Manifold Sampling for Optimizing Nonsmooth Nonconvex Compositions

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Abstract

We propose a manifold sampling algorithm for minimizing a nonsmooth composition \( f = h \circ F \), where we assume \( h \) is nonsmooth and may be inexpensively computed in closed form and \( F \) is smooth but its Jacobian may not be available. We additionally assume that the composition \( h \circ F \) defines a continuous selection. Manifold sampling algorithms can be classified as model-based derivative-free methods, in that models of \( F \) are combined with particularly sampled information about \( h \) to yield local models for use within a trust-region framework. We demonstrate that cluster points of the sequence of iterates generated by the manifold sampling algorithm are Clarke stationary. We consider the tractability of three particular subproblems generated by the manifold sampling algorithm and the extent to which inexact solutions to these subproblems may be tolerated. Numerical results demonstrate that manifold sampling as a derivative-free algorithm is competitive with state-of-the-art algorithms for nonsmooth optimization that utilize first-order information about \( f \).

1 Introduction

We consider unconstrained composite optimization problems of the form

\[
\text{minimize } \{ f(x) \colon x \in \mathbb{R}^n \} \quad \text{when } f(x) \triangleq h(F(x)),
\]

where \( h : \mathbb{R}^p \to \mathbb{R} \) is a structured, possibly nonsmooth and nonconvex function but its Clarke subdifferential \( \partial_C h(z) \) is known at any \( z \in \mathbb{R}^p \) in the domain of \( h \) and the function \( F : \mathbb{R}^n \to \mathbb{R}^p \), where \( F = [F_1 F_2 \cdots F_p]^\top \), is assumed continuously differentiable. We are especially motivated by problems where \( F \) is expensive to evaluate and the Jacobian \( \nabla F(x) \) is assumed unavailable. Such problems arise, for example, when using a nonsmooth loss function \( h \) to measure the quality of output from a function \( F \) that depends on some expensive simulation.

Manifold sampling is an approach for solving (1) that constructs models of \( F \) and combines these models using particular sampled information about \( h \). Manifold sampling was originally developed for the specific case where \( h \) is the \( \ell_1 \)-norm [39] and was later generalized to the case where \( h \) is a potentially nonconvex continuous selection of affine functions [34].

Definition 1.1. A function \( h \) is a continuous selection on \( U \subseteq \mathbb{R}^p \) if it is continuous on \( U \) and \( h(z) \in \{h_j(z) \colon h_j \in \mathcal{H} \} \) for all \( z \in U \), where \( h_j : \mathbb{R}^p \to \mathbb{R} \) and \( \mathcal{H} \) is a finite set of selection functions.

While the manifold sampling algorithm presented in [34] required every \( h_j \in \mathcal{H} \) to be an affine function, this work considers the case where each \( h_j \in \mathcal{H} \) is assumed only to be Lipschitz continuous and Lipschitz continuously differentiable. Past manifold sampling algorithms made the implicit assumption that each

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selection function was uniquely represented by its gradient; such an assumption does not hold in this more general case.

As in previous manifold sampling algorithms, the unavailability of $\nabla F(x)$ at a given $x \in \mathbb{R}^n$ is handled through standard techniques of model-based derivative-free optimization, that is, via the construction of models $m^F(x)$ of $F_i(x)$. We then employ

$$M(x) \triangleq [m^{F_1}(x) \cdots m^{F_r}(x)]^T \quad \text{and} \quad \nabla M(x) \triangleq [\nabla m^{F_1}(x) \cdots \nabla m^{F_r}(x)]$$

as approximations of $F(x)$ and $\nabla F(x)$, respectively. In the present work, we will use not only knowledge of the functions $h_j \in \mathcal{H}$ that define $h$ but also $\nabla h_j(z)$, the gradients of linearizations of $h_j$ at points $z$, in order to update iterates. For each continuously differentiable $h_j \in \mathcal{H}$, the composition $h_j(F(x))$ is also continuously differentiable, and from a simple application of the chain rule

$$\nabla h_j(F(x)) = \nabla F(x) \nabla h_j(F(x)) \approx \nabla M(x) \nabla h_j(F(x)).$$

Thus, when considering topologically connected point sets satisfying

$$\{x \in \mathbb{R}^n : h(F(x)) = h_j(F(x))\},$$

we can use standard derivative-free techniques to produce sufficiently accurate models of $h_j \circ F$ and hence sufficiently accurate models of $h \circ F$ when restricted to (3). Manifolds\footnote{Using a result such as Theorem 2 of [53], one can show that functions $h$ satisfying Definition 1.1 admit a Whitney stratification, and the resulting strata could be interpreted as manifolds in (3). See also [7, 19, 30]. Accounting for such a manifold representation would be cumbersome, however, and hence we use the notation of continuous selections.} in this manuscript refer to any topologically connected set of the form (3) and hence refer to regions where $h_j \circ M$ might be used as models of $f = h \circ F$. In each manifold sampling iteration, we construct models of $F$ and make use of $h_j \circ F$ for some $h_j \in \mathcal{H}$. These models are then assembled in a particular manner to suggest search directions within an iterative (trust-region) method.

Our work is not in the scope of optimization of functions defined on general Riemannian manifolds, which is an active, but distinct, area of research.

### 1.1 Literature review

Unconstrained nonsmooth noncomposite convex optimization given a subgradient oracle has become a classical method; see, for instance, [52] for a textbook treatment of first-order subgradient methods. A historically popular class of methods for the solution for convex nonsmooth optimization methods has been bundle methods; see [43] for a survey from 2001. Given a noncomposite nonconvex objective function but still assuming access to a subgradient oracle, various solution methodologies have been proposed. Subgradient methods tailored to the nonconvex setting are investigated in, for instance, [3, 4], while bundle methods suitable for the nonconvex setting have also been developed (see, e.g., [28, 29, 36]). The approach of [49] iteratively constructs convex second-order models of the objective and employs a line search for globalization; in [50] similar models of the objective are constructed, but a trust region is employed for globalization, yielding convergence of a subsequence to a Dini stationary point. Difference-of-convex approaches for nonsmooth composite objectives have also been studied in recent works [15, 41].

For unconstrained nonsmooth noncomposite nonconvex optimization when in the derivative-free setting, Bagirov, Karasözen, and Sezer [5] proposed the so-called discrete gradient method, which computes approximate subgradients for use in a subgradient descent framework; see also [51]. Direct-search methods in derivative-free optimization have been historically concerned with convergence to Clarke stationary points and are hence suitable for nonsmooth optimization. See the book [1] for an excellent treatment of this subject. Bundle methods, as well as trust-region bundle methods, have also been considered in the derivative-free setting; see, for instance, [31, 42].

Unconstrained nonsmooth composite optimization problems of the form (1) have been given special attention in the literature. Works from the 1980s provide fundamental analyses for the case where $h$ is...
convex and $\nabla F$ is available [21, 22, 58, 59, 60]. In a derivative-free setting, the authors in [23, 24] analyze algorithms for composite optimization where $h$ is a general convex function but $\nabla F$ is not available. To the best of our knowledge, [34] is the only work that allows for $h$ to be nonconvex and does not require access to $\nabla F$.

The case of $h$ in (1) being a general convex function has enjoyed special attention [12, 21, 22, 23, 24, 59]. Convex functions $h$ are natural in many applications. For instance, they are frequently used as penalty functions, such as $\| \cdot \|_p$ and $\max(\cdot, 0)$ (an exact penalty for inequality constraints). Thus, in the literature one sometimes sees treatments of particular convex functions $h$. For example, in [11, 57], $h$ is fixed as $\| \cdot \|^2_2$, while in [27, 44, 58], $h$ is fixed as $\max(\cdot)$. In [22, 60], $h$ is fixed as a polyhedral convex function, which is a convex piecewise-affine function. The work in [34] removes the convexity requirement to address functions $h$ that are assumed only to be continuous and piecewise-affine.

We note that the algorithmic differentiation (AD) community has analyzed methods for computing generalized derivatives of piecewise-smooth functions for use in gradient-based nonsmooth optimization methods. The authors of [26] consider the “abs-normal form” (see, e.g., [25, 55]) of local nonsmooth models of a class of piecewise-smooth functions that commonly appear in computer codes, and they demonstrate how standard AD tools can be extended to derive these models, which are then used to design bundle-type methods. The approach in [45] considers a limited class of composite functions and uses a forward-AD method to compute a subgradient of such functions for use in McCormick relaxations, which can be solved by global optimization methods; the resulting relaxation is more amenable to global optimization methods. A state-of-the-art forward-AD mode for computing generalized derivatives of composite piecewise-differentiable functions is presented in [33]. A reverse-AD method for computing the subgradients of the same class of functions as considered in [45] is derived in [6]. In [32], the authors demonstrate a practical reverse-AD mode for computing generalized derivatives of composite piecewise-differentiable functions.

Gradient sampling methods [8, 9, 10, 18, 37] are designed for noncomposite nonsmooth nonconvex optimization. We pay special attention to them because they are closest in spirit to manifold sampling algorithms. Gradient sampling methods were originally designed [9, 10] for the minimization of locally Lipschitz functions, a broader class of nonsmooth functions than those analyzed in the present paper. Gradient sampling methods compute random samples of gradients at multiple points in an $\epsilon$-neighborhood of a current point $x$ in order to approximate the Clarke $\epsilon$-subdifferential of $f(x), \partial f(x)$. In contrast to gradient sampling, we note that manifold sampling does not require access to gradient information and does not rely on randomization. By exploiting knowledge of the structure of the objective in (1) (in particular, the finiteness of the set $S$ defining $h$), manifold sampling does not depend on random sampling to identify the presence of distinct manifolds in a neighborhood of $x$. We note that Kiwiel [38] proposed a gradient sampling method for the derivative-free setting by computing approximate (finite-difference) gradients, but the method still depends on randomization.

1.2 Real-world example

While convex or piecewise-linear forms of $h$ may be common, they are far from exclusive. As one example, particle beamline scientists often seek operational parameters that produce a tightly bunched beam at some point in space. This allows a sample to be placed at this point in space in order to be hit by the tightest-possible beam. The spread of the beam is measured by the normalized emittance. A beamline simulation is run for a given set of operational parameters $x$, producing three vectors of simulation output $F_{1,j}(x)$, $F_{2,j}(x)$, and $F_{3,j}(x)$ for each position $j$ in a finite set $J$. The objective is to minimize $\min_{j \in J} \sqrt{F_{1,j}(x)F_{2,j}(x) - F_{3,j}(x)^2}$.

See [56] for greater detail. In this case, we have a nonconvex, not piecewise-linear, nonsmooth function $h(z) \triangleq \min_{j \in J} \left\{ h_j(z) \triangleq \sqrt{z_{1,j}z_{2,j} - z_{3,j}^2} \right\}$.

1.3 Notation and definitions

All norms are assumed to be $\ell_2$ norms. The closure, interior, and convex hull of a set $S$ are denoted $\cl(S)$, $\inte(S)$, and $\coh(S)$, respectively. The image of a set $S$ through $F$ is $\Im(F) \triangleq \{ F(x) : x \in S \}$. We define
\( B(x; \Delta) = \{ y : \|x - y\| \leq \Delta \} \). In the rest of this paper, we use 0 to denote both a scalar and a vector with a zero in each entry, depending on context. We define \( e \) to be the vector with a one in each entry.

We say a function \( f \) is Lipschitz continuous with constant \( L_f \) on \( \Omega \subset \mathbb{R}^n \) if \( |f(x) - f(y)| \leq L_f \|x - y\| \) for all \( x, y \in \Omega \). Recall that if \( f \) is also continuously differentiable, then Lipschitz continuity immediately implies that \( \|\nabla f(x)\| \leq L_f \) for all \( x \in \text{int} (\Omega) \). Similarly, \( f \) has a Lipschitz continuous gradient with constant \( L_{\nabla f} \) on \( \Omega \) if \( \|\nabla f(x) - \nabla f(y)\| \leq L_{\nabla f} \|x - y\| \) for all \( x, y \in \Omega \).

The generalized Clarke subdifferential of a locally Lipschitz continuous function \( f \) at a point \( x \) is defined as \( \partial_C f(x) \triangleq \text{co} \left( \{ \lim_{y' \to x} \nabla f(y') : y' \in D \} \right) \), where \( D \) is the set of points where \( f \) is differentiable. That is, \( \partial_C f(x) \) is the convex hull of the set of all limiting gradients from differentiable points that converge to \( x \). A point \( x \) is called a Clarke stationary point of \( f \) if \( 0 \in \partial_C f(x) \).

1.4 Organization

Section 2 collects assumptions about \( f, h, F \), and the models approximating \( F_i \). Section 3 presents the essential components of the manifold sampling algorithm. Section 4 contains lemmas concerning the essential components of the manifold sampling algorithm that will be used in later convergence analysis. We highlight Lemma 4.3 and Lemma 4.4, which relate to the feasibility of two particular subproblems encountered during each manifold sampling iteration. In Section 5, we demonstrate our main theoretical result, namely, that all cluster points of the sequence of iterates produced by the manifold sampling algorithm are Clarke stationary. Section 6 presents numerical experiments comparing an implementation of the proposed manifold sampling algorithm with other methods for nonsmooth optimization, all of which are given access to values of \( \nabla f(x) \). Section 7 contains some concluding remarks and discussion.

2 Problem Setting

We now present background material and assumptions. For an initial iterate \( x^0 \in \mathbb{R}^n \), we first define \( \mathcal{L}(x^0) \triangleq \{ x : f(x) \leq f(x^0) \} \). Moreover, for a constant \( \Delta_{\max} > 0 \) and point \( x^0 \), define

\[
\mathcal{L}_{\max} \triangleq \bigcup_{x \in \mathcal{L}(x^0)} B(x; \Delta_{\max}).
\]

We may now introduce some assumptions about the objective function \( f : \mathbb{R}^n \to \mathbb{R} \).

**Assumption 1.** We assume the following about \( f \) and \( F \).

- **A.** For a point \( x^0 \in \mathbb{R}^n \), the set \( \mathcal{L}(x^0) \) is bounded.
- **B.** Each \( F_i \) is Lipschitz continuous with constant \( L_{F_i} \) on \( \mathcal{L}_{\max} \).
- **C.** Each \( F_i \) is Lipschitz gradient continuous with constant \( L_{\nabla F_i} \) on \( \mathcal{L}_{\max} \).

From Assumption 1.A, we may conclude that \( \mathcal{L}_{\max} \) is bounded. In our analysis, we will demonstrate in Lemma 5.2 that all points evaluated by the manifold sampling algorithm are contained in \( \mathcal{L}_{\max} \).

We next define what it means for a given selection function \( h_j \) to be essentially active in a continuous selection; see [54] for a deeper treatment of continuous selections.

**Definition 2.1.** Suppose \( h \) is a continuous selection. We define

\[
\mathcal{S}_j \triangleq \{ z : h(z) = h_j(z) \}, \quad \mathcal{S}_j \triangleq \text{cl} (\text{int}(\mathcal{S}_j)), \quad \mathcal{A}(z) \triangleq \left\{ j : z \in \mathcal{S}_j \right\}.
\]

We refer to elements of \( \mathcal{A}(z) \) as essentially active indices. We refer to any \( h_j \) for which \( j \in \mathcal{A}(z) \) as an essentially active selection function for \( h \) at \( z \). Moreover, the function \( h_j \) is essentially active at \( z \in \text{co}(\text{Im}(\mathcal{L}_{\max})) \), provided \( h_j \) is an essentially active selection function for \( h \) at \( z \). For a finite set \( Z \), let \( \mathcal{A}(Z) = \bigcup_{z \in Z} \mathcal{A}(z). \)
Fundamentally, essentially active selection functions are those that describe the behavior of \( h \) near a point of interest. With this definition, we can make the following assumptions on \( h \) and the selection functions defining it.

**Assumption 2.** We assume the following about \( h \).

**A.** The function \( h \) satisfies Definition 1.1.

**B.** The set \( \mathcal{A}(z) \) of essentially active indices for \( h \) at \( z \) is computable for any \( z \in \text{co}(\text{Im}(L_{\text{max}})) \).

For all \( z, z' \in \text{co}(\text{Im}(L_{\text{max}})) \) and for each \( h \in \mathcal{A} \), we assume the following:

**C.** There exists \( L_{h_j} \) such that \( |h_j(z) - h_j(z')| \leq L_{h_j} \|z - z'\| \).

**D.** There exists \( L_{\nabla h_j} \) such that \( \|\nabla h_j(z) - \nabla h_j(z')\| \leq L_{\nabla h_j} \|z - z'\| \).

The models that we use to approximate the components \( F_i \) of \( F \) must be sufficiently accurate. As is standard in model-based derivative-free optimization, we employ full linearity as our standard of accuracy.

**Definition 2.2.** A function \( m^{F_i}: \mathbb{R}^n \rightarrow \mathbb{R} \) is said to be a fully linear model of \( F_i \) on \( \mathcal{B}(x; \Delta) \) with constants \( \kappa_{i,\text{ef}} \) and \( \kappa_{i,\text{eg}} \), provided

\[
|F_i(x + s) - m^{F_i}(x + s)| \leq \kappa_{i,\text{ef}} \Delta^2 \quad \forall s \in \mathcal{B}(0; \Delta),
\]

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

See, for instance, [40, 14] for a deeper treatment of the construction of fully linear models. A fully linear model of a function can be constructed on \( \mathcal{B}(x; \Delta) \), for example, by interpolating function values at \( n + 1 \) well-poised points including \( x \). Note in this example, however, that we do not need \( p \times (n + 1) \) evaluations of \( F \) in order to construct \( p \) fully linear models \( m^{F_i} \) since we assume that an evaluation of \( F(x) \) returns \( F_1(x), \ldots, F_p(x) \) simultaneously. Ultimately, the algorithm will use \( \nabla m^{F_i} \) in place of an unavailable \( \nabla F_i \).

Each iteration of the manifold sampling algorithm will ensure that the models \( m^{F_i} \) are fully linear models of \( F_i \) on \( \mathcal{B}(x^k; \Delta_k) \), where \( x^k \) and \( \Delta_k \) correspond to the current point and trust-region radius at iteration \( k \).

**Assumption 3.** There exist constants \( \{\kappa_{1,\text{ef}}, \ldots, \kappa_p,\text{ef}\} \) and \( \{\kappa_{1,\text{eg}}, \ldots, \kappa_p,\text{eg}\} \), independent of \( k \), such that for each component function \( \{F_1, \ldots, F_p\} \) of \( F \), each model \( \{m^{F_1}, \ldots, m^{F_p}\} \) is fully linear on \( \mathcal{B}(x^k; \Delta_k) \) with the corresponding constants. Moreover, each \( m^{F_i} \) is twice continuously differentiable, and there exists \( \kappa_{i,\text{mH}} \) so that \( \|\nabla^2 m^{F_i}(x)\| \leq \kappa_{i,\text{mH}} \) for all \( x \in L_{\text{max}} \).

For ease of presentation and analysis, we define the following constants.

**Definition 2.3.** For the constants in Assumption 1.C, Assumption 2.C, Definition 2.2, and Assumption 3, define

\[
L_F \triangleq \sqrt{\sum_{i=1}^p L_{F_i}^2}, \quad L_{\nabla F} \triangleq \sqrt{\sum_{i=1}^p L_{\nabla F_i}^2}, \quad L_h \triangleq \max_{j \in \{1, \ldots, p\}} \{L_{h_j}\}, \quad L_{\nabla h} \triangleq \max_{j \in \{1, \ldots, p\}} \{L_{\nabla h_j}\},
\]

\[
\kappa_\ell \triangleq \sum_{i=1}^p \kappa_{i,\text{ef}}, \quad \kappa_\kappa \triangleq \sum_{i=1}^p \kappa_{i,\text{eg}}, \quad \kappa_H \triangleq \sum_{i=1}^p \kappa_{i,\text{mH}}, \quad \text{and} \quad C \triangleq (2L_h \kappa_\kappa + 2L_{\nabla h} L_F^2 + L_h L_{\nabla F}).
\]

Proposition 4.1.2 in [54] demonstrates that \( L_h \) is in fact a Lipschitz constant for \( h \), and so our definition above is simply fixing a particular value of the Lipschitz constant.

## 3 Manifold Sampling for Piecewise-Smooth Compositions

We now outline the essential components of the manifold sampling algorithm (presented in Algorithm 1 in Section 3.6) for solving problems of the form (1) satisfying Assumption 1 and Assumption 2. We draw special attention to Section 3.2, Section 3.3, and Section 3.4, which respectively introduce three subproblems that must be solved in each iteration of the manifold sampling algorithm.
3.1 Sample set $\mathcal{Z}^k$, gradient set $\mathbb{D}^k$, and generator set $\mathcal{G}^k$

Manifold sampling is an iterative method that builds component models $m^{F_i}$ of each $F_i$ around the current point $x^k$. We place the first-order terms of each model in column $i$ of the matrix $\nabla M(x^k) \in \mathbb{R}^{n \times p}$ as in (2).

As in past manifold sampling algorithms, $\nabla M(x^k)$ will be combined with gradients of selection functions to yield generalized gradients for $f$ as in (1). But additional care must be taken when $h_j$ is assumed only to be smooth, and not assumed to be piecewise-affine. Because the value of $\nabla h_j$ need not be unique on a given manifold, the manifold sampling algorithm will maintain a finite sample set of points $\mathcal{Z}^k \subset \mathbb{R}^p$ representing points where different selection functions have been determined to be active. In the algorithm, $\mathcal{Z}^k$ will include both the vector values of $F(y)$ for previously evaluated points $y \in \mathcal{B}(x^k; \Delta_k)$ and points of the form $\alpha F(x^k) + (1 - \alpha)F(y)$ for $\alpha \in [0, 1]$. In other words, it may not always be the case that $\mathcal{Z}^k \subset \text{Im}(L_{\text{max}})$, but it is always the case that $\mathcal{Z}^k \subset \text{co(Im}(L_{\text{max}}))$.

The sample set $\mathcal{Z}^k$ yields a set of gradients of linearizations of active selection functions, $\mathbb{D}^k$. Combining elements of $\mathbb{D}^k$ with $\nabla M(x^k)$ produces a generator set $\mathcal{G}^k$ with elements of the form $\nabla M(x^k)\nabla h_j(z)$ for suitable selection functions $h_j$ that are active within $\mathcal{B}(F(x^k); L_F\Delta_k)$. The set $\text{co}(\mathcal{G}^k)$ can then be treated as a particular approximation to $\partial C f(x^k)$. These sets are defined in the following.

**Definition 3.1.** Let $\mathbb{D}^k$ denote the set of gradients of linearizations of selection functions corresponding to the finite sample set $\mathcal{Z}^k \subset \mathbb{R}^p$. That is, $\mathbb{D}^k = \{\nabla h_j(z) : z \in \mathcal{Z}^k, j \in \mathcal{A}(z)\}$. Let $\mathcal{G}^k$ denote the set of generators corresponding to the sample set $\mathcal{Z}^k$. That is, $\mathcal{G}^k = \{\nabla M(x^k)\nabla h_j(z) : z \in \mathcal{Z}^k, j \in \mathcal{A}(z)\}$. Let $\mathbb{D}^k$ be the matrix with columns that are the elements of $\mathbb{D}^k$. Let $\mathcal{G}^k$ be the matrix with columns that are the elements of $\mathcal{G}^k$. That is, $\mathcal{G}^k = \nabla M(x^k)\mathbb{D}^k$.

From Definition 3.1, we see that a generator set $\mathcal{G}^k$ is a sample of approximate gradients from various manifolds of the continuous selection that are potentially active at (or relatively near) $F(x^k)$. Ultimately, the minimum-norm element of $\text{co}(\mathcal{G}^k)$, which is the projection of the origin to $\text{co}(\mathcal{G}^k)$, denoted by

$$g^k \triangleq \text{proj}(0, \text{co}(\mathcal{G}^k)) \in \text{co}(\mathcal{G}^k),$$

will be employed as the gradient of a smooth master model that will be minimized in a trust-region $\mathcal{B}(x^k; \Delta_k)$ to suggest trial points. Lemma 4.1 will demonstrate that $\text{co}(\mathcal{G}^k)$ can approximate $\partial C f(x^k)$ sufficiently well in order to guarantee that manifold sampling converges to Clarke stationary points. When all the elements of $\mathcal{Z}^k$ are sufficiently close to $F(x^k)$ and $\|g^k\| \approx 0$, Lemma 4.1 suggests that $x^k$ is a Clarke stationary point. This reasoning provides the rough roadmap for our analysis.

We see in Definition 3.1 that different choices of sample sets $\mathcal{Z}^k$ induce different generator sets $\mathcal{G}^k$. While the manifold sampling algorithm permits some flexibility in the selection of $\mathcal{Z}^k$, our convergence results require some minimal assumptions on the construction of $\mathcal{Z}^k$.

**Assumption 4.** At every iteration $k$ of Algorithm 1, the finite set $\mathcal{Z}^k$ satisfies $F(x^k) \subseteq \mathcal{Z}^k \subset \mathcal{B}(F(x^k); L_F\Delta_k)$ for $L_F$ as in Definition 2.3.

Although Algorithm 1 does not assume access to $L_F$, ensuring that $\mathcal{Z}^k$ contains only elements of the form $F(y)$ for $y \in \mathcal{B}(x^k; \Delta_k)$ or $\alpha F(x^k) + (1 - \alpha)F(y)$ for $\alpha \in [0, 1]$ will ensure that Assumption 4 is satisfied.

An ideal sample set $\mathcal{Z}^k$ would be one such that $h(\mathcal{Z}^k) = \bigcup_{y \in \mathcal{B}(x^k; \Delta_k)} h(F(y))$; that is, $\mathcal{Z}^k$ would contain points in $\mathbb{R}^p$ so that all selection functions that define $h$ in the image of $\mathcal{B}(x^k; \Delta_k)$ under $F$ are identified. Fortunately, identifying all active selection functions near $x^k$ is not necessary; this is indeed fortunate because ensuring that all such active selection functions have been identified may be impossible in practice. In our implementation, $\mathcal{Z}^k$ is initialized in either of the following ways, both of which are consistent with Assumption 4 and are practical: $\mathcal{Z}^k = \{F(x^k)\}$ or $\mathcal{Z}^k = \{F(y) : y \in Y \subset \mathcal{B}(x^k; \Delta_k)\}$. We note that in the second case, additional evaluations of $F$ are not necessary; it is sufficient to let $Y$ consist of points in $\mathcal{B}(x^k; \Delta_k)$ where $F$ has been evaluated during previous iterations of the algorithm.


3.2 Smooth master model

As previously stated, we want the gradient of the smooth master model to satisfy \( g^k = \text{proj}(0, \mathbf{co}(G^k)) \). This projection can be computed by solving the convex quadratic optimization problem

\[
\min_{\lambda} \quad \lambda^T(G^k)^T G^k \lambda \quad \text{subject to} \quad e^T \lambda = 1, \quad \lambda \geq 0.
\]

Employing \( G^k \) and \( D^k \) defined in Definition 3.1 and \( \lambda^* \) solving (6), we can define

\[
g^k \triangleq G^k \lambda^* \quad \text{and} \quad d^k \triangleq D^k \lambda^*.
\]

While there may not be a unique \( \lambda^* \) solving (6), the values of \( g^k \) and \( d^k \) in (7) are necessarily unique.

We employ \([d^k]_i\), the \( i \)th element of \( d^k \), as weights attached to the \( p \) smooth component models \( m^F_i \) to yield the smooth master model

\[
m^f_k(x) \triangleq \sum_{i=1}^p [d^k]_i m^F_i(x).
\]

By construction, \( \nabla m^f_k(x^k) = \sum_{i=1}^p [d^k]_i \nabla m^F_i(x^k) = \nabla M(x^k) D^k \lambda^* = G^k \lambda^* = g^k \). We draw attention to the fact that the master model \( m^f_k \) is not assumed to be an accurate model of \( f \) in a Taylor approximation sense. However, Lemma 4.4 demonstrates a result resembling one direction of the definition of “order-1 subgradient accuracy,” as in [2, Section 19.4].

3.3 Sufficient decrease condition

In iteration \( k \) of the manifold sampling algorithm, the master model \( m^f_k \) in (8) will be employed in the trust-region subproblem

\[
\min_{s \in B(0, \Delta_k)} m^f_k(x^k + s).
\]

As with traditional trust-region methods, the problem (9) does not have to be solved exactly. Rather, an approximate solution \( s^k \) of (9) can be used, provided it satisfies a sufficient decrease condition quantified by an algorithmic parameter \( \kappa_d \in (0, 1) \), namely,

\[
\langle M(x^k) - M(x^k + s^k), d^k \rangle \geq \frac{\kappa_d}{\kappa_d + h} \|g^k\| \min \left\{ \|x^k - s^k\|, \frac{\|x^k - s^k\|}{L_{\max}} \right\}.
\]

(If \( h \) is constant on \( L_{\max} \) or all of the models \( m^F_i \) are linear and \( L_h \kappa_H = 0 \), \( \frac{\|x^k - s^k\|}{L_{\max}} \triangleq \infty \).)

Note that the sufficient decrease condition (10) differs from traditional conditions employed in classical trust-region methods (see, e.g., [13, Theorem 6.3.3]). Instead of measuring the decrease in \( m^f_k \) between \( x^k \) and \( x^k + s^k \), the left-hand side of (10) measures the decrease in terms of the specific convex combination, defined by \( d^k \), of the gradients of selection functions at points near \( F(x^k) \). The sufficient decrease condition (10) extends the approach from [39], where \( h = \| \cdot \|_1 \) and decrease is measured by using the sign pattern of \( F \) at \( x^k + s^k \). We will demonstrate in Lemma 4.4 that an \( s^k \) satisfying (10) always exists and can be found with a particular step choice.

Remark 3.1 (on the various uses of \( \Delta_k \)). Note that the trust-region subproblem (9), Assumption 3 on model quality, and Assumption 4 on allowable sample sets all involve the parameter \( \Delta_k \). This intentional conflation of the use of \( \Delta_k \) greatly facilitates our analysis. In analyses of derivative-free model-based methods, one commonly sees \( \Delta_k \) controlling both trust-region radii and model accuracy. In manifold sampling, \( \Delta_k \) plays a third role of the \( \epsilon \) parameter in the approximation of the Clarke \( \epsilon \)-subdifferential induced by \( G^k \). Whereas practical implementations of derivative-free model-based methods sometimes decouple \( \Delta_k \) into separate parameters controlling step sizes and model accuracy, one could also consider a third decoupling of \( \Delta_k \) from its use in Assumption 4 at the expense of an algorithm that is more difficult to analyze.
3.4 Manifold sampling loop

In the manifold sampling algorithm, the trial step $s^k$ suggested by the trust-region subproblem may not yield sufficient decrease if $\mathcal{A}(Z^k)$ is a poor sample of nearby active manifolds. Therefore, after $s^k$ has been computed and $F(x^k + s^k)$ has been evaluated, but before the ratio determining success, $\rho_k$ (defined in (14)), is computed, $Z^k$ sometimes must be augmented, resulting in a new master model and a new $s^k$. We refer to this process that occurs in each iteration as the manifold sampling loop.

Although adding indices to $Z^k$ may result in a given manifold sampling iteration requiring the solution of more than one trust-region subproblem—and, more importantly, more than one evaluation of $F$—in practice the number of function evaluations per iteration is rarely more than one. We further remark that, even in theory, this manifold sampling loop cannot cycle indefinitely because the number of selection functions defining $h$ is finite.

The termination of the manifold sampling loop hinges on a search for a sample point $z \in \text{co} \left( \{F(x^k), F(x^k + s^k)\} \right)$ and an index $j$ satisfying

$$ j \in \mathcal{A}(z), $$

$$ \nabla h_j(z)^T (F(x^k) - F(x^k + s^k)) \leq h(F(x^k)) - h(F(x^k + s^k)). $$

(11a)

(11b)

In other words, a point $z \in \mathbb{R}^p$ and an index $j$ in $\mathcal{A}(z)$ satisfy (11), provided the affine function $h(F(x^k)) + \nabla h_j(z)^T (F(x^k + s^k) - F(x^k))$ overestimates $h(F(x^k + s^k))$. We remark that (11) is less stringent than the condition in [34], which sought a manifold $j$ satisfying

$$ h_j(F(x^k)) \leq h(F(x^k)) \quad \text{and} \quad h_j(F(x^k + s^k)) \geq h(F(x^k + s^k)). $$

(12)

If $h$ is a continuous selection of affine functions, which is the special case considered in [34], then (12) is equivalent to fixing one affine function $h_j \in \mathcal{A}$ that underestimates $h$ at $F(x^k)$ but overestimates $h$ at $F(x^k + s^k)$. Between [34] and our present work, we see that the commonality lies in the overestimation of $h$ at $F(x^k + s^k)$.

We will demonstrate (in Lemma 4.2) that under our assumptions, we can compute a $(z, j)$ pair satisfying (11) for any $s^k$. As our analysis will reveal, however, we additionally require the existence of a secondary $z' \in Z^k$ satisfying

$$ j \in \mathcal{A}(z'), $$

$$ (s^k)^T \nabla M(x^k)(\nabla h_j(z') - d^k) \leq 0 $$

(13a)

(13b)

for the same $j$ employed in (11). Geometrically, (13b) requires that the trial step $s^k$ be obtuse with the vector pointing to the single generator $\nabla M(x^k)\nabla h_j(z')$ from the minimum norm of the convex hull of the generators, $\nabla M(x^k)d^k = g^k$. From the classical projection theorem (see, e.g., [52, Theorem 2.39]), a trial step $s^k$ parallel to the steepest descent direction $-g^k$ satisfies (13b). Thus, if a trial step $s^k$ obtained from the solution of (9) fails to lead to the simultaneous satisfaction of (11) and (13), then we may safely replace $s^k$ with a default scaled steepest descent direction.

3.5 $\rho_k$ test

In common with classical trust-region methods, manifold sampling employs a ratio test as a merit criterion. Whereas the value of $\rho_k$ in a classical trust-region method measures the ratio of the actual decrease $f(x^k) - f(x^k + s^k)$ to predicted model decrease $m_k^f(x^k) - m_k^f(x^k + s^k)$, the $\rho_k$ used in the manifold sampling algorithm is the ratio of actual decrease in $F$ to predicted decrease in $M$, as weighted by the convex combination of gradients $d^k$. Explicitly, given $d^k$ defined in (7) and $s^k$ satisfying (10), $\rho_k$ is the ratio

$$ \rho_k \triangleq \frac{(F(x^k) - F(x^k + s^k),d^k)}{(M(x^k) - M(x^k + s^k),d^k)}. $$

(14)

A trial step $x^k + s^k$ is accepted only if $\rho_k$ is sufficiently large.
Algorithm 1: Manifold sampling for general compositions (MSG)

1. Set $\eta_1 \in (0, 1)$, $\eta_2 \in (0, 1)$, $\kappa_H \geq 0$, $\eta_2 \in (0, \eta_{\text{max}})$, $0 < \gamma_i < 1 \leq \gamma_i$, and $\Delta_{\text{max}} > 0$
2. Choose $\Delta_0$ satisfying $\Delta_{\text{max}} \geq \Delta_0 > 0$ and initial iterate $x^0$
3. for $k = 0, 1, 2, \ldots$ do
4.   Evaluate $F$ as needed to build $p$ models $m_k^F$ satisfying Assumption 3
5.   Initialize $Z^k$ satisfying Assumption 4; form $D^k$ by Definition 3.1
6.   while true do // manifold sampling loop
7.     Form $M(x^k)$ using $\nabla m_k^F(x^k)$; set $G^k \leftarrow \nabla M(x^k)D^k$
8.     Solve (6) for $\lambda^*$; set $d^k \leftarrow D^k\lambda^*$
9.     Build master model $m_k^F$ using (8) with $\nabla m_k^F(x^k) = G^k\lambda^* = g^k$
10. if $\Delta_k < \eta_2 \|g^k\|$ then
11.     generate $\Delta_k, \Delta_{\text{sk}}, \kappa_H \text{ and } \kappa_H$ // acceptable iter.
12.     if $j \in \mathcal{A}(Z^k)$ then
13.         Calculate $\rho_k$ using (14) and break // successful iter.
14.     else
15.         Update $m_k^F$ (evaluating $F$ if needed) satisfying Assumption 3
16.         $Z^k \leftarrow Z^k \cup \{x\} \cup \{F(y) : y \in B(x; \Delta_k)\}$; form $D^k$ by Definition 3.1
17.     else
18.         $\rho_k \leftarrow 0$; break // unsuccessful iter.
19. if $\rho_k > \eta_1 > 0$ then
20.     $x^{k+1} \leftarrow x^k + s^k$; $\Delta_{k+1} \leftarrow \min\{\gamma_i\Delta_k, \Delta_{\text{max}}\}$ // successful iter.
21. else
22.     $x^{k+1} \leftarrow x^k$; $\Delta_{k+1} \leftarrow \gamma_i\Delta_k$ // unsuccessful iter.

Procedure generate $\Delta_k, \Delta_{\text{sk}}, \kappa_H \text{ and } \kappa_H$

P.1: Approximately solve (9) to obtain $s^k$ satisfying (10)
P.2: Evaluate $F(x^k + s^k)$
P.3: Find $z \in \text{co} (\{F(x^k), F(x^k + s^k)\})$ and $j$ satisfying (11)
P.4: if $j \in \mathcal{A}(Z^k)$, $\bar{x}^k \in Z^k$ satisfying (13) then
P.5: Set $s^k$ following Lemma 4.4
P.6: Evaluate $F(x^k + s^k)$; find $z \in \text{co} (\{F(x^k), F(x^k + s^k)\})$ and $j$ satisfying (11)
P.7: return $s^k, j,$ and $z$

3.6 Algorithm statement

Having introduced the various algorithmic components, we can now state the algorithm along with restrictions on algorithmic parameters in Algorithm 1.

We draw special attention to the following aspects of Algorithm 1 concerning subproblems.

Line 8: The problem (6) can be solved exactly in finite time, for example, by using the specialized active-set algorithm of [35]. Note that the direction $d^k$ produced in this line is used in (10) and (13b).

Line P.1: The existence of such an $s^k$ is guaranteed by Lemma 4.4. The proof of Lemma 4.4 also provides an explicit construction for such an $s^k$. Thus, even if a standard trust-region method applied to (9) fails to return a trial step $s^k$ satisfying (10), we can appeal to the construction in Lemma 4.4.

Line P.3: We again stress that the existence of such a $z$ is guaranteed by Lemma 4.2. Moreover, in Lemma 4.3, we will demonstrate that such a $z$ can be found in finite time without performing additional evaluations of $F$. If multiple $j \in \mathcal{A}(z)$ are identified for the given $z$, then we arbitrarily select an element in $\arg\max_{j \in \mathcal{A}(z)} \{\nabla h_j(z)^T (F(x^k + s^k) - F(x^k)) : j$ and $z$ satisfy (11) $\}$.

We additionally draw attention to other important aspects of Algorithm 1.

Line 1: We note that $\kappa_H$ is an algorithmic parameter that bounds the norms of the Hessians of the models $m^F$. For analysis, we assume that $\eta_{\text{max}} \in \mathbb{R} \cup \{\infty\}$, the upper bound on $\eta_2$, satisfies

$$\eta_{\text{max}} \triangleq \min \left\{ \frac{1}{1 - \kappa_H}, \frac{\eta_2}{\kappa_H} \right\}.$$ (15)
(Again, for ease, define either \( \frac{1}{p_h \kappa_H} \) or \( \frac{p_H}{p_h} \) to be infinite in the pathological case when \( L_h \kappa_H = 0 \) or \( C = 0 \).) If \( L_h \kappa_H \) is large, then (15) may allow iterations to be deemed acceptable only when \( \Delta_k \) is relatively small. Furthermore, as (15) contains constants that are generally unknown, Section 6.1 discusses safeguards that can be included in a numerical implementation of Algorithm 1 if \( \eta_2 > \eta_{\text{max}} \).

**Line 6:** Algorithm 1 will break out of the manifold sampling loop after at most \( |\delta| - |\mathcal{A}(F(x^k))| \) times through. The reason is that \( \{ j : h_j \in \mathcal{H} \} \supseteq \mathcal{A}(\mathbb{Z}^k) \supseteq \mathcal{A}(F(x^k)) \) and each time Line 16 is visited, the cardinality of \( \mathcal{A}(\mathbb{Z}^k) \) will be increased by at least one. In the worst case, the indices of all selection functions in \( \mathcal{H} \) must be added to \( \mathbb{Z}^k \) before \( \rho_k \) can be calculated.

**Line 15:** Depending on the means of model building being employed, one may want to incorporate the function values \( F(x^k + s^k) \) computed in this inner iteration into the models \( m^F_k \). So long as the updated models \( m^F_k \) satisfy Assumption 3, as stated in this line of the algorithm, this will not affect convergence.

**Line 20:** By (31), (32), and the updating of \( \Delta_{k+1} \) on successful iterations, all points evaluated by Algorithm 1 are in the set \( \mathcal{L}_{\text{max}} \) as defined in (4).²

**Acceptable iterations:** Because any acceptable iteration satisfies Line 10, acceptable iterations occur when \( \Delta_k < \eta_2 \| \nabla m^F_k(x^k) \| = \eta_2 \| g^k \| \). That is, acceptable iterations occur when the norm of the master model gradient is sufficiently large relative to \( \Delta_k \). On acceptable iterations,

\[
\| g^k \| \geq \min \{ L_h \kappa_H \Delta_k , \| g^k \| \} \geq L_h \kappa_H \min \{ \Delta_k , \eta_2 \| g^k \| \} = L_h \kappa_H \Delta_k .
\]  

**Successful iterations:** Successful iterations are acceptable iterations for which \( \rho_k > \eta_1 \) and \( x^{k+1} \leftarrow x^k + s^k \).

Note that on every successful iteration, the gradient of the linearization, \( d^k \), is represented in \( \text{co} (\mathbb{D}^k) \) and the decrease condition in (10) is satisfied by \( s^k \).

4 Preliminary Analysis

We now show preliminary results that will be used in the analysis of Algorithm 1. We first show a result linking elements in \( \text{co} (\mathbb{G}^k) \) to the subdifferentials of \( f \) at nearby points.

**Lemma 4.1.** Let Assumptions 1–3 hold, and let \( x, y \in \mathcal{L}_{\text{max}} \) satisfy \( \| x - y \| \leq \Delta \). For any finite subsets \( I, J \) and \( I' \) such that \( I \subseteq J \subseteq \{1, \ldots, |\delta|\} \) and \( I' \subseteq \mathbb{N} \), define

\[
\mathbb{G} \triangleq \{ \nabla M(x) \nabla h_i(z_{i'}) : i \in I, z_{i'} \in \mathcal{B}(F(x) ; L_F \Delta), i' \in I' \} \quad \text{and} \quad \mathcal{H} \triangleq \text{co} (\{ \nabla F(y) \nabla h_j(F(y)) : j \in J \}).
\]

Then for each \( g \in \text{co} (\mathbb{G}) \), there exists \( v(g) \in \mathcal{H} \) satisfying

\[
\| g - v(g) \| \leq c_2 \Delta ,
\]  

where \( c_2 \) is defined by

\[
c_2 \triangleq L_h (L_{\nabla F} + \kappa_g) + 2 L_F^2 L_{\nabla h},
\]  

for \( L_h, L_{\nabla F} \), and \( \kappa_g \) from Definition 2.3.

**Proof (adapted from [34, Lemma 4.1]).** Any \( g \in \text{co} (\mathbb{G}) \) may be expressed as

\[
g = \sum_{(i,i') \in I \times I'} \lambda_{i,i'} \nabla M(x) \nabla h_i(z_{i'}),
\]  

where \( z_{i'} \in \mathcal{B}(F(x) ; L_F \Delta) \) and \( \lambda_{i,i'} \geq 0 \) for each \( (i,i') \in I \times I' \).

By supposition, \( \nabla F(y) \nabla h_i(F(y)) \in \mathcal{H} \) for all \( i \in I \). For \( v(g) \triangleq \sum_{(i,i') \in I \times I'} \lambda_{i,i'} \nabla F(y) \nabla h_i(F(y)) \), using the same \( \lambda_{i,i'} \) as in (19) for \( (i,i') \in I \times I' \), convexity of \( \mathcal{H} \)

²This claim assumes that any additional points evaluated during model construction in Line 4 are also in \( \mathcal{L}_{\text{max}} \). Allowing for points outside of \( \mathcal{L}_{\text{max}} \) is straightforward, provided the functions are defined wherever they are evaluated.
Algorithm 2: Grid Search for $z$ and $j$

1. if $F(x)$ and some $j$ satisfy (11) then return $F(x)$ and $j$
2. if $F(x + s)$ and some $j$ satisfy (11) then return $F(x + s)$ and $j$
3. for $l = 1, 2, \ldots$ do
   4. Generate $2^{l-1}$ candidates $\{ \frac{2k+1}{2^l}; k = 1, \ldots, 2^{l-1} \}$
   5. for $k = 1, 2, \ldots, 2^{l-1}$ do
      6. $\alpha \leftarrow \frac{2k+1}{2^l}$ and set $z(\alpha)$ as in (20)
    7. if $z(\alpha)$ and some $j$ satisfy (11) then return $z(\alpha)$ and $j$

implies that $v(g) \in \mathcal{H}$. Since $y \in B(x; \Delta)$ and using Assumption 1.B, Assumption 1.C, Assumption 2.C, Assumption 2.D, and Assumption 3, we have

$$\| \nabla M(x) \nabla h_i(z_{i'}) - \nabla F(y) \nabla h_i(F(y)) \| \leq (L_h L_{\nabla F} + 2L_F^2 L_{\nabla h_i} + \kappa_h L_h) \Delta$$

for each $(i, i')$. The definition of $v(g)$ and (19) then imply

$$\| y - v(g) \| \leq \sum_{(i, i') \in I \times I'} | \lambda_{i, i'} \nabla M(x) \nabla h_i(F(x)) - \lambda_{i, i'} \nabla F(y) \nabla h_i(F(y)) | \leq c_2 \Delta.$$

For simplicity, in the rest of the paper we drop the superscripts of $x^k$ and $s^k$ when possible. The next lemma guarantees that the condition in Line P.3 of Algorithm 1 can always be attained.

**Lemma 4.2.** If Assumption 2 holds, then there exist $z \in \text{co}(\{F(x), F(x + s)\})$ and index $j$ satisfying (11).

**Proof.** We first define

$$z(\alpha) \equiv \alpha F(x) + (1 - \alpha) F(x + s)$$

and will show there exists an $\alpha \in [0, 1]$ such that $z(\alpha)$ and $j \in \mathcal{A}(z(\alpha))$ satisfy (11).

We prove by contradiction. Suppose there exists no such $\alpha$. When Assumption 2.A and Assumption 2.B hold, by Lemma A.1,

$$h(F(x)) - h(F(x + s)) \geq \int_0^1 \inf_{j \in \mathcal{A}(z(\alpha))} \{ \nabla h_j(z(\alpha))^\top (F(x) - F(x + s)) \} d\alpha$$

$$> \int_0^1 (h(F(x)) - h(F(x + s))) d\alpha = h(F(x)) - h(F(x + s)),$$

which is a contradiction. Therefore, the result is shown.

Having demonstrated an existence result in Lemma 4.2, we now show that Algorithm 2 produces a point $z$ and index $j$ satisfying (11) in finite time. In numerical experiments, we use the bisection search of Algorithm 3 (in Appendix A) instead of Algorithm 2. While we cannot show that Algorithm 3 terminates in finite time, in practice it is faster, and we have yet to encounter issues with termination.\(^3\)

**Lemma 4.3.** If Assumption 2 holds, then Algorithm 2 returns a point $z$ and index $j$ satisfying (11) in finitely many iterations.

\(^3\)One can construct more efficient approaches for identifying $z$ and $j$ when $h$ takes specific forms, but we present Algorithm 2 and Algorithm 3 because of their general applicability to functions satisfying Assumption 2.
Proof. If $F(x) = F(x + s)$, then the proof is trivial. Therefore, consider $F(x) \neq F(x + s)$. Let Assumption 2.A and Assumption 2.B hold. Suppose that for all $j \in \mathcal{A}(F(x))$,
\[
\nabla h_j(F(x))^T(F(x) - F(x + s)) > h(F(x)) - h(F(x + s)),
\]
(21)
or else it is clear that Algorithm 2 terminates at the very first line.
Recall the definition of $z(\alpha)$ in (20). By Definition 2.1, there exist index $j_1$ and $\alpha_{j_1} < 1$ such that $j_1 \in \mathcal{A}(F(x))$ and also $j_1 \in \mathcal{A}(z(\alpha))$ for all $\alpha \in [0, \alpha_{j_1}]$. Because $h_{j_1}$ is continuously differentiable, $\nabla h_{j_1}(z(\alpha))^T(F(x) - F(x + s))$ is a continuous function of $\alpha$ for $\alpha \in [0, 1]$. Combined with (21), there must exist $\tilde{\alpha}_{j_1} \in (0, \alpha_{j_1}]$ such that $\nabla h_{j_1}(z(\alpha))^T(F(x) - F(x + s)) > h(F(x)) - h(F(x + s))$ for all $\alpha \in [0, \tilde{\alpha}_{j_1}]$.

We now show by contradiction that there must exist some $\alpha \in [\tilde{\alpha}_{j_1}, 1)$ such that for some $j \in \mathcal{A}(z(\alpha))$, $\nabla h_j(z(\alpha))^T(F(x) - F(x + s)) < h(F(x)) - h(F(x + s))$. Suppose such an $\alpha$ does not exist. By Lemma A.1,
\[
h(F(x)) - h(F(x + s)) \geq \int_0^1 \inf_{j \in \mathcal{A}(z(\alpha))} \{\nabla h_j(z(\alpha))^T(F(x) - F(x + s))\} d\alpha = \int_0^{\tilde{\alpha}_{j_1}} \inf_{j \in \mathcal{A}(z(\alpha))} \{\nabla h_j(z(\alpha))^T(F(x) - F(x + s))\} d\alpha + \int_{\tilde{\alpha}_{j_1}}^1 \inf_{j \in \mathcal{A}(z(\alpha))} \{\nabla h_j(z(\alpha))^T(F(x) - F(x + s))\} d\alpha > \int_0^1 (h(F(x)) - h(F(x + s))) d\alpha = h(F(x)) - h(F(x + s)),
\]
which is a contradiction. Thus, there exist $\alpha^* \in [\tilde{\alpha}_{j_1}, 1)$ and $j^* \in \mathcal{A}(z(\alpha^*))$ satisfying $\nabla h_{j^*}(z(\alpha^*))^T(F(x) - F(x + s)) < h(F(x)) - h(F(x + s))$. Using the same arguments as previously, we have from Definition 2.1 that there exists $\epsilon_{\alpha^*} > 0$ such that at least one of $j^* \in \mathcal{A}(z(\alpha))$ for all $\alpha \in (\alpha^* - \epsilon_{\alpha^*}, \alpha^*)$ or $j^* \in \mathcal{A}(z(\alpha))$ for all $\alpha \in (\alpha^*, \alpha^* + \epsilon_{\alpha^*})$ holds. Without loss of generality, suppose $j^* \in \mathcal{A}(z(\alpha))$ for all $\alpha \in (\alpha^* - \epsilon_{\alpha^*}, \alpha^*)$. By the continuity and smoothness of $h_{j^*}$ (Assumption 2.D), there exists $\kappa_{\alpha^*} \leq \kappa_{\alpha_{j_1}}$ such that for all $\alpha \in (\alpha^* - \epsilon_{\alpha^*}, \alpha^*)$, we have $\nabla h_{j^*}(z(\alpha))^T(F(x) - F(x + s)) < h(F(x)) - h(F(x + s))$.
Algorithm 2 will evaluate a point within the interval $(\alpha^* - \epsilon_{\alpha^*}, \alpha^*)$ within at most $\lceil \log \frac{1}{\epsilon_{\alpha^*}} \rceil$ iterations. Hence, Algorithm 2 must terminate in finite time.

We now demonstrate that Line P.1 in Algorithm 1 is always satisfiable, even if the trust-region subproblem solver does not identify such a solution. We note that Line P.1 is not reached if $0 \in \text{co} \left(\mathbb{G}^k\right)$ by virtue of the acceptability criterion.

**Lemma 4.4.** Let $d^k = D^k \lambda^*$ be obtained from Line 8 of Algorithm 1, and therefore $g^k = \nabla M(x^k)d^k$. If Assumption 2.C and Assumption 3 are satisfied and (15) holds, then $s \triangleq -\Delta_k \frac{g^k}{\|g^k\|}$ satisfies (10) (in place of $s^k$).

**Proof.** From Assumption 2.C, Definition 2.3, Definition 3.1, (6), and (7), we know that
\[
\|d^k\| = \|D^k \lambda^*\| \leq \max_{d \in D^k} \|d\| \leq L_h.
\]
(22)
Moreover, from Assumption 3 and Definition 2.3, for any $s \in \mathbb{R}^n$ we have
\[
\|M(x^k) + \nabla M(x^k)^Ts - M(x^k + s)\| \leq \sum_{i=1}^p |m_{Fi}(x^k) + \nabla m_{Fi}(x^k)^Ts - m_{Fi}(x^k + s)| \leq \sum_{i=1}^p \frac{1}{2} \kappa_{i,m,H} \|s\|^2 = \frac{1}{2} \kappa_H \|s\|^2,
\]
(23)
where the last inequality comes from Taylor’s theorem. Combining (22), (23), and the definition of $s$, we have
\[
(d^k)^T(M(x^k) + \nabla M(x^k)^Ts - M(x^k + s)) \\
\geq -\|d^k\||M(x^k) + \nabla M(x^k)^Ts - M(x^k + s)|| \geq -\frac{1}{2} L_h \kappa_H \|s\|^2 = -\frac{1}{2} L_h \kappa_H \Delta_k^2.
\]
Using (15), we get (10) by
\[
\langle M(x^k) - M(x^k + \delta), d^k \rangle \geq - (d^k)^T \nabla M(x^k)^T \delta - \frac{1}{2} L_h \kappa H \Delta_k^2
\]
\[
= - (g^k)^T \delta - \frac{1}{2} L_h \kappa H \Delta_k^2 = \|g^k\| \Delta_k - \frac{1}{2} L_h \kappa H \Delta_k^2
\]
\[
\geq \|g^k\| \Delta_k - \frac{1}{2} \|g^k\| \Delta_k = \frac{1}{2} \|g^k\| \Delta_k \geq \frac{\|g^k\|}{L_h \kappa H} \min \left\{ \Delta_k, \frac{\|g^k\|}{L_h \kappa H} \right\}.
\]

\[\Box\]

Lemma 4.5 is a technical result concerning decrease in the objective function that we will employ in Section 5.

**Lemma 4.5.** Let Assumptions 1–4 hold. If iteration \( k \) of Algorithm 1 is acceptable, then
\[
h(F(x^k)) - h(F(x^k + s^k)) \geq (d^k)^T (F(x^k) - F(x^k + s^k)) - C \Delta_k^2
\]
for \( C \) as in Definition 2.3.

**Proof.** Because iteration \( k \) is acceptable, there is some point \( z \in \text{co} \{F(x^t), F(x^k + s^k)\} \) and \( j \in \mathcal{A}(\mathbb{Z}^k) \) such that (11b) holds. Furthermore, either some \( z' \in \mathbb{Z}^k \subset \mathbb{R}^p \) with \( j \in \mathcal{A}(z') \) that satisfies (13b), or \( s^k \) is generated following Lemma 4.4 with \( \nabla M(x^k) \nabla h_j(z') \in \text{co} \left\{ \mathbb{G}^k \right\} \). We show that in either case
\[
(\nabla h_j(z') - d^k)^T \nabla M(x^k)^T s^k \leq 0.
\]

When (13b) is satisfied by \( z' \in \mathbb{Z}^k \) and \( j \in \mathcal{A}(z') \), (25) follows immediately from (13b). When \( s^k \) is generated from Lemma 4.4 with \( \nabla M(x^k) \nabla h_j(z') \in \text{co} \mathbb{G}^k \), then \( s^k = -\Delta_k \frac{g^k}{\|g^k\|} \). By the classical projection theorem (see, e.g., [52, Theorem 2.39]),
\[
(\nabla h_j(z') - d^k)^T \nabla M(x^k)^T s^k = -(\nabla h_j(z') - d^k)^T \nabla M(x^k)^T \Delta_k \frac{g^k}{\|g^k\|} \leq 0,
\]
which is exactly (25).

From Assumption 1.C, \( |F_i(x^k + s^k) - F_i(x^k) - \nabla F_i(x^k)^T s^k| \leq \frac{L_{\nabla F_i}}{2} \|s^k\|^2 \) for \( i = 1, \ldots, p \). By the definition of \( L_{\nabla F} \) in Definition 2.3,
\[
\|F(x^k + s^k) - F(x^k) - \nabla F(x^k)^T s^k\| \leq \frac{L_{\nabla F}}{2} \|s^k\|^2.
\]

Therefore, by the Cauchy–Schwarz inequality,
\[
(\nabla h_j(z) - d^k)^T (F(x^k + s^k) - F(x^k))^T s^k \leq \|\nabla h_j(z) - d^k\| \|F(x^k + s^k) - F(x^k)\| \leq (2L_h) \frac{L_{\nabla F}}{2} \|s^k\|^2.
\]

Thus,
\[
h(F(x^k + s^k)) - h(F(x^k)) - (d^k)^T (F(x^k + s^k) - F(x^k))
\]
\[
\leq (\nabla h_j(z) - d^k)^T (F(x^k + s^k) - F(x^k))
\]
\[
\leq (\nabla h_j(z) - d^k)^T \nabla F(x^k)^T s^k + L_h L_{\nabla F} \|s^k\|^2
\]
\[
= (\nabla h_j(z') - d^k)^T \nabla M(x^k)^T s^k + (\nabla h_j(z) - \nabla h_j(z'))^T \nabla F(x^k)^T s^k + L_h L_{\nabla F} \|s^k\|^2
\]
\[
\leq (\nabla h_j(z') - d^k)^T (\nabla M(x^k)^T s^k + (\nabla h_j(z) - \nabla h_j(z'))^T s^k) + 2L_{\nabla h} L_{\nabla M} \Delta_k^2 + L_h L_{\nabla F} \Delta_k^2
\]
\[
= (\nabla h_j(z') - d^k)^T (\nabla M(x^k)^T s^k + (\nabla h_j(z) - d^k)^T (\nabla F(x^k) - \nabla M(x^k))^T s^k)
\]
\[
\leq 0 + 2L_{\nabla h} L_{\nabla M} \Delta_k^2 + 2L_{\nabla h} L_{\nabla M} \Delta_k^2 + L_h L_{\nabla F} \Delta_k^2 = C \Delta_k^2,
\]
where the first inequality comes from (11b); the second inequality comes from (27); the third inequality comes from Assumption 1.B, Assumption 2.D, and Assumption 4; and the last inequality comes from Assumption 2.C, Assumption 3, and (25).

Between Lemma 4.4 and Lemma 4.5, we have established that every acceptable iterate in Algorithm 1 satisfies (10) and (24) simultaneously.

5 Analysis of Manifold Sampling

We now show that cluster points of the sequence of iterates generated by Algorithm 1 are Clarke stationary. The proof uses the following sequence of results.

Lemma 5.1 shows that when the trust-region radius $\Delta_k$ is a sufficiently small multiple of $\|g^k\|$, the norm of the master model gradient, the iteration will be successful.

Lemma 5.2 shows that $\lim_{k \to \infty} \Delta_k = 0$.

Lemma 5.3 shows that as $k \to \infty$, a subsequence of master model gradients $g^k$ must go to zero as well.

Lemma 5.4 shows that zero is in the generalized Clarke subdifferential $\partial_C f(x^*)$ of any cluster point $x^*$ of any subsequence of iterates where the master model gradients go to zero.

Theorem 5.1 shows that $0 \in \partial_C f(x^*)$ for any cluster point $x^*$ of the sequence of iterates generated by Algorithm 1.

We remark that the proofs of Lemma 5.3, Lemma 5.4, and Theorem 5.1 are similar to analogous results in [34, 39], but we have included them for completeness.

We first demonstrate that a successful iteration occurs whenever the trust-region radius is smaller than a constant multiple of the norm of the master model gradient.

**Lemma 5.1.** Let Assumptions 2 and 3 hold. If an iteration is acceptable and

$$\Delta_k < \frac{\kappa_d(1 - \eta)}{4\kappa_i L_H} \|g^k\|$$

(where the pathological case of $\kappa_i = 0$ or $L_H = 0$ results in an infinite right-hand side), then $\rho_k > \eta_i$ in Algorithm 1, and the iteration is successful.

**Proof.** Because the iteration is acceptable, $g^k \neq 0$, and so the right-hand side of (28) is positive. Using the definition of $\rho_k$ in (14), we have

$$1 - \rho_k \leq |\rho_k - 1|$$

$$= \frac{|(F(x^k) - F(x^k + s^k)) \cdot d^k|}{(M(x^k) - M(x^k + s^k), d^k)} - 1$$

$$= \frac{|(F(x^k) - F(x^k + s^k)) \cdot d^k|}{(M(x^k) - M(x^k + s^k), d^k)} - 1$$

$$= \frac{|(F(x^k) - F(x^k + s^k)) \cdot d^k|}{(M(x^k) - M(x^k + s^k), d^k)}$$

$$\leq \frac{\|F(x^k) - M(x^k)\| \|d^k\| + \|F(x^k + s^k) - M(x^k + s^k)\| \|d^k\|}{(M(x^k) - M(x^k + s^k), d^k)}$$

$$\leq \frac{2\kappa_i L_H \Delta_k^2}{(M(x^k) - M(x^k + s^k), d^k)}$$

$$\leq \frac{4\kappa_i L_H \Delta_k^2}{\kappa_d \|g^k\| \min \left\{ \Delta_k, \frac{\|g^k\|}{\kappa_d L_H} \right\}}$$

(by (10))

$$= \frac{4\kappa_i L_H \Delta_k^2}{\kappa_d \|g^k\|}$$

(by (16)),

14
where the second inequality holds by Assumption 3, Assumption 2.C, and the fact that \( \|s^k\| \leq \Delta_k \) and \( \|d^k\| \leq L_h \). Applying (28) to (29) yields

\[
1 - \rho_k \leq \frac{4\eta_1 L_h \Delta_k}{\kappa_4 \|g^k\|} < 1 - \eta_1.
\]

Thus, \( \rho_k > \eta_1 \) if \( \Delta_k \) satisfies (28), and the iteration is successful.

We now show that the sequence of trust-region radii converges to zero.

**Lemma 5.2.** Let Assumptions 1–4 hold. If \( \{x^k, \Delta_k\}_{k \in \mathbb{N}} \) is generated by Algorithm 1, then the sequence \( \{f(x^k)\}_{k \in \mathbb{N}} \) is nonincreasing, and \( \lim_{k \to \infty} \Delta_k = 0 \).

**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 \( k \), by Assumptions 1–3, we know that

\[
f(x^k) - f(x^{k+1}) \geq (d^k)^T(F(x^k) - F(x^{k+1})) - C\Delta_k^2 \quad \text{[by (24)]}
\]

\[
= \rho_k(d^k)^T(M(x^k) - M(x^{k+1})) - C\Delta_k^2 \quad \text{[by (14)]}
\]

\[
\geq \rho_k \frac{4\eta_2}{\kappa_4 \max\{L_h, \gamma_d\}} \|g^k\| \min\{\Delta_k, \frac{\|g^k\|}{\kappa_4 \gamma_d}\} - C\Delta_k^2 \quad \text{[by (10)]}
\]

\[
= \rho_k \frac{4\eta_2}{\kappa_4 \gamma_d} \|g^k\| \Delta_k - C\Delta_k^2 > \eta_1 \frac{4\eta_2}{\kappa_4 \gamma_d} \|g^k\| \Delta_k - C\Delta_k^2 \quad \text{[by (15)].}
\]

Based on (30), if \( C > 0 \), we have

\[
f(x^k) - f(x^{k+1}) > \eta_1 \frac{4\eta_2}{\kappa_4 \gamma_d} \|g^k\| \Delta_k - C\Delta_k^2 \quad \text{[by (30)]}
\]

\[
> \eta_1 \frac{4\eta_2}{\kappa_4 \gamma_d} \frac{C\Delta_k^2}{\kappa_4 \gamma_d} = C\Delta_k > 0 \quad \text{[by (15)].}
\]

On the other hand, if \( C = 0 \), by (30) we have

\[
f(x^k) - f(x^{k+1}) > \eta_1 \frac{4\eta_2}{\kappa_4 \gamma_d} \|g^k\| \Delta_k > \frac{4\eta_1 \gamma_d}{2\gamma_d^2} \Delta_k^2 > 0.
\]

Thus, the sequence \( \{f(x^k)\}_{k \in \mathbb{N}} \) is nonincreasing.

To show that \( \Delta_k \to 0 \), we separately consider the cases when there are infinitely or finitely many successful iterations. 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 1.A, Assumption 1.B, and Assumption 2.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 there exists a positive constant \( \overline{C} > 0 \) such that

\[
\infty > f(x^0) - f^* \geq \sum_{j=0}^{\infty} f(x^{k_j}) - f(x^{k_j+1}) > \sum_{j=0}^{\infty} \overline{C} \Delta_{k_j}^2
\]

by (31) and (32). It follows that \( \Delta_{k_j} \to 0 \) for the sequence of successful iterations. Observe that \( \Delta_{k_j+1} \leq \gamma_1 \Delta_{k_j} \) and that \( \Delta_{k+1} = \gamma_1 \Delta_{k} < \Delta_k \) if iteration \( k \) is unsuccessful. Thus, for any unsuccessful iteration \( k > k_j \), \( \Delta_k \leq \gamma_1 \Delta_{k_j} \), where \( q \triangleq \max\{k_j: j \in \mathbb{N}, k_j < k\} \). It follows immediately that \( 0 \leq \lim_{k \to \infty} \Delta_k \leq \gamma_1 \lim_{j \to \infty} \Delta_{k_j} = 0 \), and so \( \Delta_k \to 0 \) in this case.

Next, suppose there are only finitely many successful iterations and let \( \nu \in \mathbb{N} \) be the number of successful iterations. Since \( \gamma_1 < 1 \), it follows that \( 0 \leq \Delta_k \leq \gamma_1^{\nu-k} \Delta_0 \) for each \( k \in \mathbb{N} \). Thus, \( \Delta_k \to 0 \).

We now show that the norms of the master model gradients are not bounded away from zero.

**Lemma 5.3.** Let Assumptions 1–4 hold. If the sequence \( \{x^k, \Delta_k\}_{k \in \mathbb{N}} \) is generated by Algorithm 1, then \( \lim_{k \to \infty} \|g^k\| = 0 \).
Proof. To obtain a contradiction, suppose there is an iteration \( j \) and some \( \epsilon > 0 \) for which \( \|g^k\| > \epsilon \) for all \( k \geq j \). Algorithm 1 guarantees that \( \Delta_j \geq \gamma \Delta_0 > 0 \). With Assumptions 2 and 3, any iteration where \( \Delta_k < V\|g^k\| \) for \( V \triangleq \min \left\{ \eta_2, \frac{\kappa - 1}{\kappa \ell \gamma} \right\} \) will be successful because the conditions of Lemma 5.1 are then satisfied. Therefore, by the contraction hypothesis, any \( k \geq j \) satisfying \( \Delta_k < V\epsilon \) is guaranteed to be successful, in which case \( \Delta_{k+1} = \gamma \Delta_k > \Delta_k \). On the other hand, if \( \Delta_k \geq V\epsilon \), then \( \Delta_{k+1} \geq \gamma \Delta_k \). Under Assumptions 1–3, a straightforward inductive argument then yields \( \Delta_k \geq \min(\gamma_0 V\epsilon, \Delta_j) > 0 \) for all \( k \geq j \), contradicting Lemma 5.2. Thus, no such \((j, \epsilon)\) pair exists, and so \( \liminf_{k \to \infty} \|g^k\| = 0 \).

The next lemma shows that subsequences of iterates with master model gradients converging to 0 have cluster points that are Clarke stationary. Algorithm 1 generates at least one such subsequence of iterates by Lemma 5.3.

Lemma 5.4. Let Assumptions 1–4 hold, and let \( \{x^k, \Delta_k, g^k\}_{k \in \mathbb{N}} \) be a sequence generated by Algorithm 1. For any subsequence \( \{k_j\}_{j \in \mathbb{N}} \) of acceptable iterations such that both

\[
\lim_{j \to \infty} \|g^{k_j}\| = 0
\]

and \( \{x^{k_j}\}_{j \in \mathbb{N}} \to x^* \) for some cluster point \( x^* \), then \( 0 \in \partial C f(x^*) \).

Proof. By continuity of \( F_i \) (Assumption 1.B), there exists \( \tilde{\Delta} > 0 \) so that for all \( \Delta \in [0, \tilde{\Delta}] \), the manifolds active in \( B(x^*; \Delta) \) are precisely the manifolds active at \( x^* \); that is,

\[
\kappa_i(F(x^*)) = \bigcup_{y \in B(F(x^*); L_F \Delta)} \kappa_i(y) \quad \text{for all } \Delta \leq \tilde{\Delta}.
\]

(34)

Thus, because \( \Delta_k \to 0 \) by Lemma 5.2 and because \( \{k_j\}_{j \in \mathbb{N}} \) converges to \( x^* \) by supposition, we may conclude that for \( j \) sufficiently large, \( \kappa_i(Z^{k_j}) \subseteq \kappa_i(F(x^*)) \). By Lemma 4.1, with \( I \leftarrow \kappa_i(Z^{k_j}), J \leftarrow \kappa_i(F(x^*)), x \leftarrow x^{k_j}, y \leftarrow x^* \), and \( \Delta \leftarrow \max \{\Delta_{k_j}, \|x^{k_j} - x^*\|\} \), there exists \( v \in \partial C f(x^*) \) for each \( g^{k_j} \) so that

\[
\|g^{k_j} - v(g^{k_j})\| \leq c_2 \max \{\Delta_{k_j}, \|x^{k_j} - x^*\|\}
\]

with \( c_2 \) defined by (18). By the acceptability of each iteration indexed by \( k_j \), \( \|g^{k_j} - v(g^{k_j})\| \leq c_2 \max \{\eta_2\|g^{k_j}\|, \|x^{k_j} - x^*\|\} \) holds, and so \( \|v(g^{k_j})\| \leq \max \{1 + c_2\eta_2\|g^{k_j}\|, \|g^{k_j}\| + c_2 \|x^{k_j} - x^*\|\} \). Moreover, since \( \|g^{k_j}\| \to 0 \) and \( \|x^{k_j} - x^*\| \to 0 \) by assumption, \( \|v(g^{k_j})\| \to 0 \). Proposition 7.1.4 in [20] then yields the claimed result by establishing that \( \partial C f \) is outer semicontinuous and therefore \( 0 \in \partial C f(x^*) \).

Theorem 5.1. Let Assumptions 1–4 hold. If \( x^* \) is a Clarke stationary point of a sequence \( \{x^k\} \) generated by Algorithm 1, then \( 0 \in \partial C f(x^*) \).

Proof. First, suppose that there are only finitely many successful iterations, with \( k' \) being the last. Suppose toward a contradiction that \( 0 \notin \partial C f(x^k) \). By the same reasoning used to conclude (34), there exists \( \tilde{\Delta} > 0 \) such that \( \kappa_i(F(x^k)) = \bigcup_{y \in B(F(x^k); L_F \Delta)} \kappa_i(y) \) for all \( \Delta \leq \tilde{\Delta} \).

By assumption, \( \Delta_k \) decreases by a factor of \( \gamma_0 \) in each iteration after \( k' \) since every iteration after \( k' \) is unsuccessful. Thus there is a least iteration \( k'' \geq k' \) such that \( \Delta_{k''} \leq \Delta \). By Assumption 4, for each \( k \geq k'' \), \( \kappa_i(Z^k) = \kappa_i(F(x^k)) \), and therefore \( (\nabla M(x^k)\nabla h_j(F(x^k))) \in G^k \) for all \( j \in \kappa_i(F(x^k)) \). Since \( k' \) is the last successful iteration, \( x^k = x^k \) for all \( k \geq k'' \geq k' \). Consequently, under Assumptions 1–3, the conditions for Lemma 4.1 hold for \( x \leftarrow x^k, y \leftarrow x^{k'} \) (noting that \( x^k = x^{k'} \)), \( \Delta \leftarrow 0, I \leftarrow \kappa_i(Z^k), \) and \( J \leftarrow \kappa_i(F(x^k)) \).

Thus, for each \( k \geq k'' \), \( g^k \in \partial C f(x^{k'}) \).

Since \( 0 \notin \partial C f(x^{k'}) \) by supposition, \( v^* \triangleq \text{proj}(0, \partial C f(x^{k'})) \) is nonzero, and so

\[
\|g^k\| \geq \|v^*\| > 0 \quad \text{for all } k \geq k''.
\]

(35)

Since \( \Delta_k \to 0, \Delta_k \) will satisfy the conditions of Lemma 5.1 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 \( x^{k_j} \to x^* \) and \( \|g^{k_j}\| \to 0 \). If the sequence \( \{x^k\}_{k \in \mathbb{N}} \) converges, then the subsequence \( \{x^{k_j}\}_{j \in \mathbb{N}} \) from Lemma 5.3 satisfies these two conditions. Otherwise, if the sequence \( \{x^k\} \) is not convergent, we will show that \( \lim\inf_{k \to \infty} (\max\{\|x^k - x^*\|, \|g^k\|\}) = 0 \) for each cluster point \( x^* \). Suppose toward contradiction that there exists \( \bar{\nu} > 0 \), an iteration \( k \), and a cluster point \( x^* \) of the sequence \( \{x^k\} \) such that \( \{x^k\}_{k \in \mathcal{K}} \) converges to \( x^* \) and such that \( \|g^k\| > \bar{\nu} \) for all \( k \in \mathcal{K} \), where \( \mathcal{K} \triangleq \{k: k \geq \bar{k}, \|x^k - x^*\| \leq \bar{\nu}\} \). As an intermediate step in the combination of (30) and (33), we had shown that \( \sum_{j=0}^{\infty} (\eta_1 \frac{\eta_1}{2} \|g^{k_j}\| \Delta_{k_j} - C \Delta_k^2) < \infty \). Because (33) shows that \( \sum_{j=0}^{\infty} \Delta_{k_j}^2 \) is finite, we may conclude that \( \sum_{j=0}^{\infty} \eta_1 \frac{\eta_1}{2} \|g^{k_j}\| \Delta_{k_j} < \infty \). Thus,

\[
\eta_1 \frac{\eta_1}{2} \sum_{k \in \mathcal{K}} \|g^k\| \|x^{k+1} - x^k\| \leq \eta_1 \frac{\eta_1}{2} \sum_{j=0}^{\infty} \|g^{k_j}\| \|x^{k+1} - x^{k_j}\|
\]

\[
\leq \eta_1 \frac{\eta_1}{2} \sum_{j=0}^{\infty} \|g^{k_j}\| \Delta_{k_j} < \infty.
\]

(36)

Because \( \|g^k\| > \bar{\nu} \) for all \( k \in \mathcal{K} \), we conclude from (36) that

\[
\sum_{k \in \mathcal{K}} \|x^{k+1} - x^k\| < \infty.
\]

(37)

Because \( x^k \not\to x^* \), for any choice of \( \hat{\nu} \in (0, \bar{\nu}) \) the quantity

\[
q(k') \triangleq \min\{\kappa \in \mathbb{N}: \kappa > k', \|x^\kappa - x^{k'}\| > \hat{\nu}\}
\]

is well defined for any \( k' \in \mathcal{K} \). For any \( k' \in \mathcal{K} \), \( \{k', k' + 1, \ldots, q(k') - 1\} \subset \mathcal{K} \).

From (37), there exists \( N \in \mathbb{N} \) such that \( \sum_{k \in \mathcal{K}} \|x^{k+1} - x^k\| \leq \hat{\nu} \). Letting \( k' \geq N \) be arbitrary, we arrive at

\[
\hat{\nu} < \|x^{q(k')} - x^{k'}\| \leq \sum_{i \in \{k', k'+1, \ldots, q(k')-1\}} \|x^{i+1} - x^i\| \leq \sum_{k \in \mathcal{K}} \|x^{k+1} - x^k\| \leq \hat{\nu},
\]

a contradiction. Thus, \( \lim\inf_{k \to \infty} (\max\{\|x^k - x^*\|, \|g^k\|\}) = 0 \) for all cluster points \( x^* \). By Lemma 5.4, \( 0 \in \partial_C f(x^*) \) for all such subsequences.

\section{Numerical Experiments}

We now present the performance of an implementation of Algorithm 1 for problems of the form (1).

\subsection{Implementation details}

To study its practical efficiency, we produced a MATLAB implementation of Algorithm 1, which we denote manifold sampling: general (MSG). We outline the specific choices made in our implementation.

We considered two versions of MSG, MSG-1 and MSG-2, which provide distinct approaches to initializing and updating \( \mathbb{Z}^k \) in Line 5 and Line 16 of Algorithm 1. MSG-1 implements Line 5 as \( \mathbb{Z}^k \leftarrow \{F(x^k)\} \) and Line 16 as \( \mathbb{Z}^k \leftarrow \mathbb{Z}^k \cup \{z\} \), while MSG-2 implements Line 5 as \( \mathbb{Z}^k \leftarrow \{F(x^k)\} \cup (\mathbb{Y} \cap \{F(y) \in B(x^k; \Delta_k)\}) \)
and Line 16 as $\mathbb{Z}^k \leftarrow \mathbb{Z}^k \cup \{z\} \cup \{Y \cap \{F(y) : y \in B(x^k; \Delta_j)\}\}$, where, as in Section 3.1, $Y$ is the set of all $y \in \mathbb{R}^n$ previously evaluated during the current run of Algorithm 1.

The default parameters of MSG are fixed to $\eta_1 = 0.01$, $\eta_2 = 10^4$, $\kappa_d = 10^{-4}$, $\gamma_d = 0.5$, $\gamma_1 = 2$, and $\Delta_{\max} = 10^8$. We remark that the selection of $\eta_2 = 10^4$ may violate the restriction on $\eta_{\max}$ specified in (15). The bound in (15) was derived for the sake of worst-case analysis (see, e.g., (31) and (32)), and we thus expect (15) to be an unnecessarily conservative restriction in the most general case. Therefore, for the sake of labeling iterations acceptable more frequently and thus accepting potentially larger trial steps, we relax the condition in (15). This motivates the addition of a safeguard to MSG; the criterion in Line 12 is augmented to test both that $j \in \mathbb{A}(\mathbb{Z}^k)$ and that $h(F(x^k + s^k)) < h(F(x^k))$.

We also include some termination conditions in our implementation of Algorithm 1. First, the outer for loop (Line 3) is terminated if the number of evaluations of $F$ has exceeded a fixed budget. MSG also employs a termination condition before Line 10 such that if $\|g^k\| \leq g_{tol}$ and $\Delta_k \leq \Delta_{\min}$ for some positive constants $g_{tol}$ and $\Delta_{\min}$, then MSG terminates. We fixed $g_{tol} = \Delta_{\min} = 10^{-13}$ in our experiments.

We use a MATLAB implementation of GQT [46] to compute $s^k$ in our trust-region subproblems (9). We explicitly check whether (10) is satisfied by $s^k$; if it is not, then we employ the step prescribed by Lemma 4.4 to ensure that (10) is satisfied.

For the purposes of model building in Line 4 and model updating in Line 15, we employ the minimum Frobenius norm quadratic interpolation and geometry point selection routines used in the implementation of POUNDERS [57]. As is frequently seen in practical implementations of trust-region methods, MSG additionally modifies the trust-region radius management beginning in Line 19. In particular, while trial steps are still accepted, provided $\rho_k > \eta_1$, the trust-region radius only increases provided $\rho_k > 0.5$.

### 6.2 Test problems

We benchmark our implementation of Algorithm 1 on objectives of the form $f(x) = h(F(x))$, where $F : \mathbb{R}^n \to \mathbb{R}^p$ is derived from the functions in the Moré–Wild benchmarking test set [47], which were originally intended for nonlinear least-squares minimization (that is, $h = \| \cdot \|_2^2$). This initially gives us 53 problems, as specified by combinations of definitions of $F$ and initial points $x^0$. In the test set, the functions $F$ are all differentiable, and all but four are nonconvex. The dimension of $F$ ranges from 2 to 65.

For our experiments, we define $h$ as a piecewise-quadratic function of the form

$$h(z) \triangleq \max_{j \in \{1, \ldots, l\}} \left\{ h_j(z) \triangleq \|z - z_j\|^2_{Q_j} + b_j \right\} \quad (38)$$

defined by $z_j \in \mathbb{R}^p$, $Q_j \in \mathbb{R}^{p \times p}$, and $b_j \in \mathbb{R}^l$ for $2 \leq l \in \mathbb{N}$. We use the notation that, for a given matrix $Q$, $\|y\|_{Q} \triangleq y^\top Q y$. For each of the 53 functions and starting-point pairs $(F, x^0)$, we generated a single random instance of (38) in the following manner. We first set $z^j \triangleq F(y^j)$ for $j \in \{1, \ldots, l\}$, where $y^j$ is drawn uniformly from the ball $\{y : \|y - x^0\|_\infty \leq 20\}$. We then randomly generate a positive-definite matrix $Q_1$ and negative-definite matrices $Q_2, \ldots, Q_l$. The positive-definiteness of $Q_1$ ensures that $h \circ F$ is bounded from below. We set all $b_j$ to be 0 except $b_1$, which we define as $b_1 \triangleq -2 \max_{j \in \{2, \ldots, l\}} \left\{ \|F(y^j) - F(y^1)\|_{Q_1}^2 \right\}$ in order to ensure that $h(F(y^j)) = 0$ for $j \in \{2, \ldots, l\}$. This definition of $b_j$ also guarantees that $h_j(z) = h(z)$ for at least one value of $z$ (in particular, $z = F(y^j)$); intuitively, for each $j$, we are increasing the likelihood that $j \in \mathbb{A}(F(x^k))$ for some $x^k$ evaluated during a given run of an optimization method. With this particular random construction, stationary measures ought to be small only in neighborhoods of kink points or at the global maxima of the negative definite quadratics (the latter of which are not local minima of $h(F(\cdot))$).

For each $(F, x^0)$ pair in the Moré–Wild benchmark set and for each value of $l \in \{2p, 4p, 8p, 16p\}$ we repeat our random generation scheme five times. This procedure produces $53 \times 4 \times 5 = 1060$ benchmarking problems.

Figure 1 shows the contour plot of one of our test problems. We highlight that these problems have multiple potential Clarke stationary points that have varying values of $h \circ F$. For this reason, we must compare the performance of different implementations not only in terms of the best function value obtained but also in terms of a metric designed to approximate a Clarke stationarity measure.
Figure 1: Contour plot (left) and manifold information (right) for one of our test functions. The circle shows the starting point, and the squares show the three points converged to by the five methods used in our numerical experiments.

6.3 Comparing performance

We consider two quantities of interest when comparing methods for solving problems of the form (38): the objective value $f$ and approximate stationary value $\Gamma$. With respect to $f$, we consider a method to have solved a problem $p$ to a level $\tau$ after $t$ function evaluations, provided the corresponding point $x^t$ satisfies

$$f(x^0) - f(x^t) \geq (1 - \tau) (f(x_0) - f^*),$$ (39)

where $x^0$ is a starting point common to all methods and $f^*$ is the best-found function value for all methods being compared. That is, we consider a problem solved with respect to $f$ when it has found more than $(1 - \tau)$ of the most decrease from $x^0$ found by any method being compared.

Determining an approximate stationary value $\Gamma(x^t)$ at a point $x^t$ evaluated by a method requires more care. To do so, we randomly generate $50$ points $S^t \subset B(x^t, 10^{-5}) \subset \mathbb{R}^n$ and then compute

$$G(x^t) \triangleq \{ \nabla F(s) \nabla h_j(F(s)) : j \in A(F(s)), s \in S^t \}. \quad (40)$$

We then define $\Gamma(x^t) \triangleq \text{proj}(0, \text{co}(G(x^t)))$. The gradient values in (40) can be computed (in postprocessing) because $\nabla F$ is computable in closed form for the problems considered and each $h_j$ is a quadratic function by construction. We consider a problem to be solved to a level $\tau$ with respect to $\Gamma(x^t)$ when the minimum-norm element of the convex hull of the sample of gradients $G(x^t)$ is less than $\tau$. That is,

$$\Gamma(x^t) \leq \tau. \quad (41)$$

We use data profiles [47] to compare the performance of methods for nonsmooth optimization using the problems and metrics defined above. To construct data profiles, we determine how many evaluations of $F$ are required by each method to solve a given problem to a level $\tau$ for either criterion (39) or criterion (41). Once a method satisfies the given criterion on any problem for the first time after $t$ evaluations of $F$, its data profile line is incremented by $\frac{1}{10^6}$ at the point $\frac{t}{(n_p + 1)}$ (where $n_p$ is the dimension of the problem) on the horizontal axis. The data profile therefore shows the cumulative fraction of problems solved by each method as a function of the number of evaluations of $F$ (scaled by $n_p + 1$).

6.4 Utilizing nearly active manifolds

In preliminary experiments, we identified the following practical modification that may be made to an implementation of Algorithm 1: it can be useful to slightly alter the definition of $A(z)$. For example, given
h of the form (38), consider a \( z \) such that \( h(z) = h_1(z) \) but \( |h_2(z) - h_1(z)| \approx 0 \). Although this is generally insufficient evidence to conclude the existence of \( z' \) in a neighborhood of \( z \) such that \( h(z') = h_2(z') \), it could potentially be beneficial for an implementation of Algorithm 1 to allow \( \mathcal{A}(z) = \{1, 2\} \) instead of \( \mathcal{A}(z) = \{1\} \). In the event that a \( z' \) does exist realizing \( \mathcal{A}(z') = \{2\} \), having \( \mathcal{G}_k \) include this phantom information may permit a manifold sampling loop to terminate earlier than it would have otherwise.

Altering the definition of \( \mathcal{A}(z) \) will not affect the theoretical convergence of our algorithm, provided \( \mathcal{A}(F(x^k)) \subseteq \mathcal{A}(F(x^*)) \) as \( \Delta_k \to 0 \). To demonstrate the effects of changing the definition of \( \mathcal{A}(z) \) by including nearly active manifolds in the definition of activity for problems of the form (38), we introduce a parameter \( \sigma \) and consider instead

\[
\mathcal{A}_{\sigma, \Delta_k}(z) \triangleq \{ j : |h(z) - h_j(z)| \leq \min\{\sigma, \Delta\} \}.
\]

We show in Figure 2 data profiles of both MSG-1 and MSG-2, replacing the definition of \( \mathcal{A}(z) \) with \( \mathcal{A}_{\sigma, \Delta_k}(z) \) for values \( \sigma \in \{0, 10^{-4}, 10^{-8}\} \). Notice that \( \mathcal{A}_{0, \Delta_k}(z) = \mathcal{A}(z) \) as defined in Definition 2.1.

While investigating the relatively worse behavior of MSG-1, we found that (perhaps unsurprisingly) many iterations are spent rediscovering manifolds that had been identified on previous iterations. On the other hand, MSG-2, with its memory of recent manifolds encoded in \( Y \), begins iterations with more of the manifold information it needs to find descent.

We observe a marked improvement in increasing \( \sigma \) from 0 to \( 10^{-8} \). When \( \sigma = 0 \), a sample point may be close to—but not exactly on—a place where multiple quadratics define \( h \). We hypothesize that setting \( \sigma \) to a small but nonzero value (in this case, \( 10^{-8} \)) allows MSG to exploit knowledge of multiple nearly active manifolds near kinks, which are the locations of stationary points of our test set by construction. However, setting \( \sigma \) to be too large degrades performance, likely because of too many inactive manifolds being used by MSG. Based on this initial tuning, we set the parameter \( \sigma = 10^{-8} \) for both MSG-1 and MSG-2 throughout the remainder of our numerical experiments, thus replacing \( \mathcal{A}(z) \) with \( \mathcal{A}_{10^{-8}, \Delta_k}(z) \).

### 6.5 Comparisons with other methods

We compare MSG with other nonsmooth optimization methods that require an oracle for the computation of \( \nabla F \). These are GRANSO, HANSO, and SLQP-GS. The GGradient-based Algorithm for Non-Smooth Optimization (GRANSO) employs a sequential quadratic optimization method with Broyden–Fletcher–Goldfarb–Shanno (BFGS) approximate Hessian updates [16]. GRANSO was run with its default settings. The Hybrid Algorithm for Non-Smooth Optimization (HANSO) implements BFGS and gradient sampling methods together with a bundle method [48]. HANSO is hard-coded to perform at most 100 gradient sampling iterations since such iterations can be expensive; this cap was removed. Sequential Linear or Quadratic Programming with Gradient Sampling (SLQP-GS) has two modes: the sequential linear programming mode and the se-
Figure 3: Data profiles using function values with $\tau = 10^{-3}$ (left) and using the approximate stationary measure $\Gamma$ for $\tau = 10^{-5}$ (right).

sequential quadratic programming mode, where gradient information is always obtained by a sampling process to compute search directions efficiently [17]. We use the sequential quadratic mode in our experiments.

Figure 3 (left) shows a data profile in terms of decrease in $f$; that is, the definition of solved is determined by (39). As previously remarked, however, function values may be insufficient to describe the performance of methods on our benchmarking test set, and so the right plot in Figure 3 shows data profiles in terms of $\Gamma$, and the definition of solved is determined by (41).

From Figure 3, we may conclude that MSG-2 outperforms MSG-1. It is remarkable that without requiring any values of $\nabla F$, MSG-2 exhibits competitive performance with HANSO and GRANSO. We also note that MSG-1 and MSG-2 both outperform SLQP-GS in our experiments.

7 Discussion

We note that the objective function in (1) could involve an additional summand $\psi(x)$ (that is, we could redefine $f(x) \triangleq \psi(x) + h(F(x))$ for some $\psi: \mathbb{R}^n \to \mathbb{R}$) assumed continuously differentiable and bounded below. Our analysis could easily be extended to apply to such functions.

One naturally desires a worst-case complexity rate for manifold sampling algorithms. While such analysis may be possible, it would rely critically on the per-iteration cost of the manifold sampling loop identifying the selection functions active in the current trust region. For the worst case, one can construct examples where all selection functions need to be identified. Similar concerns may explain why worst-case complexity results have not yet been demonstrated for gradient sampling methods.

A Additional Results

Here we provide an additional lemma as a reference for the proofs of the lemmas in Section 4.

Lemma A.1. Let Assumption 2 hold. Let $z(\alpha)$ be as in (20). Then $h(F(x)) - h(F(x + s)) \geq \int_0^1 \inf_{j \in A(z(\alpha))} \{\nabla h_j(z(\alpha))^T (F(x) - F(x + s))\} \, d\alpha.$

Proof. By Assumptions 2.A and 2.B, we can define sets $\mathcal{L}_1, \ldots, \mathcal{L}_N$ by $\mathcal{L}_i = \{\alpha \in [0, 1) : \exists \tau > 0 \text{ such that } i = \min\{j : j \in A(z(\beta))\} \forall \beta \in [\alpha, \alpha + \tau]\}$.

By definition, it is immediate that $\{\mathcal{L}_i\}_{i=1}^N$ form a partition of $[0, 1)$. 

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For any interval \([q, r) \subseteq [0, 1]\) such that \([q, r) \subseteq \mathcal{L}_i\) for some \(i = 1, \ldots, N\),
\[
    h(z(r)) - h(z(q)) = h_i(F(x + s) + r(F(x) - F(x + s))) - h_i(F(x + s) + q(F(x) - F(x + s)))
\]
\[
    = \int_q^r \nabla h_i(z(\alpha))^T (F(x) - F(x + s)) \, d\alpha
\]
\[
    = \int_q^r \inf_{i, \alpha \in \mathcal{L}_i} \{\nabla h_i(z(\alpha))^T (F(x) - F(x + s))\} \, d\alpha
\]
\[
    \geq \int_q^r \inf_{i \in \Lambda(z(\alpha))} \{\nabla h_i(z(\alpha))^T (F(x) - F(x + s))\} \, d\alpha.
\]

Define a maximal interval as any half-open interval \([q, r) \subseteq \mathcal{L}_i\) such that \([q - \tau, r) \not\subseteq \mathcal{L}_i\) and \([q, r + \tau) \not\subseteq \mathcal{L}_i\) for all \(\tau > 0\). Let \(\Lambda_i\) denote the union of maximal half-open intervals \([q_\ell, r_\ell) \in \mathcal{L}_i\). Then,
\[
    h(F(x) - h(F(x + s)) = \sum_{j=1}^N \sum_{\ell \in \Lambda_j} h(z(r_\ell)) - h(z(q_\ell))
\]
\[
    \geq \sum_{j=1}^N \sum_{\ell \in \Lambda_j} \int_{q_\ell}^{r_\ell} \inf_{i \in \Lambda(z(\alpha))} \{\nabla h_i(z(\alpha))^T (F(x) - F(x + s))\} \, d\alpha
\]
\[
    = \int_0^1 \inf_{i \in \Lambda(z(\alpha))} \{\nabla h_i(z(\alpha))^T (F(x) - F(x + s))\} \, d\alpha.
\]

\[\square\]

**Bisection search algorithm**

Here we provide a bisection search algorithm as an alternative to Algorithm 2 for use in Line P.3 in Algorithm 1. Although we have not been able to prove a result analogous to Lemma 4.3, Algorithm 3 is the search algorithm that we implement in practice. In our numerical experiments, Algorithm 3 always terminated successfully.

**Algorithm 3:** Bisection Search for \(\nabla h_j(z)\)

1. if \(F(x)\) and some \(j\) satisfy (11) then return \(\nabla h_j(F(x))\)
2. if \(F(x + s)\) and some \(j\) satisfy (11) then return \(\nabla h_j(F(x + s))\)
3. Set \(\alpha \leftarrow 0, \beta \leftarrow 1\)
4. while true do
5.   Set \(z(\alpha_1) \leftarrow \alpha \frac{\beta + \beta}{2} F(x) + (1 - \alpha \frac{\beta + \beta}{2}) F(x + s)\)
6.   if \(z(\alpha_1)\) and some \(j\) satisfy (11) then return \(\nabla h_j(z(\alpha_1))\)
7.   else if \(h(z(\alpha_1)) > \frac{\alpha + \beta}{2} h(F(x)) + \frac{1}{2} h(F(x + s))\) then
8.      \(\beta \leftarrow \frac{\alpha + \beta}{2}\)
9.   else
10.      \(\alpha \leftarrow \frac{\alpha + \beta}{2}\)

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