

Convergence of trust-region methods based on probabilistic models

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Abstract

In this paper we consider the use of probabilistic or random models within a classical trust-region framework for optimization of deterministic smooth general nonlinear functions. Our method and setting differs from many stochastic optimization approaches in two principal ways. Firstly, we assume that the value of the function itself can be computed without noise, in other words, that the function is deterministic. Secondly, we use random models of higher quality than those produced by usual stochastic gradient methods. In particular, a first order model based on random approximation of the gradient is required to provide sufficient quality of approximation with probability greater than or equal to $1/2$. This is in contrast with stochastic gradient approaches, where the model is assumed to be “correct” only in expectation.

As a result of this particular setting, we are able to prove convergence, with probability one, of a trust-region method which is almost identical to the classical method. Moreover, the new method is simpler than its deterministic counterpart as it does not require a criticality step. Hence we show that a standard optimization framework can be used in cases when models are random and may or may not provide good approximations, as long as “good” models are more likely than “bad” models. Our results are based on the use of properties of martingales. Our motivation comes from using random sample sets and interpolation models in derivative-free optimization. However, our framework is general and can be applied with any source of uncertainty in the model. We discuss various applications for our methods in the paper.

Keywords: Trust-region methods, unconstrained optimization, probabilistic models, derivative-free optimization, global convergence.

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1 Introduction

1.1 Motivation

The focus of this paper is the analysis of a numerical scheme that utilizes randomized models to minimize deterministic functions. In particular, our motivation comes from algorithms for minimization of so-called *black-box* functions where values are computed, e.g., via simulations. For such problems, function evaluations are costly and derivatives are typically unavailable and cannot be approximated. Such is the setting of *derivative-free optimization* (DFO), of which the list of applications—including molecular geometry optimization, circuit design, groundwater community problems, medical image registration, dynamic pricing, and aircraft design (see the references in [15]) — is diverse and growing. Nevertheless, our framework is general and is not limited to the setting of derivative-free optimization.

There is a variety of evidence supporting the claim that randomized models can yield both practical and theoretical benefits for deterministic optimization. A primary example is the recent success of stochastic gradient methods for solving large-scale machine learning problems. As another example, the randomized coordinate descent method for large-scale convex deterministic optimization proposed in [24] yields better complexity results than, e.g., cyclical coordinate descent. Most contemporary randomized methods generate random directions along which all that may be required is some minor level of descent in the objective f . The resulting methods may be very simple and enjoy low per-iteration complexity, but the practical performance of these approaches can be very poor. On the other hand, it was noted in [5] that the performance of stochastic gradient methods for large-scale machine learning improves substantially if the sample size is increased during the optimization process. Within direct search, the use of random positive spanning sets has also been recently investigated [1, 34] with gains in performance and convergence theory for nonsmooth problems. This suggests that for a wide range of optimization problems, requiring a higher level of accuracy from a randomized model may lead to more efficient methods. Thus, our primary goal is to design randomized numerical methods that do not rely on producing descent directions “eventually”, but provide accurate enough approximations so that in each iteration a sufficiently improving step is produced with high probability (in fact, probability greater than half is sufficient in our analysis). We incorporate these models into a trust-region framework so that the resulting algorithm is able to work well in practice.

Our motivation originates with model-based DFO methodology (e.g., see [14, 15]) where local models of f are built from function values sampled in the vicinity of a given iterate. To date, most algorithms of this type have relied on sample sets that are generated by the algorithm steps or added in a deterministic manner. A complex mechanism of sample set maintenance is necessary to ensure that the quality of the models is acceptable, while the expense of sampling the function values is not excessive. Various approaches have been developed for this mechanism, which achieve different trade-offs for the number of sample points required, the computational expense of the mechanism itself, and the quality of the models. One of the primary premises of this paper is the assumption that using random sample sets can yield new and better trade-offs. That is, randomized models can maintain a higher quality by using fewer sample points without complex maintenance of the sample set. One example of such a situation is described in [3], where linear or quadratic polynomial models are constructed from random sample sets. It is shown that one can build such models, meeting a Taylor type accuracy with high probability, using significantly less sample points than what is needed in the deterministic case, provided

the function being modeled has sparse derivatives.

The framework considered by us in the current paper is sufficiently broad to encompass any situation where the quality or accuracy of the trust-region models is random. In particular, such models can be built directly using some form of derivative information, as long as it is accurate with certain probability.

1.2 Trust-region framework

The trust-region method introduced and analyzed in this paper is rather simple. At each iteration one solves a trust-region subproblem, i.e., one minimizes the model within a trust-region ball. Note that one does not know whether the model is accurate or not. If the trust-region step yields a good decrease in the objective function relatively to the decrease in the model and the trust-region radius is sufficiently small relatively to the size of the model gradient, then the step is taken and the trust-region radius is possibly increased. Otherwise the step is rejected and the trust-region radius is decreased. We show that such a method always drives the trust-region radius to zero.

Based on this property we show that, provided the (first order) accuracy of the model occurs with probability no smaller than $1/2$, conditioned to the prior iteration history, then the gradient of the objective function converges to zero with probability one. Our proof technique relies on building random processes from the random events defined by the models being or not being accurate, and then making use of their submartingale-like properties. We extend the theory to the case when the models of sufficient second order accuracy occur with probability no smaller than $1/2$. We show that a subsequence of the iterates drive a measure of second order stationarity to zero with probability one. However, to demonstrate the lim-type convergence to a second order stationary point we need additional assumptions on the models.

1.3 Notation

Several constants are used in this paper to bound various quantities. These constants are denoted by κ with acronyms for the subscripts that are indicative of the quantities that they are meant to bound. We list their most used definitions here, for convenience. The actual meaning of the constants will become clear when each of them is introduced in the paper.

κ_{fcd}	“fraction of Cauchy decrease”
κ_{fod}	“fraction of optimal decrease”
κ_{Lg}	“the Lipschitz constant of the gradient of the function”
κ_{Lh}	“the Lipschitz constant of the Hessian of the function”
$\kappa_{L\tau}$	“the Lipschitz constant of the measure τ of second order stationarity of the function”
κ_{ef}	“error in the function value”
κ_{eg}	“error in the gradient”
κ_{eh}	“error in the Hessian”
$\kappa_{e\tau}$	“error in the τ measure”
κ_{bhm}	“bound on the Hessian of the models”
$\kappa_{bh,f}$	“bound on the Hessian of the function”

This paper is organized as follows. In Section 2 we briefly describe existing methods for derivative-free optimization and provide an illustrative example to motivate the use of random

models. In Section 3 we introduce the probabilistic models of the first order and the trust-region method based on such models. The convergence of the method to first order criticality points is proved in Section 4. The second order case is addressed in Section 5. Finally, in Section 6 we describe various useful random models that satisfy the conditions needed for convergence results in Sections 3 and 5.

2 Methods of derivative-free optimization

We consider in this paper the unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} f(x),$$

where the first (and second, in some cases) derivatives of the objective function $f(x)$ are assumed to exist and be Lipschitz continuous. However, as it is considered in derivative-free optimization (DFO), explicit evaluation of these derivatives is assumed to be impossible. Derivative-free methods rely on sampling the objective function at one or more points at each iteration. Some sample to explore directions, others to build models.

Directional methods. Among the methods of directional type for minimization without derivatives are the direct-search methods which were developed using a single positive spanning set or a finite number of them (see the surveys [20] and [15, Chapter 8]). The basic versions of these methods, like coordinate or compass search, are inherently slow for problems of more than a few variables, not only because they are not able to use curvature information and rarely reuse sample points, but also because they rely on few directions. They were shown to be globally convergent for smooth problems [32] and had their worst case complexity measured by global rates [33].

Not restricting direct search to a finite number of positive spanning sets was soon discovered to enhance practical performance. Approaches allowing for an infinite number of positive spanning sets were proposed in [1, 20], with results applicable to nonsmooth functions when the generation is dense in the unit sphere (see [1, 34]).

On the other hand, randomized stochastic methods recently became a popular alternative to direct-search methods. These methods are also directional, but instead of using directions from a positive spanning set, they select a search direction randomly. This can allow faster convergence because directions of significant descent may be occasionally observed, which might not be the case when insisting on using directions from a fixed positive spanning set (and the use of a randomly rotated positive spanning set may require polling all its directions to find such a direction of significant descent). The random search approach introduced in [21] samples points from a Gaussian distribution. Convergence of an improved scheme was shown in [25]. In [23], Nesterov recently presented several derivative-free random search schemes and provided bounds for their global convergence rates. Different improvements of these methods emerged in the latest literature, e.g., [19]. Although complexity results for both convex and nonsmooth nonconvex functions are available for randomized search, the practical usefulness of these methods is limited by the fixed step sizes determined by the complexity analysis and, as in direct search, by the lack of curvature information.

Model-based trust-region methods. Model-based DFO methods developed by Powell [26, 27, 28, 29], and by Conn, Scheinberg, and Toint [9, 10], introduced a class of trust-region methods that relied on *interpolation* or *regression* based quadratic approximations of the objective function instead of the usual Taylor series quadratic approximation. The regression-based method was later successfully used in [4] based on [13]. In all cases the models are built based on sample points in reasonable proximity to the current best iterate. The computational study of Moré and Wild [22] has shown that these methods are typically significantly superior in practical performance to the other existing approaches due to the use of models that effectively capture the local curvature of the objective function. While the model quality is undoubtedly essential for the performance of these methods, guaranteeing sufficient quality on specific iterations is quite expensive computationally. Randomized models, on the other hand, can offer a suitable alternative by providing a good quality approximation with high probability.

An illustration of directional and model-based methods. Consider the well known Rosenbrock function for our computational illustration

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2.$$

The function is known to be difficult for first order or zero order methods and well suited for second order methods. Nevertheless, some first/zero order methods perform reasonably, while others perform poorly. We compared the following four methods: 1) a simple variant of direct search, the coordinate or compass search method (CS) which uses the positive basis $[I \ -I]$, 2) a direct-search method using the positive basis $[Q \ -Q]$ where Q is an orthogonal matrix obtained by randomly generating the first column (DSR), 3) a random search (RS) with step size inversely proportional to the iteration count, and 4) a basic model-based trust-region method with quadratic models (TRQ). The outcome of the algorithms is summarized as follows.

1. CS: number of function evaluations: 11307, final function value: 1.0e-6.
2. DSR: number of function evaluations: 5756, final function value: 1.0e-8.
3. RS: number of function evaluations: 3724, final function value: 1.0e-8.
4. TRQ: number of function evaluations: 62, final function value: 1.0e-14.

It is evident from these results that the random directional approaches, and in particular random search, are more successful at finding good directions for descent, while the coordinate search is slow due to the fixed choice of the search directions. It is also clear, from the performance of the second order trust-region method on this problem, that using accurate models can substantially improve efficiency. It is natural, thus, to consider the effects of randomization in model-based methods. In particular we consider methods that use models built from randomly sampled points in hopes of obtaining better models.

3 First order trust-region method based on probabilistic models

Let us consider the classical trust-region method setting and notation (see [15] for a similar description). At iteration k , f is approximated by a model m_k within the ball $B(x_k, \delta_k)$ centered at x_k and of radius δ_k . Then the model is minimized (or approximately minimized) in the ball

to possibly obtain x_{k+1} . In this section we will introduce and analyze a trust-region algorithm based on probabilistic models, i.e., models m_k which are built in a random fashion. First we discuss these models and state what will be assumed from them.

3.1 The probabilistically fully linear models

For simplicity of the presentation, we consider only quadratic models, written in the form

$$m_k(x_k + s) = m_k(x_k) + s^\top g_k + \frac{1}{2} s^\top H_k s,$$

where $g_k = \nabla m_k(x_k)$ and $H_k = \nabla^2 m_k(x_k)$. Our analysis is not, however, dependent on the models being quadratic.

Let us start by introducing a measure of (linear or first order) accuracy of the model m_k .

Definition 3.1 *We say that a function m_k is a $(\kappa_{eg}, \kappa_{ef})$ -fully linear model of f on $B(x_k, \delta_k)$ if, for every $s \in B(0, \delta_k)$,*

$$\begin{aligned} \|\nabla f(x_k + s) - \nabla m_k(x_k + s)\| &\leq \kappa_{eg} \delta_k, \\ \|f(x_k + s) - m(x_k + s)\| &\leq \kappa_{ef} \delta_k^2. \end{aligned}$$

The concept of fully linear models is introduced in [14] and [15], but here we use the notation proposed in [4]. In [15, Chapter 6] there is a detailed discussion on how to construct and maintain deterministic fully linear models.

For the case of random models, the key assumption in our convergence analysis is that these models exhibit good accuracy (as in Definition 3.1) with sufficiently high probability. We will consider random models M_k , and then use the notation $m_k = M_k(\omega_k)$ for their realizations. The randomness of the models will imply the randomness of the points x_k and the trust-region radii δ_k . Thus, in the sequel, these random quantities will be denoted by X_k and Δ_k , respectively, while $x_k = X_k(\omega_k)$ and $\delta_k = \Delta_k(\omega_k)$ denote their realizations.

Definition 3.2 *We say that a sequence of random models $\{M_k\}$ is (p) -probabilistically $(\kappa_{eg}, \kappa_{ef})$ -fully linear for a corresponding sequence $\{B(X_k, \Delta_k)\}$ if the events*

$$S_k = \{M_k \text{ is a } (\kappa_{eg}, \kappa_{ef})\text{-fully linear model of } f \text{ on } B(X_k, \Delta_k)\}$$

satisfy the following submartingale-like condition

$$P(S_k | F_{k-1}^M) \geq p,$$

where $F_{k-1}^M = \sigma(M_0, \dots, M_{k-1})$ is the σ -algebra generated by M_0, \dots, M_{k-1} . Furthermore, if $p \geq \frac{1}{2}$, then we say that the random models are probabilistically $(\kappa_{eg}, \kappa_{ef})$ -fully linear.

Note that M_k is a random model that encompasses all the randomness of iteration k of our algorithm. The iterates X_k and the trust region radii Δ_k are random variables defined over the σ -algebra generated by M_0, \dots, M_{k-1} . Each M_k depends on X_k and Δ_k and hence on M_0, \dots, M_{k-1} . Definition 3.2 serves to enforce the following property: even though the accuracy of M_k may be dependent on the history, (M_1, \dots, M_{k-1}) , via its dependence on X_k and Δ_k , it is sufficiently good with probability at least p , regardless of that history. We believe this condition

is more reasonable than assuming complete independence of M_k from the past, which is difficult to ensure given that the current iterate, around which the model is built, and the trust-region radius depend on the algorithm history.

Now we discuss the corresponding assumptions on the models realizations that we use in the algorithm. The first assumption guarantees that we are able to adequately minimize (or reduce) the model at each iteration of our algorithm.

Assumption 3.1 *For every k , and for all realizations m_k of M_k (and of X_k and Δ_k), we are able to compute a step s_k such that*

$$m_k(x_k) - m_k(x_k + s_k) \geq \frac{\kappa_{fcd}}{2} \|g_k\| \min \left\{ \frac{\|g_k\|}{\|H_k\|}, \delta_k \right\}, \quad (1)$$

for some constant $\kappa_{fcd} \in (0, 1]$. We say in this case that s_k has achieved a fraction of Cauchy decrease.

The Cauchy step itself, which is the minimizer of the quadratic model within the trust region along the negative model gradient $-g_k$, trivially satisfies this property with $\kappa_{fcd} = 1$.

We also assume a uniform bound on the model Hessians:

Assumption 3.2 *There exists a positive constant κ_{bhm} , such that for every k , the Hessians H_k of all realizations m_k of M_k satisfy*

$$\|H_k\| \leq \kappa_{bhm}. \quad (2)$$

The above assumption is introduced for convenience. While it is possible to show our results without this assumption, it is not restrictive in the case of fully linear models. In particular, one can construct fully linear models with arbitrarily small $\|H_k\|$ using interpolation techniques. In the case of models that, fortuitously, have large Hessian norms, because they are not fully linear, we can simply set the Hessian to some other matrix of a smaller norm (or zero).

3.2 Algorithm and basic properties

Let us consider the following simple trust-region algorithm.

Algorithm 3.1 *Fix the positive parameters η_1 , η_2 , γ , δ_{\max} with $\gamma > 1 > \eta_1$. Select initial $k = 0$, $\delta_0 \leq \delta_{\max}$, and x_0 . At iteration k approximate the function f in $B(x_k, \delta_k)$ by m_k and then approximately minimize m_k in $B(x_k, \delta_k)$, computing s_k so that it satisfies a fraction of Cauchy decrease (1). Let*

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m(x_k) - m(x_k + s_k)}. \quad (3)$$

If $\rho_k \geq \eta_1$, then set $x_{k+1} = x_k + s_k$ and

$$\delta_{k+1} = \begin{cases} \gamma^{-1} \delta_k & \text{if } \|g_k\| < \eta_2 \delta_k, \\ \min\{\gamma \delta_k, \delta_{\max}\} & \text{if } \|g_k\| \geq \eta_2 \delta_k. \end{cases}$$

Otherwise, set $x_{k+1} = x_k$ and $\delta_{k+1} = \gamma^{-1} \delta_k$. Increase k by one and repeat the iteration.

This is a basic trust-region algorithm, with one specific modification: the trust-region radius is always increased if sufficient function reduction is achieved, that is the step is successful, *and* the trust-region radius is small compared to the norm of the model gradient. The logic behind this update follows from the line-search type intuition, where the step size is typically proportional to the norm of the model gradient, hence the trust region should be of comparable size also. Later we will show how the algorithm can be modified to allow for the trust-region radius to remain unchanged in some iterations.

Each realization of the algorithm defines a sequence of realizations for the corresponding random variables, in particular: $m_k = M_k(\omega_k)$, $x_k = X_k(\omega_k)$, $\delta_k = \Delta_k(\omega_k)$.

For the purpose of proving convergence of the algorithm to first order critical points, we assume that the function f and its gradient are Lipschitz continuous in regions considered by the algorithm realizations. To define this region we follow the process in [14]. Suppose that x_0 (the initial iterate) is given. Then all the subsequent iterates belong to the level set

$$L(x_0) = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}.$$

However, the failed iterates may lie outside this set. In the setting considered in this paper, all potential iterates are restricted to the region

$$L_{enl}(x_0) = L(x_0) \cup \bigcup_{x \in L(x_0)} B(x, \delta_{\max}) = \bigcup_{x \in L(x_0)} B(x, \delta_{\max}),$$

where δ_{\max} is the upper bound on the size of the trust regions, as imposed by the algorithm.

Assumption 3.3 *Suppose x_0 and δ_{\max} are given. Assume that f is continuously differentiable in an open set containing the set $L_{enl}(x_0)$ and that ∇f is Lipschitz continuous on $L_{enl}(x_0)$ with constant κ_{Lg} . Assume also that f is bounded from below on $L(x_0)$.*

The following lemma states that the trust-region radius converges to zero regardless of the realization of the model sequence $\{M_k\}$ made by the algorithm, as long as the fraction of Cauchy decrease is achieved by the step at every iteration.

Lemma 3.1 *For every realization of Algorithm 3.1,*

$$\lim_{k \rightarrow \infty} \delta_k = 0.$$

Proof. Suppose that $\{\delta_k\}$ does not converge to zero. Then, there exists $\epsilon > 0$ such that $\#\{k : \delta_k > \epsilon\} = \infty$. Because of the way δ_k is updated we must have

$$\#\left\{k : \delta_k > \frac{\epsilon}{\gamma}, \delta_{k+1} \geq \delta_k\right\} = \infty,$$

in other words, there must be an infinite number of iterations on which δ_{k+1} is not decreased, and, for these iterations we have $\rho \geq \eta_1$ and $\|g_k\| \geq \eta_2 \frac{\epsilon}{\gamma}$. Therefore, because (1) and (2) hold,

$$\begin{aligned} f(x_k) - f(x_k + s_k) &\geq \eta_1 (m(x_k) - m(x_k + s_k)) \\ &\geq \eta_1 \frac{\kappa_{fcd}}{2} \|g_k\| \min \left\{ \frac{\|g_k\|}{\kappa_{bhm}}, \delta_k \right\} \\ &\geq \eta_1 \frac{\kappa_{fcd}}{2} \min \left\{ \frac{\eta_2}{\kappa_{bhm}}, 1 \right\} \eta_2 \frac{\epsilon^2}{\gamma^2}. \end{aligned} \tag{4}$$

This means that at each iteration where δ_k is increased, f is reduced by a constant. Since f is bounded from below, the number of such iterations cannot be infinite, and hence we arrived at a contradiction. \square

Another result that we use in our analysis is the following fact typical of trust-region methods, stating that, in the presence of sufficient model accuracy, a successful step will be achieved, provided the trust-region radius is sufficiently small relatively to the size of the model gradient.

Lemma 3.2 *If m_k is $(\kappa_{eg}, \kappa_{ef})$ -fully linear on $B(x_k, \delta_k)$ and*

$$\delta_k \leq \min \left\{ \frac{\|g_k\|}{\kappa_{bhm}}, \frac{\kappa_{fed}(1 - \eta_1)\|g_k\|}{4\kappa_{ef}} \right\},$$

then at the k -th iteration $\rho_k \geq \eta_1$.

The proof can be found in [15, Lemma 10.6].

4 Convergence of the first order trust-region method based on probabilistic models

We now assume that the models used in the algorithm are probabilistically fully linear, and show our first order convergence results. First we will state an auxiliary result from the martingale literature that will be useful in our analysis.

Theorem 4.1 *Let G_k be a submartingale, i.e., a sequence of random variables which, for every k , are integrable ($\mathbb{E}(|G_k|) < \infty$) and*

$$\mathbb{E}[G_k | F_{k-1}^G] \geq G_{k-1},$$

where $F_{k-1}^G = \sigma(G_0, \dots, G_{k-1})$ is the σ -algebra generated by G_0, \dots, G_{k-1} and $\mathbb{E}[G_k | F_{k-1}^G]$ denotes the conditional expectation of G_k given the past history of events F_{k-1}^G .

Assume further that $|G_k - G_{k-1}| \leq M < \infty$, for every k . Consider the random events $C = \{\lim_{k \rightarrow \infty} G_k \text{ exists and is finite}\}$ and $D = \{\limsup_{k \rightarrow \infty} G_k = \infty\}$. Then $P(C \cup D) = 1$.

Proof. The theorem is a simple extension of [16, Theorem 5.3.1], see [16, Exercise 5.3.1]. \square Roughly speaking, this results shows that a random walk with bounded increments and an upward drift either converges to a finite limit or is unbounded from above. We will apply this result to $\log \Delta_k$ which, as we show, is a random walk with an upward drift that cannot converge to a finite limit.

4.1 The liminf-type convergence

As is typical in trust-region methods, we show first that a subsequence of the iterates drive the gradient of the objective function to zero.

Theorem 4.2 *Suppose that the model sequence $\{M_k\}$ is probabilistically $(\kappa_{eg}, \kappa_{ef})$ -fully linear for some positive constants κ_{eg} and κ_{ef} . Let $\{X_k\}$ be a sequence of random iterates generated by Algorithm 3.1. Then, almost surely,*

$$\liminf_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0.$$

Proof. Recall the definition of events the S_k in Definition 3.2. Let us start by constructing the following random walk

$$W_k = \sum_{i=0}^k (2(1_{S_i}) - 1),$$

where 1_{S_i} is the indicator random variable ($1_{S_i} = 1$ if S_i occurs, $1_{S_i} = 0$ otherwise). From the martingale-like property enforced in Definition 3.2, it easily follows that W_k is a submartingale. In fact, one has

$$\begin{aligned} \mathbb{E}[W_k | F_{k-1}^S] &= \mathbb{E}[W_{k-1} | F_{k-1}^S] + \mathbb{E}[2(1_{S_k}) - 1 | F_{k-1}^S] \\ &= W_{k-1} + 2\mathbb{E}[1_{S_k} | F_{k-1}^S] - 1 \\ &= W_{k-1} + 2P(S_k | F_{k-1}^S) - 1 \\ &\geq W_{k-1}, \end{aligned}$$

where $F_{k-1}^S = \sigma(1_{S_0}, \dots, 1_{S_{k-1}})$ is the σ -algebra generated by $1_{S_0}, \dots, 1_{S_{k-1}}$, in turn contained in $F_{k-1}^M = \sigma(M_0, \dots, M_{k-1})$. Since the submartingale W_k has ± 1 (and hence, bounded) increments it cannot have a finite limit. Thus, by Theorem 4.1 we have that the event $D = \{\limsup_{k \rightarrow \infty} W_k = \infty\}$ holds almost surely.

Since our objective is to show that $\liminf_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$ almost surely, we can show it by conditioning on an almost sure event. All that follows is conditioned on the event $D = \{\limsup_{k \rightarrow \infty} W_k = \infty\}$.

Suppose there exist $\epsilon > 0$ and k_1 such that, with positive probability,

$$\|\nabla f(X_k)\| \geq \epsilon,$$

for all $k \geq k_1$.

Let $\{x_k\}$ and $\{\delta_k\}$ be any realization of $\{X_k\}$ and $\{\Delta_k\}$, respectively, built by Algorithm 3.1. By Lemma 3.1, there exists k_2 such that we have $\forall k \geq k_2$

$$\delta_k < \mathbf{b} := \min \left\{ \frac{\epsilon}{2\kappa_{eg}}, \frac{\epsilon}{2\kappa_{bhm}}, \frac{\epsilon}{2\eta_2}, \frac{\kappa_{fcd}(1 - \eta_1)\epsilon}{8\kappa_{ef}}, \frac{\delta_{\max}}{\gamma} \right\}. \quad (5)$$

Consider some iterate $k \geq k_0 := \max\{k_1, k_2\}$ such that $1_{S_k} = 1$ (model m_k is fully linear). Then, from the definition of fully linear models

$$\|\nabla f(x_k) - g_k\| \leq \kappa_{eg}\delta_k < \frac{\epsilon}{2},$$

hence,

$$\|g_k\| \geq \frac{\epsilon}{2}.$$

Using Lemma 3.2 we obtain $\rho_k \geq \eta_1$. Also

$$\|g_k\| \geq \frac{\epsilon}{2} \geq \eta_2\delta_k.$$

Hence, by the construction of the algorithm, and the fact that $\delta_k \leq \frac{\delta_{\max}}{\gamma}$, we have $\delta_{k+1} = \gamma\delta_k$.

Let us consider now the random variable R_k with realization $r_k = \log_\gamma(\mathbf{b}^{-1}\delta_k)$. For every realization $\{r_k\}$ of $\{R_k\}$ we have seen that there exists k_0 such that $r_k < 0$ for $k \geq k_0$. Moreover, if $1_{S_k} = 1$ then $r_{k+1} = r_k + 1$, and if $1_{S_k} = 0$, $r_{k+1} \geq r_k - 1$ (implying that R_k is a submartingale). Hence, $r_k - r_{k_0} \geq w_k - w_{k_0}$ (w_k denoting a realization of W_k that correspond to the particular realization r_k). Since we are conditioning on the event D , we have that R_k has to be positive infinitely often with probability one, contradicting the fact that for all realizations $\{r_k\}$ of $\{R_k\}$ there exists k_0 such that $r_k < 0$ for $k \geq k_0$. Thus, conditioning on D we always have that $\liminf_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$ with probability one. Therefore

$$\liminf_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$$

almost surely. \square

4.2 The lim-type convergence

In this subsection we show that $\lim_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$ almost surely. Before stating and proving the main theorem we state and prove two auxiliary lemmas.

Lemma 4.1 *Let $\{Z_k\}_{k \in \mathbb{N}}$ be a sequence of non-negative uniformly bounded random variables and $\{B_k\}$ be a sequence of Bernoulli random variables (taking values 1 and -1) such that*

$$P(B_k = 1 | \sigma(B_1, \dots, B_{k-1}), \sigma(Z_1, \dots, Z_k)) \geq 1/2.$$

Let \mathcal{P} be the set of natural numbers k such that $B_k = 1$ and $\mathcal{N} = \mathbb{N} \setminus \mathcal{P}$ (note that \mathcal{P} and \mathcal{N} are random sequences). Then

$$\text{Prob} \left(\left\{ \sum_{i \in \mathcal{P}} Z_i < \infty \right\} \cap \left\{ \sum_{i \in \mathcal{N}} Z_i = \infty \right\} \right) = 0.$$

Proof. Let us construct the following process $G_k = G_{k-1} + B_k Z_k$. It is easy to check that G_k is a submartingale with bounded increments $\{B_k Z_k\}$. Hence we can apply Theorem 4.1 and observe that the event $\{\limsup_{k \rightarrow \infty} G_k = -\infty\}$ has probability zero. On the other hand, note that $G_k = \sum_{i \in \mathcal{P}, i \leq k} Z_i - \sum_{i \in \mathcal{N}, i \leq k} Z_i$ and hence $\{\sum_{i \in \mathcal{P}} Z_i < \infty\} \cap \{\sum_{i \in \mathcal{N}} Z_i = \infty\}$ implies that $\{\limsup_{k \rightarrow \infty} G_k = -\infty\}$. Since event $\{\limsup_{k \rightarrow \infty} G_k = -\infty\}$ happens with zero probability, then so does the event that implies it, in other words, $\{\sum_{i \in \mathcal{P}} Z_i < \infty\} \cap \{\sum_{i \in \mathcal{N}} Z_i = \infty\}$ happens with zero probability. \square

Lemma 4.2 *Let $\{X_k\}$ and $\{\Delta_k\}$ be sequences of random iterates and random trust-region radii generated by Algorithm 3.1. Fix $\epsilon > 0$ and define the sequence $\{K_i\}$ consisting of the natural numbers k for which $\|\nabla f(X_k)\| > \epsilon$ (note that K_i is a sequence of random variables). Then,*

$$\sum_{k \in \{K_i\}} \Delta_k < \infty$$

almost surely.

Proof. Let $\{m_k\}$, $\{x_k\}$, $\{\delta_k\}$, $\{k_i\}$ be realizations of $\{M_k\}$, $\{X_k\}$, $\{\Delta_k\}$, $\{K_i\}$ respectively. Let us separate $\{k_i\}$ in two subsequences: $\{p_i\}$ is the subsequence of $\{k_i\}$ such that m_{p_i} is $(\kappa_{eg}, \kappa_{ef})$ -fully linear on $B(x_{p_i}, \delta_{p_i})$, and $\{n_i\}$ is the subsequence of the remaining elements of $\{k_i\}$.

We will now show that $\sum_{j \in \{p_i\}} \delta_j < \infty$ for any such realization. If $\{p_i\}$ is finite, then this result trivially follows. Otherwise, since $\delta_k \rightarrow 0$, we have that for sufficiently large p_i , $\delta_{p_i} < \mathbf{b}$, with \mathbf{b} defined by (5). Since $\|\nabla f(x_{p_i})\| > \epsilon$, and m_{p_i} is fully linear on $B(x_{p_i}, \Delta_{p_i})$, then by the derivations in Theorem 4.2, we have $\|g_{p_i}\| \geq \frac{\epsilon}{2}$, and by Lemma 3.2 $\rho_{p_i} \geq \eta_1$. Hence, for all p_i large enough, the decrease in the function value satisfies

$$f(x_{p_i}) - f(x_{p_i+1}) \geq \eta_1 \frac{\kappa_{fcd} \epsilon}{2} \delta_{p_i}.$$

Thus

$$\sum_{j \in \{p_i\}} \delta_j \leq \frac{4(f(x_0) - f_*)}{\eta_1 \kappa_{fcd} \epsilon} < \infty,$$

where f_* is a lower bound on the values of f on $L(x_0)$.

For each k_i , the event S_{k_i} (whether the model is fully linear on iteration k_i) has probability at least $\frac{1}{2}$ conditioned on all of the history of the algorithm. Hence, we can apply Lemma 4.1 (note that $\{\Delta_k\}$ is a sequence of non-negative uniformly bounded variables and S_{k_i} are the Bernoulli random variables) and obtain

$$\text{Prob} \left(\left\{ \sum_{j \in \{P_i\}} \Delta_j < \infty \right\} \cap \left\{ \sum_{j \in \{N_i\}} \Delta_j = \infty \right\} \right) = 0.$$

This means that, almost surely,

$$\sum_{j \in \{K_i\}} \Delta_j = \sum_{j \in \{P_i\}} \Delta_j + \sum_{j \in \{N_i\}} \Delta_j < \infty.$$

□

We are now ready to prove the lim-type result.

Theorem 4.3 *Suppose that the model sequence $\{M_k\}$ is probabilistically $(\kappa_{eg}, \kappa_{ef})$ -fully linear for some positive constants κ_{eg} and κ_{ef} . Let $\{X_k\}$ be a sequence of random iterates generated by Algorithm 3.1. Then, almost surely,*

$$\lim_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0.$$

Proof. Suppose that $\lim_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$ does not hold almost surely. Then, with positive probability, there exists $\epsilon > 0$ such that $\|\nabla f(X_k)\| > 2\epsilon$, holds for infinitely many k . Without loss of generality, we assume that $\epsilon = \frac{1}{n_\epsilon}$, for some natural number n_ϵ .

Let $\{K_i\}$ be a subsequence of the iterations for which $\|\nabla f(X_k)\| > \epsilon$. We are going to show that, if such an ϵ exists then $\sum_{j \in \{K_i\}} \Delta_j$ is a divergent sum.

Let us call a pair of integers (W', W'') an ‘‘ascent’’ pair if $0 < W' < W''$, $\|\nabla f(X_{W'})\| \leq \epsilon$, $\|\nabla f(X_{W'+1})\| > \epsilon$, $\|\nabla f(X_{W''})\| > 2\epsilon$ and, moreover, for any $w \in (W', W'')$, $\epsilon < \|\nabla f(X_w)\| \leq$

2ϵ . Each such ascent pair forms a nonempty interval of integers $\{W'+1, \dots, W''\}$ which is a subset of the sequence $\{K_i\}$. Since $\liminf_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$ holds almost surely (by Theorem 4.2), it follows that there are infinitely many such intervals. Let us consider the sequence of these intervals $\{(W'_\ell, W''_\ell)\}$. The idea is now to show (with positive probability) that, for any ascent pair (W'_ℓ, W''_ℓ) with ℓ sufficiently large, $\sum_{j=W'_\ell+1}^{W''_\ell-1} \Delta_j$ is uniformly bounded away from 0 (and hence $W'_\ell+1 < W''_\ell$), which implies that $\sum_{j \in \{K_i\}} \Delta_j = \infty$ since $\sum_\ell \sum_{j=W'_\ell+1}^{W''_\ell-1} \Delta_j \leq \sum_{j \in \{K_i\}} \Delta_j$, because the sequence $\{K_i\}$ contains all intervals $\{W'_\ell, W''_\ell\}$.

Let $\{x_k\}$ and $\{\delta_k\}$ be realizations of $\{X_k\}$ and $\{\Delta_k\}$, for which $\|\nabla f(x_k)\| > \epsilon$ for $k \in \{k_i\}$. By the triangular inequality, for any ℓ ,

$$\epsilon < \left| \|\nabla f(x_{w'_\ell})\| - \|\nabla f(x_{w''_\ell})\| \right| \leq \sum_{j=w'_\ell}^{w''_\ell-1} \left| \|\nabla f(x_j)\| - \|\nabla f(x_{j+1})\| \right|.$$

Since ∇f is Lipschitz continuous (with constant κ_{Lg}),

$$\epsilon \leq \sum_{j=w'_\ell}^{w''_\ell-1} \left| \|\nabla f(x_j)\| - \|\nabla f(x_{j+1})\| \right| \tag{6}$$

$$\leq \kappa_{Lg} \sum_{j=w'_\ell}^{w''_\ell-1} \|x_j - x_{j+1}\| \tag{7}$$

$$\leq \kappa_{Lg} \left(\delta_{w'_\ell} + \sum_{j=w'_\ell+1}^{w''_\ell-1} \delta_j \right). \tag{8}$$

From the fact that δ_k converges to zero, then, for any ℓ large enough, $\delta_{w'_\ell} < \frac{\epsilon}{2\kappa_{Lg}}$, and hence $\sum_{j=w'_\ell+1}^{w''_\ell-1} \delta_j > \frac{\epsilon}{2} > 0$, which gives us $\sum_{j \in \{k_i\}} \delta_j = \infty$.

We have thus proved that if, $\lim_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$ does not hold almost surely, then, with positive probability, there exists n_ϵ such that $\{K_i\}$ defined as above based on n_ϵ , satisfies $\sum_{j \in \{K_i\}} \Delta_j = \infty$. On the other hand, Lemma 4.2 guarantees that, for every n_ϵ , the probability of $\sum_{j \in \{K_i\}} \Delta_j = \infty$ is zero. The set of all $n_\epsilon \in \mathbb{N}$ is countable hence the probability of one of these countable events occurring is still zero, because the union of a countable number of rare events is itself a rare event. In other words, the probability of the existence of a value n_ϵ for which $\sum_{j \in \{K_i\}} \Delta_j = \infty$ is zero, which contradicts the initial assumption that $\lim_{k \rightarrow \infty} \|\nabla f(X_k)\| = 0$ does not hold almost surely. \square

4.3 Modified trust-region schemes

The trust-region radius update of Algorithm 3.1 may be too restrictive as it only allows for this radius to be increased or decreased. In practice typically two separate thresholds are used, one for the increase of the trust-region radius and another for its decrease. In the remaining cases the trust-region radius remains unchanged. Hence, here we propose an algorithm similar to Algorithm 3.1 but slightly more appealing in practice.

Algorithm 4.1 Fix the positive parameters $\eta_1, \eta_2, \eta_3, \gamma, \delta_{\max}$, with $\gamma > 1 > \eta_1$ and $\eta_3 \leq \eta_2$. Select initial $k = 0$, $\delta_0 \leq \delta_{\max}$, and x_0 . At iteration k approximate the function f in $B(x_k, \delta_k)$ by m_k and then approximately minimize m_k in $B(x_k, \delta_k)$, computing s_k so that it satisfies a fraction of Cauchy decrease (1). Let ρ_k be defined as in (3).

If $\rho_k \geq \eta_1$, then set $x_{k+1} = x_k + s_k$ and

$$\delta_{k+1} = \begin{cases} \gamma^{-1}\delta_k & \text{if } \|g_k\| < \eta_3\delta_k, \\ \delta_k & \text{if } \eta_3\delta_k \leq \|g_k\| < \eta_2\delta_k, \\ \min\{\gamma\delta_k, \delta_{\max}\} & \text{if } \eta_2\delta_k \leq \|g_k\|. \end{cases}$$

Otherwise, set $x_{k+1} = x_k$ and $\delta_{k+1} = \gamma^{-1}\delta_k$.

Increase k by one and repeat the iteration.

It is straightforward to adapt the proofs of Lemma 3.1 and Theorems 4.2 and 4.3 to show the convergence for this new algorithm. Additionally, one can consider two different thresholds, $0 < \eta_0 < 1$ for decrease of the trust region radius, and $\eta_1 > \eta_0$ for the increase of the trust region radius.

5 Second order trust-region method based on probabilistic models

In this section we present the analysis of the convergence of a trust-region algorithm to second order stationary points under the assumption that the random models are likely to provide second order accuracy.

5.1 The probabilistically fully quadratic models

Let us now introduce a measure of second order quality or accuracy of the models m_k (see [14, 15, 4] for more details).

Definition 5.1 We say that a function m_k is a $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic model of f on $B(x_k, \delta_k)$ if, for every $s \in B(0, \delta_k)$,

$$\begin{aligned} \|\nabla^2 f(x_k + s) - H_k\| &\leq \kappa_{eh}\delta_k, \\ \|\nabla f(x_k + s) - \nabla m_k(x_k + s)\| &\leq \kappa_{eg}\delta_k^2, \\ \|f(x_k + s) - m(x_k + s)\| &\leq \kappa_{ef}\delta_k^3. \end{aligned}$$

As in the fully linear case, we assume that the models used in the algorithms are fully quadratic with a certain probability.

Definition 5.2 We say that a sequence of random models $\{M_k\}$ is (p) -probabilistically $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic for a corresponding sequence $\{B(X_k, \Delta_k)\}$ if the events

$$S_k = \{M_k \text{ is a } (\kappa_{eh}, \kappa_{eg}, \kappa_{ef})\text{-fully quadratic model of } f \text{ on } B(X_k, \Delta_k)\}$$

satisfy the following submartingale-like condition

$$P(S_k | F_{k-1}^M) \geq p,$$

where $F_{k-1}^M = \sigma(M_0, \dots, M_{k-1})$ is the σ -algebra generated by M_0, \dots, M_{k-1} . Furthermore, if $p \geq \frac{1}{2}$, then we say that the random models are probabilistically $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic.

We now need to discuss the algorithmic requirements and problem assumptions which will be needed for global convergence to second order critical points. In terms of problems assumptions we will need one more order of smoothness.

Assumption 5.1 *Suppose x_0 and δ_{\max} are given. Assume that f is twice continuously differentiable in an open set containing the set $L_{\text{enl}}(x_0)$ and that $\nabla^2 f$ is Lipschitz continuous with constant κ_{Lh} and that $\|\nabla^2 f\|$ is bounded by a constant κ_{bhf} on $L_{\text{enl}}(x_0)$. Assume also that f is bounded from below on $L(x_0)$.*

We will no longer assume that the Hessian H_k of the models is bounded in norm, since we cannot simply disregard large Hessian model values without possibly affecting the chances of the model being fully quadratic. However, a simple analysis can show that $\|H_k\|$ is uniformly bounded from above for any fully quadratic model m_k (although we may not know what this bound is and hence may not be able to use it in an algorithm).

Lemma 5.1 *Given constants κ_{eh} , κ_{eg} , κ_{ef} , and δ_{\max} , there exists a constant κ_{bmh} such that for every k and every realization m_k of M_k which is a $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic model of f on $B(x_k, \delta_k)$ with $x_k \in L(x_0)$ and $\delta_k \leq \delta_{\max}$ we have*

$$\|H_k\| \leq \kappa_{bmh}.$$

Proof. The proof follows trivially from the definition of fully quadratic models and the assumption that $\|\nabla^2 f\|$ is bounded by a constant κ_{bhf} on $L_{\text{enl}}(x_0)$. \square

It will also be necessary to assume that the minimization of the model achieves a certain level of second order improvement (an extension of the Cauchy decrease).

Assumption 5.2 *For every k , and for all realizations m_k of M_k (and of X_k and Δ_k), we are able to compute a step s_k so that*

$$m_k(x_k) - m_k(x_k + s_k) \geq \frac{\kappa_{fod}}{2} \max \left\{ \|g_k\| \min \left[\frac{\|g_k\|}{\|H_k\|}, \delta_k \right], \max\{-\lambda_{\min}(H_k), 0\} \delta_k^2 \right\}. \quad (9)$$

for some constant $\kappa_{fod} \in (0, 1]$. We say in this case that s_k has achieved a fraction of optimal decrease.

A step satisfying this assumption is given, for instance, by computing both the Cauchy step and, in the presence of negative curvature in the model, the eigenstep, and by choosing the one that provides the largest reduction in the model. The eigenstep is the minimizer of the quadratic model in the trust region along an eigenvector corresponding to the smallest (negative) eigenvalue of H_k .

The measure of proximity to a second order stationary point for the function f is slightly different from the traditional, and is given by

$$\tau(x) = \max \left\{ \min \left[\|\nabla f(x)\|, \frac{\|\nabla f(x)\|}{\|\nabla^2 f(x)\|} \right], -\lambda_{\min}(\nabla^2 f(x)) \right\}.$$

The model approximation of this measure is defined similarly:

$$\tau^m(x) = \max \left\{ \min \left[\|\nabla m(x)\|, \frac{\|\nabla m(x)\|}{\|\nabla^2 m(x)\|} \right], -\lambda_{\min}(\nabla^2 m(x)) \right\}.$$

We consider the additional terms $\|\nabla f(x)\|/\|\nabla^2 f(x)\|$ and $\|\nabla m(x)\|/\|\nabla^2 m(x)\|$ given that we no longer assume a bound in the model Hessians as we did in the first order case. We show now that $\tau(x)$ is Lipschitz continuous under Assumption 5.1.

Lemma 5.2 *Suppose that Assumption 5.1 holds. Then there exists a constant $\kappa_{L\tau}$ such that for all $x_1, x_2 \in L_{enl}(x_0)$*

$$|\tau(x_1) - \tau(x_2)| \leq \kappa_{L\tau} \|x_1 - x_2\|. \quad (10)$$

Proof. First we note that under Assumption 5.1 there must exist an upper bound $\kappa_{bfg} > 0$ on the norm of the gradient of f , $\|\nabla f(x)\| \leq \kappa_{bfg}$ for all $x \in L_{enl}(x_0)$.

Then let us see that $h(x) = \min\{\|\nabla f(x)\|, \|\nabla f(x)\|/\|\nabla^2 f(x)\|\}$ is Lipschitz continuous. Given $x, y \in L_{enl}(x_0)$, one consider four cases: (i) The case $\|\nabla^2 f(x)\| \geq 1$ and $\|\nabla^2 f(y)\| \geq 1$ results from the Lipschitz continuity and boundedness above of the gradient and the Hessian. (ii) The case $\|\nabla^2 f(x)\| < 1$ and $\|\nabla^2 f(y)\| < 1$ results from the Lipschitz continuity of the gradient. (iii) The argument is the same for the other two cases, so let us choose one of them, say $\|\nabla^2 f(x)\| < 1$ and $\|\nabla^2 f(y)\| \geq 1$. In this case, using these inequalities, one has

$$\begin{aligned} |h(x) - h(y)| &\leq \left| \|\nabla f(x)\| - \frac{\|\nabla f(y)\|}{\|\nabla^2 f(y)\|} \right| \leq \left| \|\nabla f(x)\| - \frac{\|\nabla f(x)\|}{\|\nabla^2 f(y)\|} \right| + \frac{\kappa_{Lg} \|x - y\|}{\|\nabla^2 f(y)\|} \\ &\leq \|\nabla f(x)\| (\|\nabla^2 f(y)\| - \|\nabla^2 f(x)\|) + \kappa_{Lg} \|x - y\|. \end{aligned}$$

Thus, $|h(x) - h(y)| \leq (\kappa_{bfg}\kappa_{Lh} + \kappa_{Lg})\|x - y\|$.

The proof then results from the fact the maximum of two Lipschitz continuous functions is Lipschitz continuous and the fact that eigenvalues are Lipschitz continuous functions of the entries of a matrix. \square

The following lemma shows that the difference between the problem measure $\tau(x)$ and the model measure $\tau^m(x)$ is of the order of δ if $m(x)$ is a fully quadratic model on $B(x, \delta)$ (thus extending the error bound on the Hessians given in Definition 5.1).

Lemma 5.3 *Suppose that Assumption 5.1 holds. Given constants κ_{eh} , κ_{eg} , κ_{ef} , and δ_{\max} there exists a constant $\kappa_{e\tau}$ such that for any m_k which is $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic model of f on $B(x_k, \delta_k)$ with $x_k \in L(x_0)$ and $\delta_k \leq \delta_{\max}$ we have*

$$|\tau(x_k) - \tau^m(x_k)| \leq \kappa_{e\tau} \delta_k. \quad (11)$$

Proof. From the definition of fully quadratic models and the upper bounds on $\|\nabla f\|$ and $\|\nabla^2 f\|$ on $L_{enl}(x_0)$, we conclude that both $\|\nabla m(x_k)\|$ and $\|\nabla^2 m(x_k)\|$ are also bounded from above with constants independent of x_k and δ_k .

For a given x_k several situation may occur depending on which terms dominate in the expressions for $\tau(x_k)$ and $\tau^m(x_k)$. In particular, if $\|\nabla^2 f(x_k)\| \leq 1$ and $\|\nabla^2 m(x_k)\| \leq 1$, then

$$\tau(x_k) = \max \{ \|\nabla f(x_k)\|, -\lambda_{\min}(\nabla^2 f(x_k)) \}$$

and

$$\tau^m(x_k) = \max \{ \|\nabla m(x_k)\|, -\lambda_{\min}(\nabla^2 m(x_k)) \}$$

and the proof of the lemma is the same as in the case of the usual criticality measure, analyzed in [15]. Let us consider the case, when $\|\nabla^2 f(x_k)\| \geq 1$ and $\|\nabla^2 m(x_k)\| \geq 1$. From the fact that m_k is $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic we have that

$$\begin{aligned} \left| \frac{\|\nabla m(x_k)\|}{\|\nabla^2 m(x_k)\|} - \frac{\|\nabla f(x_k)\|}{\|\nabla^2 f(x_k)\|} \right| &\leq \left| \|\nabla m(x_k)\| \|\nabla^2 f(x_k)\| - \|\nabla f(x_k)\| \|\nabla^2 m(x_k)\| \right| \\ &\leq \|\nabla^2 f(x_k)\| \kappa_{eg} \delta_k^2 + \|\nabla f(x_k)\| \kappa_{eh} \delta_k \leq \kappa_{e\tau} \delta_k, \end{aligned}$$

for some large enough $\kappa_{e\tau}$, independent of x_k and δ_k .

The other two cases that need consideration are

- $\tau^m(x_k) = \frac{\|\nabla m(x_k)\|}{\|\nabla^2 m(x_k)\|}$, $\tau(x_k) = \|\nabla f(x_k)\|$, and
- $\tau(x_k) = \frac{\|\nabla f(x_k)\|}{\|\nabla^2 f(x_k)\|}$, $\tau^m(x_k) = \|\nabla m(x_k)\|$.

Let us consider the first case. We know that $\|\nabla^2 f(x_k)\| \leq 1 \leq \|\nabla^2 m(x_k)\|$ and hence $\|\nabla^2 m(x_k)\| - 1 \leq \|\nabla^2 m(x_k) - \nabla^2 f(x_k)\| \leq \kappa_{eh} \delta_k$. Now we can write,

$$\begin{aligned} |\tau(x_k) - \tau^m(x_k)| &= \left| \|\nabla f(x_k)\| - \frac{\|\nabla m(x_k)\|}{\|\nabla^2 m(x_k)\|} \right| \leq \left| \|\nabla f(x_k)\| - \frac{\|\nabla f(x_k)\|}{\|\nabla^2 m(x_k)\|} \right| + \frac{\kappa_{eg} \delta_k^2}{\|\nabla^2 m(x_k)\|} \\ &\leq \|\nabla f(x_k)\| (\|\nabla^2 m(x_k)\| - 1) + \kappa_{eg} \delta_k^2 \leq \|\nabla f(x_k)\| \kappa_{eh} \delta_k + \kappa_{eg} \delta_k^2 \leq \kappa_{e\tau} \delta_k, \end{aligned}$$

for some large enough $\kappa_{e\tau}$, independent of x_k and δ_k . The proof of the second case is derived in a similar manner. Combining these results with standard steps of analysis, such as the one in [15] we conclude the proof of this lemma. \square

Let us now define $\tau_k = \tau(x_k)$ and $\tau_k^m = \tau^m(x_k)$. From the assumption that $\nabla^2 f(x)$ is bounded on $L_{enl}(x_0)$, it is clear that if $\tau_k \rightarrow 0$ (when $k \rightarrow \infty$), then $\nabla f(x_k) \rightarrow 0$ and $\max\{-\lambda_{\min}(\nabla^2 f(x_k)), 0\} \rightarrow 0$. We next present an algorithm for which we will then analyze the convergence of τ_k .

5.2 Algorithm and liminf-type convergence

Consider the following modification of Algorithm 3.1.

Algorithm 5.1 Fix the positive parameters $\eta_1, \eta_2, \gamma, \delta_{\max}$, with $\gamma > 1 > \eta_1$. Select initial $k = 0$, $\delta_0 \leq \delta_{\max}$, and x_0 . At iteration k approximate the function f in $B(x_k, \delta_k)$ with m_k

and then approximately minimize m_k in $B(x_k, \delta_k)$, computing s_k so that it satisfies a fraction of optimal decrease (9). Let ρ_k be defined as in (3).

If $\rho_k \geq \eta_1$, set $x_{k+1} = x_k + s_k$ and

$$\delta_{k+1} = \begin{cases} \gamma^{-1} \delta_k & \text{if } \tau_k < \eta_2 \delta_k, \\ \min\{\gamma \delta_k, \delta_{\max}\} & \text{if } \tau_k \geq \eta_2 \delta_k. \end{cases}$$

Otherwise, set $x_{k+1} = x_k$ and $\delta_{k+1} = \gamma^{-1} \delta_k$.

Increase k by one and repeat the iteration.

The analysis of this method is similar to that of the first order method described in Section 3. The main difference lies in a replacement of the use of assumptions and in the lack of proof of the lim-type result. First, we will follow the steps of Section 3 to analyze the behavior of the trust-region radius.

Lemma 5.4 *For every realization of Algorithm 5.1,*

$$\lim_{k \rightarrow \infty} \delta_k = 0.$$

Proof. Suppose that $\{\delta_k\}$ does not converge to zero. Then, there exists $\epsilon > 0$ such that $\#\{k : \delta_k > \epsilon\} = \infty$. We are going to consider the following subsequence $\{k : \delta_k > \frac{\epsilon}{\gamma}, \delta_{k+1} \geq \delta_k\}$. By assumption this subsequence is infinite and due to the way δ_k is updated we have $\rho_k \geq \eta_1$ and $\tau_k^m \geq \eta_2 \frac{\epsilon}{\gamma}$ for each k in this subsequence.

First assume that $\min\{\|g_k\|, \frac{\|g_k\|}{\|H_k\|}\} \geq \eta_2 \frac{\epsilon}{\gamma}$. Therefore, from (9) we have

$$\begin{aligned} f(x_k) - f(x_k + s_k) &\geq \eta_1 (m(x_k) - m(x_k + s_k)) \\ &\geq \eta_1 \frac{\kappa_{fod}}{2} \|g_k\| \min\left\{\frac{\|g_k\|}{\|H_k\|}, \delta_k\right\} \\ &\geq \eta_1 \frac{\kappa_{fod}}{2} \eta_2 \frac{\epsilon^2}{\gamma^2} \min\{\eta_2, 1\}. \end{aligned}$$

Now assume that $-\lambda_{\min}(H_k) \geq \eta_2 \frac{\epsilon}{\gamma}$. Therefore, from (9) we have

$$\begin{aligned} f(x_k) - f(x_k + s_k) &\geq \eta_1 (m(x_k) - m(x_k + s_k)) \\ &\geq -\eta_1 \frac{\kappa_{fod}}{2} \lambda_{\min}(H_k) \delta_k^2 \\ &\geq \eta_1 \frac{\kappa_{fod}}{2} \eta_2 \frac{\epsilon^3}{\gamma^3}. \end{aligned}$$

This means that at iteration k the function f decreases by an amount bounded away from zero. Since we have assumed that there is an infinite number of such iterations, we obtain a contradiction with the assumption that f is bounded from below. \square

The next step is to extend Lemma 3.2 to the second order context.

Lemma 5.5 *If m_k is $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic on $B(x_k, \delta_k)$ and*

$$\delta_k \leq \min\left\{\tau_k^m, \sqrt{\frac{\kappa_{fod}(1-\eta_1)\tau_k^m}{4\kappa_{ef}}}, \frac{\kappa_{fod}(1-\eta_1)\tau_k^m}{4\kappa_{ef}}\right\},$$

then at the k -th iteration $\rho_k \geq \eta_1$.

The proof is a trivial extension of the proof of [15, Lemma 10.17] taking into account our modified definition of τ_k^m .

We can now prove the following convergence result which states that a subsequence of iterates approaches second order stationarity almost surely.

Theorem 5.1 *Suppose that the model sequence $\{M_k\}$ is probabilistically $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic for some positive constants κ_{eh} , κ_{eg} , and κ_{ef} . Let $\{X_k\}$ be a sequence of random iterates generated by Algorithm 5.1. Then, almost surely,*

$$\liminf_{k \rightarrow \infty} \tau(X_k) = 0.$$

Proof. As in Theorem 4.2, let us consider the random walk $W_k = \sum_{i=0}^k (2 \cdot 1_{S_i} - 1)$ (where 1_{S_i} is the indicator random variable, now based on the event S_i of Definition 5.2). All that follows is also conditioned on the almost sure event $D = \{\limsup_{k \rightarrow \infty} W_k = \infty\}$.

Suppose there exist $\epsilon > 0$ and k_1 such that, with positive probability, $\tau_k \geq \epsilon$, for all $k \geq k_1$. Let $\{x_k\}$ and $\{\delta_k\}$ be any realization of $\{X_k\}$ and $\{\Delta_k\}$, respectively, built by Algorithm 5.1. From Lemma 5.1, there exists k_2 such that we have $\forall k \geq k_2$

$$\delta_k < \mathbf{b} := \min \left\{ \frac{\epsilon}{2\kappa_{e\tau}}, \frac{\epsilon}{2}, \frac{\epsilon}{2\eta_2}, \sqrt{\frac{\kappa_{fod}(1-\eta_1)\epsilon}{8\kappa_{ef}}}, \frac{\kappa_{fod}(1-\eta_1)\epsilon}{8\kappa_{ef}}, \frac{\delta_{\max}}{\gamma} \right\} > 0. \quad (12)$$

Let $k \geq k_0 := \max\{k_1, k_2\}$ such that $1_{S_k} = 1$. Then, $|\tau_k - \tau_k^m| \leq \kappa_{e\tau}\delta_k < \frac{\epsilon}{2}$, and thus $\tau_k^m \geq \frac{\epsilon}{2}$. Now, using Lemma 5.5, we obtain $\rho_k \geq \eta_1$. We also have $\tau_k^m \geq \frac{\epsilon}{2} \geq \eta_2\delta_k$. Hence, by the construction of the algorithm, and the fact that $\delta_k \leq \frac{\delta_{\max}}{\gamma}$, we have $\delta_{k+1} = \gamma\delta_k$.

The rest of the proof is derived exactly as the proof of Theorem 4.2 (defining the random variable R_k with realization $r_k = \log_\gamma(\mathbf{b}^{-1}\delta_k)$, but with \mathbf{b} now given by (12)). Conditioning on D we obtain $\liminf_{k \rightarrow \infty} \tau(X_k) = 0$, and thus $\liminf_{k \rightarrow \infty} \tau(X_k) = 0$ almost surely. \square

5.3 The lim-type convergence

Let us summarize what we know about the convergence of Algorithm 5.1. Clearly all results that hold for Algorithm 3.1 also hold for Algorithm 5.1, hence as long as the probabilistically fully linear (or fully quadratic) models are used, almost surely, the iterates of Algorithm 5.1 form a sequence $\{x_k\}$, such that $\nabla f(x_k) \rightarrow 0$ as $k \rightarrow \infty$, in other words, the sequence $\{x_k\}$ converges to a set of first order stationary points. Moreover, as we just showed in the previous section, as long as the probabilistically fully quadratic models are used, there exists a subsequence of iterates $\{x_k\}$ which converges to a second order stationary point with probability one. Note that under certain assumptions, for instance, assuming that the Hessian of $f(x)$ is strictly positive definite at every second order stationary point, we can conclude from the results shown so far (and similarly to [8, Theorem 6.6.7]) that, almost surely, all limit points of the sequence of iterates of Algorithm 5.1 are second order stationary points.

There are however cases, when the set of first order stationary points is connected, and contains both second order stationary points and points with negative curvature of the Hessian. An example of such a function is

$$f(x) = xy^2.$$

All points such that $y = 0$ for a set of first order stationary points, while any $x \geq 0$ gives us second order stationary points, while $x < 0$ does not. In theory our algorithm may produce two subsequences of iterates, one converging to a point with $y = 0$ and $x > 0$ (a second order stationary point), and another converging to a point for which $y = 0$ and $x < 0$ (a first order stationary point with negative curvature of the Hessian).

Theorem 6.6.8 in [8] shows that all limit points of a trust-region algorithm are second order stationary without the assumption on these limit points being isolated, but under the condition that the trust-region radius is increased at successful iterations. The results in [15] show that all limit points of a trust-region framework based on deterministic fully quadratic models are second order stationary under slightly modified trust-region maintenance conditions. While the same result may be true for Algorithm 5.1 using probabilistically fully quadratic models, we were unable to extend the results in [15] to this case. Below we present explanations where such an extension fails, but the key lies in the fact that successful iterations and hence increase in the trust region are no longer guaranteed.

Conjecture 5.1 *Suppose that the model sequence $\{M_k\}$ is probabilistically $(\kappa_{eh}, \kappa_{eg}, \kappa_{ef})$ -fully quadratic for some positive constants κ_{eh} , κ_{eg} and κ_{ef} . Let $\{X_k\}$ be a sequence of random iterates generated by Algorithm 5.1. Then, almost surely,*

$$\lim_{k \rightarrow \infty} \tau(X_k) = 0.$$

Let us attempt to follow the same logic as in the proof of Theorem 4.3. The first part of the proof applies immediately after substituting $\|\nabla f(x)\|$ by $\tau(x)$ wherever is appropriate.

Indeed, suppose that $\lim_{k \rightarrow \infty} \tau(X_k) = 0$ does not hold almost surely. Then, with positive probability, there exists $\epsilon > 0$ such that $\tau(X_k) > 2\epsilon$, holds for infinitely many k 's. Without loss of generality, we assume that $\epsilon = \frac{1}{n_\epsilon}$, for some natural number n_ϵ .

Let $\{K_i\}$ be a subsequence of the iterations for which $\tau(X_k) > \epsilon$. We are going to show that, if such an ϵ exists then $\sum_{j \in \{K_i\}} \Delta_j$ is a divergent sum.

Let us call a pair of integers (W', W'') an ‘‘ascent’’ pair if $0 < W' < W''$, $\tau(X_{W'}) \leq \epsilon$, $\tau(X_{W'+1}) > \epsilon$, $\tau(X_{W''}) > 2\epsilon$ and, moreover, for any $w \in (W', W'')$, $\epsilon < \tau(X_w) \leq 2\epsilon$. Each such ascent pair forms a nonempty interval of integers $\{W' + 1, \dots, W''\}$ which is a subset of the sequence $\{K_i\}$. Since $\liminf_{k \rightarrow \infty} \tau(X_k) = 0$ holds almost surely (by Theorem 5.1), it follows that there are infinitely many such intervals. Let us consider the sequence of these intervals $\{(W'_\ell, W''_\ell)\}$. The idea is now to show (with positive probability) that, for any ascent pair (W'_ℓ, W''_ℓ) with ℓ sufficiently large, $\sum_{j=W'_\ell+1}^{W''_\ell-1} \Delta_j$ is uniformly bounded away from 0 (and hence $W'_\ell + 1 < W''_\ell$), which implies that $\sum_{j \in \{K_i\}} \Delta_j = \infty$ since $\sum_\ell \sum_{j=W'_\ell+1}^{W''_\ell-1} \Delta_j \leq \sum_{j \in \{K_i\}} \Delta_j$, because the sequence $\{K_i\}$ contains all intervals $\{W'_\ell, W''_\ell\}$.

Let $\{x_k\}$ and $\{\delta_k\}$ be realizations of $\{X_k\}$ and $\{\Delta_k\}$, for which $\tau_k > \epsilon$ for $k \in \{k_i\}$. By the triangle inequality, for any ℓ ,

$$\epsilon < \left| \tau_{w'_\ell} - \tau_{w''_\ell} \right| \leq \sum_{j=w'_\ell}^{w''_\ell-1} |\tau_j - \tau_{j+1}|.$$

Since $\tau(x)$ is Lipschitz continuous (with constant $\kappa_{L\tau}$),

$$\epsilon \leq \sum_{j=w'_\ell}^{w''_\ell-1} |\tau_j - \tau_{j+1}| \quad (13)$$

$$\leq \kappa_{L\tau} \sum_{j=w'_\ell}^{w''_\ell-1} \|x_j - x_{j+1}\| \quad (14)$$

$$\leq \kappa_{L\tau} \left(\delta_{w'_\ell} + \sum_{j=w'_\ell+1}^{w''_\ell-1} \delta_j \right). \quad (15)$$

From the fact that δ_k converges to zero, then, for any ℓ large enough, $\delta_{w'_\ell} < \frac{\epsilon}{2\kappa_{L\tau}}$, and hence $\sum_{j=w'_\ell+1}^{w''_\ell-1} \delta_j > \frac{\epsilon}{2} > 0$, which gives us $\sum_{j \in \{k_i\}} \delta_j = \infty$.

We have thus proved that if, $\lim_{k \rightarrow \infty} \tau(X_k) = 0$ does not hold almost surely, then, with positive probability, there exists n_ϵ such that $\{K_i\}$ defined as above based on n_ϵ , satisfies $\sum_{j \in \{K_i\}} \Delta_j = \infty$.

The second part of the proof should rely on providing the contradiction to the statement that $\sum_{j \in \{K_i\}} \Delta_j = \infty$ can happen with positive probability. In the case of Theorem 4.3 the proof utilized the fact that the sum of all δ_j , for all $j \in \{p_i\}$ such that m_j is fully linear, has to be finite, because it appears as a term in the lower bound on the total decrease of the objective function (see Lemma 4.2). However, in the second order case the total decrease of the objective function is bounded from below by a factor of $\sum_{j \in \{p_i\}} \delta_j^2$. Hence it is possible that $\sum_{j \in \{k_i\}} \delta_j^2 < \infty$, while $\sum_{j \in \{k_i\}} \delta_j = \infty$. In the deterministic case the proof of the fact that $\sum_{j \in \{k_i\}} \delta_j < \infty$ relies on the trust-region maintenance strategy. In particular if the model m_j is fully quadratic for every $j \in \{k_i\}$ then the trust-region radius is increased at each iteration $j \in \{k_i\}$. In other words, for large enough ℓ , $\delta_{w'_\ell+2} = \gamma \Delta_{w'_\ell+1}$ and so on until $\delta_{w''_\ell-1} = \gamma \delta_{w''_\ell-2}$. Hence

$$\sum_{j=w'_\ell+1}^{w''_\ell-1} \delta_j < M \delta_{w''_\ell-1}. \quad (16)$$

This then implies that $\sum_{j=w'_\ell+1}^{w''_\ell-1} \delta_j \rightarrow 0$ as $\ell \rightarrow \infty$ because $\delta_{w''_\ell-1} \rightarrow 0$.

The difficulty in the probabilistic case comes from the fact that the trust region only increases with some high probability, but not necessarily at each iteration. In general it is possible to construct examples of random walks, which satisfy the conditions on the maintenance of δ_j , but for which with positive probability there exist arbitrarily large indices w'_ℓ and w''_ℓ , such that $w''_\ell - w'_\ell$ is arbitrarily large, and such that (16) does not hold. In other words, under the current conditions we are not able to show that (16) holds with probability one for all ℓ , hence we cannot prove the conjecture. The proof can be established under the additional assumption that the probability of occurrence of fully quadratic models increases in some cases as the algorithm progresses. However, this scenario essentially leads to deterministic schemes and hence is of no interest for this paper.

6 Examples of probabilistically fully linear and fully quadratic models in DFO

In the previous section we described an algorithmic framework that is based on models whose approximation quality is random and is sufficiently good with probability more than $1/2$ (conditioned on the past). We called such models probabilistically fully linear or fully quadratic, depending on the quality of approximation that they provide. In this section, we discuss how such models can be generated (for some large enough values of the κ constants) and outline future research in this direction.

6.1 Fully linear and fully quadratic polynomial interpolation models and Λ -poised sample sets

Let \mathcal{P}_n^d denote the set of polynomials of degree $\leq d$ in \mathbb{R}^n and let $q_1 = q + 1$ denote the dimension of this space. It is clear that the dimension of \mathcal{P}_n^1 is $q_1 = n + 1$ and the dimension of \mathcal{P}_n^2 is $q_1 = \frac{1}{2}(n + 1)(n + 2)$. A basis $\Phi = \{\phi_0(x), \phi_1(x), \dots, \phi_q(x)\}$ for \mathcal{P}_n^d is a set of q_1 polynomials of degree $\leq d$ that span \mathcal{P}_n^d . For any such basis Φ , any polynomial $m(x) \in \mathcal{P}_n^d$ can be written as

$$m(x) = \sum_{j=0}^q \alpha_j \phi_j(x), \quad (17)$$

where the α_j 's are real coefficients. Given a set of $p_1 = p + 1$ points $Y = \{y_0, y_1, \dots, y_p\} \subset \mathbb{R}^n$, $m(x)$ is said to be the interpolation polynomial of $f(x)$ on Y if it satisfies

$$M(\Phi, Y)\alpha = f(Y), \quad (18)$$

where $M(\Phi, Y)$ is defined as follows

$$M(\Phi, Y) = \begin{bmatrix} \phi_0(y^0) & \phi_1(y^0) & \cdots & \phi_q(y^0) \\ \phi_0(y^1) & \phi_1(y^1) & \cdots & \phi_q(y^1) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_0(y^p) & \phi_1(y^p) & \cdots & \phi_q(y^p) \end{bmatrix} \quad (19)$$

and $f(Y)$ is the p_1 dimensional vector whose entries are $f(y_i)$ for $i = 0, \dots, p$. The interpolation polynomial $m(x)$ exists and is unique if and only if $p = q$ and the set Y is *poised* [27], which essentially means that $M(\Phi, Y)$ is nonsingular. When the number of points p_1 is smaller than the number of elements in Φ the matrix $M(\Phi, Y)$ has more columns than rows and the system (18) is underdetermined. In this case there are several choices of interpolating polynomials, which we will discuss later. If, on the other hand, $p > q$, then the system (18) is overdetermined and one can apply least squares regression instead of interpolation. Other polynomial approximations are also possible. If Y is such that the condition number of $M(\Phi, \hat{Y})$ is bounded by Λ , where $\hat{Y} = \{(y_0 - x_k)/\Delta, \dots, (y_p - x_k)/\Delta\}$ is a scaled version of Y , then we say that Y is Λ -poised (see [15]). It is shown in [12, 13, 15] that if Y is Λ -poised and $p_1 \geq n + 1$, then one can build a model which is $(\kappa_{ef}, \kappa_{eg})$ -fully linear, with κ_{ef} and κ_{eg} both equal to $\mathcal{O}(p\Lambda)$. Analogously, it is shown that if $p_1 \geq (n + 1)(n + 2)/2$, then one can also build a $(\kappa_{ef}, \kappa_{eg}, \kappa_{eh})$ -fully quadratic polynomial model with κ_{ef} , κ_{eg} , and κ_{eh} equal to $\mathcal{O}(p\Lambda)$. Hence, to build a fully quadratic model in n dimensions one may require $(n + 1)(n + 2)/2$ sample points (within reasonable proximity

of the current iterate x_k). If such a sample set is already available, estimating the condition number of the matrix $M(\Phi, Y)$ may require up to $\mathcal{O}(n^6)$ arithmetic operations. This dependency on the dimension limits the use of fully quadratic models to small dimensional problems.

There are two main ways to improve the per-iteration complexity of DFO algorithms. One approach, to only change the sample set by one point at a time, has been very successful in practice, as it not only reduces the number of function evaluations, but also the linear algebra involved [11, 18, 29, 35]. However, in [31] it was shown that such algorithms still require computing a Λ -poised set in the criticality step of the trust-region framework. Hence computation of up to n new sample points is required if fully linear models are used, while for fully quadratic models up to $(n+1)(n+1)/2 - 1$ new sample points have to be evaluated.

The other, complementary, approach is to use quadratic models based on fewer than $(n+1)(n+2)/2$ sample points, which also reduces both the cost of the linear algebra and the number of function evaluations. In practical DFO applications, incomplete quadratic models have been used very successfully.

Let $Y = \{y_0, y_1, \dots, y_p\}$ be a set of $p+1$ sample points with $p < q$ and let $\Phi = \{1, x_1, x_2, \dots, x_n, x_1^2/2, x_1x_2, \dots, x_{n-1}x_nx_n^2/2\}$. The interpolating polynomial for f on the set Y is given by (17), where α satisfies the undetermined interpolation system (18). Since this system admits multiple solutions we have some freedom in selecting α . In [11, 15, 35] the minimum Frobenius norm (MFN) models are considered, i.e., the models for which the Frobenius norm of the Hessian, or $\|\alpha_Q\|_2 = \|(\alpha_{n+1}, \alpha_{n+2}, \dots, \alpha_q)\|_2$, is minimized subject to (18). In [29] Powell selects the model based on minimizing the Frobenius norm of the update of the Hessian. Both these methods are successful in practice, and provide useful second order information. However, so far theoretically they are not shown to be superior to simple linear models. Indeed as we will show in the example below the MFN models may be nearly as bad as simple linear models, but the use of random sample sets can provide a significant practical improvement in this case.

6.2 Random sample sets

In the cases when function evaluations are not very expensive or can be obtained in parallel, there is less incentive to reuse old sample points for model building, because ensuring the model quality can become the bottleneck of the computations. Instead, one can simply use well-poised deterministic sample sets, chosen in advance. However this is not always the best approach, because the pattern is chosen without any consideration for the shape of the function and may be a very poor fit. In Section 2 we have seen examples where random directions provided better decrease on average than those from a fixed pattern. Similarly, random sample sets can automatically provide good quality models with high enough probability, yet they do not suffer from the worst case behavior of the deterministic sample sets. We consider another example.

Example of comparison of using underdetermined quadratic models based on random and deterministic sample sets. Let us consider the function $f(x) = 10(x_2 - x_1^2)^2 + (1 - x_1)^2$, which is a version of the Rosenbrock function used in Section 2, but with smaller curvature and Hessian condition number. We apply a trust-region method [3] to this function with models based on 5 points at each iteration and construct MFN models based on the sample sets. Note that a fully quadratic model requires 6 points. In one case we choose deterministic models with the sample set selected as the current iterate plus the coordinate steps of length δ , i.e., $Y = \{y^0, y^0 \pm \delta e_1, y^0 \pm \delta e_2\}$ — a very well poised set. In other words, the set Y is generated

Iter. #	success	f value	Δ	ρ
1687	0	+3.67420711e-04	+3.12e-02	-1.66e+00
1688	1	+3.67418778e-04	+6.25e-02	+8.13e+02
1689	0	+3.67418778e-04	+3.12e-02	-1.66e+00
1690	1	+3.67409693e-04	+6.25e-02	+3.92e+03
1691	0	+3.67409693e-04	+3.12e-02	-1.66e+00
1692	1	+3.67407812e-04	+6.25e-02	+8.34e+02
1693	0	+3.67407812e-04	+3.12e-02	-1.66e+00
1694	1	+3.67398959e-04	+6.25e-02	+4.03e+03
1695	0	+3.67398959e-04	+3.12e-02	-1.66e+00

Table 1: The illustration of the oscillating behavior of a trust-region method based on deterministic underdetermined sample set.

around the current iterate y^0 by adding coordinate steps of size δ . For the second method we generate the set Y by picking 4 random points in a ball of radius δ around the current iterate. The results are as follows: the method based on deterministic sample sets achieved the final function value of 10^{-4} in 8500 function evaluations, while the method based on random sample sets achieved (on average over ten runs) the function value of 10^{-6} in 2500 function evaluations (with largest deviation of under 200 function evaluations and less than one order of magnitude in accuracy). Clearly, using random sample sets enhances the performance of the MFN models here. In particular, one can observe the slow progress of the deterministic method in Table 6.2 which represents iteration output. It is clear from the table that iterations follow a pattern (which starts at around iteration 1000) where δ_k increased and decreased according to alternating successful and unsuccessful steps, while the progress is slow overall. We have repeated the experiments 10 times with the fixed pattern which a randomly rotated equivalent of Y defined above. The cyclic behavior and significant slow down did not occur for every pattern, but for about half of these patterns. The variance in the number of function values was in the order of thousands and the final accuracy varied from 3 to 8 digits, a very non-robust behavior. The purpose of this example is to illustrate the effect of random sample sets. Note, that if instead of fixed well-posed deterministic sample sets, we had used sample sets which included some recent old sample points, then the behavior of the MFN method would have matched that of the method based on random sample sets. We believe that this is due to the fact that the sets of (recent) old sample points have essentially random behavior (although theoretically this cannot be proved, of course).

Analysis of poisedness of random sample sets. Let us consider a sample set $Y = \{0, y^1, \dots, y^p\} \subset \mathbb{R}^n$ with a fixed point at the origin and the remaining n points being generated randomly from a standard Gaussian distribution (with zero mean and covariance matrix equal to the identity matrix, with the case of a scaled identity matrix being a simple extension of what we present below). Let us consider $\Phi(x) = \{1, x_1, x_2, \dots, x_n\}$. Hence $M(\Phi, Y)$ is simply a matrix whose first column is all 1's, the first row is zero except the first element and the remaining $p \times n$ matrix is a Gaussian random matrix. Under a simple transformation, the condition number of $M(\Phi, Y)$ is equal to the condition number of a random Gaussian $p \times n$

matrix. From results in random matrix theory [7, 17] we have the following bound

$$P(\text{cond}(M(\Phi, Y)) > \Lambda) \leq C(n, p) \frac{1}{\Lambda^{|n-p|+1}},$$

where $C(n, p)$ is a constant dependent on p and n . In particular, for $p = n$ the result in [7] implies

$$P(\text{cond}(M(\Phi, Y)) > \Lambda) \leq \frac{1}{\sqrt{2\pi}} \frac{Cn}{\Lambda}.$$

where C is a universal constant smaller than 6.5. This result implies that given n and p , there exists Λ large enough such that $P(\text{cond}(M(\Phi, Y)) < \Lambda) > \frac{1}{2}$. Hence there exist constants κ_{ef} and κ_{eg} such that the linear interpolation (or regression) polynomials based on Gaussian sample sets are probabilistically $(\kappa_{ef}, \kappa_{eg})$ -fully linear.

A more complicated, but important class of models are the quadratic models based on sample sets of $p + 1 > n + 1$ sample points. In this case the basis Φ is constructed from first and second order polynomials and $M(\Phi, Y)$ no longer has the simple structure of a Gaussian matrix. Matrices of this form have been studied in [30] and are referred to as structured random matrices. The bounds derived in [30] show that the condition number of $M(\Phi, Y)$ is small with sufficiently high probability if p is large enough (but still scales pseudo-linearly with the number of columns in $M(\Phi, Y)$). We believe that these results can be used to show that for a fixed p , the condition number of $M(\Phi, Y)$ is bounded with sufficiently high probability. Explicit derivations of such bounds and conditions is subject for future research.

Sparse models based on random sample sets. A natural question that arises in our context is whether we can build accurate, i.e., fully quadratic models, without requiring $(n + 1)(n + 2)/2$ sample points. For instance, in larger dimensional cases it often happens that the Hessian of the objective function is sparse. Clearly, if we know in advance that some elements of the Hessian (coefficients of α_Q) are zero, then we can reduce the number of variables in system (18). However, in a typical situation of a black-box optimization, the information about the sparsity of the Hessian is not available. It has been shown recently in [3] that by minimizing $\|\alpha_Q\|_1$ instead of $\|\alpha_Q\|_2$ it is possible to recover fully quadratic interpolation models of a function with sparse Hessian by using fewer sample points than $(n + 1)(n + 2)/2$. This is the first result that shows that fully quadratic model recovery with incomplete sample sets is possible. This result relies on the theory of sparse recovery in compressed sensing [6] and on results in random matrix theory [30]. In particular these models are shown to be fully quadratic with probability larger than $1 - n^{-\gamma \log p}$, for some universal constant $\gamma > 0$, as long as the number of sample points satisfies $p \geq \mathcal{O}(n(\log n)^4)$ and a sparse fully quadratic model exists.

Similar, but much simpler results can be obtained for recovery of a sparse fully linear model, if such a model exists. In this case, the sample set Y can be generated by a Gaussian distribution around the current iterate and the random matrix $M(\Phi, Y)$ can be viewed as a Gaussian matrix, just as it described above. Sparse signal recovery can be applied in this well-known case to show that if the number of nonzeros in the gradient is s and the number of sample points is

$$p \geq Cs \log(n/s),$$

then a sparse fully linear model can be recovered with probability greater than $1 - c_1 e^{-c_2 p}$, for some universal constants c_1, c_2 , and C . In fact the constants also depend on the error between the function values $f(y_i)$ and the sparse model values $m(y_i)$, but we omit these details here for simplicity.

Nonuniform recovery and martingale property. In the examples we considered so far the sample sets are generated to provide high quality of the models independently of the past history of the algorithm. However, our theory allows the probability of a good model to be dependent on the past. In some cases taking this into account may provide a more efficient approach to building models. Here we discuss one possible example.

The results of recovery of sparse models which we considered so far from compressed sensing imply, the so-called, uniform recovery, where the matrix $M(\Phi, Y)$ is designed in such a way that *any* sparse model can be recovered. However, in our case, it is sufficient to recover the specific model that happens to approximate the objective function f sufficiently well in a trust region. Thus, the *nonuniform* recovery results can apply. Some of these results, including the ones for the Gaussian matrices, can be found in [2, 30]. The key is that if only one fixed signal needs to be recovered with high probability, then it is sufficient to generate the random matrix $M(\Phi, Y)$ using fewer samples than what is necessary for the uniform recovery. The probability of generating a fully linear or fully quadratic model can be made sufficiently high, conditioned on the model itself. This fact, in our setting, means that the probability of a “good” model is high, conditioned on the current iterate and trust-region radius, in other words, on the past behavior of the algorithm. In short, we observe that such a setting will satisfy the submartingale property, but not complete independence on the past.

Example of comparing performance of sparse model recovery vs. other underdetermined second order models. Consider the following function again, $f(x) = 10(x_2 - x_1^2)^2 + (1 - x_1)^2$, but this time $x \in \mathbb{R}^{10}$, which means that we have a 10-dimensional problem, but only the first two dimensions are important. Note that to build a fully linear model without applying sparse recovery we need to sample 11 points, and to build a fully quadratic model we need 66 sample points. We apply three variants of the trust-region algorithm discussed in this paper to this problem which only differ by the choice of the models. In the first case, the models are built based on a fixed number n_Y of random points that are distributed in a small hypercube around the current iterate, and we call this method RSTR. In the second case, we build sparse models based on “greedy” sample sets of up to a given number of points n_Y , which only use points generated in the course of the trust-region steps, in other words, reusing old points, and we call it GSTR. The third algorithm uses the same greedy sample sets, but constructs MFN models, rather than sparse models, we call this method MFN. We repeated the experiments for each method for n_Y ranging from 16 to 40, for RSTR we report results averages over 5 runs, since the outcome is random. The resulting numbers of function evaluations and iterations are illustrated in Table 6.2.

The number of function evaluations taken by GSTR and MFN are roughly the same as the number of iterations, because only one function value is computed per iteration, except for the first iteration. From the number of iterations required by each algorithm it is evident that RSTR clearly recovers the fully quadratic models of f , with as few as 20 sample points, while the other two methods do not. While the first algorithm performs more function evaluations, they can be obtained in parallel, and the achieved accuracy is by far better than that of the other methods. We want to note that while the outcome of RSTR is random, we observed very little variance in the number of iterations, and hence, function evaluations, in our experiments. It is also interesting to observe that the number of iterations of RSTR does not get smaller after the size of the n_Y exceeds 20, hence, it appears that while larger number of sample points per iteration may allow for more reliable recovery, it is not necessary for fast convergence. Computational

n_Y	# of iter. RSTR	# of iter. GSTR	# of iter. MFN	# of fun. eval. RSTR
16	189	318	767	3027
17	99	247	1048	1693
18	38	158	925	680
19	30	157	646	585
20	27	137	1086	536
21	20	144	919	424
22	21	145	778	462
23	24	149	848	547
24	19	150	962	515
25	20	152	636	504
26	19	144	414	513
27	19	125	456	509
28	18	166	401	568
29	20	137	659	570
30	19	122	503	607
31	20	154	349	627
32	20	157	390	646
33	20	164	484	528
34	18	175	442	605
35	18	164	362	637
36	20	139	301	727
37	20	162	328	754
38	20	136	439	652
39	18	183	316	702
40	19	152	536	760

Table 2: The comparison of the number of iterations and function evaluations for RSTR, averaged over 5 runs, (accuracy for $n_Y \geq 20$ is $1.0e - 11$), GSTR (accuracy $1.0e - 9$), and MFN (accuracy $1.0e - 5$) methods.

trade-offs in optimization using sparse models is a subject of a separate study.

Other random models. Additional settings where relying on random models may give an advantage for an optimization scheme occur in a parallel environment when full synchronization is not needed. We may wish to consider the following asynchronous setting: each processor takes different, random amount of time to compute a function value. Let us consider a time budget τ . Let us now assume that a sufficiently large number of function evaluations are computed in less than τ time, with some sufficiently high probability. If we assign function evaluations to processors randomly, then the resulting sample set is random and the resulting model is well-poised with high probability.

Alternatively, one may consider a setting where the objective function is evaluated approximately for each sample point, with some high probability of this approximation being accurate, but yet some small probability of a bad approximation. In this case the resulting interpolation/regression model will provide a good approximation with high probability. Note that when computing the function value at the potential new iterate (rather than a sample point) one is still assuming that an accurate value is computed. Relaxing this condition is also a subject for future study.

Reusing sample points. In a sequential computational setting with expensive function evaluations it is efficient to reuse existing sample points in the vicinity of the current iteration. The success of the second method in the example above indicates that sparse models based on greedy sample sets are useful, even though the sparse recovery properties are unlikely to hold for such sets. Hence the random sample models may be dependent in some practical approaches. An obvious example of a method which reuses sample points and relies on sample models would be as follows. At each iteration the interpolation model is build based on up to $n + 1$ existing sample points and an additional number of random sample points. The past points are picked so that they are in a reasonable vicinity of the current iterate and so that they form a well-poised set. For various technique of selecting such a set, see [15]. The random points are selected to enrich the current set of sample points. The resulting sample set clearly depends on the history of the algorithm, on the other hand, if the set of re-used sample points is well poised, then the whole set is well-poised with sufficiently high probability. Investigating general cases of models when the submartingale property holds, or relaxing the submartingale property in a controlled way, and deriving new convergence results is a subject of our future research. Before more detailed analysis is derived it is essential to identify classes of random models that best perform in practice.

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References

- [1] C. Audet and J. E. Dennis Jr. Mesh adaptive direct search algorithms for constrained optimization. *SIAM J. Optim.*, 17:188–217, 2006.

- [2] U. Ayaz and H. Rauhut. Nonuniform sparse recovery with subgaussian matrices. *ETNA*, 2013, to appear.
- [3] A. S. Bandeira, K. Scheinberg, and L. N. Vicente. Computation of sparse low degree interpolating polynomials and their application to derivative-free optimization. *Math. Program.*, 134:223–257, 2012.
- [4] S. C. Billups, J. Larson, and P. Graf. Derivative-free optimization of expensive functions with computational error using weighted regression. *SIAM J. Optim.*, 23:27–53, 2013.
- [5] R. Byrd, G. M. Chin, J. Nocedal, and Y. Wu. Sample size selection in optimization methods for machine learning. *Math. Program.*, 134:127–155, 2012.
- [6] E. J. Candès. Compressive sampling. *Proceedings of the International Congress of Mathematicians Madrid 2006*, Vol. III, 2006.
- [7] Z. Chen and J. J. Dongarra. Condition numbers of Gaussian random matrices. *SIAM J. Matrix Anal. Appl.*, 27:603–620, 2005.
- [8] A. R. Conn, N. I. M. Gould, and Ph. L. Toint. *Trust-Region Methods*. MPS-SIAM Series on Optimization. SIAM, Philadelphia, 2000.
- [9] A. R. Conn, K. Scheinberg, and Ph. L. Toint. On the convergence of derivative-free methods for unconstrained optimization. In M. D. Buhmann and A. Iserles, editors, *Approximation Theory and Optimization, Tributes to M. J. D. Powell*, pages 83–108. Cambridge University Press, Cambridge, 1997.
- [10] A. R. Conn, K. Scheinberg, and Ph. L. Toint. Recent progress in unconstrained nonlinear optimization without derivatives. *Math. Program.*, 79:397–414, 1997.
- [11] A. R. Conn, K. Scheinberg, and Ph. L. Toint. A derivative free optimization algorithm in practice. In *Proceedings of the 7th AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, St. Louis, Missouri, September 2-4*, 1998.
- [12] A. R. Conn, K. Scheinberg, and L. N. Vicente. Geometry of interpolation sets in derivative free optimization. *Math. Program.*, 111:141–172, 2008.
- [13] A. R. Conn, K. Scheinberg, and L. N. Vicente. Geometry of sample sets in derivative free optimization: Polynomial regression and underdetermined interpolation. *IMA J. Numer. Anal.*, 28:721–748, 2008.
- [14] A. R. Conn, K. Scheinberg, and L. N. Vicente. Global convergence of general derivative-free trust-region algorithms to first and second order critical points. *SIAM J. Optim.*, 20:387–415, 2009.
- [15] A. R. Conn, K. Scheinberg, and L. N. Vicente. *Introduction to Derivative-Free Optimization*. MPS-SIAM Series on Optimization. SIAM, Philadelphia, 2009.
- [16] R. Durrett. *Probability: Theory and Examples*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, Cambridge, fourth edition, 2010.
- [17] A. Edelman. Eigenvalues and condition numbers of random matrices. *SIAM J. Matrix Anal. Appl.*, 9:543–560, 1988.
- [18] G. Fasano, J. L. Morales, and J. Nocedal. On the geometry phase in model-based algorithms for derivative-free optimization. *Optim. Methods Softw.*, 24:145–154, 2009.
- [19] S. Ghadimi and G. Lan. Stochastic first- and zeroth-order methods for nonconvex stochastic programming. Technical report, University of Florida, 2012.
- [20] T. G. Kolda, R. M. Lewis, and V. Torczon. Optimization by direct search: New perspectives on some classical and modern methods. *SIAM Rev.*, 45:385–482, 2003.
- [21] J. Matyas. Random optimization. *Automation and Remote Control*, 26:246–253, 1965.
- [22] J. J. Moré and S. M. Wild. Benchmarking derivative-free optimization algorithms. *SIAM J. Optim.*, 20:172–191, 2009.
- [23] Y. Nesterov. Random gradient-free minimization of convex functions. Technical Report 2011/1, CORE, 2011.
- [24] Y. Nesterov. Efficiency of coordinate descent methods on huge-scale optimization problems. *SIAM J. Optim.*, 22:341–362, 2012.
- [25] B. T. Polyak. *Introduction to Optimization*. Optimization Software, 1987.

- [26] M. J. D. Powell. A direct search optimization method that models the objective and constraint functions by linear interpolation. In S. Gomez and J.-P. Hennart, editors, *Advances in Optimization and Numerical Analysis, Proceedings of the Sixth Workshop on Optimization and Numerical Analysis, Oaxaca, Mexico*, volume 275 of *Math. Appl.*, pages 51–67. Kluwer Academic Publishers, Dordrecht, 1994.
- [27] M. J. D. Powell. On the Lagrange functions of quadratic models that are defined by interpolation. *Optim. Methods Softw.*, 16:289–309, 2001.
- [28] M. J. D. Powell. On trust region methods for unconstrained minimization without derivatives. *Math. Program.*, 97:605–623, 2003.
- [29] M. J. D. Powell. Least Frobenius norm updating of quadratic models that satisfy interpolation conditions. *Math. Program.*, 100:183–215, 2004.
- [30] H. Rauhut. Compressive sensing and structured random matrices. In M. Fornasier, editor, *Theoretical Foundations and Numerical Methods for Sparse Recovery*, Radon Series Comp. Appl. Math., pages 1–92. 2010.
- [31] K. Scheinberg and Ph. L. Toint. Self-correcting geometry in model-based algorithms for derivative-free unconstrained optimization. *SIAM J. Optim.*, 20:3512–3532, 2010.
- [32] V. Torczon. On the convergence of pattern search algorithms. *SIAM J. Optim.*, 7:1–25, 1997.
- [33] L. N. Vicente. Worst case complexity of direct search. *EURO Journal on Computational Optimization*, 1, 2013.
- [34] L. N. Vicente and A. L. Custódio. Analysis of direct searches for discontinuous functions. *Math. Program.*, 133:299–325, 2012.
- [35] S. M. Wild. MNH: A derivative-free optimization algorithm using minimal norm Hessians. In *Tenth Copper Mountain Conference on Iterative Methods*, April 2008.