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EXPEDITING STOCHASTIC DERIVATIVE-FREE OPTIMIZATION

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ABSTRACT

Adaptive sampling-based trust-region optimization has emerged as an efficient solver for nonlinear and nonconvex problems in noisy derivative-free environments. This class of algorithms proceeds by iteratively constructing local models on objective function estimates that use a carefully chosen number of calls to the stochastic oracle. To expedite this class of algorithms, we introduce four refinements: (a) quadratic local models with diagonal Hessian, (b) a direct search, (c) a reusing strategy, and (d) common random numbers. We have substantiated that the introduced refinements enable the algorithm to achieve accelerated convergence, both in numerical simulations and in theoretical analyses.

1 INTRODUCTION

In the artificial intelligence era, stochastic derivative-free optimization (SDFO) is receiving much attention for allowing users to specify functions involved in non-explicit forms. As a result, SDFO has many applications, such as hyper-parameter tuning, reinforcement learning, and simulation-based optimization. An essential characteristic of SDFO is that the evaluation of the function is only accessible via a stochastic simulation, consuming significant time. Consequently, obtaining a sufficiently viable solution through solving SDFO will also require a significant amount of time. In this paper, we aim to develop a sample-efficient iterative algorithm for solving unconstrained SDFO of a nonconvex, smooth, bounded-below function $f : \mathbb{R}^d \to \mathbb{R}$ defined in $\mathbb{R}^d$. The problem is of the form

$$\min_{\boldsymbol{x}\in\mathbb{R}^d} \left\{ f(\boldsymbol{x}) := \mathbb{E}[F(\boldsymbol{x},\xi)] = \int_{\Xi} F(\boldsymbol{x},\xi)dP \right\}, \tag{1}$$

where $F : \mathbb{R}^d \times \Xi \to \mathbb{R}$ is a function defined on a probability space $(\Xi, \mathcal{F}, P)$. To estimate $f(\boldsymbol{x})$, we generate independent and identically distributed copies of the random variable $F(\boldsymbol{x},\xi)$ allowing us to compute the sample average. We assume access to zeroth-order stochastic oracles, meaning that direct derivative information is unattainable. Consequently, to solve (1) using a model-based method such as trust-region optimization (TRO) (Conn et al. 2000), we must implicitly approximate the gradient.

Trust-region (TR) algorithms are a family of iterative methods for solving smooth nonconvex stochastic optimization problems that have recently gained in popularity due primarily to the robustness stemming their self-tuning nature. The random sequence of iterates $\{\boldsymbol{X}_k\}$ recommended by a single run of TRO in a stochastic setting, as described for Problem (1), leverages local approximations of the function and their minimizers within neighborhoods of dynamic sizes. In a derivative-free setting, the approximation is often done with interpolation or regression using estimated function values at adjacent points around the incumbent solution, indicating that the computational load escalates alongside the growth in problem dimension. To address this issue, we suggest four refinements for the adaptive sampling-based trust-region optimization, called ASTRO-DF (Shashaani et al. 2018): (a) quadratic local models with diagonal Hessian (coordinate basis), (b) a direct search, (c) a reusing strategy, and (d) common random numbers (CRN).

2 REFINED ASTRO-DF

In this section, we introduce four refinements aiming to design a more efficient algorithm tailored for addressing high-dimensional SDFO problems (Table 1). Note that an iteration complexity (IC) is defined as $T_\epsilon := \min\{k : \|\nabla f(\boldsymbol{X}_k)\| \leq \epsilon\}$ and a work complexity (WC) is defined as $\sum_{k=1}^{T_\epsilon} W_k$, with W_k tracking the total calls to the stochastic oracle during iteration k.

Table 1: Refinements for ASTRO-DF.

Design Set Selection		IC	WC
Coordinate Basis (CB)	· Constructing local model within the TR using the CB	$\mathcal{O}(\epsilon^{-2})$	$\widetilde{\mathcal{O}}(\epsilon^{-6})$
Direct Search	· Updating the candidate as the best point within the TR		
Reusing Strategy	· Reusing the farthest point from $\boldsymbol{X}_k$ within the TR · Constructing the local model with a rotated CB		
Sampling Strategy		**IC**	**WC**
CRN	· Querying the oracle with the same random number · Using same sample sizes for any point per iteration	$\mathcal{O}(\epsilon^{-2})$	$\widetilde{\mathcal{O}}(\epsilon^{-4})$

In what follows, we summarize the principal advantages of each refinements.

1. **(Coordinate Basis)** The use of interpolation in the CB enhances gradient accuracy, lowers linear algebra cost, and imparts curvature insight through the diagonal Hessian.
2. **(Direct Search)** By integrating direct search into the trust-region framework, leveraging existing information at no extra cost to enhance solution quality and increase successful iteration likelihood, vital for sustaining larger steps and minimizing simulation oracle calls.
3. **(Reusing Strategy)** The suggested reusing strategy possesses the ability to not only alleviate computational load but also inherently explore the direction (via the direct search method in the current iteration) that demonstrated the most promising reduction in the previous iteration.
4. **(CRN)** CRN can facilitate SDFO algorithm efficiency by preserving structure inherent to the objective function sample-path. We unveiled that ASTRO-DF achieves $\widetilde{\mathcal{O}}(\epsilon^{-4})$ for the work complexity when combined with CRN and the continuous sample path, a significant improvement over $\widetilde{\mathcal{O}}(\epsilon^{-6})$.

3 CONCLUDING REMARKS

We make two remarks in closing.

- In the context of SO, a critical inquiry arises: "How can the number of necessary simulation oracle calls be minimized while still attaining a good enough solution?" We suggested four refinements to answer such question both numerically and theoretically, while still achieving the strong convergence.
- Most existing stochastic TR algorithms assume independence between the local models to obtain the convergence, which implies that the reusing strategy and CRN are not applicable. We proved that ASTRO-DF with CRN converges to the stationary point almost surely. As for the analysis of ASTRO-DF with the reusing strategy, we leave it to future research to explore further.

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