{x}, \mathbf{y}) \quad (14)$$

where $\mathbf{x} \in \mathbb{R}^{d_x}$ and $\mathbf{y} \in \mathbb{R}^{d_y}$ are optimization variables (for ease of notation, let $d_x = d_y = d$), f is a black-box objective function, and \mathcal{X} and \mathcal{Y} are compact convex sets. One motivating application behind problem (14) is the design of *black-box poisoning attack* [52], where the attacker deliberately influences the training data (by injecting poisoned samples) to manipulate the results of a black-box predictive model. To solve the

problem posed in (14), the work [52], [53] presented efficient ZO min-max algorithms for stochastic and deterministic bi-level optimization with nonconvex outer minimization over \mathbf{x} and strongly concave inner maximization over \mathbf{y} . They proved the convergence rate to be sub-linear when gradient estimation is integrated with alternating (projected) stochastic gradient descent-ascent methods.

3) *ZO distributed optimization*: Consider the minimization of a network cost, given by the sum of local objective functions $\{f_i\}$ at multiple agents

$$\begin{aligned} & \underset{\{\mathbf{x}_i \in \mathcal{X}\}}{\text{minimize}} \quad \sum_{i=1}^N f_i(\mathbf{x}_i) \\ & \text{subject to} \quad \mathbf{x}_i = \mathbf{x}_j, \quad \forall j \in \mathcal{N}(i). \end{aligned} \quad (15)$$

Here $\mathcal{N}(i)$ denotes the set of neighbors of agent/node i , and the underlying network/graph is connected, namely, there exists a path between every pair of distinct nodes. Some recent works have started to tackle the distributed optimization problem (15) with black-box objectives. In [54], a distributed Kiefer Wolfowitz type ZO algorithm was proposed along with convergence analysis, for the case that the objective functions $\{f_i\}$ are strongly convex. In [55], [56], the ZO distributed (sub)gradient algorithm and the ZO distributed mirror descent algorithm were developed for nonsmooth convex optimization. In [57], [58], the convergence of consensus-based distributed ZO algorithms was established for nonconvex (unconstrained) optimization.

4) *Structured high-dimensional optimization*: Compared to FO algorithms, ZO algorithms typically suffer from a slowdown (proportional to the problem size d) in convergence. Thus, some recent works attempt to mitigate this limitation when solving high-dimensional (large d) problems. The work [59] explored the functional sparsity structure, under which the objective function f depends only on a subset of d coordinates. This assumption also implies the gradient sparsity, which enabled the development of a LASSO based algorithm for gradient estimation, and eventually yielded poly-logarithmic dependence on d when f is convex. And the work [41] established the convergence rate of ZO-SGD which depends on d only poly-logarithmically under the assumption of gradient sparsity. In addition, the work [60] proposed a direct search based algorithm, which yields the convergence rate that is poly-logarithmically dependent on dimensionality for any monotone transform of a smooth and strongly convex objective with a low-dimensional structure. That is, the objective function $f(\mathbf{x})$

is supported on a low dimensional manifold \mathcal{X} . Another work [61] studied the problem of ZO optimization on Riemannian manifolds, and proposed algorithms that only depend on the intrinsic dimension of the manifold by using ZO Riemannian gradient estimates.

C. Convergence rates

We first elaborate on the criteria used to analyze the convergence rate of ZO algorithms under different problem settings.

1) *Convex optimization*: The convergence error is measured by the *optimality gap of function values* $\mathbb{E}[f(\mathbf{x}_T) - f(\mathbf{x}^*)]$ for a convex objective f , where \mathbf{x}_T denotes the updated point at the final iteration T , \mathbf{x}^* denotes the optimal solution, and the expectation is taken over the full probability space, e.g., random gradient approximation and stochastic sampling.

2) *Online convex optimization*: The *cumulative regret* [62] is typically used in place of the optimality gap, namely, $\mathbb{E}\left[\sum_{t=1}^T f_t(\mathbf{x}_t) - \min_{\mathbf{x}} \sum_{t=1}^T f_t(\mathbf{x})\right]$ for an online convex cost function f_t , e.g., $f_t(\cdot) = f(\cdot; \xi_t)$ in problem (8).

3) *Unconstrained nonconvex optimization*: The convergence is evaluated by the first-order stationary condition in terms of the *squared gradient norm* $\frac{1}{T} \sum_{t=1}^T \mathbb{E}[\|\nabla f(\mathbf{x}_t)\|_2^2]$ for the nonconvex objective f . Since first-order stationary points could be saddle points of a nonconvex optimization problem, the *second-order stationary condition* is also used to ensure the local optimality of a first-order stationary point (namely, escaping saddle-points) [41], [63]. The work [41] and [63] focused on stochastic optimization and deterministic optimization, respectively.

4) *Constrained nonconvex optimization*: The criterion for convergence is commonly determined by detecting a sufficiently small squared norm of the *gradient mapping* [43], [64], $P_{\mathcal{X}}(\mathbf{x}_t, \nabla f(\mathbf{x}_t), \eta_t) := \frac{1}{\eta_t} [\mathbf{x}_t - \Pi_{\mathcal{X}}(\mathbf{x}_t - \eta_t \nabla f(\mathbf{x}_t))]$, where the notation follows (11). $P_{\mathcal{X}}(\mathbf{x}_t, \nabla f(\mathbf{x}_t), \eta_t)$ can naturally be interpreted as the projected gradient, which offers a feasible update from the previous point \mathbf{x}_t . The *Frank-Wolfe duality gap* is another commonly-used convergence criterion [41], [44], [46], [47], given by $\max_{\mathbf{x} \in \mathcal{X}} \langle \mathbf{x} - \mathbf{x}_t, -\nabla f(\mathbf{x}_t) \rangle$. It is always non-negative, and becomes 0 if and only if $\mathbf{x}_t \in \mathcal{X}$ is a stationary point.

More generally, given a convergence measure $\mathcal{M}(\cdot)$, \mathbf{x} is called an ϵ -optimal solution if $\mathcal{M}(\mathbf{x}) \leq \epsilon$. The convergence

error is typically expressed as a function of the number of iterations T , relating the convergence rate to the iteration complexity. Since the convergence analysis of existing ZO algorithms varies under different problem domains and algorithmic parameter settings, in Table I we compare the convergence performance of ZO algorithms covered in this section from 5 perspectives: problem structure, type of gradient estimates, smoothing parameter, convergence error, and function query complexity.

IV. APPLICATION: ADVERSARIAL EXAMPLE GENERATION

In this section, we present the application of ZO optimization to the generation of prediction-evasive *adversarial examples* to fool DL models. Adversarial examples, also known as evasion attacks, are inputs corrupted with imperceptible adversarial perturbations (to be designed) toward misclassification (namely, prediction different from true image labels) [22], [65].

Most studies on adversarial vulnerability of DL have been restricted to the *white-box* setting where the adversary has complete access and knowledge of the target system (e.g., DNNs) [22], [65]. However, it is often the case that the internal states/configurations and the operating mechanism of DL systems are not revealed to the practitioners (e.g., Google Cloud Vision API). This gives rise to the problem of *black-box adversarial attacks* [23], [24], [66]–[69], where the only mode of interaction of the adversary with the system is via submission of inputs and receiving the corresponding predicted outputs.

More formally, let \mathbf{z} denote a legitimate example, and $\mathbf{z}' := \mathbf{z} + \mathbf{x}$ denote an adversarial example with the adversarial perturbation \mathbf{x} . Given the learned ML/DL model θ , the problem of adversarial example generation can be cast as an optimization problem of the following generic form [49], [65]

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^d}{\text{minimize}} && f(\mathbf{z} + \mathbf{x}; \theta) + \lambda g(\mathbf{x}) \\ & \text{subject to} && \|\mathbf{x}\|_{\infty} \leq \epsilon, \mathbf{z}' \in [0, 1]^d, \end{aligned} \quad (16)$$

where $f(\mathbf{z}'; \theta)$ denotes the (black-box) attack loss function for fooling the model θ using the perturbed input \mathbf{z}' (see [23] for a specific formulation), $g(\mathbf{x})$ is a regularization function that penalizes the sparsity or the structure of adversarial perturbations, e.g., group sparsity in [70], $\lambda \geq 0$ is a regularization parameter, the ℓ_{∞} norm enforces similarity between \mathbf{z}' and \mathbf{z} , and the input space of ML/DL systems is normalized to $[0, 1]^d$. If $\lambda \neq 0$, then problem (16) is in the

Method	Problem structure	Gradient estimation	Smoothing parameter μ	Convergence error (T iterations)	Query complexity (T iterations)
ZO-GD [19]	NC, UnCons ¹	2-point GauGE ²	$O\left(\frac{1}{\sqrt{dT}}\right)$	$O\left(\frac{d}{T}\right)$	$O(\mathcal{D} T)^3$
ZO-SGD [18]	NC, UnCons	2-point GauGE	$O\left(\frac{1}{d\sqrt{T}}\right)$	$O\left(\frac{\sqrt{d}}{\sqrt{T}}\right)$	$O(T)$
ZO-SCD [34]	NC, UnCons	2-point CooGE ²	$O\left(\frac{1}{\sqrt{T}} + \frac{1}{(dT)^{1/4}}\right)$	$O\left(\frac{\sqrt{d}}{\sqrt{T}}\right)$	$O(T)$
ZO-signSGD [36]	NC, UnCons	b -point UniGE ²	$O\left(\frac{1}{\sqrt{dT}}\right)$	$O\left(\frac{\sqrt{d}}{\sqrt{T}} + \frac{\sqrt{d}}{\sqrt{b}}\right)^4$	$O(bT)$
ZO-SVRG [32]	NC, UnCons	b -point UniGE	$O\left(\frac{1}{\sqrt{dT}}\right)$	$O\left(\frac{d}{T} + \frac{1}{b}\right)$	$O(\mathcal{D} s + bsm)$ $T = sm$
ZO-Hess [40]	SC, UnCons	b -point GauGE	$O\left(\frac{1}{d}\right)$	$O\left(e^{-bT/d}\right)$	$O(bT)$
ZO-ProxSGD / ZO-PSGD [43]	NC, Cons	b -point GauGE	$O\left(\frac{1}{\sqrt{dT}}\right)$	$O\left(\frac{d^2}{bT} + \frac{d}{b}\right)$	$O(bT)$
ZO-SMD [21]	C, Cons	2-point GauGE	$O\left(\frac{1}{dt}\right)$	$O\left(\frac{\sqrt{d}}{\sqrt{T}}\right)$	$O(T)$
ZO-SCG [41]	NC, Cons	b -point GauGE	$O\left(\frac{1}{\sqrt{d^3T}}\right)$	$O\left(\frac{1}{\sqrt{T}} + \frac{d\sqrt{T}}{b}\right)$	$O(bT)$
ZO-AdaMM [45]	NC, Cons	b -point GauGE	$O\left(\frac{1}{\sqrt{dT}}\right)$	$O\left(\frac{d}{T} + \frac{d}{b}\right)$	$O(b^2T)$
ZO-ADMM [27]	C, Composite	b -point UniGE	$O\left(\frac{1}{d^{1.5t}}\right)$	$O\left(\frac{\sqrt{d}}{\sqrt{bT}}\right)$	$O(bT)$
ZO-Min-Max [52]	NC, Cons	b -point UniGE	$O\left(\frac{1}{d\sqrt{T}}\right)$	$O\left(\frac{1}{T} + \frac{d}{b}\right)$	$O(b^2T)$
Dist-ZO [58]	NC, UnCons	2-point UniGE	$\frac{1}{\sqrt{dt}}$	$O\left(\frac{\sqrt{d}}{\sqrt{T}}\right)$	$O(T)$
ZO-SCRN [41]	NC, UnCons	b -point UniGE	$\frac{1}{d^{5/2}T^{1/3}}$	$O\left(\frac{1}{T^{4/3}}\right)$ $b = O\left(dT^{4/3}\right)$	$O(bT)$

¹ Problem setting: NC, C, SC, UnCons, Cons and Composite represent nonconvex, convex, strongly convex, unconstrained, constrained and composite optimization respectively.

² GauGE and UniGE represent the gradient estimates using random direction vectors drawn from $\mathcal{N}(\mathbf{0}, \mathbf{I})$ and $\mathcal{U}(\mathcal{S}(0, 1))$, respectively. CooGE represents the coordinate-wise partial derivative estimate.

³ \mathcal{D} denotes the entire dataset.

TABLE I: Comparison of different ZO algorithms in problem setting, gradient estimation, smoothing parameter, convergence error, and function query complexity.

form of composite optimization, and ZO-ADMM is a well-suited optimizer. If $\lambda = 0$, a solution to problem (16) is known as a black-box ℓ_∞ attack [24], which can be obtained using ZO methods for constrained optimization.

In Table II, we present black-box ℓ_∞ attacks with respect to 5 ImageNet images against the Inception V3 model [71]. The adversarially perturbed images are obtained from 4 ZO methods including ZO-PSGD, ZO-SMD, ZO-AdaMM, and ZO-NES (a projected version of ZO-signSGD that is used in practice [24]). We demonstrate the attack performance of different ZO algorithms in terms of the ℓ_2 norm of the generated perturbations and the number of queries needed to achieve a first successful black-box attack. As we can see, ZO-PSGD typically has the fastest speed of converging to a valid adversarial example, while ZO-AdaMM has the best convergence accuracy in terms of the smallest distortion required to fool the neural network.

V. APPLICATION: ONLINE SENSOR MANAGEMENT

ZO optimization is also advantageous when it is *difficult* to compute the first-order gradient of an objective function. Online sensor management provides an example of such a scenario [27], [72]. Sensor selection for parameter estimation is a fundamental problem in smart grids, communication systems, and wireless sensor networks [73]. The goal is to seek the optimal tradeoff between sensor activations and the estimation accuracy over a time period.

We consider the cumulative loss for online sensor selection [27]

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^d}{\text{minimize}} && \frac{1}{T} \sum_{t=1}^T \left[-\log \det \left(\sum_{i=1}^d x_i \mathbf{a}_{i,t} \mathbf{a}_{i,t}^T \right) \right] \\ & \text{subject to} && \mathbf{1}^T \mathbf{x} = m_0, \quad \mathbf{0} \leq \mathbf{x} \leq \mathbf{1}, \end{aligned} \quad (17)$$

where $\mathbf{x} \in \mathbb{R}^d$ is the optimization variable, d is the number of sensors, $\mathbf{a}_{i,t} \in \mathbb{R}^n$ is the observation coefficient of sensor i at time t , and m_0 is the number of selected sensors. The objective function of (17) can be interpreted as the log determinant of the error covariance matrix associated with the maximum likelihood

























True label:	brambling	cannon	pug-dog	fly	armadillo	balloon
Perturbed image (ZO-PSGD):						
Prediction label:	goldfinch	plow	bucket	longicorn	croquet ball	parachute
ℓ_2 Distortion:	35.2137	87.7304	72.3397	111.068	172.719	35.9330
# of queries:	7640	150	130	50	210	5830
Perturbed image (ZO-SMD):						
Prediction label:	goldfinch	plow	bucket	cicada	croquet ball	parachute
ℓ_2 distortion:	8.9708	26.0126	20.9504	30.0968	45.097	10.9023
# of queries:	29980	350	260	140	570	15830
Perturbed image (ZO-AdaMM):						
Prediction label:	goldfinch	plow	bucket	cicada	croquet ball	parachute
ℓ_2 distortion:	8.0502	5.7359	4.5753	4.4456	6.3149	7.7405
# of queries:	53300	1710	790	540	2780	32900
Perturbed image (ZO-NES):						
Prediction label:	goldfinch	plow	bucket	cicada	croquet ball	parachute
ℓ_2 distortion:	54.9956	34.5852	28.7035	28.9158	40.1483	51.7116
# of queries:	22110	1080	830	430	2280	15340

TABLE II: Comparison of various ZO methods for generating untargeted adversarial attacks against Inception V3 model over 5 ImageNet images. Row 1: true labels of given images. Row 2-4: Results obtained using ZO-SMD, which include perturbed images, corresponding prediction labels, ℓ_2 norm of perturbations, and the number of queries when achieving the first successful black-box attack. A similar explanation holds for other rows, except that different ZO methods are used.

estimator for parameter estimation [74]. The constraint $\mathbf{0} \leq \mathbf{x} \leq \mathbf{1}$ is a relaxed convex hull of the Boolean constraint $\mathbf{x} \in \{0, 1\}^m$, which encodes whether or not a sensor is selected.

Conventional methods such as projected gradient (first-order) and interior-point (second-order) algorithms can be used to solve problem (17). However, both methods involve the calculation of inverses of large matrices that are necessary to evaluate the gradient of the cost function. The matrix inversion step is usually a bottleneck while acquiring the gradient information in high dimensions and it is particularly problematic in the online optimization setting. Since problem (17) involves mixed equality and inequality constraints, it has been shown [27] that ZO-ADMM is an effective ZO optimization method for circumventing the computational bottleneck.

In Figure 2, we compare the performance of ZO-ADMM and that of FO-ADMM [75] for sensor selection. In the top plots, we demonstrate the primal-dual residuals in ADMM against the number of iterations. As we can see, ZO-ADMM has a slower convergence rate than FO-ADMM, and it approaches the

accuracy of FO-ADMM as the number of iterations increases. In the bottom plots, we show the mean squared error (MSE) of parameter estimation using different number of selected sensors m_0 in (17). As we can see, ZO-ADMM yields almost the same MSE as FO-ADMM in the context of parameter estimation using m_0 activated sensors, determined by the hard thresholding of continuous sensor selection schemes, i.e., solutions of problem (17) obtained from ZO-ADMM and FO-ADMM.

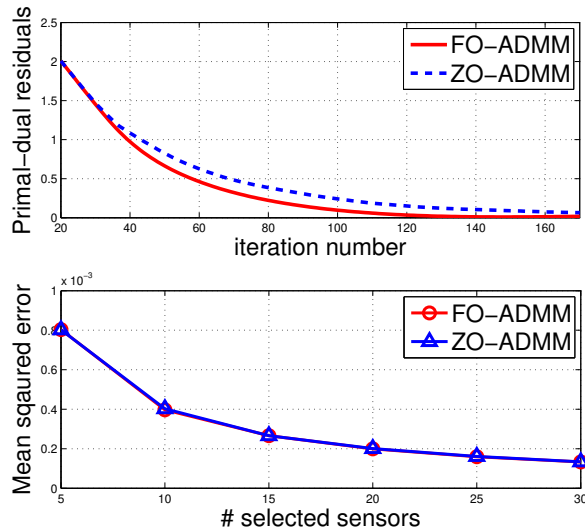


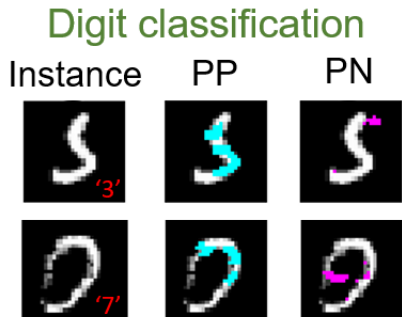
Fig. 2: Comparison between ZO-ADMM and FO-ADMM for solving the sensor selection problem (17). Top: ADMM primal-dual residuals versus number of iterations. Bottom: Mean squared error of activated sensors for parameter estimation versus the total number of selected sensors.

VI. OTHER RECENT APPLICATIONS

In this section we discuss some other recent applications of ZO optimization in signal processing and machine learning.

A. Model-agnostic contrastive explanations. Explaining the decision making process of a complex ML model is crucial to many ML-assisted high-stakes applications, such as job hiring, financial loan application and judicial sentence. When generating local explanations for the prediction of an ML model on a specific data sample, one common practice is to leverage the information of its input gradient for sensitivity analysis of the model prediction. For ML models that do not have explicit functions for computing input gradients, such as access-limited APIs or rule-based systems, ZO optimization enables the generation of local explanations using model queries without the knowledge of the gradient information. Moreover, even when the input gradient can be obtained via ML platforms

such as TensorFlow and PyTorch, the gradient computation is platform-specific. In this case, ZO optimization has the advantage of alleviating platform dependency when developing multi-platform explanation methods, as it only depends on model inference results.



(a)

Credit loan approval

Alice's loan application would be approved if
Consolidated risk markers changes from 65 to **72** AND
Average age of accounts in months changes from 52 to **68** AND
Months since most recent credit inquiry not within the last 7 days
 changes from 2 to **3**

(b)

Fig. 3: Contrastive explanations generated by ZO optimization methods. (a) For hand-written digit classification, the red digit class on the corner of an input sample shows the model prediction of the instance. The pixels highlighted by the cyan color are the pertinent positive (PP) supporting the original prediction. The pixels highlighted by the purple color are the pertinent negative (PN) that will alter the model prediction when added to the original instance. (b) For the credit loan application, the PN of an applicant (Alice) is used to explain the necessary modifications on a subset of the original features in order to change the model prediction from ‘denial’ to ‘approval’.

Here, we apply ZO optimization to generating contrastive explanations [76] for two ML applications – handwritten digit classification and loan approval. Contrastive explanations consist of two components derived from a given data sample for explaining the model prediction, i.e., a pertinent positive (PP) that is minimally and sufficiently present to keep the same prediction of the original input sample, and a pertinent negative (PN) that is minimally and necessarily absent to alter the model prediction. The process of finding PP and PN is formulated as a sparsity-driven and data-perturbation based optimization problem guided by the model prediction outcomes [25], which can be solved by ZO optimization methods. Fig. 3 shows the contrastive explanations generated from black-box neural network models by ZO-GD using the objective functions in [25]. For hand-written digit classification, the PP identifies a subset of pixels such that their presence is minimally sufficient for model

prediction. Moreover, the PN identifies a subset of pixels such that their absence is minimally necessary for altering model prediction. The PP and PN together constitute a contrastive explanation for interpreting model prediction. Similarly, for credit loan approval task trained on the FICO explainable machine learning challenge dataset¹ based on a neural network model, the PN generated for an applicant (Alice) can be used to explain how the model would alter the recommendation from ‘denial’ to ‘approval’ based on Alice’s loan application profile².

B. Policy search in reinforcement learning. Reinforcement learning aims to determine given a state which action to take (or policy) in order to maximize the reward. One of the most popular policy search approaches is the model-free policy search, where agent learns parameterized policies from sampled trajectories without needing to learn the model of the underlying dynamics. Model-free policy search updates the parameters such that trajectories with higher reward are more likely to be obtained when following the updated policy [77]. Traditional policy search methods, such as REINFORCE [78], rely on randomized exploration in the action space to compute an estimated direction of improvement. These methods (referred to as policy gradient methods) then leverage the first order information of the policy (or Jacobian) to update its parameters to maximize the reward. Note that the chance of finding a sequence of actions resulting in high total reward decreases as the horizon length increases and thus policy gradient methods often exhibit high variance and result in large sample complexity [79].

To alleviate these problems, ZO policy search methods, which directly optimize over policy parameter space, have emerged as an alternative to policy gradient. More specifically, ZO policy search methods seek to directly optimize the total reward in the space of parameters by employing finite-difference methods to compute estimates of the gradient with respect to policy parameters [77], [80]–[83]. These methods are fully zeroth-order, i.e., they do not exploit first-order information of the policy, the reward, or the dynamics. Interestingly, it has been observed that although policy gradient methods leverage more information, ZO policy search methods often perform better empirically. In particular, the work [82] characterized

¹<https://community.fico.com/s/explainable-machine-learning-challenge>

²Please refer to <https://aix360.mybluemix.net> for more details.

the convergence rate of ZO policy optimization when applied to linear-quadratic systems. And the work [83] theoretically showed that the complexity of exploration in the action space (using policy gradients) depends on both the dimensionality of the action space and the horizon length, as opposed to, the complexity of exploration in the parameter space (using ZO methods) depends only on the dimensionality of the parameter space.

C. Automated ML. The success of ML relies heavily on selecting the right pipeline algorithms for the problem at hand, and on setting its hyperparameters. Automated ML (AutoML) automates the process of model selection and hyperparameter optimization. It offers the advantages of producing simpler solutions, faster creation of those solutions, and models that often outperform hand-designed machine learning models. One could view AutoML as the process of optimization of an unknown black-box function. Recently, several Bayesian optimization (BO) approaches have been proposed for AutoML [26], [84]. BO works by building a probabilistic surrogate via Gaussian process (GP) for the objective function, and then using an acquisition function defined from this surrogate to decide where to sample. However, BO suffers from a computational bottleneck: an internal first-order solver is required to determine the parameters of the GP model by maximizing the log marginal likelihood of the current function evaluations at each iteration of BO. The first-order solver is slow due to the difficulty of computing the gradient of the log-likelihood function with respect to the parameters of GP. To circumvent this difficulty, the ZO optimization algorithm can be used to determine the hyperparameters and thus to accelerate BO in AutoML [26]. In the context of meta-learning, ZO optimization has also been leveraged to obviate the need for determining computationally-intensive high-order derivatives during meta-training [29]. Lastly, we note that ZO optimization can be integrated with learning-to-optimize (L2O), which models the optimizer through a trainable DNN-based meta-learner [85], [86].

VII. OPEN QUESTIONS AND DISCUSSIONS

Although there has been a great deal of progress on the design, theoretical analysis, and applications of ZO optimization, many questions and challenges still remain.

A. ZO optimization with non-smooth objectives. There exists a gap between the theoretical analysis of ZO optimizers and practical ML/DL applications with non-smooth objectives, where the former usually requires the smoothness of the objective function. There are two possible means of relaxing the smoothness assumption. First, the randomized smoothing technique ensures that the convolution of two functions is at least as smooth as the smoothest of the two original functions. Thus, f_μ is smooth even if f is non-smooth in (2). This motivates the technique of *double randomization* that approximates a subgradient of a non-smooth objective function [21], where an extra randomized perturbation is introduced to prevent drawing points from non-smooth regions of f . The downside of double randomization is the increase of function query complexity. Second, a model-based trust region method can be leveraged to approximate the subgradient/gradient using linear or quadratic interpolation [6], [31]. This leads to the general approach of gradient estimation without imposing extra assumptions on the objective function. However, it increases the computation cost due to the need to solve nested regression problems.

B. ZO optimization with black-box constraints. The current work on ZO optimization is restricted to black-box objective functions with white-box constraints. In the presence of black-box constraints, the introduction of barrier functions (instead of constraints) [87] in the objective could be a potential solution. One could also employ the method of multipliers to reformulate black-box constraints as regularization functions in the objective function [26].

C. ZO optimization for privacy-preserving distributed learning. To protect the sensitive information of data in the context of distributed learning, it is common to add ‘noise’ (randomness) into gradients of individual cost functions of agents, known as message-perturbing privacy strategy [88]. The level of privacy is often evaluated by differential privacy (DP). A high degree of DP prevents the adversary from gaining meaningful personal information of any individuals. Similarly, ZO optimization also conceals the gradient information and allows the use of noisy gradient estimates that are constructed from function values. Thus, one interesting question is: can ZO optimization be designed with privacy guarantees? In a more general sense, it would be worthwhile to examine what roles ZO optimization plays in the privacy-preserving and

Byzantine-tolerant federated learning setting.

D. ZO optimization and automatic differentiation. Automatic differentiation (AD) provides a way for efficiently and accurately evaluating derivatives of numeric functions, which are expressed as computer programs [89]. The backpropagation algorithm, used for training neural networks, can be regarded as a specialized instance of AD under the reverse mode. AD decomposes the derivative of the complex function into sub-derivatives of constituent operations through the chain rule. When a sub-derivative is infeasible or difficult to compute, the ZO gradient estimation techniques could be integrated with AD. In particular, when the high-order derivatives (beyond gradient) are required, e.g., model-agnostic meta-learning [90], ZO optimization could help to overcome the derivative bottleneck.

E. ZO optimization for discrete variables. Many machine learning and signal processing tasks involve handling discrete variables, such as texts, graphs, sets and categorical data. In addition to the technique of relaxation to continuous values, it is worthwhile to explore and design ZO algorithms that directly operate on discrete domains.

F. Tight convergence rates of ZO methods. Although the optimal rate for ZO unconstrained convex optimization was studied in [21], there remain many open questions on seeking the optimal rates, or associated tight lower bounds, for general cases of ZO constrained nonconvex optimization.

VIII. CONCLUSIONS

In this survey paper, we discussed various variants of ZO gradient estimators and focused on their statistical modelling as this leads to general ZO algorithms. We also provided an extensive comparison of ZO algorithms and discussed their iteration and function query complexities. Furthermore, we presented numerous emerging applications of ZO optimization in signal processing and machine learning. Finally, we highlighted some unsolved research challenges in ZO optimization research and presented some promising future research directions.

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REFERENCES

- [1] J. Kiefer, J. Wolfowitz, et al., “Stochastic estimation of the maximum of a regression function,” *The Annals of Mathematical Statistics*, vol. 23, no. 3, pp. 462–466, 1952.
- [2] J. C. Spall, “A stochastic approximation technique for generating maximum likelihood parameter estimates,” in *American Control Conference*, 1987, pp. 1161–1167.
- [3] J. Nocedal and S. Wright, *Numerical optimization*, Springer Science & Business Media, 2006.
- [4] A. R. Conn, K. Scheinberg, and L. N. Vicente, *Introduction to derivative-free optimization*, vol. 8, SIAM, 2009.
- [5] L. M. Rios and N. V. Sahinidis, “Derivative-free optimization: a review of algorithms and comparison of software implementations,” *Journal of Global Optimization*, vol. 56, no. 3, pp. 1247–1293, 2013.
- [6] J. Larson, M. Menickelly, and S. M. Wild, “Derivative-free optimization methods,” *Acta Numerica*, vol. 28, pp. 287–404, May 2019.
- [7] J. A. Nelder and R. Mead, “A simplex method for function minimization,” *The Computer Journal*, vol. 7, no. 4, pp. 308–313, 1965.
- [8] E. Fermi and N. Metropolis, “Numerical solution of a minimum problem,” *Technical Report LA-1492*, <https://hdl.handle.net/2027/mdp.39015086487645>, 1952.
- [9] V. Torczon, “On the convergence of the multidirectional search algorithm,” *SIAM Journal on Optimization*, vol. 1, no. 1, pp. 123–145, 1991.
- [10] D. M. Bortz and C. T. Kelley, “The simplex gradient and noisy optimization problems,” in *Computational Methods for Optimal Design and Control*, pp. 77–90. Springer, 1998.
- [11] A. R. Conn, N. I. Gould, and P. L. Toint, *Trust region methods*, vol. 1, SIAM, 2000.
- [12] A. I. F. Vaz and L. N. Vicente, “PSwarm: a hybrid solver for linearly constrained global derivative-free optimization,” *Optimization Methods & Software*, vol. 24, no. 4-5, pp. 669–685, 2009.
- [13] D. E. Goldberg and J. H. Holland, “Genetic algorithms and machine learning,” *Machine Learning*, vol. 3, no. 2-3, pp. 95–99, 1988.
- [14] B. Shahriari, K. Swersky, Z. Wang, R. P. Adams, and N. De Freitas, “Taking the human out of the loop: A review of bayesian optimization,” *Proceedings of the IEEE*, vol. 104, no. 1, pp. 148–175, 2016.
- [15] M. J. D. Powell, “A direct search optimization method that models the objective and constraint functions by linear interpolation,” in *Advances in optimization and numerical analysis*, pp. 51–67. Springer, 1994.
- [16] E. Jones, T. Oliphant, P. Peterson, et al., “SciPy: Open source scientific tools for Python,” 2001.
- [17] J. Deng, W. Dong, R. Socher, L.-J. Li, K. Li, and F.-F. Li, “Imagenet: A large-scale hierarchical image database,” in *IEEE CVPR*, 2009, pp. 248–255.
- [18] S. Ghadimi and G. Lan, “Stochastic first-and zeroth-order methods for nonconvex stochastic programming,” *SIAM Journal on Optimization*, vol. 23, no. 4, pp. 2341–2368, 2013.
- [19] Y. Nesterov and V. Spokoiny, “Random gradient-free minimization of convex functions,” *Foundations of Computational Mathematics*, vol. 2, no. 17, pp. 527–566, 2015.
- [20] A. D. Flaxman, A. T. Kalai, and H. B. McMahan, “Online convex optimization in the bandit setting: Gradient descent without a gradient,” in *Proc. 16th Annual ACM-SIAM Symposium on Discrete algorithms*, 2005, pp. 385–394.
- [21] J. C. Duchi, M. I. Jordan, M. J. Wainwright, and A. Wibisono, “Optimal rates for zero-order convex optimization: The power of two function

- evaluations,” *IEEE Trans. Inf. Theory*, vol. 61, no. 5, pp. 2788–2806, 2015.
- [22] I. Goodfellow, J. Shlens, and C. Szegedy, “Explaining and harnessing adversarial examples,” *ICLR*, 2015.
- [23] P.-Y. Chen, H. Zhang, Y. Sharma, J. Yi, and C.-J. Hsieh, “Zoo: Zeroth order optimization based black-box attacks to deep neural networks without training substitute models,” in *Proc. 10th ACM Workshop on Artificial Intelligence and Security*, 2017, pp. 15–26.
- [24] A. Ilyas, K. Engstrom, A. Athalye, and J. Lin, “Black-box adversarial attacks with limited queries and information,” in *ICML*, July 2018.
- [25] A. Dhurandhar, T. Pedapati, A. Balakrishnan, et al., “Model agnostic contrastive explanations for structured data,” *arXiv preprint arXiv:1906.00117*, 2019.
- [26] S. Liu, P. Ram, D. Vijaykeerthy, et al., “An ADMM based framework for AutoML pipeline configuration,” *AAAI*, 2019.
- [27] S. Liu, J. Chen, P.-Y. Chen, and A. O. Hero, “Zeroth-order online ADMM: Convergence analysis and applications,” in *AISTATS*, 2018, vol. 84, pp. 288–297.
- [28] S.-M. Moosavi-Dezfooli, A. Fawzi, J. Uesato, and P. Frossard, “Robustness via curvature regularization, and vice versa,” in *IEEE CVPR*, 2019, pp. 9078–9086.
- [29] X. Song, W. Gao, Y. Yang, K. Choromanski, A. Pacchiano, and Y. Tang, “Es-maml: Simple hessian-free meta learning,” in *ICLR*, 2020.
- [30] Y.-Y. Tsai, P.-Y. Chen, and T.-Y. Ho, “Transfer learning without knowing: Reprogramming black-box machine learning models with scarce data and limited resources,” *ICML*, 2020.
- [31] A. S. Berahas, L. Cao, K. Choromanski, and K. Scheinberg, “A theoretical and empirical comparison of gradient approximations in derivative-free optimization,” *arXiv preprint arXiv:1905.01332*, 2019.
- [32] S. Liu, B. Kailkhura, P.-Y. Chen, P. Ting, S. Chang, and L. Amini, “Zeroth-order stochastic variance reduction for nonconvex optimization,” *NeurIPS*, 2018.
- [33] J. C. Spall et al., “Multivariate stochastic approximation using a simultaneous perturbation gradient approximation,” *IEEE transactions on automatic control*, vol. 37, no. 3, pp. 332–341, 1992.
- [34] X. Lian, H. Zhang, C.-J. Hsieh, Y. Huang, and J. Liu, “A comprehensive linear speedup analysis for asynchronous stochastic parallel optimization from zeroth-order to first-order,” in *NeurIPS*, 2016, pp. 3054–3062.
- [35] O. Shamir, “An optimal algorithm for bandit and zero-order convex optimization with two-point feedback,” *JMLR*, vol. 18, no. 52, pp. 1–11, 2017.
- [36] S. Liu, P.-Y. Chen, X. Chen, and M. Hong, “signSGD via zeroth-order oracle,” in *ICLR*, 2019.
- [37] B. Gu, Z. Huo, and H. Huang, “Zeroth-order asynchronous doubly stochastic algorithm with variance reduction,” *arXiv preprint arXiv:1612.01425*, 2016.
- [38] L. Liu, M. Cheng, C.-J. Hsieh, and D. Tao, “Stochastic zeroth-order optimization via variance reduction method,” *arXiv preprint arXiv:1805.11811*, 2018.
- [39] K. Ji, Z. Wang, Y. Zhou, and Y. Liang, “Improved zeroth-order variance reduced algorithms and analysis for nonconvex optimization,” in *ICML*, 2019, vol. 97, pp. 3100–3109.
- [40] H. Ye, Z. Huang, C. Fang, C. J. Li, and T. Zhang, “Hessian-aware zeroth-order optimization for black-box adversarial attack,” *arXiv preprint arXiv:1812.11377*, 2018.
- [41] K. Balasubramanian and S. Ghadimi, “Zeroth-order nonconvex stochastic optimization: Handling constraints, high-dimensionality, and saddle-points,” *arXiv preprint arXiv:1809.06474*, pp. 651–676, 2019.
- [42] M. Cheng, S. Singh, P.-Y. Chen, S. Liu, and C.-J. Hsieh, “Sign-OPT: A query-efficient hard-label adversarial attack,” *ICLR*, 2020.
- [43] S. Ghadimi, G. Lan, and H. Zhang, “Mini-batch stochastic approximation methods for nonconvex stochastic composite optimization,” *Mathematical Programming*, vol. 155, no. 1-2, pp. 267–305, 2016.
- [44] K. Balasubramanian and S. Ghadimi, “Zeroth-order (non)-convex stochastic optimization via conditional gradient and gradient updates,” in *NeurIPS*, 2018, pp. 3455–3464.
- [45] X. Chen, S. Liu, K. Xu, X. Li, X. Lin, M. Hong, and D. Cox, “ZO-AdaMM: Zeroth-order adaptive momentum method for black-box optimization,” in *NeurIPS*, 2019, pp. 7202–7213.
- [46] J. Chen, J. Yi, and Q. Gu, “A Frank-Wolfe framework for efficient and effective adversarial attacks,” in *AAAI*, 2020.
- [47] A. K. Sahu, M. Zaheer, and S. Kar, “Towards gradient free and projection free stochastic optimization,” *AISTATS*, 2019.
- [48] X. Chen, S. Liu, R. Sun, and M. Hong, “On the convergence of a class of adam-type algorithms for non-convex optimization,” in *ICLR*, 2019.
- [49] P. Zhao, S. Liu, P.-Y. Chen, N. Hoang, K. Xu, B. Kailkhura, and X. Lin, “On the design of black-box adversarial examples by leveraging gradient-free optimization and operator splitting method,” in *ICCV*, 2019.
- [50] X. Gao, B. Jiang, and S. Zhang, “On the information-adaptive variants of the ADMM: an iteration complexity perspective,” *Optimization Online*, vol. 12, 2014.
- [51] F. Huang, S. Gao, S. Chen, and H. Huang, “Zeroth-order stochastic alternating direction method of multipliers for nonconvex nonsmooth optimization,” *IJCAI*, 2019.
- [52] S. Liu, S. Lu, X. Chen, Y. Feng, K. Xu, A. Al-Dujaili, M. Hong, and U.-M. O’Reilly, “Min-max optimization without gradients: Convergence and applications to adversarial ML,” in *ICML*, 2020.
- [53] Z. Wang, K. Balasubramanian, S. Ma, and M. Razaviyayn, “Zeroth-order algorithms for nonconvex minimax problems with improved complexities,” *arXiv preprint arXiv:2001.07819*, 2020.
- [54] A. K. Sahu, D. Jakovetic, D. Bajovic, and S. Kar, “Distributed zeroth order optimization over random networks: A kiefer-wolfowitz stochastic approximation approach,” in *IEEE CDC*, 2018, pp. 4951–4958.
- [55] D. Yuan, D. W. C. Ho, and S. Xu, “Zeroth-order method for distributed optimization with approximate projections,” *IEEE Trans. Neural Netw.*, vol. 27, no. 2, pp. 284–294, 2015.
- [56] Z. Yu, D. W. C. Ho, and D. Yuan, “Distributed randomized gradient-free mirror descent algorithm for constrained optimization,” *arXiv preprint arXiv:1903.04157*, 2019.
- [57] D. Hajinezhad, M. Hong, and A. Garcia, “Zone: Zeroth-order nonconvex multiagent optimization over networks,” *IEEE Trans. Autom. Control*, vol. 64, no. 10, pp. 3995–4010, 2019.
- [58] Y. Tang and N. Li, “Distributed zero-order algorithms for nonconvex multi-agent optimization,” in *Allerton*, 2019, pp. 781–786.
- [59] Y. Wang, S. Du, S. Balakrishnan, and A. Singh, “Stochastic zeroth-order optimization in high dimensions,” in *AISTATS*. April 2018, vol. 84, pp. 1356–1365, PMLR.
- [60] D. Golovin, J. Karro, G. Kochanski, C. Lee, X. Song, and Q. Zhang, “Gradientless descent: High-dimensional zeroth-order optimization,” in *ICLR*, 2020.
- [61] J. Li, K. Balasubramanian, and S. Ma, “Zeroth-order optimization on Riemannian manifolds,” *arXiv preprint arXiv:2003.11238*, 2020.

- [62] E. Hazan, “Introduction to online convex optimization,” *Foundations and Trends® in Optimization*, vol. 2, no. 3-4, pp. 157–325, 2016.
- [63] E.-V. Vlastakis-Gkaragkounis, L. Flokas, and G. Piliouras, “Efficiently avoiding saddle points with zero order methods: No gradients required,” in *NeurIPS*, 2019, pp. 10066–10077.
- [64] S. J. Reddi, S. Sra, B. Póczos, and A. J. Smola, “Proximal stochastic methods for nonsmooth nonconvex finite-sum optimization,” in *NeurIPS*, 2016, pp. 1145–1153.
- [65] N. Carlini and D. Wagner, “Towards evaluating the robustness of neural networks,” in *IEEE Symposium on Security and Privacy*, 2017, pp. 39–57.
- [66] C.-C. Tu, P. Ting, P.-Y. Chen, S. Liu, H. Zhang, J. Yi, C.-J. Hsieh, and S.-M. Cheng, “Autozoom: Autoencoder-based zeroth order optimization method for attacking black-box neural networks,” in *AAAI*, 2019.
- [67] W. Brendel, J. Rauber, and M. Bethge, “Decision-based adversarial attacks: Reliable attacks against black-box machine learning models,” *ICLR*, 2018.
- [68] M. Cheng, T. Le, P.-Y. Chen, J. Yi, H. Zhang, and C.-J. Hsieh, “Query-efficient hard-label black-box attack: An optimization-based approach,” *ICLR*, 2019.
- [69] P. Zhao, P.-Y. Chen, S. Wang, and X. Lin, “Towards query-efficient black-box adversary with zeroth-order natural gradient descent,” *AAAI*, 2020.
- [70] K. Xu, S. Liu, P. Zhao, et al., “Structured adversarial attack: Towards general implementation and better interpretability,” in *ICLR*, 2019.
- [71] C. Szegedy, V. Vanhoucke, S. Ioffe, J. Shlens, and Z. Wojna, “Rethinking the inception architecture for computer vision,” in *IEEE CVPR*, 2016, pp. 2818–2826.
- [72] T. Chen and G. B. Giannakis, “Bandit convex optimization for scalable and dynamic IoT management,” *IEEE Internet of Things Journal*, 2018.
- [73] A. O. Hero and D. Cochran, “Sensor management: Past, present, and future,” *IEEE Sensors J.*, vol. 11, no. 12, pp. 3064–3075, 2011.
- [74] S. Joshi and S. Boyd, “Sensor selection via convex optimization,” *IEEE Trans. Signal Process.*, vol. 57, no. 2, pp. 451–462, 2009.
- [75] T. Suzuki, “Dual averaging and proximal gradient descent for online alternating direction multiplier method,” in *ICML*, 2013, pp. 392–400.
- [76] A. Dhurandhar, P.-Y. Chen, et al., “Explanations based on the missing: Towards contrastive explanations with pertinent negatives,” in *NeurIPS*, 2018, pp. 592–603.
- [77] J. Kober, J. A. Bagnell, and J. Peters, “Reinforcement learning in robotics: A survey,” *The International Journal of Robotics Research*, vol. 32, no. 11, pp. 1238–1274, 2013.
- [78] R. J. Williams, “Simple statistical gradient-following algorithms for connectionist reinforcement learning,” *Machine learning*, vol. 8, no. 3-4, pp. 229–256, 1992.
- [79] T. Zhao, H. Hachiya, G. Niu, and M. Sugiyama, “Analysis and improvement of policy gradient estimation,” in *NeurIPS*, 2011, pp. 262–270.
- [80] T. Salimans, H. Ho, X. Chen, S. Sidor, and I. Sutskever, “Evolution strategies as a scalable alternative to reinforcement learning,” *arXiv preprint arXiv:1703.03864*, 2017.
- [81] F. Schnke, C. Osendorfer, Thomas Rückstieß, A. Graves, J. Peters, and J. Schmidhuber, “Parameter-exploring policy gradients,” *Neural Networks*, vol. 23, no. 4, pp. 551–559, 2010.
- [82] D. Malik, A. Pananjady, K. Bhatia, K. Khamaru, P. Bartlett, and M. Wainwright, “Derivative-free methods for policy optimization: Guarantees for linear quadratic systems,” in *Proceedings of Machine Learning Research*, 16–18 Apr 2019, vol. 89, pp. 2916–2925.
- [83] A. Vemula, W. Sun, and J. A. Bagnell, “Contrasting exploration in parameter and action space: A zeroth-order optimization perspective,” in *Proceedings of Machine Learning Research*, 16–18 Apr 2019, vol. 89, pp. 2926–2935.
- [84] J. Snoek, H. Larochelle, and R. P. Adams, “Practical bayesian optimization of machine learning algorithms,” in *NeurIPS*, 2012, pp. 2951–2959.
- [85] Y. Ruan, Y. Xiong, S. Reddi, S. Kumar, and C.-J. Hsieh, “Learning to learn by zeroth-order oracle,” in *ICLR*, 2020.
- [86] Y. Cao, T. Chen, Z. Wang, and Y. Shen, “Learning to optimize in swarms,” in *NeurIPS*, 2019, pp. 15044–15054.
- [87] S. Boyd and L. Vandenberghe, *Convex optimization*, Cambridge university press, 2004.
- [88] S. Song, K. Chaudhuri, and A. D. Sarwate, “Stochastic gradient descent with differentially private updates,” in *IEEE GlobalSIP*, 2013, pp. 245–248.
- [89] A. G. Baydin, B. A. Pearlmutter, A. A. Radul, and J. M. Siskind, “Automatic differentiation in machine learning: A survey,” *JMLR*, vol. 18, no. 1, pp. 5595–5637, Jan. 2017.
- [90] C. Finn, P. Abbeel, and S. Levine, “Model-agnostic meta-learning for fast adaptation of deep networks,” in *ICML*, 2017, pp. 1126–1135.