Structure-Aware Methods for Expensive Derivative-Free Nonsmooth Composite Optimization

Jeffrey Larson and Matt Menickelly

1Mathematics and Computer Science Division, Argonne National Laboratory
jmlarson@anl.gov; mmenickelly@anl.gov (both authors contributed equally)

March 21, 2023

Abstract

We present new methods for solving a broad class of bound-constrained nonsmooth composite minimization problems. These methods are specially designed for objectives that are some known mapping of outputs from a computationally expensive function. We provide accompanying implementations of these methods: in particular, a novel manifold sampling algorithm (MS-P) with subproblems that are in a sense primal versions of the dual problems solved by previous manifold sampling methods and a method (GOOMBAH) that employs more difficult optimization subproblems. For these two methods, we provide rigorous convergence analysis and guarantees. We demonstrate extensive testing of these methods. Open-source implementations of the methods developed in this manuscript can be found at github.com/P0ptUS/IBCDF0/.

Keywords: Derivative-free optimization, Nonsmooth optimization, Composite optimization, Continuous selections, Manifold sampling.

1 Introduction

We consider optimization problems of the form

\[
\min_{x \in \Omega} \quad f(x),
\]

where \( f : \mathbb{R}^n \to \mathbb{R} \), and \( \Omega \) is a subset of the \( n \)-fold Cartesian product of the extended reals defined by bound constraints, namely, \( \Omega \equiv \{ x : \ell \leq x \leq u \} \). We additionally assume \( f \) in (1) is a composite function, that is, \( f \) satisfies the following.

Assumption 1. The function \( f \) in (1) has the form \( f(x) \triangleq h(F(x)) \), where \( h : \mathbb{R}^p \to \mathbb{R} \) and \( F : \mathbb{R}^n \to \mathbb{R}^p \).

In particular, we are interested in the case where \( h \) is a known function that is cheap to evaluate (with a known subdifferential) but a single evaluation of \( F \) requires considerable time or computational resources. In this paper we consider \( h \) in Assumption 1 to be from a fairly broad family of functions called continuous selections.

Definition 1. The function \( h \) is a continuous selection on a set \( U \) if it is continuous on \( U \) and

\[
h(z) \in \{ h_j(z) : h_j \in \mathcal{H} \}, \quad \forall z \in U,
\]

where \( \mathcal{H} \) is a finite set of functions \( h_j : \mathbb{R}^p \to \mathbb{R} \), called selection functions.
The composite functions represented by continuous selections are extensive, encapsulating virtually all practical use cases of composite optimization. For example, \( h \) can be the 1-norm [1], a quantile function (e.g., a minimum or maximum of entries in \( F \)) [2–4], a piecewise-affine function [5–7], or even a piecewise-nonlinear function [8]. As one example of the latter, most general case, particle accelerator physicists often seek parameters \( x \) that minimizes the minimum spread of a simulated beam over a finite set of locations \( J \) along a beam line [9]. High-fidelity simulations of such beam lines may require many thousands of compute hours, producing copious amounts of output. One way of quantifying the beam spread is the normalized emittance [10], which takes some computed quantities \( F_{1,j}(x), F_{2,j}(x), F_{3,j}(x) \) for each \( j \in J \) and combines them with the mapping \( \sqrt{F_{1,j}(x)F_{2,j}(x) - F_{3,j}(x)^2} \). Therefore, the outer function is \( h(z) \triangleq \min_{j \in J} \sqrt{z_{1,j}^2 - z_{2,j}^2 - z_{3,j}^2} \).

In this paper we provide convergence results for—and implementations of—various methods for solving (1). We begin by extending past work in manifold sampling methods, providing an empirically superior “primal variant” (MS-P) of the manifold sampling algorithm proposed in [8]. That algorithm was developed for only the unconstrained version of (1), and involves subproblems that are dual to the subproblems involved in the present work. We will demonstrate theoretical convergence results for this new primal variant of manifold sampling under reasonable assumptions. Additionally, we will demonstrate a method (GOOMBAAH) that uses more difficult trust-region subproblems than are typically analyzed; in general, there are no guarantees that these subproblems can be solved in finite time. However, by safeguarding this optimization method with the primal variant, we will yield a provably convergent method that we find to perform exceptionally well in practice, particularly when function evaluations are expensive.

**Terminology and notation** Before proceeding, we record the following definition of essentially active selection functions pertinent to continuous selections.

**Definition 2** (adapted from [11]). If \( h \) is a continuous selection function on \( U \), define

\[
S_i \triangleq \{ z : h(z) = h_j(z) \}, \quad \bar{S}_i \triangleq \text{cl}(\text{int}(S_i)), \quad \mathcal{A}(z) \triangleq \{ i : z \in \bar{S}_i \}.
\]

Elements of \( \mathcal{A}(z) \) are called essentially active indices; any \( h_j \) for which \( j \in \mathcal{A}(z) \) is an essentially active selection function for \( h \) at \( z \).

With these definitions, we can make assumptions on \( h \). Of course, these assumptions need hold only at points where \( h \) could possibly be evaluated over the course of an optimization run. For a constant \( \Delta_{\text{max}} > 0 \) bounding the possible trust-region radii \( \Delta > 0 \) and a starting point \( x^0 \), define

\[
L_{\text{max}} \triangleq \bigcup_{x \in L(x^0)} B(x; \Delta_{\text{max}}), \tag{2}
\]

where \( B(x; \Delta) \triangleq \{ y : \| x - y \| \leq \Delta \} \) and \( L(x^0) \) is the \( f(x^0) \) level set of \( f \): \( L(x^0) \triangleq \{ x \in \mathbb{R}^n : f(x) \leq f(x^0) \} \).

**Assumption 2.** With Definitions 1–2 we assume the following about \( h \).

A. The function \( h \) is a continuous selection\(^1\) on \( \text{Im}_F (L_{\text{max}} \cap \Omega) \).

B. For any \( z \in \text{Im}_F (L_{\text{max}} \cap \Omega) \), the essentially active indices \( \mathcal{A}(z) \) are computable.

**Remark 1.** In Assumption 2B, we use the word “computable” because in many instances of continuous selections, some computation—ideally not much more than \( \mathcal{O}(p) \) arithmetic operations and much less than the cost of evaluating \( F \)—is likely required to determine \( \mathcal{A}(z) \). For a simple example, if \( h(z) \triangleq \max_{j \in \{1, \ldots, p\}} h_j(z) \), then to determine \( \mathcal{A}(z) \), the obvious way to implement the continuous selection is to sort \( \{ h_j(z) \}_{j \in \{1, \ldots, p\}} \) in ascending order—an \( \mathcal{O}(p \log p) \) computation—and then return the sorted index (or indices, in the case of a tie) corresponding to the maximum value among the values of \( h_j(z) \).

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\(^1\)For practical purposes, one should attempt to define/construct \( \bar{S} \) such that \( \bar{S} \) contains only functions that are essentially active somewhere in the domain of \( h \), \( \text{Im}_F (L_{\text{max}} \cap \Omega) \).
In this manuscript we use subscripts to index scalars and superscripts to index vectors. All norms are assumed to be Euclidean unless otherwise stated. The closure, interior, and convex hull of a set $S$ are denoted $\text{cl}(S)$, $\text{int}(S)$, and $\text{co}(S)$, respectively. For ease of reference, we maintain a glossary of notation in the supplemental material in Appendix A.

## 2 Motivation and Background

In this section we first discuss the foundational definitions and assumptions for model-based derivative-free optimization (DFO) methods. We then present and discuss specialized trust-region subproblems for use in algorithms solving (1). Furthermore we provide a high-level overview of the methods to be analyzed and contrast them with other methods for nonsmooth optimization.

### 2.1 Model-based methods

Manifold sampling methods belong to the class of model-based trust-region methods. Although manifold sampling methods need not be derivative-free methods (see [4, 12, 13]), the inspiration and analysis are heavily influenced by these model-based trust-region methods from DFO (see [14] for a complete treatment). The software attached to this paper is intended for DFO, but all that is needed is that models of each component function $F_i$ satisfy the following definition.

**Definition 3.** A function $m^{F_i}: \mathbb{R}^n \rightarrow \mathbb{R}$ is said to be a gradient-accurate model of $F_i$ on $\mathcal{B}(x; \Delta)$ if there exists a constant $\kappa_{i,\text{eg}}$ independent of $x$ and $\Delta$, so that

$$
\|\nabla F_i(x + s) - \nabla m^{F_i}(x + s)\| \leq \kappa_{i,\text{eg}} \Delta \quad \forall s \in \mathcal{B}(0; \Delta).
$$

Definition 3 is similar to the definition of fully linear models that is common in model-based DFO (e.g., [15, Definition 6.1]) except it does not require accuracy of function values. As we will see, our method’s subproblems requires only accurate gradients. Definition 3 also resembles the concept of “order-1 subgradient accuracy” in [16, Definition 4.2] with the exception that Definition 3 is a statement about gradient (as opposed to arbitrary subgradient) accuracy. In model-based DFO, algorithms exist for constructing fully linear (and hence, gradient-accurate) models $m^{F_i}$ by interpolation or regression on values of $F_i$. Our software will maintain gradient-accurate models by employing the same interpolation/regression subroutines as found in the software POUNDERS [17].

### 2.2 Manifold sampling subproblems

Manifold sampling methods (e.g., [1, 7, 8]) evaluate $F$ at various points $y$ in the domain $\Omega$. Because the evaluation of $F$ is assumed to involve a non-negligible expense, all past points $y$ and their corresponding values $F(y)$ are typically stored in memory for the purpose of model building. Given that the continuous selection structure of $h$ is known (via Assumption 2), the values of $h_j(z)$ and $\nabla h_j(z)$ (for any $h_j \in \mathcal{H}$) are readily available at any point $z$, even if $h_j$ is not an essentially active selection function for $h$ at $z$. Various manifold sampling implementations differ in how they determine which indices $j$ corresponding to $h_j \in \mathcal{H}$ to employ in subproblems, and how the information $h_j(F(y))$ and $\nabla h_j(F(y))$ are used to produce putative iterates. We will now describe how, in the novel manifold sampling method introduced in this paper, we choose indices of selection functions and subsequently choose putative iterates.

Over the run of our manifold sampling method, we will include any point $y \in \mathbb{R}^n$ for which $f(y)$ has been previously evaluated in a set $Y$, along with the corresponding indices $\mathcal{A}(F(y))$. On each iteration of the method, we will use an algorithmically determined current iterate $x^k$, an algorithmically updated radius $\Delta_k$, and this set $Y$ to determine a set of indices $\mathbb{G}^k$. As shorthand notation, let $f_j(\cdot) \triangleq h_j(F(\cdot))$ for a given selection index $j$. Moreover, with the model Jacobian $\nabla m_k(\cdot)$ obtained by concatenating the model gradients $\nabla m^{F_i}_k$ in the $k$th iteration, we abbreviate $g_j^k \triangleq \nabla M_k(x^k)\nabla h_j(F(x^k))$. Then, we define $\mathbb{G}^k$ via

$$
\mathbb{G}^k \triangleq \left\{ j : j \in \mathcal{A}(F(y)) \text{ for some } y \in Y, f_j(x^k) > f(x^k), \text{ and } \|x^k - y\| \leq c_1\Delta_k^2 \right\} \\
\cup \left\{ j : j \in \mathcal{A}(F(y)) \text{ for some } y \in Y, f_j(x^k) \leq f(x^k), \text{ and } \|x^k - y\| \leq c_2\Delta_k \right\},
$$

(3)

3
where \(c_1, c_2 \geq 0\) are algorithmic parameters. The presence of the term \(c_1 \Delta_k^2\) in (3) is different from past manifold sampling work; previous work would simply include \(j \in \mathbb{G}^k\) provided there existed \(y \in Y \cap B(x^k; c_1 \Delta_k)\) such that \(j \in \mathcal{A}(F(y))\). It will become clear in the proof of Lemma 4 why this choice was made in the present work.

Note that in the extreme case where \(c_1 = c_2 = 0\) in (3), \(\mathbb{G}^k\) includes indices corresponding only to selection functions active at \(F(x^k)\). This extreme case corresponds to the generator set construction employed in CMS of [1]. The extreme choice of \(c_1 = c_2 = 0\) corresponds to an approximation of the Clarke subdifferential \(\partial_C f(x^k)\). By allowing strictly positive values of \(c_1, c_2\), we are in principle constructing an inner approximation of the Clarke \(\epsilon\)-subdifferential \(\partial_C f(x^k)\).

With this set of indices \(\mathbb{G}^k\), we can now define a subproblem for use in the \(k\)th iteration to compute trial steps. Additionally defining

\[
\beta_{j,k} \triangleq \max\{0, f_j(x^k) - f(x^k)\},
\]

we define a primal model via

\[
m_k(s) = \max_{j \in \mathbb{G}^k} \{f_j(x^k) + (g^k_j)\top s - \beta_{j,k}\} + \frac{1}{2} s\top H^k s - f(x^k),
\]

where \(H^k \in \mathbb{R}^{n \times n}\) is a symmetric matrix. The subproblem employed in each iteration is then given by

\[
\begin{array}{ll}
\text{minimize} & m_k(s) \\
\text{subject to:} & ||s|| \leq \Delta_k \\
& \ell \leq x^k + s \leq u.
\end{array}
\]

We now provide some intuition concerning (5) — in particular, explaining why the model of an arbitrary selection function \(h\) is replaced with a piecewise maximum (4) — and connect it with past manifold sampling work. We first equivalently reformulate (5) as

\[
\begin{array}{ll}
\text{minimize} & v + \frac{1}{2} s\top H^k s - f(x^k) \\
\text{subject to:} & v \geq f_j(x^k) + (g^k_j)\top s - \beta_{j,k} \quad \forall j \in \mathbb{G}^k \\
& ||s|| \leq \Delta_k \\
& \ell \leq x^k + s \leq u.
\end{array}
\]

To handle bounds \(\ell, u \in (\mathbb{R} \cup \{\infty\})^n\), we introduce two sets,

\[
\mathbb{L}_\infty \triangleq \{i \in 1, \ldots, n : \ell_i = -\infty\}, \quad \mathbb{U}_\infty \triangleq \{i \in 1, \ldots, n : u_i = \infty\}.
\]

We also introduce, for brevity, a bilinear function

\[
\Lambda(\lambda; x, a) \triangleq \lambda_a\top a + \lambda_\ell\top (x - \ell) + \lambda_u\top (u - x),
\]

where \(a^k \in \mathbb{R}^{\mathbb{G}^k}\) is defined entrywise by

\[
a^k_{j} = f(x^k) - f_j(x^k) + \beta_{j,k}.
\]

With this notation, one can show (see [12, Proposition 6]) for the case where \(\Omega = \mathbb{R}^n\) that the strong Lagrangian dual of (5) is

\[
\begin{array}{ll}
\text{maximize} & \frac{1}{2} \nu\top (G^k \lambda_a - \lambda_\ell + \lambda_u) - \mu \frac{\Delta_k^2}{2} - \Lambda(\lambda; x^k, a^k) \\
\text{subject to:} & \lambda_a, \lambda_\ell, \lambda_u, \mu \geq 0 \\
& [\lambda_\ell]_i = 0, \quad i \in \mathbb{L}_\infty \\
& [\lambda_u]_i = 0, \quad i \in \mathbb{U}_\infty \\
& \epsilon\top \lambda_a = 1 \\
& H^k + \mu I_n \succeq 0 \\
& (H^k + \mu I_n)\nu = -G^k \lambda_a + \lambda_\ell - \lambda_u,
\end{array}
\]

\footnote{For later reference, observe that in the special case of \(\mathbb{G}^k\) where \(c_1 = c_2 = 0\), a null step \(s = 0\) in (5) implies that \(v = f(x^k)\), which in turn implies the objective value of (5) is 0.}
where $G^k \in \mathbb{R}^{n \times [G]}$ is the matrix with columns $\{g^k_j : j \in \mathcal{G}^k\}$, $I_n \in \mathbb{R}^{n \times n}$ is an identity matrix, and $e \in \mathbb{R}^{[G]}$ is the vector of all ones. As one might expect, our manifold sampling method derives a stationary measure from (7); in particular, by setting $\Delta_k = 1$ and $H^k = 0$, we arrive at a stationary measure $\chi_k$ given by

$$
\chi_k \triangleq \minimize_{\lambda_\ell, \lambda_u, \lambda_a} \left\{ \|G^k\lambda_a - \lambda_\ell + \lambda_u\| + \Lambda(\lambda; x^k, a^k) : \lambda_a, \lambda_\ell, \lambda_u \geq 0, e^\top \lambda_a = 1, \left[\lambda_\ell\right]_i = 0 \in \mathbb{L}_\infty, \left[\lambda_u\right]_i = 0 \in \mathbb{U}_\infty \right\}. \quad (8)
$$

Because $H_k = 0$, the constraint $\mu I_n \succeq 0$ coupled with the maximization of $-\mu \frac{\Delta^2}{2}$ in (7) implies that $\mu = 0$. As a sanity check, notice that each entry of $a^k$ satisfies $f(x^k) - f_j(x^k) + \beta_{j,k} \geq 0$. This, coupled with the observation that $\lambda_u, \lambda_\ell, \lambda_a, x^k - \ell, u - x^k \geq 0$ for any $x^k$ feasible with respect to the constraints of (5), gives the expected characteristic that $\chi_k \geq 0$.

We observe that (9) is precisely the direction-finding subproblem employed in previous manifold sampling works [1, 7, 8]; the $\lambda^*$ solving (9) would be used to define a master model gradient $g^k = G^k\lambda^*$, which in turn would be used to define a smooth master model

$$
m^D_k(s) \triangleq (g^k)^\top s + \frac{1}{2} s^\top H^k s. \quad (10)
$$

For this reason we refer to the model $m_k(s)$ in (4) as the primal model, while we refer to $m^D_k(s)$ in (10) as the dual model.

Having established this connection between previous and present work, we next address the question of what the primal model (4) is actually modeling. We illustrate in Figure 1 the difference between (4) and the dual model (10) in the context of a trust-region subproblem. We remark (importantly!) that the cartoon function $h$ in Figure 1 is the piecewise maximum function, and as such, (4) is a particularly good model of $h \circ F$. Although, as we will show, employing the primal model (4) in the subproblem (5) leads to desirable convergence properties, the primal model need not be a great local model of $h \circ F$ on any given iteration of a manifold sampling problem in general. These considerations motivate our solver GOOMBAH, discussed in the next section.

### 2.3 High-level discussion of MS-P

Each iteration of MS-P consists of a pass through the MS-P loop. In the MS-P loop, we first construct $\mathcal{G}^k$ according to (3) and ensure that for each $j \in \mathcal{G}^k$, $f_j(x^k) + (g^k)^\top s$ is a gradient-accurate model of $f_j$ on $\mathcal{B}(x^k; \Delta_k)$. We remark that, given a method to construct fully linear (and, therefore, gradient-accurate) models $M$ of $F$, it is straightforward to show under Assumption 4 that $h(M(x))$ is a gradient-accurate model of $h(F(x))$; see [18, Theorem 32]. We then (approximately) solve the subproblem (6) to obtain $(v_k, s^k)$. We also solve the subproblem (8) to measure stationarity $\chi_k$. Provided $\Delta_k$ is sufficiently small relative to $\chi_k$ ($\Delta_k \leq \eta_2 \chi_k$ for an algorithmic parameter $\eta_2$), we continue the iteration; otherwise we abort the iteration early, shrinking the trust region and keeping the incumbent $x^{k+1} = x^k$. We note that, in general, we require $\eta_2 \in (0, 1/\kappa_H)$, where $\kappa_H$ is a fixed constant satisfying $\|H^k\| \leq \kappa_H$ for all $k$. Thus, in the special case where $\kappa_H = 0$—which is the case in our numerical experiments—$\eta_2 = \infty$ is an acceptable setting, and thus this early termination will never happen.

Provided the MS-P loop did not terminate early because of an overly large $\Delta_k$, we evaluate $F(x^k + s^k)$ and compute the ratio

$$
\rho_k \triangleq \frac{f(x^k) - f(x^k + s^k)}{f(x^k) - v_k - \frac{1}{2} s^k^\top H^k s^k} = \frac{f(x^k) - f(x^k + s^k)}{m_k(0) - m_k(s^k)}. \quad (11)
$$

3 The necessary conditions on approximate solution quality are given in Assumption 5
Figure 1: In the top row, with $Y = \{y^1\}$, the primal model (4) employed by the manifold sampling method of this paper and the dual model (10) of previous manifold sampling methods are identical. With this common model, the minimizer of the subproblem (5) is $y^2$. Because the function $F_2$ is essentially active at $y^2$ (but not at $y^1$), the manifold sampling loop needs to include this information before proceeding. However, the primal and dual models differ when $Y = \{y^1, y^2\}$, as shown in the bottom row. The minimizer of (5) provides a decrease in $h \circ F$, while (9) produces a model gradient with a norm of zero, so no progress is made on the given iteration.

If $\rho_k \geq \eta_1$ for some algorithmic parameter $\eta_1 > 0$, then the $k$th iteration is deemed **successful**, and we update $x^{k+1}$ with $x^k + s^k$ and possibly increase $\Delta_k$ by a factor $\gamma_i \geq 1$ and end the $k$th iteration.

On the other hand, if $\rho_k$ is too small and some new manifold was identified when evaluating $F(x^k + s^k)$, we recompute $G^k$ as in (3). If $G^k$ is unchanged by the addition of $x^k + s^k$ to $Y$, we shrink $\Delta_k$ by a positive factor $\gamma_i < 1$ and remain in the **MS-P loop** if $G^k \cap A(F(x^k + s^k))$ is empty. If $G^k \cap A(F(x^k + s^k))$ is nonempty, the iteration is declared **unsuccessful**, and we set $x^{k+1}$ to $x^k$ and decrease $\Delta_k$. If $G^k$ is in fact changed, we update models and $G^k$, resolve (5) and (8) with the new $G^k$, reevaluate $\rho_k$, and recheck for success. Note that Lemma 1 will show that the **MS-P loop** will terminate in finite time.

### 2.4 High-level discussion of **GOOMBAH**

As noted previously, any primal model (4) used by **MS-P** can potentially be a poor model of $h(F(x))$. However, the primal model captures the local first-order information necessary to attain a convergence result in the limit of the $\{x^k\}$ generated by **MS-P**. Given that a closed form of $h$ is known and
available, one can consider a modification of MS-P with a trust-region subproblem of the form

$$\begin{align*}
\text{minimize} & \quad h(M(x^k + s)) \\
\text{subject to:} & \quad \|s\| \leq \Delta_k,
\end{align*}$$

where $M$ remains a gradient-accurate model of $F$ on $B(x^k; \Delta_k)$. If, for example, $M$ contains quadratic models for components of $F$ and if $h$ is a general selection function, (approximately) solving (12) may require considerable computational effort, and no certificate of (approximate) optimality may be available. Importantly for deriving convergence results, there may be no known methods that can ensure Cauchy-like decrease in finite time given general forms of (12). Therefore, assuming that approximate solutions to (12) are available (as is done in Assumption 5 for the subproblem (6)) would be a somewhat hollow assumption. Depending on the computational expense of evaluating $F$, however, deploying a global optimization solver on (12) with an appropriate time budget may be justified. Thus, we propose to use the machinery of the MS-P loop with its stationary measure $\chi_k$ to ensure sufficient decrease in each iteration with respect to the stationary measure, thereby guaranteeing global convergence. Pseudocode for this proposed algorithm is given in GOOMBAH, so named because it employs a trust-region subproblem that is a glassbox optimization of a model of a blackbox in a hypersphere.

After computing the solution to (12) in each iteration, GOOMBAH computes the quantity

$$\tilde{\rho}_k = \frac{f(x^k) - f(x^k + \tilde{s}^k)}{\Delta_k^{1+\omega}}$$

for an algorithmic constant $\omega > 0$. If $\tilde{\rho}_k > \eta_1$, then we accept the subproblem (12) solution as the next iterate as in a standard trust-region method; if, on the other hand, the sufficient decrease suggested by (13) is not attained, then we enter the MS-P loop. We study the utility of such recourse in the numerical section by studying GOOMBAH that does not resort to manifold sampling when the candidate (12) solution is poor.

### 2.5 Comparing/contrasting with other approaches

Nonsmooth general (i.e., noncomposite) optimization methods—that is, methods that are suitable for minimizing continuous selections but that do not assume knowledge of $h$ as in Assumption 2—that assume access to an oracle capable of computing $f(x)$ and a(n arbitrary) subgradient $\xi(x) \in \partial f(x)$ are plentiful. Most fundamentally, there exist counterparts of classical gradient descent methods, usually termed subgradient descent methods; see [19] for a textbook treatment of such methods.

An alternative class of methods for the solution of nonsmooth optimization methods has been bundle methods; see [20] for a survey. Originally designed for convex nonsmooth optimization, bundle methods maintain a bundle of cutting planes and iteratively solve a subproblem involving a piecewise-affine model,

$$\min_{s \in \mathbb{R}^n} \max_{y \in Y_k} f(y) + \xi(y)^\top (x^k + s - y),$$

where, in the notation developed so far, $Y_k \subseteq Y$ is algorithmically determined and $\xi(y)$ still refers to the arbitrary subgradient returned by an oracle. We observe that the inner maximization in (14) is clearly related to the affine functions involved in the primal model (4). Notably, however, the affine functions of (14) are first-order models of $f$ centered at individual points $y \in Y_k$, whereas the affine models in (4) are (approximate) first-order models of individual $f_j$ centered at $x^k$. That is, the piecewise-affine model (4) of manifold sampling directly exploits knowledge of the continuous selection, whereas the piecewise-affine model in (14) does not.

While both subgradient and bundle methods were originally intended for convex nonsmooth optimization, there exist extensions suitable for nonconvex optimization. For more recent work in nonconvex subgradient descent methods, see [21, 22]; for more recent work in nonconvex bundle methods, see [23–25].
A third class of methods for the solution of noncomposite nonsmooth (nonconvex) optimization problems given access to gradients is gradient sampling methods [26–30]. Gradient sampling methods are applicable to the minimization of locally Lipschitz functions, a class of nonsmooth functions broader than that analyzed in the present paper. By Rademacher’s theorem, a function that is locally Lipschitz on $\mathcal{R}^n$ admits a gradient almost everywhere, and hence one can compute $\nabla f(x)$ for almost all $x \in \mathcal{R}^n$; we will call the full measure set of differentiable points $\mathcal{D} \subseteq \mathcal{R}^n$. At each iteration, gradient sampling methods maintain a finite sample of gradients $\nabla$ that is locally Lipschitz on functions broader than that analyzed in the present paper. By Rademacher’s theorem, a function methods are applicable to the minimization of locally Lipschitz functions, a class of nonsmooth optimization problems given access to gradients is

$$\min_{s \in \mathcal{R}^n} f(x^k) + \max_{g \in \mathcal{G}^k} \left\{ g^\top s + \frac{1}{2} s^\top H_k s \right\}, \quad (15)$$

where $H_k$ is a (positive-definite) matrix. Importantly, the dual problem to (15) can be written as

$$\min_{\lambda \in \mathcal{R}^{||G_k||^2}} \frac{1}{2} ||G_k\lambda||^{2}_{H_k^{-1}} : e^\top \lambda = 1, \lambda \geq 0, \quad (16)$$

where $G_k$ is a matrix with columns given by the sampled gradients in $\mathcal{G}^k$. The dual problem (16) reveals when $H_k = I_n$, and as $\mathcal{G}^k$ becomes dense in $\mathcal{B}(x^k; \Delta_k)$, the search direction $s^k$ approaches a steepest descent direction for the locally Lipschitz function $f$. It is clear that when we assume (1) is an unconstrained problem (so that $\lambda_k = \lambda_n = 0$), (7) similarly provides a steepest descent direction for $f$. However, because continuous selections involve only finitely many selection functions (those indexed by $\mathcal{S}$), a manifold sampling method never needs to sample densely in $\mathcal{B}(x^k; \Delta_k)$ in order to obtain arbitrarily good approximations to the steepest descent direction: only finitely many selection functions in $\mathcal{S}$ active at (or near) $x^k$ must ever be sampled.

All three of these classes of methods (subgradient descent methods, bundle methods, gradient sampling methods) admit derivative-free variants, whereby the subgradient oracle required for these methods is replaced with approximate (e.g., finite-difference-based) approximations. Notably, in a derivative-free setting, Bagirov et al. [31] proposed the so-called discrete gradient method, which computes approximate subgradients for use in a subgradient descent framework; see also [32]. Derivative-free bundle methods have also been proposed; see [33]. Even closer to our proposed method is a derivative-free bundle method employing a trust region—as opposed to a proximal point mechanism—proposed in [34]. Kiwiel [35] proposed a gradient sampling method for the derivative-free setting by computing approximate (finite-difference) gradients. Moreover, as a fourth class of methods most practical for DFO, direct-search methods have been historically concerned with convergence to Clarke stationary points and are hence suitable for nonsmooth optimization; see the book [36] for an excellent treatment of these methods.

Special attention has been paid to composite optimization in the literature, that is, for cases where $h$ in Assumption 1 is known and an oracle exists for computing $F(x)$ and $\nabla F(x)$. Works from the 1980s provide fundamental analyses for the case where $h$ is convex and $\nabla F$ is available [2, 5, 6, 37, 38]. A bundle method for composite nonsmooth optimization with convex $h$ was proposed in [39]. Recently, Bareilles et al. [40] proposed a peculiar algorithm that identifies a smooth manifold (see also [2]) via a subproblem involving a known proximal operator for $h$ and then solves a second-order subproblem restricted to that manifold. The use of the term manifold in [40] is more formal than that employed here, and the assumptions imposed on $h$ and the manifold structure it creates are nontrivial when compared with the generality and simplicity of continuous selections.

In the derivative-free setting, the authors in [41, 42] analyze algorithms for composite optimization where $h$ is a general convex function but $\nabla F$ is not available. To the best of our knowledge, [7] was the first derivative-free work to consider a nonconvex $h$ (piecewise-linear), while [8] was the first derivative-free work to consider a general nonconvex continuous selection $h$. 

8
3 Analysis

We now state the algorithms below and the provide assumptions (Section 3.1) used in the analyses of convergence of MS-P (Section 3.2) and GOOMBAH (Section 3.3).

**MS-P Loop**: Manifold sampling primal loop

```
input: Iterate \( x^k \), radius \( \Delta_k \), set of points \( Y \)
output: \( x^{k+1} \), \( \Delta_{k+1} \), \( Y \)
1 Set \( c_1, c_2 \geq 0 \), \( \kappa_H \geq 0 \), \( \eta_1 > 0 \), \( \eta_2 \in (0, 1/\kappa_H) \), \( 0 < \gamma_d < 1 < \gamma_i \)
2 Store \( \Delta \leftarrow \Delta_k \)
3 while true do
   4 Ensure \( M \) is a gradient-accurate model of \( F \) on \( \mathcal{B}(x^k; \Delta_k) \) using \( Y \) (this may require evaluating \( F \) at additional points and adding them to \( Y \))
   5 Construct \( G^k \) according to (3) with \( Y \), \( \Delta_k \), \( c_1 \), and \( c_2 \)
   6 Choose \( H^k \) such that \( \| H^k \| \leq \kappa_H \)
   7 (Approximately) solve subproblem (6) to obtain \( (v_k, s^k) \)
   8 Solve subproblem (8) to obtain \( x_k \)
   9 if \( \Delta_k > \eta_2 \gamma_i \) then
      10 \( x^{k+1} \leftarrow x^k, \Delta_{k+1} \leftarrow \gamma_d \Delta \) \hspace{1cm} // unsuccessful iteration
   11 return
   12 Evaluate \( F(x^k + s^k) \) and set \( Y \leftarrow Y \cup x^k + s^k \)
   13 Compute \( \rho_k \) according to (11)
   14 if \( \rho_k \geq \eta_1 \) then
      15 \( x^{k+1} \leftarrow x^k, \Delta_{k+1} \leftarrow \gamma_i \Delta \) \hspace{1cm} // successful iteration
   16 return
   17 else
      18 Compute temporary \( G^k \) according to (3)
   19 if \( G^k = G^k \) then
      20 if \( G^k \cap A(F(x^k + s^k)) \neq \emptyset \) then
         21 \( x^{k+1} \leftarrow x^k, \Delta_{k+1} \leftarrow \gamma_d \Delta \) \hspace{1cm} // unsuccessful iteration
      22 return
      23 else
         24 \( \Delta_k \leftarrow \gamma_d \Delta_k \)
   25 else
      26 \( G^k \leftarrow G^k \)
```

**GOOMBAH**: Glassbox Optimization Of Model of Blackbox in A Hypersphere

```
1 Choose initial iterate and radius, \( x^0, \Delta_0 > 0 \)
2 Initialize history of evaluated points \( Y \) (at least with \( x^0 \))
3 for \( k = 0, 1, 2, \ldots \) do
   4 \( x^{k+1}, \Delta_{k+1}, Y \leftarrow MS-P\text{ loop} (x^k, \Delta^k, Y) \)
```

3.1 Additional assumptions

We first state additional regularity assumptions on \( h \) and \( F \) that we make in order to provide rigorous convergence guarantees about MS-P. We note that even if these assumptions were violated,
**MS-P** would be well defined, but convergence guarantees may not hold, even on a computer with infinite precision.

We first assume some regularity conditions on $F$ using some constants from Definition 4.

**Assumption 3.**

A. Each component $F_i$ of $F$ is Lipschitz continuous with some constant $K_{F_i}$.

B. Each component $F_i$ of $F$ has a Lipschitz continuous gradient with constant $K_{\nabla F_i}$.

C. For a point $x^0 \in \mathbb{R}^n$, assume the set $L(x^0) \triangleq \{ x : f(x) \leq f(x^0) \}$ is bounded.

We additionally cast the following assumptions concerning selection functions that comprise the outer function $h$:

**Assumption 4.** On $\mathbf{im}_F(L_{\text{max}} \cap \Omega)$, each $h_j \in \mathcal{H}$ is Lipschitz continuous, is Lipschitz continuously differentiable, and has bounded gradients. That is, for all $z, z' \in \mathbf{im}_F(L_{\text{max}} \cap \Omega)$:

A. There exists $K_{h_j}$ such that $|h_j(z) - h_j(z')| \leq K_{h_j} \|z - z'\|.$

B. There exists $K_{\nabla h_j}$ such that $\|\nabla h_j(z) - \nabla h_j(z')\| \leq K_{\nabla h_j} \|z - z'\|.$

C. There exists $K_{\nabla h}$ such that $\|\nabla h(z)\| \leq K_{\nabla h}.$

We define the following terms for convenience.

**Definition 4.** For the constants in Assumption 1.B, Definition 3, and Assumption 4, define

$$K_h \triangleq \max_{j \in \{1, \ldots, |\mathcal{H}|\}} \{ K_{h_j} \}, \quad K_F \triangleq \max_{i \in \{1, \ldots, p\}} \{ K_{F_i} \}, \quad K_{\nabla F} \triangleq \max_{i \in \{1, \ldots, p\}} \{ K_{\nabla F_i} \},$$

$$K_{\nabla h} \triangleq \max_{j \in \{1, \ldots, |\mathcal{H}|\}} \{ K_{\nabla h_j} \}, \quad \kappa_k \triangleq \sum_{i=1}^p \kappa_{i, \text{eg}}.$$

Our final assumption requires that the method used to solve the subproblem (6) returns a solution that satisfies a Cauchy-like decrease property. This assumption is reasonable because there exist finite-time algorithms for producing such an approximate solution (see, e.g., [12] and [43, Section 12.2])

**Assumption 5.** The approximate solution $(v_k, s^k)$ to (6) satisfies the constraints of (6) and moreover satisfies

$$- (v_k - f(x^k) + \frac{1}{2} s^k \top H_k s^k) \geq \kappa_{fcd} \lambda_k \min \left\{ \frac{\lambda_k}{\kappa_H}, \Delta_k, 1 \right\}$$

for an algorithmic parameter $\kappa_{fcd} \in (0, 1)$.

### 3.2 Convergence of MS-P

We begin by demonstrating that the **MS-P loop** must terminate finitely.

**Lemma 1.** If Assumptions 1–4 hold, the **MS-P loop** will terminate.

**Proof.** If either $\Delta_k > \eta_2 \lambda_k$ or $\rho_k \leq \eta_1$, then the loop terminates. Suppose that for a given $k$, on every pass through the **MS-P loop**, $\Delta_k \leq \eta_2 \lambda_k$ and $\rho_k < \eta_1$; hence, exactly one of Line 24 or Line 26 will be reached on each pass. After finitely many (at most $|\mathcal{H}|$) consecutive passes through the **MS-P loop**, $G_k$ must equal $G_0$ and so, Line 24 will be reached, and $\Delta_k$ will be decreased. By Assumptions 2–4, $f$ is piecewise-differentiable in the sense of Scholtes [11] so there exists $\hat{\Delta} > 0$ such that for all $\Delta \leq \hat{\Delta}$

$$\mathcal{A}(F(x^k)) = \bigcup_{y \in \mathcal{B}(x^k : \Delta)} \mathcal{A}(F(y)).$$

For all such $\Delta \leq \hat{\Delta}$, we also have that $G_k \cap \mathcal{A}(F(x^k + s^k)) \neq \emptyset$, because $\mathcal{A}(F(x^k)) \subset G_k$ by (3). Thus, once $\Delta_k \leq \hat{\Delta}$, iteration $k$ will be deemed unsuccessful and the loop will terminate. □ □
We now show that the convex hull of model gradients indexed by \( I \sim \mathbb{G}^k \) in some sense approximates part of the Clarke subdifferential \( \partial_C f(x^k) \). The proof is virtually identical to \([7, \text{Lemma 4.1}]\) up to differences in notation and is included for completeness.

**Lemma 2.** Let Assumption 1 and Assumption 3, hold, and let \( x, y \in L_{\text{max}} \) satisfy \( \|x - y\| \leq \Delta \). Choose arbitrary subsets \( I \subseteq J \subseteq \{1, \ldots, |\mathbb{Y}|\} \), and define

\[
\mathcal{G} \triangleq \text{co} \left( \{ \nabla M(x)\nabla h_i(F(x)) : i \in I \} \right) \quad \text{and} \quad \mathcal{H} \triangleq \text{co} \left( \{ \nabla F(y)\nabla h_j(F(y)) : j \in J \} \right),
\]

where \( M \) is a gradient-accurate model of \( F \) on \( \mathcal{B}(x; \Delta) \). Then for each \( g \in \mathcal{G} \), there exists some \( \sigma(g) \in \mathcal{H} \) satisfying

\[
\|g - \sigma(g)\| \leq B\Delta,
\]

where \( B \) is defined with the constants from Definition 4 by

\[
B \triangleq K_h(K_{\text{V}} + \kappa_h) + K_FK_{\text{V}},
\]

**Proof (adapted from \([7, \text{Lemma 4.1}]\)).** Any \( g \in \mathcal{G} \) may be expressed as

\[
g = \sum_{i \in I} \lambda_i \nabla M(x)\nabla h_i(F(x)),
\]

where \( \sum_{i \in I} \lambda_i = 1 \) and \( \lambda_i \geq 0 \) for each \( i \).

By supposition, \( \nabla F(y)\nabla h_i(F(y)) \in \mathcal{H} \) for all \( i \in I \). For

\[
\sigma(g) \triangleq \sum_{i \in I} \lambda_i \nabla F(y)\nabla h_i(F(y))
\]

using the same \( \lambda_i \) as in (20) for \( i \in I \), convexity of \( \mathcal{H} \) implies that \( \sigma(g) \in \mathcal{H} \). Since \( y \in \mathcal{B}(x; \Delta) \), the triangle inequality, Assumption 3.A, Assumption 3.B, Assumption 4.A, and the definition of gradient-accurate give

\[
\|
abla M(x)\nabla h_i(F(x)) - \nabla F(y)\nabla h_i(F(y))\| \leq \|
abla F(y) - \nabla F(x)\| \|
abla h_i(F(y))\|
\]

\[
+ \|
abla F(x)\| \|
abla h_i(F(x)) - \nabla h_i(F(y))\|
\]

\[
+ \|
abla F(x) - \nabla M(x)\| \|
abla h_i(F(x))\|
\]

\[
\leq (K_hK_{\text{V}} + K_FK_{\text{V}} + \kappa_hK_h)\Delta,
\]

for each \( i \). Using this along with (20) and the definition of \( \sigma(g) \) yields

\[
\|g - \sigma(g)\| \leq \sum_{i \in I} [\lambda_i \|
abla M(x)\nabla h_i(F(x)) - \lambda_i \nabla F(y)\nabla h_i(F(y))\|]
\]

\[
\leq \sum_{i \in I} \lambda_i \|
abla M(x)\nabla h_i(F(x)) - \nabla F(y)\nabla h_i(F(y))\| \leq B\Delta.
\]

\( \square \)

We next provide a brief proposition bounding the distance between values of distinct selection functions.

**Proposition 3.** Let Assumptions 1–2 hold and suppose on iteration \( k \) of \( \text{MS-P} \) that \( \bar{j} \in \mathbb{G}^k \) and \( f_j(x^k) > f(x^k) \). Then,

\[
|f(x^k) - f_j(x^k)| \leq 2K_hc_1\Delta_k^2.
\]

**Proof.** Because \( j \in \mathbb{G}^k \), there exists some corresponding \( \bar{y} \in Y \cap \mathcal{B}(x^k; c_1\Delta_k^2) \) so that \( f(\bar{y}) = f_j(\bar{y}) \). Then,

\[
|f(x^k) - f_j(x^k)| \leq |f(x^k) - f(\bar{y})| + |f(\bar{y}) - f_j(x^k)|
\]

\[
= |f(x^k) - f(\bar{y})| + |f_j(\bar{y}) - f_j(x^k)|
\]

\[
\leq 2K_h\|x^k - \bar{y}\| \leq 2K_hc_1\Delta_k^2.
\]

\( \square \)
The next lemma demonstrates that iteration $k$ of MS-P will be successful if the trust region $\Delta_k$ is sufficiently small with respect to the stationarity measure $\lambda_k$.

**Lemma 4.** Let Assumptions 1–5 hold, and define

$$\bar{C} \triangleq \frac{\kappa_{\text{fed}}(1 - \eta_1)}{K_{\mathcal{V}_h}K_h + \kappa_gK_{\mathcal{V}_h} + \frac{\alpha}{2} + 2c_1K_h}.$$

If in the $k$th iteration of MS-P, $\mathcal{A}(x^k + s^k) \cap \mathcal{G}^k \neq \emptyset$, and

$$\Delta_k \leq \min \{1, C\lambda_k\}, \quad (21)$$

where

$$C \triangleq \min \left\{ \eta_2, \bar{C}, \sqrt{\kappa_H^{-1}C} \right\}, \quad (22)$$

then $\rho_k \geq \eta_1$ in MS-P. That is, the $k$th iteration is successful.

**Proof.** Let $j \in \mathcal{A}(x^k + s^k) \cap \mathcal{G}^k$ be arbitrary, if the intersection is not a singleton. Then there are two cases to analyze:

**Case 1** $h_j(F(x^k)) \leq f(x^k)$: In this case, $\beta_{j,k} = 0$ and so

$$1 - \rho_k = \frac{f(x^k) - v_k - \frac{1}{2}s^T H_k s_k - [f(x^k) - f(x^k + s^k)]}{f(x^k) - v_k - \frac{1}{2}s^T H_k s_k}$$

$$= \frac{f(x^k + s^k) - v_k - \frac{1}{2}s^T H_k s_k}{f(x^k) - v_k - \frac{1}{2}s^T H_k s_k}$$

$$= \frac{f(x^k + s^k) - f_j(x^k) - g_j^T s_k - \frac{1}{2}s^T H_k s_k}{f(x^k) - v_k - \frac{1}{2}s^T H_k s_k}$$

$$= \frac{\Delta_j(F(x^k + s^k)) - (\nabla M(x^k)\nabla h_j(F(x^k)))^T s_k - \frac{1}{2}s^T H_k s_k}{\Delta_j(F(x^k)) - v_k - \frac{1}{2}s^T H_k s_k},$$

where the last equality is because $j \in \mathcal{A}(x^k + s^k)$. Note that

$$\Delta_j(F(x^k + s^k)) - \Delta_j(F(x^k)) = h_j(F(x^k + s^k) - h_j(F(x^k))$$

$$= h_j(F(x^k) + s^k) - h_j(F(x^k)) - [\nabla M(x^k)\nabla h_j(F(x^k))]^T s_k$$

$$+ [\nabla F(x^k)\nabla h_j(F(x^k))]^T s_k - [\nabla F(x^k)\nabla h_j(F(x^k))]^T s_k$$

$$\leq h_j(F(x^k) + s^k) - h_j(F(x^k)) + [\nabla F(x^k)\nabla h_j(F(x^k))]^T s_k$$

$$+ \|\nabla F(x^k) - \nabla M(x^k)\|\nabla h_j(F(x^k))\| \Delta_k$$

$$\leq K_{\mathcal{V}_F}K_{\mathcal{V}_h} \Delta^2_k + \kappa_g K_{\mathcal{V}_h} \Delta^2_k = (K_{\mathcal{V}_F}K_{\mathcal{V}_h} + \kappa_g K_{\mathcal{V}_h}) \Delta^2_k,$$

where the last inequality is due to Taylor’s theorem, Assumption 3.B, Assumption 4.B, Assumption 4.C, and the definition of gradient-accurate. Thus, continuing,

$$1 - \rho_k \leq \frac{(K_{\mathcal{V}_F}K_{\mathcal{V}_h} + \kappa_g K_{\mathcal{V}_h} + \frac{\alpha}{2}) \Delta^2_k}{f(x^k) - v_k - \frac{1}{2}s^T H_k s_k} \leq \frac{(K_{\mathcal{V}_F}K_{\mathcal{V}_h} + \kappa_g K_{\mathcal{V}_h} + \frac{\alpha}{2}) \Delta^2_k}{\kappa_{\text{fed}} \lambda_k \min \left\{ \frac{\lambda_k}{\kappa_H}, \Delta_k, 1 \right\}}$$

$$\leq \frac{(K_{\mathcal{V}_F}K_{\mathcal{V}_h} + \kappa_g K_{\mathcal{V}_h} + \frac{\alpha}{2}) \Delta^2_k}{\kappa_{\text{fed}} \Delta_k \min \left\{ \frac{\Delta_k}{C\kappa_H}, 1 \right\}}$$

$$= \frac{(K_{\mathcal{V}_F}K_{\mathcal{V}_h} + \kappa_g K_{\mathcal{V}_h} + \frac{\alpha}{2}) \Delta^2_k}{\kappa_{\text{fed}} \min \left\{ \frac{1}{C\kappa_H}, 1 \right\}} \leq 1 - \eta_1,$$
where the second inequality uses Assumption 5 and the last inequality uses the fact that $\Delta_k \leq \min \{1, C\Delta_k\}$. Thus, in this case, $\rho_k \geq \eta_1$, and the $k$th iteration is successful.

**Case 2** $h_j(F(x^k)) > f(x^k)$: In this case, $\beta_{j,k} = h_j(F(x^k)) - f(x^k) > 0$. Thus,

$$1 - \rho_k = \frac{f(x^k + s^k) - v_k - \frac{1}{2}s^k^TH^k s^k}{f(x^k) - v_k - \frac{1}{2}s^k^TH^k s^k} = \frac{f(x^k + s^k) - h_j(F(x^k)) - \frac{1}{2}s^k^TH^k s^k + h_j(F(x^k)) - f(x^k)}{f(x^k) - v_k - \frac{1}{2}s^k^TH^k s^k} = \frac{f(x^k + s^k) - h_j(F(x^k)) - \frac{1}{2}s^k^TH^k s^k + h_j(F(x^k)) - f(x^k)}{f(x^k) - v_k - \frac{1}{2}s^k^TH^k s^k} \leq \frac{(K_{\chi F} K_{\chi h} + \kappa_{c} K_{\chi h} + \frac{\eta_2}{2} + 2c_1 K_h) \Delta_k^2}{\kappa_{\text{fed}} \frac{1}{C} \min \left\{ \frac{\Delta_k}{C \kappa H}, 1 \right\}} \leq \frac{(K_{\chi F} K_{\chi h} + \kappa_{c} K_{\chi h} + \frac{\eta_2}{2} + 2c_1 K_h)}{\kappa_{\text{fed}} \frac{1}{C} \min \left\{ \frac{1}{C \kappa H}, 1 \right\}} = 1 - \eta_1,$$

where the second-to-last inequality uses the fact that $j \in G^k$ and Proposition 3. Thus, in this case, $\rho_k \geq \eta_1$ if $\Delta_k$ satisfies (21), and iteration $k$ is again successful.

The next lemma shows that the sequence of trust-region radii converges to zero.

**Lemma 5.** Let Assumptions 1–5 hold. If $\{x^k, \Delta_k\}_{k \in \mathbb{N}}$ is generated by MS-P, then $\lim_{k \to \infty} \Delta_k = 0$.

**Proof.** If iteration $k$ is unsuccessful, then $\Delta_{k+1} < \Delta_k$, and $x^{k+1} = x^k$; therefore, $f(x^{k+1}) = f(x^k)$. On successful iterations $k$, $\rho_k \geq \eta_1 > 0$ ensures that $f(x^{k+1}) < f(x^k)$. Thus, the sequence $\{f(x^k)\}_{k \in \mathbb{N}}$ is nonincreasing.

To show that $\Delta_k \to 0$, we consider the cases in which there are infinitely many or finitely many successful iterations separately. First, suppose that there are infinitely many successful iterations, indexed by $\{k_j\}_{j \in \mathbb{N}}$. Since $f(x^k)$ is nonincreasing in $k$ and $f$ is bounded below (by Assumption 3.C), the sequence $\{f(x^k)\}_{k \in \mathbb{N}}$ converges to some limit $f^* \leq f(x^0)$. Thus, having infinitely many successful iterations (indexed $\{k_j\}_{j \in \mathbb{N}}$) implies that

$$\infty > f(x^0) - f^* \geq \sum_{j=0}^{\infty} f(x^{k_j}) - f(x^{k_j+1}) > \sum_{j=0}^{\infty} \eta_1 \kappa_{\text{fed}} \chi_{k_j} \min \left\{ \frac{\chi_{k_j}}{\kappa H}, 1 \right\} > \sum_{j=0}^{\infty} \eta_1 \kappa_{\text{fed}} \Delta_{k_j} \min \left\{ \frac{\Delta_{k_j}}{\eta_2 \kappa H}, 1 \right\},$$

where the second-to-last inequality is due to the definition of success and Assumption 5 and the last inequality is because every successful iteration must satisfy $\Delta_{k_j} \leq \eta_2 \chi_{k_j}$. We note that if $1$ were the minimizer infinitely often in the right-hand side of (23), then a contradiction would immediately result, because this would imply $\chi_{k_j} > \kappa H$ for all such infinitely many $j$, violating the finiteness of the sum. Thus, we conclude from (23) that

$$\infty > \sum_{j=0}^{\infty} \eta_1 \kappa_{\text{fed}} \Delta_{k_j}^2 \min \left\{ \frac{1}{\eta_2 \kappa H}, 1 \right\}.$$

It follows that $\Delta_{k_j} \to 0$ for the sequence of successful iterations. Observe that while multiple decreases of $\Delta_k$ may occur inside the MS-P loop during the $k$th iteration of MS-P, the presence of
\( \Delta \) in the **MS-P loop** ensures that \( \Delta_{k+1} \in \{ \gamma_d \Delta_k, \gamma_i \Delta_k \} \). Hence, \( \Delta_{k+1} \leq \gamma_i \Delta_k \), and moreover, \( \Delta_{k+1} = \gamma_d \Delta_k \) if iteration \( k \) is unsuccessful. Thus, for any unsuccessful iteration \( k > k_j \), \( \Delta_k \leq \gamma_i \Delta_q \), where \( q \equiv \max \{ j : j \in \mathbb{N}, k_j < k \} \). It follows immediately that

\[
0 \leq \lim_{k \to \infty} \Delta_k \leq \gamma_i \lim_{j \to \infty} \Delta_{k_j} = 0,
\]

and so \( \Delta_k \to 0 \) as required.

Next, suppose there are only finitely many successful iterations; let \( N \in \mathbb{N} \) be the number of successful iterations. Since \( \gamma_d < 1 \leq \gamma_i \), it follows that \( 0 \leq \Delta_k \leq \gamma_i^N \gamma_d^{k-N} \Delta_0 \) for each \( k \in \mathbb{N} \). Thus, \( \Delta_k \to 0 \).

We now show that the sequence \( \{ \chi_k \} \) is not bounded away from zero.

**Lemma 6.** Let Assumptions 1–5 hold. If the sequence \( \{ x^k, \Delta_k, \chi_k \}_{k \in \mathbb{N}} \) is generated by **MS-P**, then \( \lim_{k \to \infty} \chi_k = 0 \).

**Proof.** To obtain a contradiction, suppose there is an iteration \( \tilde{K} \) and some \( \epsilon > 0 \) for which \( \chi_k \geq \epsilon \), for all \( k \geq \tilde{K} \). Any iteration \( k > \tilde{K} \) that witnesses both \( \Delta_k \leq C \chi_k \) and \( \mathbb{G}_k \cap \mathcal{A}(x^k + s^k) = \emptyset \) is guaranteed to be successful by Lemma 4, and so Line 21 of the **MS-P loop** cannot be reached. Coupled with the fact that the **MS-P loop** must terminate eventually (Lemma 1), we have that for all \( k \geq \tilde{K} \) such that \( \Delta_k \leq C \chi_k \), the **MS-P loop** must yield a successful iteration, and so \( \Delta_{k+1} \geq \gamma_i \Delta > \Delta_k \).

Therefore, \( \Delta_k > \gamma_d C \epsilon \) for all \( k \geq \tilde{K} \), contradicting Lemma 5. Thus, no such \(( \tilde{K}, \epsilon )\) pair exists, and so \( \lim_{k \to \infty} \chi_k = 0 \).

The next lemma shows that any convergent subsequence \( \{ k_j \} \) of \( \{ k \} \) on which \( \chi_{k_j} \to 0 \) admits a Clarke stationary cluster point. **MS-P** generates at least one such subsequence of iterates by **Lemma 6**.

**Lemma 7.** Let Assumptions 1–5 hold. Let \( \{ x^k, \Delta_k, g^k \}_{k \in \mathbb{N}} \) be a sequence generated by **MS-P**. For any subsequence \( \{ k_j \}_{j \in \mathbb{N}} \) iterations such that both

\[
\lim_{j \to \infty} \chi_{k_j} = 0,
\]

and \( \{ x^{k_j} \}_{j \in \mathbb{N}} \to x^* \) for some cluster point \( x^* \), then \( 0 \in \partial_C \mathcal{L}(x^*) \), where \( \mathcal{L}(x) \) is the Lagrangian of (1),

\[
\mathcal{L}(x) \equiv f(x) + \lambda_f^\top (f - x) + \lambda_u^\top (x - u).
\]

**Proof.** Let \( \| k \| \equiv \mathbb{G}^k \), and let \( \| k \| \equiv \mathcal{A}(x^*) \). Because

- \( \Delta_k \to 0 \) by **Lemma 5**,  
- \( \{ x^{k_j} \}_{j \in \mathbb{N}} \) converges to \( x^* \) by assumption,
- \( f \) is piecewise-differentiable [11] due to ??–??, and
- the definition of \( \mathbb{G}^k \) in (3),

we conclude that for \( j \) sufficiently large, only selection functions that are essentially active at \( x^* \) are represented in \( \mathbb{G}^{k_j} \). Consequently, \( \| k \| \subseteq \| k \| \) for all \( j \) sufficiently large. Hence, in the definition of \( \chi_k \) (8), we see that \( a^{k_j} = 0 \) for all \( j \) sufficiently large.

Let \( (\lambda^{k_j}_a, \lambda^{k_j}_f, \lambda^{k_j}_u) \) denote the minimizing \((\lambda_a, \lambda_f, \lambda_u)\) in the definition of \( \chi_k \) (8), and define

\[
g^{k_j} \equiv C^{k_j} \lambda^{k_j}_f.
\]

By **Lemma 2** with \( l \leftarrow k_j, \) \( l \leftarrow j^{k_j}, \) \( x \leftarrow x^{k_j}, \) \( y \leftarrow x^* \), and \( \Delta \leftarrow \Delta_{k_j} \), there exists \( \sigma(g^{k_j}) \in \partial_C f(x^*) \) for each \( g^{k_j} \) so that

\[
\| g^{k_j} - \sigma(g^{k_j}) \| \leq B \Delta_{k_j},
\]

with \( B \) defined by (19). Thus,

\[
\| g^{k_j} - \lambda^{k_j}_f + \lambda^{k_j}_u - (\sigma(g^{k_j}) - \lambda^{k_j}_f + \lambda^{k}_u) \| \leq B \Delta_{k_j},
\]
and so
\[ \|g(k_j) - \lambda_{k_j}^f + \lambda_{k_j}^u\| \leq B\Delta_{k_j} + \|g(k_j) - \lambda_{k_j}^f + \lambda_{k_j}^u\| = B\Delta_{k_j} + \lambda_{k_j}, \]
where the latter equality is true for all \( j \) sufficiently large since we have shown that \( a^{k_j} = 0 \) for \( j \) sufficiently large. Since \( \lambda_{k_j} \to 0 \) and \( \Delta_{k_j} \to 0 \) by assumption, we conclude that \( \|\sigma(g(k_j)) - \lambda_{k_j}^f + \lambda_{k_j}^u\| \to 0 \). Because \( \sigma(g(k_j)) - \lambda_{k_j}^f + \lambda_{k_j}^u \in \partial C(L(x_k)) \), Proposition 7.1.4 in [44] yields the claimed result, by establishing that \( \partial C L \) is outer-semicontinuous and therefore \( 0 \in \partial C L(x^*) \).

We can now present our final result: that the limit of any subsequence of \( MS-P \) iterates is a Clarke stationary point of the Lagrangian of (1).

**Theorem 8.** Let Assumptions 1–5 hold. If \( x^* \) is a cluster point of a sequence \( \{x^k\} \) generated by \( MS-P \), then \( 0 \in \partial C L(x^*) \).

**Proof.** First, suppose that there are only finitely many successful iterations and \( k' \) is the last. Suppose for contradiction that \( 0 \notin \partial C L(x^{k'}) \). By continuity of \( F_i \) (Assumption 1), there exists \( \Delta > 0 \) so that for all \( \Delta \in [0, \Delta] \), the manifolds active in \( B(x^{k'}; \Delta) \) are precisely the manifolds active at \( x^{k'} \); that is,
\[ A(F(x^{k'})) = \bigcup_{y \in B(x^{k'}; \Delta)} A(F(y)) \quad \text{for all } \Delta \leq \Delta. \]

By assumption, \( \Delta_k \) decreases by a factor of \( \gamma_0 \) in each iteration after \( k' \) because every iteration after \( k' \) is unsuccessful. Thus there is a least iteration \( k'' \geq k' \) so that \( \Delta_{k''} \leq \Delta \). By the definition of \( G^k \) in (3), for each \( k \geq k'' \), \( G^k \) contains all manifolds at \( x^{k'} \), and therefore \( \nabla M(x^{k'}) \nabla h_i(F(x^{k})) \in G^k \) for all \( j \in A(F(x^{k})) \). Since \( k' \) is the last successful iteration, \( x^k = x^{k'} \) for all \( k \geq k'' \geq k' \). Consequently, the conditions for Lemma 2 hold for \( x \leftarrow x^k, y \leftarrow x^{k'} \) (noting that \( x^k = x^{k'} \)) \( \Delta \leftarrow 0, G \leftarrow G^k \), and \( H \leftarrow \partial C f(x^k) \); thus, for each \( k \geq k'' \), \( g^k - \lambda_{k}^f + \lambda_{k}^u \in \partial C L(x^{k'}) \).

Since \( 0 \notin \partial C L(x^{k'}) \) by supposition, \( \pi^* \triangleq \text{proj} (0, \partial C L(x^{k'})) \) is nonzero, and so
\[ \|g^k - \lambda_{k}^f + \lambda_{k}^u\| \geq \|\pi^*\| > 0 \quad \text{for all } k \geq k''. \]

Since \( \Delta_k \to 0 \), \( \Delta_k \) will satisfy the conditions of Lemma 4 for \( k'' \) sufficiently large: there will be a successful iteration contradicting \( k' \) being the last.

Next, suppose there are infinitely many successful iterations. We will demonstrate that there exists a subsequence of successful iterations \( \{k_j\} \) that simultaneously satisfies both
\[ x^{k_j} \to x^* \quad \text{and} \quad \|g^{k_j} - \lambda_{k_j}^f + \lambda_{k_j}^u\| \to 0. \]

If the sequence \( \{x^k\}_{k \in \mathbb{N}} \) converges, then the subsequence \( \{x^{k_j}\}_{j \in \mathbb{N}} \) from Lemma 6 satisfies (25). Otherwise, if the sequence \( \{x^k\}_k \) is not convergent, we will show that \( \liminf_{k \to \infty} (\max(\|x^k - x^*\|, \|g^k - \lambda_{k}^f + \lambda_{k}^u\|)) = 0 \) for each cluster point \( x^* \). Suppose for contradiction that there exist \( \bar{\theta} > 0 \), an iteration \( \bar{k} \), and a cluster point \( x^* \) of the sequence \( \{x^k\} \) with the following property: given the infinite set
\[ K \triangleq \{k : k \geq \bar{k}, \|x^k - x^*\| \leq \bar{\theta}\}, \]
the subsequence \( \{x^k\}_{k \in K} \) converges to \( x^* \) and \( \|g^k - \lambda_{k}^f + \lambda_{k}^u\| > \bar{\theta} \) for all \( k \in K \). Thus,
\[ \eta_1 \sum_{k \in K} \|g^k - \lambda_{k}^f + \lambda_{k}^u\| \leq \|x^{k+1} - x^k\| \leq \eta_1 \sum_{k=0}^{\infty} \|g^k - \lambda_{k}^f + \lambda_{k}^u\| \|x^{k+1} - x^k\| < \infty, \]

since on successful iterations, \( \|x^{k+1} - x^k\| \leq \Delta_k \), while on unsuccessful iterations, \( \|x^{k+1} - x^k\| = 0 \). Since \( \|g^k - \lambda_{k}^f + \lambda_{k}^u\| > \bar{\theta} \) for all \( k \in K \), we conclude from (26) that
\[ \sum_{k \in K} \|x^{k+1} - x^k\| < \infty. \]
Since \( x^k \not\to x^* \), there exists some \( \hat{\theta} \in (0, \bar{\theta}) \) for which, for each \( k' \in \mathbb{K} \), there exists
\[
q(k') \triangleq \min \{ \kappa \in \mathbb{N} : \kappa > k', \| x^\kappa - x^{k'} \| > \hat{\theta} \}.
\]
From this construction, since \( \hat{\theta} \leq \bar{\theta} \), then \( \{ k', k' + 1, \ldots, q(k') - 1 \} \subset \mathbb{K} \).

By (27), for \( \theta \) there exists \( N \in \mathbb{N} \) such that
\[
\sum_{k \in \mathbb{K}, k \geq N} \| x^{k+1} - x^k \| \leq \hat{\theta}.
\]

Taking \( k' \geq N \), by the triangle inequality, we have
\[
\hat{\theta} < \| x^{q(k')} - x^{k'} \| \leq \sum_{i \in \{ k', k' + 1, \ldots, q(k') - 1 \}} \| x^{i+1} - x^i \| \leq \sum_{k \in \mathbb{K}, k \geq N} \| x^{k+1} - x^k \| \leq \hat{\theta}.
\]

Therefore, \( \hat{\theta} < \bar{\theta} \), a contradiction. Therefore \( \liminf_{k \to \infty} (\max \{ \| x^k - x^* \|, \| g^k - \lambda^k_H + \lambda^k_C \| \}) = 0 \) for all cluster points \( x^* \), and there is a subsequence satisfying (25). By Lemma 7, \( 0 \in \partial_C L(x^*) \) for all such subsequences.

3.3 Convergence of GOOMBAH

Because GOOMBAH essentially reverts to a manifold sampling step whenever the (approximate) solution to (12) does not provide sufficient decrease according to (13), GOOMBAH retains all the same convergence properties as guaranteed by Theorem 8 for MS-P. To see why (13) works as a sufficient decrease measure, look at (23) in the proof of Lemma 5. Partition the infinite set of successful iterations \( \{ k_j \} \) into the set of successful iterations that are solutions of (12), \( \mathbb{K}_1 \), and the set of successful iterations from the manifold sampling loop, \( \mathbb{K}_2 \). That is, \( \{ k_j \} = \mathbb{K}_1 \cup \mathbb{K}_2 \). With this partition,
\[
\infty > f(x^0) - f^* \geq \sum_{j=0}^{\infty} f(x^{k_j}) - f(x^{k_j+1})
\geq \sum_{k \in \mathbb{K}_1} \bar{\eta}_1 \Delta^1_k + \sum_{k \in \mathbb{K}_2} \eta_1 \kappa_{fcd} \chi_k \min \left\{ \frac{\lambda_k}{\kappa_H}, \Delta_k, 1 \right\}
\geq \sum_{k \in \mathbb{K}_1} \bar{\eta}_1 \Delta^1_k + \sum_{k \in \mathbb{K}_2} \eta_1 \kappa_{fcd} \min \left\{ \frac{\Delta^2_k}{\kappa_H^2}, \frac{\Delta^2_k}{C^2} \right\}.
\]

Regardless of the cardinalities of \( \mathbb{K}_1 \) and \( \mathbb{K}_2 \) (both infinite, or exactly one infinite), we still conclude that \( \Delta_{k_j} \to 0 \), and so the proof of Lemma 5 still follows. The remaining proofs are unaffected.

4 Testing

We now discuss the performance of implementations of the numerical optimization methods presented in this manuscript. We compare MS-P, GOOMBAH, and the previous manifold sampling code, which we denote MS-D because it employs the dual model (10). In inspecting some GOOMBAH runs, we observed that the recourse to using the MS-P loop occurred on relatively few iterations. This motivates the inclusion in our set of benchmarked implementations of a modified GOOMBAH that does not resort to any manifold sampling logic but instead shrinks \( \Delta_k \) on iterations in which
\[
\frac{h(F(x^k)) - h(F(x^k + s^k))}{h(M(x^k)) - h(M(x^k + s^k))} \leq \eta_1.
\]

The theory and implementation of MS-D have been developed only for unconstrained problems. And, because of the relatively poor performance of MS-D shown below, we did not seek to extend
MS-D to address bound-constrained problems. We also tested but do not present the (relatively poor) performance of other general-purpose nonsmooth optimization methods for both bound-constrained and unconstrained problems. Because such methods do not exploit the composite problem structure, their performance was understandably poor, and we find such a comparison to be unfair.

4.1 Test problems

We test the four manifold sampling implementations on problems of the form

$$\minimize_{x \in \Omega} h(F(x))$$

with variously defined $\Omega$, $h$, $F$, and starting points $x^0$. The specific values of $F$ and $x^0$ are defined by the 53 vector-mapping problems in the Moré–Wild [45] benchmark set; the dimension of the domain $F$ is between 2 and 12 and its output is between 2 and 65 dimensions. The mappings of $F$ are smooth with known gradients (which are used only for benchmarking purposes).

For $h$ we consider the following four nonsmooth mappings:

$$h_1 \triangleq \min_i z_i^2 \quad h_3 \triangleq \sum_{i=1}^{p} |d_i - \max \{z_i, c_i\}|$$

$$h_2 \triangleq \max_i z_i^2 \quad h_4 \triangleq \max_{i \in \{1, \ldots, l\}} \|z - z_i\|_{Q_i} + b_i.$$  

The $h_3$ mapping is the piecewise-linear, censored-L1 loss function [46] that measures how far $z_i$ is from target data $d_i$, but only if $z_i$ is more than the censor value $c_i$. The values for $c_i$ and $d_i$ are randomly generated for each for a given $(F, x^0)$ pair following the approach outlined in [7, Section 5.1]. Similarly, the $l$ quadratics defining the nonconvex mapping $h_4$ are randomly generated for each $(F, x^0)$ pair following the approach in [8, Section 6.2]. While 10 instances of $h_3$ and 20 instances of $h_4$ were originally generated for each $(F, x^0)$ pair, we used only the first instance for the current benchmark studies. These four $h$ mappings have known subdifferentials.

We consider an unconstrained setting ($\Omega \triangleq \mathbb{R}^n$) and a bound-constrained setting $\Omega \triangleq \{x : \ell \leq x \leq u\}$, where $\ell$ and $u$ are defined for each $(F, x^0)$ pair via the following procedure. We first run all the unconstrained experiments and record for each $(F, x^0)$ pair the approximate minimizer $\tilde{x}$ from among the three solvers \{MS-P, GOOMBAH, GOOMBAH w/o MS-P\} that minimizes $h(F(x))$. We then identify the midpoint $x^\text{mid}$ on the line segment $[x^0, \tilde{x}]$ and define, coordinate-wise for $i = 1, \ldots, n$,

$$\ell_i = x_i^0 - \max\{x_i^0 - x_i^\text{mid}, x_i^\text{mid} - x_i^0\} \quad u_i = x_i^0 + \max\{x_i^0 - x_i^\text{mid}, x_i^\text{mid} - x_i^0\}. \quad (28)$$

Choosing the bounds as in (28) guarantees that on at least one solver per $(F, x^0)$ pair, at least one bound must become active at some point in a run.

Thus, in total, we have 424 benchmark problem instances from 53 choices of $(F, x^0)$, 4 choices of $h$, and bound-constrained and unconstrained settings.

4.2 Implementation details

Implementations of the four tested methods were developed in Matlab$^4$. All methods used the same parameters (e.g., $\Delta_0$, $\eta_1$) where possible. The MS-D implementation was run (only for the unconstrained problems) using the default settings and subproblem solvers outlined in [8]. Each method was given a budget of $100(n+1)$ evaluations of $F$ with tolerances set to be as small as possible. For GOOMBAH, $\omega = 1$ was used. Our implementations of both GOOMBAH versions and MS-P do not explicitly verify whether Assumption 5 is satisfied since we have not found it necessary in practice. Finally, we set $c_1 = c_2 = 1.0 + 10^{-8}$ in the definition of $G_k$, see (3).

The GOOMBAH solutions to (12) were produced by calling various GAMS 38.3 solvers via the Matlab-GAMS GDXMRW interface [47]. The particular GAMS models that encode our four nonsmooth mappings

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$^4$All software is available at https://github.com/P0ptUS/IBCDFO/
can be viewed in our linked repository. Unfortunately, we were unable to find one solver that worked universally for all the subproblems and all the functions $h$. Some of this is due to limitations on the forms of nonsmoothness supported by the various optimization solvers. We also found that numerical issues occasionally arose when $\Delta$ was tiny or when models $m^{\ell_i}$ were poorly scaled. As a remedy, we attempted to solve each instance of (12) by multiple GAMS solvers, including CONOPT [48], MINOS [49], KNITRO [50], and BARON [51]. All solvers were limited to 30 seconds for each subproblem solve, but rarely did any solve take more than a few seconds in its entirety. These solvers were also used to compute $\chi$ in MS-P. All model Hessians $H_k$ were set to zero; therefore $n_2$ in the MS-P loop was effectively chosen to be $\infty$. We remark that because of this choice, the if conditional beginning in Line 9 of the MS-P loop is never entered, and hence there is no need to compute $\chi_k$. Nevertheless, we compute $\chi_k$ in our implementation anyway, for the sake of being able to monitor a stationarity measure.

### 4.3 Comparing implementations with approximate stationarity

We observe that many of the compositions $h \circ F$ have numerous stationary points. Since the methods being compared are all local optimization methods, therefore, we find that comparing performance in terms of objective value to be possibly misleading. That is, we believe a local optimization method should get credit for solving a problem when it has identified an (approximate) stationary point, even if that point has a worse function value than some other stationary point.

To measure a method’s progress, we find it necessary to have an approximate stationary value for each point $x^t$ evaluated by a given method. Obtaining this quantity is somewhat difficult, with various concerns that must be addressed. To begin, we randomly generate 50 points uniformly for each point $x$, even if that point has a worse function value than some other stationary point.

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To measure a method’s progress, we find it necessary to have an approximate stationary value for each point $x^t$ evaluated by a given method. Obtaining this quantity is somewhat difficult, with various concerns that must be addressed. To begin, we randomly generate 50 points uniformly within $B(x^t; 10^{-5}) \subset \mathbb{R}^n$ and denote them $S^t$. The same initial random seed is used when comparing all methods on a given problem so the starting pattern of points is equal for all methods. We add to $S^t$ all points evaluated by the method within $B(x^t; 10^{-5})$. These points include $x^t$ and possibly any points that were used by the method to determine approximate stationarity.

With $S^t$ in hand, we can then compute

$$D(x^t) \triangleq \{\nabla F(s) \nabla h_j(F(s)) : j \in \mathbb{A}(F(s)), s \in S^t\}$$

and the corresponding

$$a(x^t) \triangleq \{h_j(F(s)) : j \in \mathbb{A}(F(s)) s \in S^t\}.$$  

(30)

The gradient values in (29) can be computed (in postprocessing) because $\nabla F$ is computable in closed form for the problems considered and each $h_j$ has a known gradient. We consider a problem to be solved to an absolute level $\tau$ when the optimal value of (8) with problem data $D(x^t)$ and $a(x^t)$ in place of $G^k$ and $a^k$, respectively, denoted $\chi_t$, satisfies

$$\chi_t \leq \tau.$$  

(31)

We used the same routines used to compute $\chi_k$ in MS-P to compute $\chi_t$ for benchmarking. Data profiles [45] are used to compare the performance of the tested methods. Data profiles display how many evaluations of $F$ are required by each method to solve a certain fraction of the benchmark set of problems to a level $\tau$ for criterion (31). If a method satisfies (31) on any problem for the first time after $t$ evaluations of $F$, the data profile is incremented by $\frac{1}{\ell t}$ at the point $(\frac{t}{n_p+1})$ (where $n_p$ is the dimension of the problem) on the horizontal axis. In other words, a method’s data profile displays the cumulative fraction of problems solved by that method as a function of the number of evaluations of $F$ (scaled by $n_p + 1$).

**Remark 2.** The condition in (30) was chosen for testing stationarity because it was the stationary measure used in the analysis of MS-P. One also can consider a projection onto zero of the convex hull of $D(x^t)$ and active constraint normals as an analogous stationary condition. For unconstrained problems, this latter stationary measure would be the same as tested in, for instance, [8]. We found no meaningful difference between the data profiles when using either metric.

The performance of the four benchmarked implementations is presented in Figure 2. For the most part, we see that the GOOMBAH implementations considerably outperform the manifold sampling
implementations on both bound-constrained and unconstrained problems. We observe that the (infrequent) recourse to manifold sampling logic helps GOOMBAH solve approximately 5% of the benchmark problems.

As mentioned, MS-D is seen to be outperformed by its primal counterpart MS-P for unconstrained problems for all levels of $\tau$ that we considered. The supplemental material in Appendix B provides a greater dissection of these results for each of the $h$ functions considered. We do note that MS-D and MS-P are seen to have nearly identical performance for the $h_1$-problems. This may be explained by the fact that the pointwise minimum structure of $h_1$ can still be addressed by the MS-P analysis, but it is clear that (4), which involves a pointwise maximum, is a poor model of such an $h_1$.

5 Discussion and Future Directions

Many open research questions are related to the methods presented in this manuscript. One of the most obvious is the need to quantify and empirically study the trade-off between the cost of
producing the next iterate \(x^k + s^k\) and the cost of performing objective evaluations \(F(x^k + s^k)\). While many derivative-free optimization papers may make a blanket statement that the cost of the objective is assumed to outweigh any cost of the operations of the optimization method itself, such an assumption seems less reasonable for the GOOMBAH method, especially if \(h\) is complicated, \(m_{Fi}\) are nonlinear models, and a global optimization method is being called to produce iterates. The development of a “convention” or “rule” for limiting such algorithmic effort does not appear obvious. It seems natural to limit the wall-clock time used to solve (12)—which may need to invoke global optimization solvers—to less than some fraction (say, one-tenth) of the expected time required to evaluate \(F\) on a given computational resource. From another vantage, such a limitation may not be proper, especially if the simulation uses massive amounts of parallel compute resources and the trust-region subproblem solver cannot utilize such resources as efficiently. In fact, one could argue that more time should be spent on the solution of (12) when \(F\) requires considerable computational resources; the time spent improving the next iterate \(x^k + s^k\) could greatly reduce the required number of calls to \(F\). Such a trade-off calculation is even further confused by the fact that, in practice, global optimization methods often find high-quality solutions quickly; additional effort does not improve the solution quality but instead only reduces the gap between a lower and upper bound on the best possible objective value.

Another feature we seek to add to the implementation of MS-P or GOOMBAH is the ability to use (approximate) derivatives of \(F\) when they are available. Because MS-P requires only gradient-accurate models via Definition 3, we remark that given access to computable gradients \(\nabla F_i(x)\), we have only to define \(m_{Fi}(x)\) as the first-order Taylor model centered at the current iterate \(x^k\), namely,

\[
m_{Fi}(x^k + s) = F_i(x^k) + \nabla F_i(x^k)^\top s.
\]

Such a choice of \(m_{Fi}\) is automatically gradient-accurate with constant \(\kappa_{i,eg} = K_{\nabla F_i}\). Although we have not yet implemented or tested a gradient-based method, this is a trivial extension, and we intend to release it eventually.

In future work, we can also investigate nontrivial model Hessians \(H_k\) in (5). In our experiments, we employed only \(H_k = 0\), but our analysis permits the use of any model Hessian satisfying \(\|H_k\| \leq \kappa_H\). Practical experience (and limited theoretical results; see, e.g., \([52]\)) leads one to believe that BFGS matrices may be appropriate choices for \(H_k\). Alternatively, in a (primal) gradient sampling context, Curtis and Que \([29]\) employed an overestimating Hessian strategy that may prove useful in the context of the subproblem (5). Additionally, at the expense of even more difficult subproblems (QCQPs), Schichl and Fendl \([53]\) proposed—in a bundle method context—incorporating Hessians that approximate \(\nabla^2 F_i(x)\) into the constraints of (5). Although this would require a more computationally difficult subproblem, this is in line with our discussion acknowledging tradeoffs between subproblem difficulty and the expense of evaluating \(F\). All these Hessian-building methods are of interest to us in future testing and releases of software.

In closing, gentle reader, we’d like to thank you. What’s that, you say? Us thanking you? No, it’s not a misprint. For you see, we enjoyed writing this manuscript as much as you enjoyed reading it. The end.

Acknowledgments

We thank Geovani Nunes Grapiglia for initial discussions of convergence analysis results. This work was supported in part by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research and Office of High-Energy Physics, Scientific Discovery through Advanced Computing (SciDAC) Program through the FASTMath Institute and the CAMPA Project under Contract No. DE-AC02-06CH11357.

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A Table of notation

A(z): Set of indices of essentially active functions at a point z ...................... Definition 2
B: Euclidean ball .......................................................... Page 2
D: Sampled gradients of f used in numerical tests ................................. Equation (29)
F: Expensive inner function, with components F_i ................................. Assumption 1
G: Matrix with columns of vectors from g_j^k ...................................... Equation (7)
G: Set of indices used to generate \( G \) .......................... Eq. (3)
H: Model Hessian \( H^k \) ............................................ Eq. (4)
\( \mathcal{S} \): Set of selection functions ................................ Definition 1
\( I_n \): The identity for \( \mathbb{R}^n \) ................................. Eq. (7)
\( K \): Used for Lipschitz constants, (e.g., \( K_{\mathcal{V}_F}, K_{\mathcal{V}_F'} \)) ................................. e.g., Definition 4
\( \mathbb{K} \): Special sets of iterates ................................................. Page 15
\( L \): Level set ............................................................... Page 2
\( L_{\text{max}} \): Level set plus \( \Delta_{\text{max}} \) padding ................................. Page 2
\( \mathcal{L} \): The Lagrangian function ......................................... Page 14
\( \mathbb{L}_\infty \): \( \{ i \in 1, \ldots, n : \ell_i = -\infty \} \) ................................................. Page 4
\( M \): Vector mapping of the \( n \) models \( m^{F_i} \) ................................. Page 3
\( \mathbb{N} \): The set of Integers
\( Q \): \( Q_i \) is used to define quadratics in test functions ................. Page 17
\( \mathcal{R} \): The set of real numbers
\( S \): Set of points \( S^l \) sampled around each \( x \) evaluated by a method ................................ Page 18
\( \mathbb{U}_\infty \): \( \{ i \in 1, \ldots, n : u_i = \infty \} \) ................................................. Page 4
\( Y \): A collection of points \( y \) from the domain of \( F \) that have been evaluated ................. Page 3

\( a \): The value \( [a^k]_j \triangleq f(x^k) - f_j(x^k) + \beta_{j,k} \) ........................................ Page 4
\( b \): \( b_i \) is used to define quadratics in test functions ......................... Page 17
\( c \): \( c_i \) are the censors for the censored-L1 loss function, Also \( c_1, c_2 \) are algorithmic constants Page 17 and Eq. (3)
\( d \): \( d_i \) are the data for the censored-L1 loss function ......................... Page 17
\( e \): Vector of all ones
\( f \): Composite objective function \( f \triangleq h \circ F \). Also, sometimes \( f_j \triangleq h_j \circ F \) ........ Assumption 1
\( g \): The generators, \( g_j^F = [\nabla m_{F_i}^F] \nabla h_j(F(x^k)) \) ........................................ Page 3
\( h \): Nonsmooth, outer piecewise-selection function ................................. Assumption 1
\( h_j \): Smooth selection functions defining \( h \) ................................. Definition 1
\( i \): General index
\( j \): General index
\( k \): Iteration of the algorithm
\( l \): Lower bounds .......................................................... Page 1
\( m^{F_i} \): A model of \( F_i \) ........................................................ Definition 3
\( n \): Dimension of domain of \( F \) (and \( f \) ............................................. Assumption 1
\( p \): Dimension of domain of \( h \) .................................................. Assumption 1
\( s \): The trust-region subproblem step, sometimes \( s^* \) or \( s^k \) or \( s^k \) .... Eq. (6) or Eq. (12)
\( t \): Index for points evaluated by methods (not necessarily the iterate \( k \) ................. Page 18
\( u \): Upper bound on domain ..................................................... Page 1
\( v \): Primal variables for the problem ................................................. Eq. (6)
\( x \): Points in the domain of \( F \)
\( y \): Points in the domain of \( F \)
\( z \): Points in the domain of \( h \)

\( \beta \): A nonnegative offset added to affine functions in primal model \( \text{Equation (4)} \)

\( \gamma_d \): Trust-region decrease factor \( \text{Page 6} \)

\( \gamma_i \): Trust-region increase factor \( \text{Page 6} \)

\( \Delta \): Trust region radius \( \text{Page 2} \)

\( \Delta_{\text{max}} \): Upper bound on trust region radius \( \text{Page 2} \)

\( \eta \): Algorithmic acceptability tolerances \( \text{Page 6, Page 5} \)

\( \kappa \): Bounds on errors (between models/functions, fraction of Cauchy decrease) \( \kappa_{i,e}, \kappa_{g}, \kappa_{H}, \kappa_{fcd} \) Definition 3, Definition 4, Page 5, Assumption 5

\( \lambda \): Dual variables \( (\lambda_a, \lambda_{\ell}, \lambda_{u}) \) Equation (7)

\( \pi \): Used to denote projection problem solution Page 15

\( \rho \): Ratio of actual-versus-predicted decrease \( \text{Equation (11), Equation (13)} \)

\( \sigma \): A mapping between two convex sets \( \text{Lemma 2} \)

\( \tau \): Tolerance used for data profiles \( \text{Equation (31)} \)

\( \chi \): Stationary measure \( \text{Equation (8)} \)

\( \Omega \): Domain of test problems, either \( \mathbb{R}^n \) or \( [\ell, u] \) \( \text{Page 1} \)

\( \partial C \): Clarke subdifferential \( \text{Page 4} \)

Operations:

\( \text{cl}(S) \): Closure of a set \( S \)

\( \text{int}(S) \): Interior of a set \( S \)

\( \text{co}(S) \): Convex hull of a set \( S \)

\( \text{proj}(0,S) \): Projection of zero onto a set \( S \)

\( \text{im}_F(S) \): Image of set \( S \) under \( F \)

B Additional data profiles
Figure 3: Data profiles on the pointwise-minimum-squared function $h_1$, constrained and unconstrained, for three values of $\tau$. 

(a) $\tau = 10^{-1}$, unconstrained 
(b) $\tau = 10^{-1}$, constrained 
(c) $\tau = 10^{-3}$, unconstrained 
(d) $\tau = 10^{-3}$, constrained 
(e) $\tau = 10^{-5}$, unconstrained 
(f) $\tau = 10^{-5}$, constrained
Figure 4: Data profiles on the pointwise-maximum-squared function $h_2$, constrained and unconstrained, for three values of $\tau$. 
Figure 5: Data profiles on the censored-L1-loss function $h_3$, constrained and unconstrained, for three values of $\tau$. 
Figure 6: Data profiles on the piecewise-quadratic function $h_4$, constrained and unconstrained, for three values of $\tau$. 