Sharp worst-case evaluation complexity bounds for arbitrary-order nonconvex optimization with inexpensive constraints

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Abstract

We provide sharp worst-case evaluation complexity bounds for nonconvex minimization problems with general inexpensive constraints, i.e. problems where the cost of evaluating/enforcing of the (possibly nonconvex or even disconnected) constraints, if any, is negligible compared to that of evaluating the objective function. These bounds unify, extend or improve all known upper and lower complexity bounds for unconstrained and convexly-constrained problems. It is shown that, given an accuracy level ϵ, a degree of highest available Lipschitz continuous derivatives p and a desired optimality order q between one and p, a conceptual regularization algorithm requires no more than $O(\epsilon^{-\frac{p+1}{p-q+1}})$ evaluations of the objective function and its derivatives to compute a suitably approximate q-th order minimizer. With an appropriate choice of the regularization, a similar result also holds if the p-th derivative is merely Hölder rather than Lipschitz continuous. We provide an example that shows that the above complexity bound is sharp for unconstrained and a wide class of constrained problems; we also give reasons for the optimality of regularization methods from a worst-case complexity point of view, within a large class of algorithms that use the same derivative information.

1 Introduction

Since the seminal paper by Vavasis [21] on the complexity of finding first-order critical points in unconstrained nonlinear optimization was published 25 years ago, the question of the optimal worst-case complexity of optimization methods has been of interest to mathematicians and also, because of its strong connection with deep learning, to computer scientists. Of late, there has been a growing interest in this research field, both for convex and nonconvex problems. This paper focusses on the latter class and follows a now subtantial[(1)] trend of research where bounds on the worst-case evaluation complexity (or oracle complexity) of obtaining first- and

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[(1)]See [12] for a more complete list of references.

(more rarely) second-order-necessary minimizers[(2)] for nonlinear nonconvex unconstrained optimization problems [21, 17, 14, 19, 5]. These papers all provide *upper* evaluation complexity bounds: they show that, to obtain an ϵ-approximate first-order-necessary minimizer (for unconstrained problem, this is a point at which the gradient of the objective function is less than ϵ in norm), *at most* $O(\epsilon^{-2})$ evaluations of the objective function[(3)] are needed if a model involving first derivatives is used, and *at most* $O(\epsilon^{-3/2})$ evaluations are needed if using second derivatives is permitted. This result was extended to convexly-constrained problems in [6]. A broader framework allowing the use of Taylor series of degree p was more recently proposed in [2], in which case the worst-case evaluation complexity bound for ϵ-first-order-necessary unconstrained minimizer is shown to be $O(\epsilon^{-\frac{p+1}{p}})$, thereby generalizing the previous results for this case. Complexity for obtaining ϵ-approximate second-order-necessary unconstrained minimizers was considered in [19, 5], where a bound of $O(\epsilon^{-3})$ evaluations was proved to obtain an ϵ-second-order-necessary minimizer using a Taylor's model of degree two, and a bound of $O(\epsilon^{-\frac{p+1}{p-1}})$ evaluations was shown in [8] for the case where a Taylor model of degree p is used. Defining q-th-order-necessary minimizers for $q > 2$ was considered in [11], where the difficulty of stating and verifying necessary optimality was discussed. In particular, it was concluded in this latter reference that defining and computing ϵ-approximate q-th-order-necessary minimizers for $q > 2$ is likely to remain elusive, essentially because of the nonlinearity and lack of continuity of the kernels of the derivatives involved. A more general Taylor-based definition of optimality was introduced instead, which allowed to show an upper bound of $O(\epsilon^{-(q+1)})$ on evaluation complexity for convexly-constrained problems, in particular improving on the bound of $O(\epsilon^{-9/2})$ stated in [1] for the case $p = q = 3$.

The unconstrained and convexly-constrained cases where the assumption of Lipschitz continuity is replaced by the weaker β-Hölder continuity ($\beta \in (0, 1]$) have also been studied for $q = 1$ in [18, 7, 9]. These references show that *at most* $O(\epsilon^{-\frac{p+\beta}{p-1+\beta}})$ evaluations are needed for obtaining an ϵ-first-order-necessary minimizer.

While upper complexity bounds are important as they provide a handle on the intrinsic difficulty of the considered problem, they do so at the condition of not being overly pessimistic. To address this last point, *lower* bounds on the evaluation complexity of unconstrained nonconvex optimization problems and methods were derived in [4, 17] and [12], where it was shown that the known upper complexity bounds are sharp (irrespective of problem's dimension) for most known methods using Taylor's models of degree one or two. That is to say that there are examples for which the complexity order predicted by the upper bound is actually achieved. More recently, Carmon *et al.* [3] provided an elaborate construction showing that *at least* a multiple of $\epsilon^{-\frac{p+1}{p}}$ function evaluations may be needed to obtain an ϵ-first-order-necessary unconstrained minimizer where derivatives of order at most p are used. This result, which matches in order the upper bound of [2], covers a very wide class of potential optimization methods[(4)] but has the drawback of being only valid for problems whose dimension essentially exceeds the number of iterations needed, which can be very large and quickly grows when ϵ tends to zero.

Contributions. The present paper aims at unifying and generalizing all the above results in a single framework, providing, for problems with inexpensive or no constraints, provably

(2) That is points satisfying the first- or second-order necessary optimality conditions for minimization.

(3) And its available derivatives.

(4) In particular, it covers randomized methods, which we do not consider in this paper.

optimal evaluation complexity bounds for arbitrary optimality order, all relevant model degrees and levels of smoothness of the objective function. By "inexpensive constraints", we mean general set constraints whose enforcement and evaluation(5) cost is negligible compared to the cost of evaluating the objective function. As a consequence, the evaluation complexity for such problems is meaningfully captured by focusing of the number of evaluations of this latter function. This class of minimization problems contains important cases such as bound-constrained problems and convexly-constrained problems (when the projection onto the feasible set is inexpensive), but also allows possibly nonconvex or even disconnected feasible sets.

In order to achieve these objectives, we first revisit the Taylor-based optimality measure of [11] and define (ϵ,δ)-q-th-order-necessary minimizers, a notion extending the standard ϵ-first- and ϵ-second-order cases to arbitrary orders. We then present a conceptual regularization algorithm using degree p models and show that this algorithm requires at most $O(\epsilon^{-\frac{p+\beta}{p-q+\beta}})$ evaluations of f and its derivatives to find such an (ϵ,δ)-q-th-order-necessary minimizer when the p-th derivative of f is assumed to be β-Hölder continuous. (If the p-th derivative is assumed to be Lispchitz continuous, the bound becomes $O(\epsilon^{-\frac{p+1}{p-q+1}})$.) This bound matches the best known lower bounds for first- and second-order, and improves on the bound in $O(\epsilon^{-(q+1)})$ given by [11]. We then show that this bound is sharp in order for unconstrained problems with Lipschitz continuous p-th derivative by completing and extending the result of [3] in two ways. The first is to show that the lower worst-case bound of order $\epsilon^{-\frac{p+1}{p}}$ evaluations for obtaining a first-order-necessary minimizer using at most p derivatives is also valid for problems of every dimension, and the second is to show that this bound can be generalized to a multiple of $\epsilon^{-\frac{p+1}{p-q+1}}$ for obtaining a q-th-order-necessary minimizer of any order q. In particular, this result matches in order the upper bound obtained in the first part of the paper and subsumes or improves known lower bounds for first- and second-order-necessary minimizers. While our lower bounds are derived for regularization algorithms applied to unconstrained problems, we also indicate that they may be extended to a much wider class of minimization methods and to a significant class of constrained problems.

The paper is organized as follows. Section 2 introduces the (possibly constrained) minimization problem of interest and the concept of (ϵ,δ)-approximate q-th-order-necessary minimizers. It also presents a variant of the Adaptive Regularization algorithm using degree p Taylor's models (ARp) whose purpose is to find such minimizers. Section 3 then provides an upper bound on the evaluation complexity for the ARp algorithm to achieve this task. Section 4 then discusses specialization of this result to the case where ϵ-approximate second-order-necessary minimizers are sought. The complexity upper bound of Section 3 is then proved to be sharp in Section 5 for the Lipschitz-continuous cases where the feasible set contains a ray. Some conclusions are finally presented in Section 6.

Notation. Throughout the paper, $\|v\|$ denotes the standard Euclidean norm of a vector $v \in \mathbb{R}^n$. For a symmetric tensor S of order p, $S[v_1,\ldots,v_p]$ is the result of applying S to the vectors $v_1,\ldots,v_p$, $S[v]^p$ is the result of applying S to p copies of the vector v and

$$\|S\|_{[p]} \stackrel{\rm def}{=} \max_{\|v\|=1} |S[v]^p| = \max_{\|v_1\|=\cdots=\|v_p\|=1} |S[v_1,\ldots,v_p]| \tag{1.1}$$

(where the second equality results from Theorem 2.1 in [23]) is the associated induced norm for such tensors. If S_1 and S_2 are tensors, $S_1 \otimes S_2$ is their tensor product and $S_1^{k\otimes}$ is the

(5)Constraint's values and that of their derivatives, if relevant.

product of S_1 k times with itself. For a real, sufficiently differentiable univariate function f, $f^{(i)}$ denotes its i-th derivative and $f^{(0)}$ is a synonym for f. For an integer k and a real $\beta \in (0,1]$, we define $(k+\beta)! \stackrel{\rm def}{=} \prod_{\ell=1}^{k}(\beta+\ell)$ (this coincides with the standard factorial if $\beta = 1$). As is usual, we also define $0! = 1$. If M is a symmetric matrix, $\lambda_{\min}(M)$ is its left-most eigenvalue. If α is a real, $\lceil \alpha \rceil$ and $\lfloor \alpha \rfloor$ denote the smallest integer not smaller than α and the largest integer not exceeding α, respectively. Finally $\mathrm{globmin}_{x\in\mathcal{S}} f(x)$ denotes the smallest value of $f(x)$ over $x \in \mathcal{S}$.

2 High-order necessary conditions for optimality and the ARp algorithm

Given $p \geq 1$, this paper considers the set-constrained optimization problem

$$\min_{x\in\mathcal{F}} f(x), \tag{2.1}$$

where we assume that $\mathcal{F} \subseteq \mathbb{R}^n$ is closed and nonempty, and where $f \in \mathcal{C}^{p,\beta}(\mathbb{R}^n)$, namely, that:

- f is p-times continuously differentiable,
- f is bounded below by $f_{\rm low}$, and
- the p-th derivative tensor of f at x is globally Hölder continuous, that is, there exist constants $L \geq 0$ and $\beta \in (0,1]$ such that, for all $x, y \in \mathbb{R}^n$,

$$\|\nabla_x^p f(x) - \nabla_x^p f(y)\|_{[p]} \leq L\|x-y\|^{\beta}. \tag{2.2}$$

Observe that convexity or even connectedness of $\mathcal{F}$ is not requested. Observe also that the more usual case of *Lipschitz continuous p-th derivative corresponds to* $\beta = 1$. We note that our assumption covers the continuous range of objective function's smoothness from Hölder continuous gradients to Lipschitz continuous p-th derivatives. In what follows, we assume that β is known.

If $T_p(x,s)$ is the standard p-th degree Taylor's expansion of f about x computed for the increment s, that is

$$T_p(x,s) \stackrel{\rm def}{=} f(x) + \sum_{\ell=1}^{p} \frac{1}{\ell!}\nabla_x^{\ell} f(x)[s]^{\ell}, \tag{2.3}$$

(2.2) provides crucial approximation bounds, whose proof can be found in the appendix.

Lemma 2.1 Let $f \in C^{p,\beta}(\mathbb{R}^n)$, and $T_p(x,s)$ be the Taylor approximation of $f(x+s)$ about x given by (2.3). Then for all $x, s \in \mathbb{R}^n$,

$$f(x+s) \leq T_p(x,s) + \frac{L}{(p+\beta)!}\,\|s\|^{p+\beta}, \tag{2.4}$$

$$\|\nabla_x^j f(x+s) - \nabla_s^j T_p(x,s)\|_{[j]} \leq \frac{L}{(p-j+\beta)!}\|s\|^{p-j+\beta}. \quad (j = 1,\ldots,p). \tag{2.5}$$

In order to characterize minimizers of (2.1), we follow [11] and introduce, for given $\delta \in (0,1]$ and $j \le p$,

$$\phi_{f,j}^{\delta}(x) \stackrel{\rm def}{=} f(x) - \mathop{\rm globmin}_{\substack{x+d\in\mathcal{F}\\ \|d\|\le\delta}} T_j(x,d), \tag{2.6}$$

which can be interpreted as the *magnitude of the largest decrease achievable on the Taylor's expansion of degree j within the intersection a ball of radius δ with the feasible set.* It was shown in [11] that $\phi_{f,j}^{\delta}(x)$ is a proper generalization of well-known unconstrained optimality measures for low orders, in that, for $\delta = 1$,

$$\phi_{f,1}^{\delta}(x) = \|\nabla_x^1 f(x)\|\,\delta, \tag{2.7}$$

$$\phi_{f,2}^{\delta}(x) = \left|\min[0, \lambda_{\min}\left(\nabla_x^2 f(x)\right)\right|\,\delta^2 \tag{2.8}$$

provided $\nabla_x^1 f(x) = 0$, and also, if additionally $\nabla_x^2 f(x)$ is positive semi-definite, that

$$\phi_{f,3}^{\delta} = \|\text{ projection of } \nabla_x^3 f(x) \text{ onto the nullspace of } \nabla_x^2 f(x)\,\|\,\delta^3. \tag{2.9}$$

At variance with other optimality measures, $\phi_{j,f}^{\delta}(x)$ is well-defined for any order $j \ge 1$ and varies continuously when x varies continuoulsy in $\mathcal{F}$. The role of the "optimality radius" δ in (2.6) merits some discussion. While the choice of $\delta = 1$ is adequate for retrieving known optimality conditions in the unconstrained case for $j = 1$, $j = 2$ provided $\nabla_x^1 f(x) = 0$, and $j = 3$ provided additionnaly $\nabla_x^2 f(x)$ is positive semi-definite (as we have just seen), δ becomes important in other cases. Corollary 3.6 in [11] indicates that, when $\mathcal{F}$ is convex, q-th-order necessary "path-based" optimality conditions hold if

$$\lim_{\delta\to 0} \frac{\phi_{f,j}^{\delta}(x)}{\delta^j} = 0 \quad \text{for} \quad j = 1, \ldots, q. \tag{2.10}$$

The limit for $\delta \to 0$ is necessary to capture the notion of local minimizer for (2.1). However, considering $\phi_{f,j}^{\delta}(x)$ for non-vanishing δ has substantial advantages from the point of view of optimization: while it may fail to indicate that x is a local minimizer, it does so only by providing a direction leading to values of f below $f(x)$, thereby helping to avoid local but non-global approximate solutions. We refer the reader to [11] for a further discussion, but conclude that considering fixed δ has strong advantages when solving (2.1).

A special case is when x is an isolated feasible point, that is a point which is the sole intersection between $\mathcal{F}$ and any sufficiently small neighbourhood of x. Such a point is clearly a local minimizer, and this is reflected by the fact that $\phi_{f,q}^{\delta}(x) = 0$ for any f, any q and any sufficiently small δ.

The main drawback of using $\phi_{f,j}^{\delta}(x)$ is, of course, that its computation requires the global minimization of $T_p(x,d)$ in the intersection of the ball of radius δ with $\mathcal{F}$. We are not aware of an easy way to do this in general(6) when $n > 1$, which is why our analysis remains of an essentially theoretical nature, as was the case for [11]. Note however that, albeit potentially very difficult, solving this global minimization problem does not involve calculating the value of f or of any of its derivatives. In that sense, this drawback is thus irrelevant for the worst-case evaluation complexity which solely focuses on these evaluations.

(6) A small value of δ might help, but this computation remains NP-hard in most cases.

Observe now that, if we were to relax the first-order condition $\nabla_x^1 f(x) = 0$ for unconstrained problems to $\|\nabla_x^1 f(x)\| \le \epsilon$ and, at the same time, relax the second-order condition to $\left|\min[0, \lambda_{\min}\left(\nabla_x^2 f(x)\right)\right| \le \epsilon$, we then deduce that

$$\phi_{f,2}^{\delta}(x) \le \epsilon\delta + \tfrac{1}{2}\epsilon\delta^2 = \epsilon \sum_{\ell=1}^{2} \frac{\delta^\ell}{\ell!}. \tag{2.11}$$

A natural generalization of this observation is to define an (ϵ, δ)-*approximate q-th-order-necessary minimizer* of f as a point x such that

$$\phi_{f,q}^{\delta}(x) \le \epsilon \chi_q(\delta) \tag{2.12}$$

where

$$\chi_q(\delta) \stackrel{\rm def}{=} \sum_{\ell=1}^{q} \frac{\delta^\ell}{\ell!}. \tag{2.13}$$

Because (2.12) is a new way to look at approximate optimality and is crucial for the rest of this paper, it is worthwhile to motivate and discuss it further.

1. When $\epsilon = 0$, (2.12) implies that the complicated path-based necessary optimality conditions derived in [11] do hold. This results from the fact that these latter conditions merely express that the Taylor's model of order q cannot decrease close enough to x along any feasible polynomial path emanating from x, which is clearly the case if x is a global minimizer of the same models in the intersection of the feasible set and a ball of radius δ centered at x. By continuity, these path-based conditions must therefore hold in the limit under (2.12) when ϵ tends to zero. The role of (2.12) as a condition for approximate minimization is thus coherent and consistent with known necessary conditions.

2. Inspired by (2.10), the stronger approximate optimality condition

$$\phi_{f,j}^{\delta}(x) \le \epsilon\, \delta^j \quad \text{for} \quad j \in \{1, \ldots, q\} \tag{2.14}$$

   was used in [11] instead of (2.12). Our main reason to prefer (2.12) is the following. Observe that (2.14) implies in particular that $\phi_{f,q}^{\delta}(x) \le \epsilon\delta^q$, which in turn implies, for δ small enough for the first-order term to dominate, that $\phi_{f,1}^{\delta}(x) \le \epsilon\delta^q$. In the unconstrained case (for example), this requires $\|\nabla_x^1 f(x_k)\| \le \epsilon\delta^{q-1}$, imposing an inordinate level of first-order optimality, much stronger than the standard condition $\|\nabla_x^1 f(x_k)\| \le \epsilon$. No such difficulty arises with (2.12) because the right-hand side of the condition involves all powers of δ, which is not the case of the right-hand side of (2.14). Note however that the vital continuity properties of $\phi_{f,q}^{\delta}$ are not affected by the choice of the right-hand side, and are thus inherited by (2.12).

3. For given $\delta \in (0, 1]$, (2.12) does not imply that $\phi_{f,j}^{\delta}(x) \le \epsilon\chi_j(\delta)$ for $j \in \{1, \ldots, q-1\}$, although the violation of this condition tends to zero with δ[7]. This slight blemish can be cured by requiring that $\phi_{f,j}^{\delta}(x) \le \epsilon\chi_j(\delta)$ for $j \in \{1, \ldots, q\}$ instead of (2.12), but we claim that the benefit of this stronger definition is outweighted by the need to perform $q-1$ additional constrained global minimizations, and therefore focus our exposition to the case using the simpler (2.12).

[7] When δ tends to zero, the terms of orders $j+1$ and higher in the Taylor's expansion defining $\phi_{f,q}^{\delta}(x)$ and $\chi_q(\delta)$ become negligible compared to the first j.

In order to further justify (2.12), we now make more explicit the "minimizing guarantees" provided by this approximate optimality condition, by formulating a result analogous to Theorem 3.7 in [11]. This result gives a lower bound on the value of $f(x)$ in the feasible neighbourhood of an (ϵ,δ)-approximate q-th-order-necessary minimizer.

Theorem 2.2 Suppose that f is p times continuouly differentiable and that $\nabla_x^q f$ is β-Hölder continuous with constant L (in the sense of (2.2) with $p = q$) in an open neighbourhood of radius $\delta \in (0,1]$ of some $x \in \mathcal{F}$. Suppose also that x is an (ϵ,δ)-approximate q-th-order-necessary minimizer of f in the sense of (2.12). Then

$$f(x+d) \geq f(x) - 2\epsilon\chi_q(\delta) \quad \text{for all } d \text{ with } \quad x+d \in \mathcal{F} \;\text{ and }\; \|d\| \leq \min\left[\delta, \left(\frac{(q+1)!\epsilon}{L}\right)^{\frac{1}{q+\beta-1}}\right]. \tag{2.15}$$

Proof. Using the triangle inequality, (2.2), (2.4) and (2.12), we obtain that

$$\begin{aligned} f(x+d) &\geq f(x+d) - T_q(x,d) + T_q(x,d) \\ &\geq -|f(x+d) - T_q(x,d)| + T_q(x,0) - \phi_{f,q}^{\delta}(x) \\ &\geq -\frac{L}{(q+1)!}\|d\|^{q+\beta} + f(x) - \epsilon\chi_q(\delta). \end{aligned}$$

Thus, if $\|d\| \leq \delta$,

$$f(x+d) \geq f(x) - \frac{L}{(q+1)!}\|d\|^{q+\beta-1}\,\delta - \epsilon\chi_q(\delta)$$

and the desired bound follows from the fact that $\delta \leq \chi_q(\delta)$. □

In order to find (ϵ,δ)-approximate q-th-order-necessary minimizers, we consider applying a variant of the ARp algorithm to (2.1). This algorithm, described as Algorithm 2.1 on the following page, is of the regularization type in that, at each iterate x_k, a step s_k is computed which approximately minimizes (in a sense defined below) the model

$$m_k(s) = T_p(x_k,s) + \frac{\sigma_k}{(p+\beta)!}\|s\|^{p+\beta} \tag{2.16}$$

subject to $x_k + s \in \mathcal{F}$, where p in an integer such that $p \geq q$ and $\sigma_k \geq \sigma_{\min}$ is a "regularization parameter".

A few comments are useful at this stage.

1. Since $\sigma_k \geq \sigma_{\min}$ by (2.22), we have that $m_k(s)$ is bounded below as a function of s and the existence of a constrained global minimizer s_k^* is guaranteed.
2. Step 2 requires, that, for $s_k \neq 0$, we also compute δ_k. This is easy for orders one and two. If $q = 1$, the formula for a global minimizer s_k^* is analytic and $\delta_k = 1$ is

Algorithm 2.1: ARp for (ϵ, δ)-approximate q-th-order-necessary minimizers

Step 0: Initialization. An initial point $x_0 \in \mathcal{F}$ and an initial regularization parameter $\sigma_0 > 0$ are given, as well as an accuracy level $\epsilon \in (0,1)$. The constants δ_{-1}, ϖ, θ, η_1, η_2, γ_1, γ_2, γ_3 and $\sigma_{\min}$ are also given and satisfy

$$\varpi \in (0,1], \quad \theta > 0, \quad \delta_{-1} \in (0,1], \quad \sigma_{\min} \in (0, \sigma_0], \quad 0 < \eta_1 \le \eta_2 < 1 \\ \text{and} \quad 0 < \gamma_1 < 1 < \gamma_2 < \gamma_3. \tag{2.17}$$

Compute $f(x_0)$ and set $k = 0$.

Step 1: Test for termination. Evaluate $\{\nabla_x^i f(x_k)\}_{i=1}^q$. If (2.12) holds with $\delta = \delta_{k-1}$, terminate with the approximate solution $x_\epsilon = x_k$. Otherwise compute $\{\nabla_x^i f(x_k)\}_{i=q+1}^p$.

Step 2: Step calculation. Attempt to compute a step s_k such that $x_k + s_k \in \mathcal{F}$ and an optimality radius $\delta_k \in (0,1]$ by approximately minimizing the model $m_k(s)$ in the sense that

$$m_k(s_k) < m_k(0) \tag{2.18}$$

and either

$$\|s_k\| \ge \varpi \epsilon^{\frac{1}{p-q+\beta}} \tag{2.19}$$

or

$$\phi_{m_k,q}^{\delta_k}(s_k) \le \frac{\theta \|s_k\|^{p-q+\beta}}{(p-q+\beta)!} \, \chi_q(\delta_k). \tag{2.20}$$

If no such step exist, terminate with the approximate solution $x_\epsilon = x_k$.

Step 3: Acceptance of the trial point. Compute $f(x_k + s_k)$ and define

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{T_p(x_k, 0) - T_p(x_k, s_k)}. \tag{2.21}$$

If $\rho_k \ge \eta_1$, then define $x_{k+1} = x_k + s_k$; otherwise define $x_{k+1} = x_k$.

Step 4: Regularization parameter update. Set

$$\sigma_{k+1} \in \begin{cases} [\max(\sigma_{\min}, \gamma_1 \sigma_k), \sigma_k] & \text{if } \rho_k \ge \eta_2, \\ [\sigma_k, \gamma_2 \sigma_k] & \text{if } \rho_k \in [\eta_1, \eta_2), \\ [\gamma_2 \sigma_k, \gamma_3 \sigma_k] & \text{if } \rho_k < \eta_1. \end{cases} \tag{2.22}$$

Increment k by one and go to Step 1 if $\rho_k \ge \eta_1$, or to Step 2 otherwise.

always acceptable. The situation is similar for $q = 2$, where s_k^* can be assessed using a trust-region method whose radius is $\delta_k = 1$ (more details are provided at the end of Section 3). The task is more difficult for higher orders where one may have to rely on the arguments of Lemma 2.5 below, or use different subproblems with decreasing values of δ. However, none of these computations involve the evaluation of f or its derivatives, and therefore the evaluation complexity bound discussed in this paper is unaffected.

3. That one needs to consider the second case in Step 2 (where no step exists satisfying (2.18) – (2.20)) can be seen by examining the following one-dimensional example. Let $p = q = 3$ and $\beta = 1$, and suppose that $\delta_{k-1} = 1$, $T_q(x_k, s) = s^2 - 2s^3$ and $\sigma_k = 4! = 24$. Then $m_k(s) = s^2 - 2s^3 + s^4 = s^2(s-1)^2$ and the origin is a global minimizer of the model (and a local minimizer of $T_q(x_k, s)$) but yet $T_q(x_k, \delta) = -1$, yielding that $\phi_{f,q}^{\delta_{k-1}}(x_k) = 1 > \epsilon\chi_q(1)$ for $\epsilon \leq 1/\chi_q(1) = \frac{4}{7}$. Thus, Step 1 with $\delta_{k-1} = 1$ has failed to identify that termination was possible. In addition, we see that, at variance with the cases $q = 1$ and $q = 2$, a global minimizer of the model (2.16) may not, for $q \geq 3$, be a global minimizer of its q-th order Taylor's expansion in the intersection of $\mathcal{F}$ and a ball of arbitrary radius: we may have to restrict this radius (to $\delta_{k-1} = \frac{1}{2}$ in our example) for this important property to hold (see Lemma 2.5 below).

4. If (2.19) holds, the possibly expensive computation of $\phi_{m_k,q}^{\delta_k}(s_k)$ in (2.20) is unnecessary and δ_k may be chosen arbitrarily in $(0, 1]$.

5. We assume the availability of a feasible starting point, which is without loss of generality for inexpensive constraints.

6. Before termination, each successful iteration requires the evaluation of f and its first p derivative tensors, while only the evaluation of f is needed at unsuccessful ones.

7. The mechanism of the algorithm ensures the non-increasing nature of the sequence $\{f(x_k)\}_{k\geq 0}$.

Iterations for which $\rho_k \geq \eta_1$ (and hence $x_{k+1} = x_k + s_k$) are called "successful" and we denote by $\mathcal{S}_k \stackrel{\rm def}{=} \{0 \leq j \leq k \mid \rho_j \geq \eta_1\}$ the index set of all successful iterations between 0 and k. We immediately observe that the total number of iterations (successful or not) can be bounded as a function of the number of successful ones (and include a proof in the appendix).

Lemma 2.3 [2, Theorem 2.4] The mechanism of Algorithm 2.1 guarantees that, if

$$\sigma_k \leq \sigma_{\max}, \tag{2.23}$$

for some $\sigma_{\max} > 0$, then

$$k + 1 \leq |\mathcal{S}_k| \left(1 + \frac{|\log \gamma_1|}{\log \gamma_2}\right) + \frac{1}{\log \gamma_2} \log\left(\frac{\sigma_{\max}}{\sigma_0}\right). \tag{2.24}$$

We also verify that the algorithm is well-defined in the sense that either a step s_k satisfying (2.18)–(2.20) can always be found, or termination is justified. For unconstrained problems with $q \in \{1,2\}$, the first possibility directly results from the observation that $\phi^{\delta}_{m_k,j}(s_k)$ (as given by (2.7)-(2.9) for $f = m_k$ and $j \in \{1,2,3\}$) can be made suitably small at a global minimizer of the model. The situation is more complicated for other cases. In order to clarify it, we first state a useful technical lemma, whose proof is in the appendix.

Lemma 2.4 Let s be a vector of $\mathbb{R}^n$. Then

$$\| \nabla_s^j \big(\|s\|^{p+\beta} \big) \|_{[j]} = \frac{(p+\beta)!}{(p-j+\beta)!} \|s\|^{p-j+\beta} \;\; \text{for} \;\; j \in \{0,\ldots,p\} \tag{2.25}$$

and

$$\| \nabla_s^{p+1} \big(\|s\|^{p+\beta} \big) \|_{[p+1]} = \beta\,(p+\beta)!\,\|s\|^{\beta-1}. \tag{2.26}$$

We now provide reasonable sufficient conditions for a nonzero step s_k and an optimality radius δ_k to satisfy (2.18)–(2.20).

Lemma 2.5 Suppose that s_k^* is a global minimizer of $m_k(s)$ under the constraint that $x_k + s \in \mathcal{F}$, such $m_k(s_k^*) < m_k(0)$. Then there exist a neighbourhood of s_k^* and a range of sufficiently small δ such that (2.18) and (2.20) hold for any s_k in the intersection of this neighbourhood with $\mathcal{F}$ and any δ_k in this range.

Proof. Let s_k^* be the global minimizer of the model $m_k(s)$ over all s such that $x_k + s \in \mathcal{F}$. Since $m_k(s_k^*) < m_k(0)$, we have that $s_k^* \neq 0$. By Taylor's theorem, we have that, for all d,

$$0 \le m_k(s_k^*+d) - m_k(s_k^*) = \sum_{\ell=1}^{p} \frac{1}{\ell!} \nabla_s^\ell m_k(s_k^*)[d]^\ell + \frac{1}{(p+1)!} \nabla_s^{p+1} m_k(s_k^*+\xi d)[d]^{p+1}$$

for some $\xi \in (0,1)$. Thus, using the triangle inequality, (2.16) and (2.26),

$$\begin{aligned} -\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell m_k(s_k^*)[d]^\ell &\le \sum_{\ell=q+1}^{p} \frac{\|d\|^\ell}{\ell!} \|\nabla_s^\ell m_k(s_k^*)\|_{[\ell]} + \frac{\|d\|^{p+1}}{(p+1)!} \|\nabla_s^{p+1} m_k(s_k^*+\xi d)\|_{[p+1]} \\ &= \sum_{\ell=q+1}^{p} \frac{\|d\|^\ell}{\ell!} \|\nabla_s^\ell m_k(s_k^*)\|_{[\ell]} + \beta\sigma_k \frac{\|d\|^{p+1}}{(p+1)!} \|s_k^*+\xi d\|^{\beta-1}. \end{aligned} \tag{2.27}$$

Since $s_k^* \neq 0$, we may then choose $\delta_k < \|s_k^*\|$ such that, for every d with $\|d\| \le \delta_k$, $\|s_k^* + \xi d\| \ge \frac{1}{2}\|s_k^*\| > 0$ and

$$\sum_{\ell=q+1}^{p} \frac{\|d\|^\ell}{\ell!} \|\nabla_s^\ell m_k(s_k^*)\|_{[\ell]} + 2^{1-\beta}\beta\sigma_k \frac{\|d\|^{p+1}}{(p+1)!} \|s_k^*\|^{\beta-1} \le \frac{\theta \|s_k^*\|^{p-q+\beta}}{2(p-q+\beta)!}\,\|d\|. \tag{2.28}$$

Hence we deduce from (2.27) and (2.28) that, for $\|d\| \le \delta_k$,

$$-\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell m_k(s_k^*)[d]^\ell \le \frac{\theta \|s_k^*\|^{p-q+\beta}}{2(p-q+\beta)!}\,\delta_k \le \frac{\theta \|s_k^*\|^{p-q+\beta}}{2(p-q+\beta)!}\,\chi_q(\delta_k),$$

where the last inequality follows from (2.13). Continuity of m_k and its derivatives and the inequality $m_k(s_k^*) < m_k(0)$ then imply that there exists a neighbourhood of $s_k^* \neq 0$ such that (2.18) holds and

$$-\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell m_k(s)[d]^\ell \leq \frac{\theta \|s\|^{p-q+\beta}}{(p-q+\beta)!} \chi_q(\delta_k).$$

for all s in this neighbourhood and all d with $\|d\| \leq \delta_k$. This yields that, for all such s with $x_k + s \in \mathcal{F}$,

$$\phi_{m_k,q}^{\delta_k}(s) = \max\left[0, \operatorname*{globmax}_{\substack{\|d\|\leq\delta_k \\ x_k+d\in\mathcal{F}}} \left(-\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell m_k(s_k)[d]^\ell \right)\right] \leq \frac{\theta \|s\|^{p-q+\beta}}{(p-q+\beta)!} \chi_q(\delta_k),$$

as requested. □

As can be seen in the proof of this lemma, δ_k may need to be small if any of the tensors

$$\nabla_s^\ell m_k(s_k^*) = \sum_{j=\ell}^{p} \frac{1}{j!} \nabla_s^j m_k(0)[s_k^*]^{j-\ell}$$

for $\ell \in \{1, \ldots, p+1\}$ has a large norm. This may occur in particular if β and $\|s_k^*\|$ are both close to zero, as is shown by the last term in the left-hand side of (2.28). We also note that (2.20) obviously holds for $s_k = s_k^*$ if $x_k + s_k^*$ is an isolated feasible point. It now remains to verify that it is justified to terminate in Step 2 when no suitable nonzero step can be found.

Lemma 2.6 Suppose that the algorithm terminates in Step 2 of iteration k with $x_\epsilon = x_k$. Then there exists a $\delta \in (0, 1]$ such that (2.12) holds for $x = x_\epsilon$ and x_ϵ is an (ϵ, δ)-approximate qth-order-necessary minimizer.

Proof. Given Lemma 2.5, if the algorithm terminates within Step 2, it must be because every global minimizer s_k^* of $m_k(s)$ under the constraints $x_k + s \in \mathcal{F}$ is such that $m_k(s_k^*) \geq m_k(0)$. In that case, $s_k^* = 0$ is one such global minimizer and we have that, for all d,

$$0 \leq m_k(d) - m_k(0) = \sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_x^j f(x_k)[d]^j + \sum_{\ell=q+1}^{p} \frac{1}{\ell!} \nabla_x^j f(x_k)[d]^j + \frac{\sigma_k}{(p+\beta)!} \|d\|^{p+\beta}.$$

We may now choose $\delta \in (0, 1]$ small enough to ensure that, for all d with $\|d\| \leq \delta$,

$$\left| \sum_{\ell=q+1}^{p} \frac{1}{\ell!} \nabla_x^j f(x_k)[d]^j + \frac{\sigma_k}{(p+\beta)!} \|d\|^{p+\beta} \right| \leq \epsilon \|d\| \leq \epsilon\, \chi_q(\delta), \tag{2.29}$$

which in turn implies that, for all d with $\|d\| \leq \delta$,

$$\phi_{f,q}^{\delta}(x_k) = \max\left[0, \operatorname*{globmax}_{\substack{\|d\|\leq\delta \\ x_k+d\in\mathcal{F}}} \left(-\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_x^\ell f(x_k)[d]^\ell \right)\right] \leq \epsilon\, \chi_q(\delta_k),$$

concluding the proof. □

Observe that, in this proof, we could have chosen δ small enough to ensure

$$\frac{\sigma_k}{(p+\beta)!}\|d\|^{p+\beta} \le \epsilon\chi_p(\delta)$$

instead of (2.29), yielding $\phi_{f,p}^{\delta}(x_k) \le \epsilon\chi_p(\delta)$, which is a stronger necessary optimality condition than (2.12). Together, Lemmas 2.5 and 2.6 ensure that Algorithm 2.1 is well-defined.

3 An upper bound on the evaluation complexity

The proofs of the following two lemmas are very similar to corresponding results in [2] and hence we again defer them to the appendix (but still include them for completeness, as the algorithm has changed).

Lemma 3.1 The mechanism of Algorithm 2.1 guarantees that, for all $k \ge 0$,

$$T_p(x_k, 0) - T_p(x_k, s_k) \ge \frac{\sigma_k}{(p+\beta)!}\|s_k\|^{p+\beta}, \tag{3.1}$$

and so (2.21) is well-defined.

Lemma 3.2 Let $f \in \mathcal{C}^{p,\beta}(\mathbb{R}^n)$. Then, for all $k \ge 0$,

$$\sigma_k \le \sigma_{\max} \stackrel{\rm def}{=} \max\left[\sigma_0, \frac{\gamma_3 L}{1-\eta_2}\right]. \tag{3.2}$$

We are now in position to prove the crucial lower bound on the step length.

Lemma 3.3 Let $f \in \mathcal{C}^{p,\beta}(\mathbb{R}^n)$. Then, for all $k \ge 0$ such that Algorithm 2.1 does not terminate at iteration $k+1$,

$$\|s_k\| \ge \kappa_s \epsilon^{\frac{1}{p-q+\beta}}, \tag{3.3}$$

where

$$\kappa_s \stackrel{\rm def}{=} \min\left[\varpi, \left(\frac{(p-q+\beta)!}{(L+\sigma_{\max}+\theta)}\right)^{\frac{1}{p-q+\beta}}\right]. \tag{3.4}$$

Proof. If $\|s_k\| > \varpi\epsilon^{\frac{1}{p-q+\beta}}$, the result is obvious. Suppose now that $\|s_k\| \le \varpi\epsilon^{\frac{1}{p-q+\beta}}$. Since the algorithm does not terminate at iteration $k+1$, we have that

$$\phi_{f,q}^{\delta_k}(x_{k+1}) > \epsilon\chi_q(\delta_k) \tag{3.5}$$

Let the global minimum in the definition of $\phi_{f,q}^{\delta_k}(x_{k+1})$ be achieved at d with $\|d\| \le \delta_k$. Since $\phi_{f,q}^{\delta_k}(x_{k+1}) > 0$, we have from (2.6) that

$$\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_x^\ell f(x_{k+1})[d]^\ell < 0$$

Then, successively using (2.6) for f at x_{k+1}, the triangle inequality, (2.16), (1.1) and (2.25), we deduce that

$$\begin{aligned}
\phi_{f,q}^{\delta_k}(x_{k+1}) &= -\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_x^\ell f(x_{k+1})[d]^\ell \\
&= -\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_x^\ell f(x_{k+1})[d]^\ell + \sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell T_p(x_k, s_k)[d]^\ell - \sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell T_p(x_k, s_k)[d]^\ell \\
&\quad - \frac{\sigma_k}{(p+\beta)!} \sum_{k=\ell}^{q} \frac{1}{\ell!} \left(\nabla_s^\ell \left[\|s\|^{p+\beta} \right](s_k) \right) [d]^\ell + \frac{\sigma_k}{(p+\beta)!} \sum_{k=\ell}^{q} \frac{1}{\ell!} \left(\nabla_s^\ell \left[\|s\|^{p+\beta} \right](s_k) \right) [d]^\ell \\
&\le \left| \sum_{\ell=1}^{q} \frac{1}{\ell!} \left[\nabla_x^\ell f(x_{k+1}) - \nabla_s^\ell T_p(x_k, s_k) \right] [d]^\ell \right| \\
&\qquad - \sum_{\ell=1}^{q} \frac{1}{\ell!} \left(\nabla_s^\ell \left[T_p(x_k, s) + \frac{\sigma_k}{(p+\beta)!} \|s\|^{p+\beta} \right]_{s=s_k} \right) [d]^\ell \\
&\qquad + \frac{\sigma_k}{(p+\beta)!} \left| \sum_{k=\ell}^{q} \frac{1}{\ell!} \left(\nabla_s^\ell \left[\|s\|^{p+\beta} \right]_{s=s_k} \right) [d]^\ell \right| \\
&\le \sum_{\ell=1}^{q} \frac{L}{\ell!(p-\ell+\beta)!} \|s_k\|^{p-\ell+\beta} \delta_k^\ell \\
&\qquad - \sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell m_k(s_k)[d]^\ell + \sum_{\ell=1}^{q} \frac{\sigma_k}{\ell!(p-\ell+\beta)!} \|s_k\|^{p-\ell+\beta} \delta_k^\ell
\end{aligned} \tag{3.6}$$

Now, since $\|d\| \le \delta_k$, and using (2.6) for m_k at s_k,

$$-\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell m_k(s_k)[d]^\ell \le \max \left[0, -\sum_{\ell=1}^{q} \frac{1}{\ell!} \nabla_s^\ell m_k(s_k)[d]^\ell \right] \le \phi_{m_k,q}^{\delta_k}(s_k).$$

Therefore, using (2.20) and (3.6), we have that

$$\begin{aligned}
\phi_{f,q}^{\delta_k}(x_{k+1}) &\le \sum_{\ell=1}^{q} \frac{L}{\ell!(p-\ell+\beta)!} \|s_k\|^{p-\ell+\beta} \delta_k^\ell + \frac{\theta\, \chi_q(\delta_k)}{(p-q+\beta)!} \|s_k\|^{p-q+\beta} \\
&\qquad + \sum_{\ell=1}^{q} \frac{\sigma_k}{\ell!(p-\ell+\beta)!} \|s_k\|^{p-\ell+\beta} \delta_k^\ell \\
&\le \frac{\left[L + \sigma_k + \theta \right] \chi_q(\delta_k)}{(p-q+\beta)!} \|s_k\|^{p-q+\beta},
\end{aligned} \tag{3.7}$$

where we have used the fact that $\|s_k\| \le \varpi \epsilon^{\frac{1}{p-q+\beta}} \le 1$ to deduce the last inequality. As a consequence, (3.5) implies that

$$\|s_k\| \ge \left[\frac{\epsilon(p-q+\beta)!}{(L+\sigma_k+\theta)} \right]^{\frac{1}{p-q+\beta}}$$

and (3.3) then immediately follows from (3.2). □

The bound given by this lemma is another indication that choosing θ of the order of L (when this is known a priori) makes sense.

We now combine all the above results to deduce an upper bound on the maximum number of successful iterations, from which a final complexity bound immediately follows.

Theorem 3.4 Let $f \in \mathcal{C}^{p,\beta}(\mathbb{R}^n)$. Then, given $\epsilon \in (0,1)$, Algorithm 2.1 needs at most

$$\left\lfloor \kappa_p(f(x_0) - f_{\rm low}) \left(\epsilon^{-\frac{p+\beta}{p-q+\beta}}\right) \right\rfloor + 1$$

successful iterations (each involving one evaluation of f and its p first derivatives) and at most

$$\left\lfloor \left\lfloor \kappa_p(f(x_0) - f_{\rm low}) \left(\epsilon^{-\frac{p+\beta}{p-q+\beta}}\right) + 1 \right\rfloor \left(1 + \frac{|\log \gamma_1|}{\log \gamma_2}\right) + \frac{1}{\log \gamma_2} \log\left(\frac{\sigma_{\max}}{\sigma_0}\right) \right\rfloor \tag{3.8}$$

iterations in total to produce an iterate x_ϵ such that (2.12) holds, where $\sigma_{\max}$ is given by (3.2) and where

$$\kappa_p \stackrel{\rm def}{=} \frac{(p+\beta)!}{\eta_1 \sigma_{\min}} \max\left\{ \varpi^{-(p+\beta)}, \left[\frac{(L + \sigma_{\max} + \theta)}{(p-q+\beta)!}\right]^{\frac{p+\beta}{p-q+\beta}} \right\}.$$

Proof. At each successful iteration k before termination, we have the guaranteed decrease

$$f(x_k) - f(x_{k+1}) \ge \eta_1 (T_p(x_k, 0) - T_p(x_k, s_k)) \ge \frac{\eta_1 \sigma_{\min}}{(p+\beta)!} \|s_k\|^{p+\beta} \tag{3.9}$$

where we used (2.21), (3.1) and (2.22). Moreover we deduce from (3.9), (3.3) and (3.2) that

$$f(x_k) - f(x_{k+1}) \ge \kappa_p^{-1} \epsilon_j^{\frac{p+\beta}{p-q+\beta}} \quad \text{where} \quad \kappa_p^{-1} \stackrel{\rm def}{=} \frac{\eta_1 \sigma_{\min} \kappa_s}{(p+\beta)!}. \tag{3.10}$$

Thus, since $\{f(x_k)\}$ decreases monotonically,

$$f(x_0) - f(x_{k+1}) \ge \kappa_p^{-1} \epsilon_j^{\frac{p+\beta}{p-q+\beta}} |\mathcal{S}_k|.$$

Using that f is bounded below by $f_{\rm low}$, we conclude

$$|\mathcal{S}_k| \le \frac{f(x_0) - f_{\rm low}}{\kappa_p^{-1}} \epsilon_j^{-\frac{p+\beta}{p-q+\beta}} \tag{3.11}$$

until termination. The desired bound on the number of successful iterations follows from combining (3.11). Lemma 2.3 is then invoked to compute the upper bound on the total number of iterations. □

In particular, if the p-th derivative of f is assumed to be globally Lipschitz rather than merely Hölder continuous (i.e. if $\beta = 1$), the bound (3.8) on the maximum number of evaluations becomes

$$\left\lfloor \left\lfloor \kappa_p (f(x_0) - f_{\rm low}) \left(\epsilon^{-\frac{p+1}{p-q+1}}\right) + 1 \right\rfloor \left(1 + \frac{|\log \gamma_1|}{\log \gamma_2}\right) + \frac{1}{\log \gamma_2} \log\left(\frac{\sigma_{\max}}{\sigma_0}\right) \right\rfloor \tag{3.12}$$

where

$$\kappa_p \stackrel{\rm def}{=} \frac{(p+1)!}{\eta_1 \sigma_{\min}} \max\left\{ \varpi^{p+\beta}, \left[\frac{q!(L+\sigma_{\max}+\theta)(e-1)}{(p-q+1)!}\right]^{\frac{p+1}{p-q+1}} \right\}.$$

This worst-case evaluation bound generalizes known bounds for $q = 1$ (see [2]) or $q = 2$ (see[8]) and significantly improve upon the bounds in $O(\epsilon^{-(q+1)})$ given by [11] for a more stringent termination rule. It also extends the results obtained in [6] for convexly-constrained problems with $q = 1$ by allowing the significantly broader class of inexpensive constraints.

We also note that it is possible to weaken the assumption that $\nabla_x^p f$ must satisfy the Hölder inequality (2.2) for every $x, y \in \mathbb{R}^n$ (as required in the beginning of Section 2). The weakest possible smoothness assumption is to require that (2.2) holds only for points belonging to the same segment of the "path of iterates" $\cup_{k\geq 0}[x_k, x_{k+1}]$ (this is necessary for the proof of Lemma 2.1). As this path joining feasible iterates may be hard to predict a priori, one may instead use the monotonic character of Algorithm 2.1 and require (2.2) to hold for all x, y in the intersection of $\mathcal{F}$ with the level set $\{x \in \mathbb{R}^n \mid f(x) \leq f(x_0)\}$. Again, it may be hard to determine this set and to ensure that it contains the path of iterates, and one may then resort to requiring (2.2) to hold in the whole of $\mathcal{F}$, which must then be convex to ensure the desired Hölder property on every segment $[x_k, x_{k+1}]$.

4 Seeking ϵ-approximate second-order-necessary minimizers

We now discuss the particular and much-studied case where second-order minimizers are sought for unconstrained problems with Lipschitz continuous Hessians (that is $p \geq q = 2$, $\mathcal{F} = \mathbb{R}^n$ and $\beta = 1$). As we now show, a specialization of Algorithm 2.1 to this case is very close (but not identical) to well-known methods. Let us consider Step 1 first. The computation of $\phi_{f,2}^{\delta_{k-1}}(x_k)$ then reduce to

$$\phi_{f,2}^{\delta_{k-1}}(x_k) = \max\left[0, -\mathop{\rm globmin}_{\|d\|\leq\delta_{k-1}} \left(\nabla_x^1 f(x_k)^T d + \tfrac{1}{2} d^T \nabla_x^2 f(x_k) d\right)\right], \tag{4.1}$$

which amounts to solving a standard trust-region subproblem with radius δ_{k-1} (see [13]). Hence verifying (4.1) or testing the more usual approximate second-order criterion

$$\|\nabla_x^1 f(x_k)\| \leq \epsilon \;\text{ and }\; \lambda_{\min}\Big(\nabla_x^2 f(x_k)\Big) \geq -\epsilon, \tag{4.2}$$

have very similar numerical costs (remember that finding the leftmost eigenvalue of the Hessian is the same as finding the global minimizer of the associated Rayleigh quotient). If we now turn to the computation of s_k in Step 2, Algorithm 2.1 then computes such a step by attempting to minimize the model

$$T_p(x_k, s) + \frac{\sigma_k}{(p+1)!}\|s\|^{p+1}, \tag{4.3}$$

as has already been proposed before for general p [2, 8]. Moreover, the failure of (2.12) in Step 1 is enough, when $q \leq 2$, to guarantee the existence of nonzero global minimizers of $T_p(x_k, s)$ and $m_k(s)$, and thus to ensure that a nonzero s_k is possible. The approximate model minimization is stopped as soon as (2.19) or (2.20) holds, the latter then reducing to checking that

$$\phi^{\delta}_{m_k,2}(x_k) = \max\left[0, -\operatorname*{globmin}_{\|d\|\leq\delta}\left(\nabla^1_s m_k(s_k)^T d + \tfrac{1}{2} d^T \nabla^2_s m_k(s_k) d\right)\right] \leq \frac{\theta\|s_k\|^{p-1}}{(p-1)!}\,\chi_2(\delta) \quad (4.4)$$

for some $\delta \in (0,1]$. For each potential s_k, finding $\delta \in (0,1]$ requires solving (possibly approximately)

$$-\operatorname*{globmin}_{\|d\|\leq\delta}\left(\nabla^1_s m_k(s_k)^T d + \tfrac{1}{2} d^T \nabla^2_s m_k(s_k) d\right) \leq \frac{\theta\|s_k\|^{p-1}}{(p-1)!}\,\chi_2(\delta).$$

While this could be acceptable without affecting the overall evaluation complexity of the algorithm, a simpler alternative is available for $q = 2$. We may consider terminating the model minimization when either (2.19) holds, or

$$0 > \operatorname*{globmin}_{\|d\|\leq 1}\left(\nabla^1_s m_k(s_k)^T d + \tfrac{1}{2} d^T \nabla^2_s m_k(s_k) d\right) \geq -\frac{\theta\|s_k\|^{p-1}}{(p-1)!}\,\chi_2(1) = -\frac{3\theta\|s_k\|^{p-1}}{2(p-1)!}. \quad (4.5)$$

The inequality is guaranteed to hold when s_k is close enough to s_k^*, a global minimizer of the model $m_k(s)$, since then $\nabla^1_s m_k(s_k^*) = 0$ and $\nabla^2_s m_k(s_k^*)$ is positive semi definite, and then $d = 0$ provides the global minimizer of the second-order Taylor model of $m_k(s)$ around s_k. Verifying (4.5) only requires at most one trust-region calculation for each potential step and ensures (4.4) with $\delta = 1$, making the choice $\delta_k = 1$ acceptable. The cost this technique is comparable to that that proposed in [8] where an eigenvalue computation is required for each potential step. Combining these observations, Algorithm 2.1 then becomes Algorithm 4.1.

If $p = q = 2$, computing s_k in Step 2 amounts to approximately minimizing the now well-known cubic model of [15, 19, 22, 5]. In addition, if s_k is the exact global minimizer of this model, the above argument shows that (4.5) automatically holds at s_k and checking this inequality by solving a trust-region subproblem is thus unnecessary. The only difference between our proposed algorithm and the more usual cubic regularization (ARC) method with exact global minimization is that the latter would check (4.2) for termination, while the algorithm presented here would instead check (4.1) with $\delta_{k-1} = 1$ by solving a trust-region subproblem. As observed above, both techniques have comparable numerical cost.

The bound (3.12) then ensures that Algorithm 4.1 terminates in at most $O\left(\epsilon^{-\frac{p+1}{p-1}}\right)$ evaluations of f, its gradient and Hessian. This algorithm thus shares(8) the upper complexity bounds stated in [8] for general p with different values of ϵ fpr fisrt- and second-order, and in [19, 5] for $p = 2$.

(8) For a marginally weaker (see footnote (7) and Theorem 2.2) but still necessary and, in our view, more sensible approximate optimality condition.

Algorithm 4.1: ARp for ϵ-approximate second-order-necessary minimizers

Step 0: Initialization. An initial point $x_0 \in \mathcal{F}$ and an initial regularization parameter $\sigma_0 > 0$ are given, as well as an accuracy level $\epsilon \in (0,1)$. The constants ϖ, θ, η_1, η_2, γ_1, γ_2, γ_3 and $\sigma_{\min}$ are also given and satisfy (2.17). Compute $f(x_0)$ and set $k = 0$.

Step 1: Test for termination. Evaluate $\{\nabla_x^i f(x_k)\}_{i=1}^2$. If (2.12) holds with $\phi_{f,2}^1(x_k)$ given by (4.1) and $\delta_{k-1} = 1$, terminate with the approximate solution $x_\epsilon = x_k$. Otherwise compute $\{\nabla_x^i f(x_k)\}_{i=3}^p$.

Step 2: Step calculation. Compute a step $s_k \neq 0$ by approximately minimizing the model (4.3) in the sense that (2.18) holds and

$$\|s_k\| \geq \varpi \epsilon^{\frac{1}{p-2+\beta}} \quad \text{or (4.5) holds.}$$

Step 3: Acceptance of the trial point. Compute $f(x_k + s_k)$ and define ρ_k as in (2.21). If $\rho_k \geq \eta_1$, then define $x_{k+1} = x_k + s_k$; otherwise define $x_{k+1} = x_k$.

Step 4: Regularization parameter update. Compute σ_{k+1} as in (2.22). Increment k by one and go to Step 1 if $\rho_k \geq \eta_1$, or to Step 2 otherwise.

5 A matching lower bound on the evaluation complexity for the Lipschitz continuous case

We now intend to show that the upper bound on evaluation complexity of Theorem 3.4 is tight in terms of the order given for unconstrained and a broad class of constrained problems with Lipschitz continuous p-th derivative (i.e. $\beta = 1$[9]). This objective is attained by defining a variant of the high-degree Hermite interpolation technique developed in [11], and then using this technique to build, for any number p of available derivatives of the objective function and any optimality order q, an unconstrained univariate example of suitably slow convergence (i.e. for which the order in ϵ given by (3.12) is achieved). This example is then embedded in higher dimensions to provide general lower bounds.

5.1 High-degree univariate Hermite interpolation

We start by investigating some useful properties of Hermite interpolation. Let us assume that we wish to construct a univariate Hermite interpolant π of degree $2(p+1)$ of the form

$$\pi(\tau) = \sum_{i=0}^{2p+1} c_i \, \tau^i \tag{5.1}$$

on the interval $[0, s]$ satisfying the $2(p+1)$ conditions

$$\pi^{(i)}(0) = f_0^{(i)}, \quad \pi^{(i)}(s) = f_1^{(i)} \text{ for } i \in \{0, \ldots, p\}, \tag{5.2}$$

(9) A example of slow convergence for general β and $p > 1 + \beta$ is provided in [9].

where $f_0^{(i)}$ and $f_1^{(i)}$ are given. The values of the coefficients $c_0,\ldots,c_p$ may then be obtained by

$$c_i = \frac{f_0^{(i)}}{i!} \quad \text{for} \quad i \in \{0,\ldots,p\}$$

while the remaining ones satisfy the linear system

$$\begin{pmatrix} a_{0,0}s^{p+1} & a_{0,1}s^{p+2} & \cdots & a_{0,p-1}s^{2p} & a_{1,p}s^{2p+1} \\ a_{1,0}s^{p} & a_{2,2}s^{p+1} & \cdots & a_{2,p-1}s^{2p-1} & a_{2,p}s^{2p} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{p,0}s & a_{p,1}s^{2} & \cdots & a_{p,p-1}s^{p} & a_{p,p}s^{p+1} \end{pmatrix} \begin{pmatrix} c_{p+1} \\ c_{p+2} \\ \vdots \\ c_{2p+1} \end{pmatrix} = \begin{pmatrix} f_1^{(0)} - T_p^{(0)}(0,s) \\ f_1^{(1)} - T_p^{(1)}(0,s) \\ \vdots \\ f_1^{(p)} - T_p^{(p)}(0,s)) \end{pmatrix} \tag{5.3}$$

where

$$T_p(0,s) = \sum_{i=0}^{p} \frac{f_0^{(i)}}{i!} s^i \quad \text{and} \quad a_{i,j} = \frac{(p+j+1)!}{(p+j+1-i)!} \quad (i,j=0,\ldots,p).$$

Observe that (5.3) can be rewritten as

$$\begin{pmatrix} s^p & & & \\ & s^{p-1} & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} A_p \begin{pmatrix} s & & & \\ & s^2 & & \\ & & \ddots & \\ & & & s^{p+1} \end{pmatrix} \begin{pmatrix} c_{p+1} \\ c_{p+2} \\ \vdots \\ c_{2p+1} \end{pmatrix} = \begin{pmatrix} f_1^{(0)} - T_p^{(0)}(0,s) \\ f_1^{(1)} - T_p^{(1)}(0,s) \\ \vdots \\ f_1^{(p)} - T_p^{(p)}(0,s)) \end{pmatrix}$$

with A_p is the matrix whose (i,j)-th entry is $a_{i,j}$, which only depends on p. It was show in [11, Appendix] that A_p is nonsingular. Therefore

$$\begin{pmatrix} c_{p+1}\, s \\ c_{p+2}\, s^2 \\ \vdots \\ c_{2p+1}\, s^{p+1} \end{pmatrix} = A_p^{-1} \begin{pmatrix} \frac{1}{s^p}[f_1^{(0)} - T_p^{(0)}(0,s)] \\ \frac{1}{s^{p-1}}[f_1^{(1)} - T_p^{(1)}(0,s)] \\ \vdots \\ f_1^{(p)} - T_p^{(p)}(0,s) \end{pmatrix}.$$

We therefore deduce that, for any $\tau \in [0,s]$,

$$\begin{aligned} |\pi^{(p+1)}(\tau)| &= \left| \sum_{i=0}^{p} \frac{(p+1+i)!}{i!} c_{p+1+i}\, \tau^i \right| \\ &\leq \sum_{i=0}^{p} \frac{(p+1+i)!}{i!} \left(|c_{p+1+i}|\, s^{i+1}\right) s^{-1} \\ &\leq \frac{(p+1)(2p+1)!}{p!} \|A_p^{-1}\|_\infty \max_{j=0,\ldots,p} \left| \frac{f_1^{(j)} - T_p^{(j)}(0,s)}{s^{p-j+1}} \right|. \end{aligned}$$

The mean-value theorem then implies that, for any $0 \leq \tau_2 \leq \tau_1 \leq s$ and some $\xi \in [\tau_2,\tau_1] \subseteq [0,s]$,

$$\begin{aligned} \frac{|\pi^{(p)}(\tau_1) - \pi^{(p)}(\tau_2)|}{|\tau_1 - \tau_2|} &= |\pi^{(p+1)}(\xi)| \\ &\leq \max_{\tau\in[0,s]} |\pi^{(p+1)}(\tau)| \\ &\leq \frac{(p+1)(2p+1)!}{p!} \|A_p^{-1}\|_\infty \max_{j=0,\ldots,p} \left| \frac{f_1^{(j)} - T_p^{(j)}(0,s)}{s^{p-j+1}} \right|. \end{aligned} \tag{5.4}$$

This development thus leads us to the following conclusion.

Theorem 5.1 Suppose that $\{f_\ell^{(j)}\}$ are given for $\ell \in \{1,2\}$ and $j \in \{0,\ldots,p\}$. Suppose also that there exists a constant $\kappa_f \geq 0$ such that, for all $j \in \{0,,\ldots,p\}$,

$$|f_1^{(j)} - T_p^{(j)}(0,s)| \leq \kappa_f \, s^{p-j+1}. \tag{5.5}$$

Then the Hermite interpolation polynomial $\pi(\tau)$ on $[0,s]$ given by (5.1) and satisfying (5.2) admits a Lipschitz continuous p-th derivative on $[0,s]$, with Lipschitz constant given by

$$L_p \stackrel{\rm def}{=} \frac{(p+1)(2p+1)!}{p!} \|A_p^{-1}\|_\infty \kappa_f,$$

which only depends on p and κ_f.

Proof. Directly results from (5.4) and (5.5). □

Observe that (5.5) is identical to (2.5) when $\beta = 1$ and $n = 1$. This means that the conditions of Theorem 5.1 automatically hold if the interpolation data $\{f_i^{(j)}\}$ is itself extracted from a function having a Lipschitz continuous p-th derivative.

Applying the above results to several interpolation intervals then yields the existence of a smooth Hermite interpolant.

Theorem 5.2 Suppose that, for some integer $k_e > 0$ and $p > 0$, the data $\{f_k^{(j)}\}$ and $\{x_k\}$ is given for $k \in \{0,\ldots,k_e\}$ and $j \in \{0,\ldots,p\}$. Suppose also that $s_k = x_{k+1} - x_k \in (0,\kappa_s]$ for $k \in \{0,\ldots,k_e\}$ and some $\kappa_s > 0$, and that, for some constant $\kappa_f \geq 0$ and $k \in \{0,\ldots,k_e-1\}$,

$$|f_{k+1}^{(j)} - T_{k,p}^{(j)}(x_k,s_k)| \leq \kappa_f \, s_k^{p-j+1}. \tag{5.6}$$

where $T_{k,p}(x_k,s) = \sum_{i=0}^p f_k^{(i)} \, s^i/i!$. Then there exists a p times continuously differentiable function f from $\mathbb{R}$ to $\mathbb{R}$ with Lipschitz continuous p-th derivative such that, for $k \in \{0,\ldots,k_e\}$,

$$f^{(j)}(x_k) = f_k^{(j)} \quad \text{for} \quad j \in \{0,\ldots,p\}.$$

Moreover, the range of f only depends on p, κ_f, $\max_k f_k^{(0)}$ and $\min_k f_k^{(0)}$.

Proof. We first use Theorem 5.1 to define a Hermite interpolant $\pi_k(s)$ of the form (5.1) on each interval $[x_k,x_{k+1}] = [x_k, x_k+s_k]$ ($k \in \{0,\ldots,k_e\}$) using $f_0^{(j)} = f_k^{(j)}$ and $f_1^{(j)} = f_{k+1}^{(j)}$ for $j \in \{0,\ldots,p\}$, and then set

$$f(x_k+s) = \pi_k(s)$$

for any $s \in [0,s_k]$. We may then smoothly prolongate f for $x \in \mathbb{R}$ by defining two additional interpolation intervals $[x_{-1}, x_0] = [-s_{-1}, 0]$ and $[x_{k_e}, x_{k_e} + s_{k_e}]$ with end conditions

$$f_{-1} = f_0^{(0)}, \quad f_{k_e+1} = f_{k_e}^{(0)} \text{ and } f_{-1}^{(j)} = f_{k_e+1}^{(j)} = 0 \text{ for } j \in \{1, \ldots, p\},$$

and where s_{-1} and s_{k_e} are chosen sufficiently large to ensure that (5.6) also holds on intervals -1 and k_e. We next set

$$f(x) = \begin{cases} f_0^{(0)} & \text{for } x \leq x_{-1}, \\ \pi_k(x - x_k) & \text{for } x \in [x_k, x_{k+1}] \text{ and } k \in \{-1, \ldots, n\}, \\ f_{k_e}^{(0)} & \text{for } x \geq x_{k_e} + s_{k_e}. \end{cases}$$

□

5.2 Slow convergence to (ϵ,δ)-approximate q-th-order-necessary minimizers

We now consider an unconstrained univariate instance of problem (2.1). Our aim is first to show that, for each choice of $p \geq 1$ and $q \in \{1, \ldots, p\}$, there exists an objective function f for problem (2.1) with $f \in C^{p,1}(\mathbb{R})$ (i.e. $\beta = 1$) such that obtaining an (ϵ, δ)-approximate q-th-order-necessary minimizer may require at least

$$\epsilon^{-\frac{p+1}{p-q+1}}$$

evaluations of the objective function and its derivatives using Algorithm 2.1, matching, in order of $\epsilon \in (0, 1]$, the upper bound (3.12). Our development follows the broad outline of [12] but extends it to approximate minimizers of arbitrary order. Given a model degree $p \geq 1$ and an optimality order $q \in \{1, \ldots, p\}$, we first define the sequences $\{f_k^{(j)}\}$ for $j \in \{0, \ldots, p\}$ and $k \in \{0, \ldots, k_\epsilon\}$ with

$$k_\epsilon = \left\lceil \epsilon^{-\frac{p+1}{p-q+1}} \right\rceil \tag{5.7}$$

by

$$\omega_k = \epsilon \, \frac{k_\epsilon - k}{k_\epsilon}. \tag{5.8}$$

as well as

$$f_k^{(j} = 0 \text{ for } j \in \{1, \ldots, q-1\} \cup \{q+1, \ldots, p\} \tag{5.9}$$

and

$$f_k^{(q)} = -(\epsilon + \omega_k)\, q!\, \chi_q(1) < 0. \tag{5.10}$$

Thus

$$T_p(x_k, s) = \sum_{j=0}^{p} \frac{f_k^{(j)}}{j!} s^j = f_k^{(0)} - (\epsilon + \omega_k)\chi_q(1) s^q \tag{5.11}$$

and, assuming $\delta_{k-1} = 1$ for all k (we verify below that this is acceptable),

$$\phi_{f,q}^{\delta_{k-1}}(x_k) = (\epsilon + \omega_k)\chi_q(\delta_{k-1}) \tag{5.12}$$

We also set $\sigma_k = p!$ for all $k \in \{0, \ldots, k_\epsilon\}$ (we again verify below that is acceptable). Note that

$$\omega_k \in (0, \epsilon] \quad \text{and} \quad \phi_{f,q}^{\delta_{k-1}} > \epsilon \chi_q(\delta_{k-1}) \text{ for } k \in \{0, \ldots, k_\epsilon - 1\}, \tag{5.13}$$

(and (2.12) fails at x_k), while

$$\omega_{k_\epsilon} = 0 \quad \text{and} \quad \phi_{f,q}^{\delta_{k-1}}(x_{k_\epsilon}) = \epsilon\chi_q(\delta_{k-1}) \tag{5.14}$$

(and (2.12) holds at x_{k_ϵ}). It is easy to verify using (5.11) that the model (2.16) is then globally minimized for

$$s_k = \left[\frac{|f_k^{(q)}|}{(q-1)!}\right]^{\frac{1}{p-q+1}} = [q(\epsilon+\omega_k)\chi_q(1)]^{\frac{1}{p-q+1}} > \epsilon^{\frac{1}{p-q+1}} \quad (k \in \{0,\ldots,k_\epsilon\}). \tag{5.15}$$

Hence this step satisfies (2.19) if we choose $\varpi = 1$. Because of this fact, we are free to choose δ_k arbitrarily in $(0,1]$ and we choose $\delta_k = 1$. Thus, provided we make the choice $\delta_{-1} = 1$ ensuring (5.12) for $k = 0$, the value $\delta_k = 1$ is admissible for all k. The step (5.15) yields that

$$\begin{aligned} m_k(s_k) &= f_k^{(0)} - (\epsilon+\omega_k)\chi_q(\delta_k)[q(\epsilon+\omega_k)\chi_q(\delta_k)]^{\frac{q}{p-q+1}} + \tfrac{1}{p+1}[q(\epsilon+\omega_k)\chi_q(\delta_k)]^{\frac{p+1}{p-q+1}} \\ &= f_k^{(0)} - \zeta(q,p)[q(\epsilon+\omega_k)\chi_q(\delta_k)]^{\frac{p+1}{p-q+1}} \end{aligned} \tag{5.16}$$

where

$$\zeta(q,p) \stackrel{\rm def}{=} \frac{p-q+1}{q(p+1)} \in (0,1). \tag{5.17}$$

Thus $m_k(s_k) < m_k(0)$ and (2.18) holds. We then define

$$f_0^{(0)} = 2[2q\chi_q(1)]^{\frac{p+1}{p-q+1}} \quad \text{and} \quad f_{k+1}^{(0)} = f_k^{(0)} - \zeta(q,p)[q(\epsilon+\omega_k)\chi_q(\delta_k)]^{\frac{p+1}{p-q+1}}, \tag{5.18}$$

which provides the identity

$$m_k(s_k) = f_{k+1}^{(0)} \tag{5.19}$$

(ensuring that iteration k is successful because $\rho_k = 1$ in (2.21) and thus that our choice of a constant σ_k is acceptable). In addition, using (5.18), (5.13), (5.17), the equality $\delta_k = 1$ and the inequality $k_\epsilon \le 1 + \epsilon^{-\frac{p+1}{p-q+1}}$ from (5.7) gives that, for $k \in \{0,\ldots,k_\epsilon\}$,

$$\begin{aligned} f_0^{(0)} \ge f_k^{(0)} &\ge f_0^{(0)} - k\zeta(q,p)[2q\epsilon\chi_q(\delta_k)]^{\frac{p+1}{p-q+1}} \\ &\ge f_0^{(0)} - k_\epsilon \epsilon^{\frac{p+1}{p-q+1}}[2q\chi_q(1)]^{\frac{p+1}{p-q+1}} \\ &\ge f_0^{(0)} - \left(1+\epsilon^{\frac{p+1}{p-q+1}}\right)[2q\chi_q(1)]^{\frac{p+1}{p-q+1}} \\ &\ge f_0^{(0)} - 2[2q\chi_q(1)]^{\frac{p+1}{p-q+1}}, \end{aligned}$$

and hence that

$$f_k^{(0)} \in \left[0, 2[2q\chi_q(1)]^{\frac{p+1}{p-q+1}}\right] \quad \text{for} \quad k \in \{0,\ldots,k_\epsilon\}. \tag{5.20}$$

We also set

$$\delta_{-1} = 1, \quad x_0 = 0 \quad \text{and} \quad x_k = \sum_{i=0}^{k-1} s_i.$$

Then (5.19) and (2.16) give that

$$|f_{k+1}^{(0)} - T_p(x_k,s_k)| = \frac{1}{p+1}|s_k|^{p+1}. \tag{5.21}$$

Now note that, using (5.11) and the first equality in (5.15),

$$T_p^{(j)}(x_k,s_k) = \frac{f_k^{(q)}}{(q-j)!}\, s_k^{q-j}\, \delta_{[j\le q]} = -\frac{(q-1)!}{(q-j)!}\, s_k^{p-j+1}\, \delta_{[j\le q]}$$

where $\delta_{[\cdot]}$ is the standard indicator function. We may now verify that, for $j\in\{1,\ldots,q-1\}$,

$$|f_{k+1}^{(j)} - T_p^{(j)}(x_k,s_k)| = |0 - T_p^{(j)}(x_k,s_k)| \le \left|\frac{(q-1)!}{(q-j)!}\right| |s_k|^{p-j+1} \le (q-1)!\, |s_k|^{p-j+1}, \quad (5.22)$$

while, for $j=q$, we have that

$$|f_{k+1}^{(q)} - T_p^{(q)}(x_k,s_k)| = |-(q-1)!\, s_k^{p-q+1} + (q-1)!\, s_k^{p-q+1}| = 0 \quad (5.23)$$

and, for $j\in\{q+1,\ldots,p\}$,

$$|f_{k+1}^{(j)} - T_p^{(j)}(x_k,s_k)| = |0-0| = 0. \quad (5.24)$$

Combining (5.21), (5.22), (5.23) and (5.24), we deduce that (5.6) holds with $\kappa_f = (q-1)!$. We may thus apply Theorem 5.2 with $\beta=1$, $\kappa_f=(q-1)!$ and $\kappa_s=1$, and deduce the existence of a p times continuously differentiable function f from $\mathbb{R}$ to $\mathbb{R}$ with Lipschitz continuous derivatives of order 0 to p which interpolates the $\{f_k^{(j)}\}$ at $\{x_k\}$ for $k\in\{0,\ldots,n\}$ and $j\in\{0,\ldots,p\}$. Moreover, (5.20) and Theorem 5.2 imply that the range of f only depends on p and q. In addition, (5.19) ensures that every iteration is successful and thus, because of (2.22), that the value $\sigma_k = p!$ may be used at all iterations.

This argument allows us to state the following lower bound on the complexity of the regularization algorithm using a p-th degree model.

Lemma 5.3 Given any $p\in\mathbb{N}_0$ and $q\in\{1,\ldots,p\}$, there exists a p times continuoulsy differentiable function f from $\mathbb{R}$ to $\mathbb{R}$ with range only depending on p and q and Lipschitz continuous p-th derivative such that, when the regularization algorithm with p-th degree model (Algorithm 2.1) is applied to minimize f without constraints, it takes exactly

$$k_\epsilon = \left\lceil \epsilon^{-\frac{p+1}{p-q+1}} \right\rceil$$

iterations (and evaluations of the objective function and its derivatives) to find an (ϵ,δ)-approximate q-th-order-necessary minimizer.

This implies the following important consequence for higher dimensional problems.

Theorem 5.4 Given any $n \in \mathbb{N}_0$, $p \in \mathbb{N}_0$ and $q \in \{1, \ldots, p\}$, there exists a p times continuoulsy differentiable function f from $\mathbb{R}^n$ to $\mathbb{R}$ with range only depending on p and q and Lipschitz continuous p-th derivative tensor such that, when the regularization algorithm with p-th degree model (Algorithm 2.1) is applied to minimize f without constraints, it takes exactly

$$k_\epsilon = \left\lceil \epsilon^{-\frac{p+1}{p-q+1}} \right\rceil \tag{5.25}$$

iterations (and evaluations of the objective function and its derivatives) to find an (ϵ, δ)-approximate q-th-order-necessary minimizer. Furthermore, the same conclusion holds if the optimization problem under consideration involves constraints provided the feasible set $\mathcal{F}$ contains a ray.

Proof. The first conclusion directly follows from Lemma 5.3 since it is always possible to include the unimodal example as an independent component of a multivariate one.

The second conclusion follows from the observation that our univariate example of slow convergence is only defined on $\mathbb{R}^+$ (even if Theorem 5.2 provides an extension to the complete real line). As a consequence, it may be used on any feasible ray. □

We now make a few observations.

1. Theorem 5.4 generalizes to arbitrary q the bound obtained in [3] for the case $q = 1$ and also shows that, at variance with the result derived in this reference, the generalized bound applies for arbitrary problem's dimension, but depends on ϵ, p and q.

2. For simplicity, we have chosen, in the above example, to minimize the model $m_k(s)$ globally at every iteration, but we might consider other pairs (s_k, δ_k). A similar example of slow convergence may in fact be constructed along the lines used above[(10)] for any sequence of acceptable[(11)] model reducing steps and associated optimality radii (in the sense of Lemma 2.5), provided the optimality radii remain bounded away from zero. This means that our example of slow convergence applies not only to Algorithm 2.1 but also to a much broader class of minimization methods. Moreover, it is also possible to weaken the constraints on the step further by relaxing (5.19) and only insisting on acceptable decrease of the objective function value in Step 3 of the algorithm.

   In [3], the authors derive their upper bound for $q = 1$ for the general class of "zero-preserving" algorithms, which are algorithms that "never explore (from x_k) coordinates which appear not to affect the function", that is directions d along which $T_p(x_k, \cdot)$ is constant. This property is obviously shared by Algorithm 2.1 because it attempts to reduce the Taylors' expansion of f around the current iterate (the presence of the isotropic regularization term is irrelevant for this).

3. Our example does not apply, for instance, to a linesearch method using global univariate minimization in a direction of search computed from the Taylor's expansion of f, which

[(10)] At the price of possibly larger constants.

[(11)] Remember that $\delta = 1$ is always possible for $q = 1$. It thus unsurprising that no such condition appears in [3].

is another zero-preserving method. Note however that this method, just as every other linesearch method (including possibly randomized coordinate searches), is bound to fail when attempting to compute approximate minimizers of order beyond three, because the Taylor's expansion at a non-optimal point then needs no longer decrease along lines. This is demonstrated by the following old example [16, 20]. Let

$$f(x_1, x_2) = (\tfrac{1}{2}x_1^2 - x_2)(x_1^2 - x_2).$$

Then $f(0,0) = 0$ and the origin is not a minimizer since f decreases along the arc $x_2 = \frac{3}{4}x_1$. Yet the origin is the global minimizer along every line passing through the origin, preventing any linesearch method to progress away from $(0,0)$.

Let us now consider an alternative unconstrained minimization method which would attempt to reduce the *unregularized* model (that is (2.16) with $\sigma_k = 0$) in order to find an unconstrained first-order minimizer. It is easy to see that if one chooses

$$f_k^{(1)} = -(\epsilon + \omega_k), \quad f_k^{(i)} = 0 \ \text{ for } \ i \in \{2, \dots, p-1\} \ \text{ and } \ f_k^{(p)} = p!,$$

the same reasoning as above yields that the largest obtainable decrease with this model occurs at

$$s_k = \left(\frac{\epsilon + \omega_k}{p}\right)^{\frac{1}{p-1}}$$

and is given by

$$f_k^{(0)} - m_k(s_k) = (p-1)\left(\frac{\epsilon + \omega_k}{p}\right)^{\frac{p}{p-1}}.$$

This then implies that at least a multiple of $\epsilon^{-\frac{p}{p-1}}$ evaluations may be needed to find approximate first-order-necessary minimizers, which is worse than the bound in $\epsilon^{-\frac{p+1}{p}}$ holding for the regularized algorithm. This is consistent with the known lower $O(\epsilon^{-2})$ bound for first-order points that holds for the (unregularized) Newton method (and hence the trust-region method), both of which use $p = 2$. Adding the regularization term thus not only provides a mechanism to limit the stepsize and make the step well-defined when $T_p(x_k, s)$ is unbounded below, but also amounts to increasing the 'useful degree' of the model by one, improving the worst-case complexity bound.

Summing up the above discussion, we conclude that an example of slow convergence requiring at least (5.25) evaluations can be built for any method whose steps decrease the regularized ($\sigma_k \geq \sigma_{\min}$) or unregularized ($\sigma_k = 0$) model (2.16) and whose approximate local optimality can be measured by (2.20) for some constant θ and $\delta_k = 1$ (which we can always enforce by adapting ϖ and (5.9)). For orders up to two, this includes most variants of steepest-descent and Newton's methods including those globalized with regularization, trust-region, a linesearch or a mixture of these (see [12] for a discussion). General linesearch methods are excluded for high-order optimization as they may fail to converge to approximate minimizers of order four and beyond.

Finally, one may wonder at what would happen if, for the interpolation data (5.9)-(5.10), the model

$$m_k(s) = T_p(x_k, s) + \frac{\sigma_k}{m!}|s|^m$$

were used for some $m > p+1$, resulting in a shorter step. The global model minimizer would then occur at $s = [q(\epsilon + \omega_k)\chi_q(1)]^{1/(m-1)}$ and give an optimal model decrease equal to

$[q(\epsilon+\omega_k)\chi_q(1)]^{m/(m-1)}(m-q)/m$. However, (5.6) would then fail for $j=0$ and the argument leading to an example of slow convergence would break down.

6 Summary, further comments and open questions

For any optimality order $q \geq 1$, we have provided the concept of an (ϵ, δ)-approximate q-th-order-necessary minimizer for the very general set-constrained problem (2.1). We have then proposed a conceptual regularization algorithm to find such approximate minimizers and have shown that, if $\nabla_x^p f$ is β-Hölder continuous, this algorithm requires at most $O(\epsilon^{-\frac{p+\beta}{p-q+\beta}})$ evaluations of the objective function and its p first derivatives to terminate. When $\nabla_x^p f$ is Lipschitz continuous, we have used an unconstrained univariate version of the problem to show that this bound is sharp in terms of the order in ϵ for any feasible set containing a ray and any problem dimension.

In view of the results in [7, 18], one may wonder at what would happen if the regularization power (i.e. the power of $\|s\|$ used in the last term of the model (2.16)) is allowed to differ from $p+\beta$. The theory presented above must then be re-examined and the crucial point is whether a global upper bound $\sigma_{\max}$ on the regularization parameter can still be ensured as in Lemma 3.2. One easily verifies that this is the case for regularization powers $r \in (p, p+\beta]$. Arguments parallel to those presented above then yield an upper bound of $O(\epsilon^{-\frac{r}{r-q}})$ evaluations(12), recovering the bound given in Section 3.3 of [7] for $q=1$. The situation is however more complicated (and beyond the scope of the present paper) for $r > p+\beta$ and the determination of a suitable general complexity upper bound for this latter case has not been formalized at this stage, but the analysis for $q=1$ discussed in Section 3.2 of [7] suggests that an improvement of the bound for larger r is unlikely.

Although the results presented essentially solve the question of determining the optimal evaluation complexity for unconstrained problems and problems with general inexpensive constraints, some interesting issues remain open at this stage. A first such issue is whether an example of slow convergence for all $\epsilon \in (0,1)$ can be found for feasible domains not containing a ray. A second is to extend the general complexity theory for problems whose constraints are not inexpensive: the discussion in [10] indicates that this is a challenging research area.

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Appendix A

A.1 Proof of Lemmas in Section 2

Proof of Lemma 2.1. We first establish the identity

$$I_{k-1,\beta} \stackrel{\rm def}{=} \int_0^1 \xi^\beta (1-\xi)^{k-1}\,d\xi = \frac{(k-1)!}{(k+\beta)!}, \quad \text{where} \quad (k+\beta)! \stackrel{\rm def}{=} \prod_{i=1}^k (i+\beta). \tag{A.1}$$

To see this, integrating by parts, we have that

$$I_{k-1,\beta} = \Big[-(k-1)\xi^\beta(1-\xi)^{k-2}\Big]_0^1 + \frac{(k-1)}{(1+\beta)}\xi^{1+\beta}(1-\xi)^{k-2}\,d\xi = \frac{(k-1)}{(1+\beta)}I_{k-2,1+\beta}$$

and thus, recursively, that

$$I_{k-1,\beta} = \frac{(k-1)!}{(k-1+\beta)!}I_{0,k-1+\beta} = \frac{(k-1)!}{(k-1+\beta)!}\int_0^1 \xi^{k-1+\beta}\,d\xi = \frac{(k-1)!}{(k+\beta)!}.$$

As in [11], consider the Taylor identity

$$\psi(1) - \tau_k(1) = \frac{1}{(k-1)!}\int_0^1 (1-\xi)^{k-1}[\psi^{(k)}(\xi) - \psi^{(k)}(0)]\,d\xi \tag{A.2}$$

involving a given univariate C^k function $\psi(t)$ and its k-th order Taylor approximation

$$\tau_k(t) = \sum_{i=0}^k \psi^{(i)}(0)\frac{t^i}{i!}$$

expressed in terms of the value $\psi^{(0)} = \psi$ and ith derivatives $\psi^{(i)}$, $i = 1, \ldots, k$. Then, picking $\psi(t) = f(x+ts)$, for given $x, s \in \mathbb{R}^n$, and $k = p$, the identity (A.2), and the relationships $\psi^{(p)}(t) = \nabla_x^p f(x+ts)[s]^p$ and $\tau_p(1) = T_p(x,s)$ give that

$$f(x+s) - T_p(x,s) = \frac{1}{(p-1)!}\int_0^1 (1-\xi)^{k-1}\left(\nabla_x^p f(x+\xi s) - \nabla_x^p f(x)\right)[s]^p\,d\xi,$$

and thus from the definition of the tensor norm (1.1), the Hölder bound (2.2) and the identity (A.1) when $k = p$ that

$$\begin{aligned}
f(x+s) - T_p(x,s) &\le \frac{1}{(p-1)!}\int_0^1 (1-\xi)^{k-1}\left|(\nabla_x^p f(x+\xi s) - \nabla_x^p f(x))\left[\frac{s}{\|s\|}\right]^p\right|\|s\|^p\,d\xi \\
&\le \frac{1}{(p-1)!}\int_0^1 (1-\xi)^{k-1}\max_{\|v\|=1}|(\nabla_x^p f(x+\xi s) - \nabla_x^p f(x))\,[v]^p|\,\|s\|^p\,d\xi \\
&= \frac{1}{(p-1)!}\int_0^1 (1-\xi)^{k-1}\|\nabla_x^p f(x+\xi s) - \nabla_x^p f(x))\|_{[p]}d\xi\cdot\|s\|^p \\
&\le \frac{1}{(p-1)!}\int_0^1 \xi^\beta(1-\xi)^{p-1}\,d\xi\cdot L\|s\|^{p+\beta} = \frac{L}{(p+\beta)!}\|s\|^{p+\beta}
\end{aligned}$$

for all $x, s \in \mathbb{R}^n$, which is the required (2.4).

Likewise, for arbitrary unit vectors $v_1, \ldots, v_j$, choosing $\psi(t) = \nabla_x^j f(x+ts)[v_1, \ldots, v_j]$ and $k = p-j$,it follows from (A.2), the relationships $\psi^{(p-j)}(t) = \nabla_x^p f(x+ts)[v_1, \ldots, v_j][s]^{p-j}$ and $\tau_{p-j}(1) = \nabla_s^j T_p(x,s)$ that

$$\begin{aligned}
&(\nabla_x^j f(x+s) - \nabla_s^j T_p(x,s))[v_1, \ldots, v_j] \\
&\quad = \frac{1}{(p-j-1)!}\int_0^1 (1-\xi)^{p-j-1}\left(\nabla_x^p f(x+\xi s) - \nabla_x^p f(x)[\,v_1, \ldots, v_j][s]^{p-j}\,d\xi.\right.
\end{aligned} \tag{A.3}$$

Then picking $v_1,\ldots,v_j$ to maximize the absolute value of left-hand size of (A.3) and using the tensor norm (1.1), the Hölder bound (2.2) and the identity (A.1) when $k=p-j$, we find that

$$\begin{aligned}
&\|\nabla_x^j f(x+s)-\nabla_s^j T_p(x,s)\|_{[j]}\\
&\quad\le \frac{1}{(p-j-1)!}\int_0^1(1-\xi)^{p-j-1}\left|(\nabla_x^p f(x+\xi s)-\nabla_x^p f(x))[v_1,\ldots,v_j]\left[\frac{s}{\|s\|}\right]^{p-j}\right|\|s\|^{p-j}\,d\xi\\
&\quad\le \frac{1}{(p-j-1)!}\int_0^1(1-\xi)^{p-j-1}\max_{\|v_1\|=\cdots=\|v_p\|=1}|(\nabla_x^p f(x+\xi s)-\nabla_x^p f(x))\,[v_1,\ldots,v_p]|\,\|s\|^{p-j}\,d\xi\\
&\quad= \frac{1}{(p-j-1)!}\int_0^1(1-\xi)^{p-j-1}\|\nabla_x^p f(x+\xi s)-\nabla_x^p f(x)\|_{[p]}\,d\xi\cdot\|s\|^{p-j}\\
&\quad\le \frac{1}{(p-j-1)!}\int_0^1\xi^\beta(1-\xi)^{p-j-1}\,d\xi\cdot L\|s\|^{p-j+\beta}=\frac{L}{(p-j+\beta)!}\|s\|^{p-j+\beta}
\end{aligned}$$

for all $x,s\in\mathbb{R}^n$, which gives (2.5). □

Proof of Lemma 2.3. The regularization parameter update (2.22) gives that, for each k,

$$\gamma_1\sigma_j\le\max[\gamma_1\sigma_j,\sigma_{\min}]\le\sigma_{j+1},\quad j\in\mathcal{S}_k,\quad\text{and}\quad\gamma_2\sigma_j\le\sigma_{j+1},\quad j\in\mathcal{U}_k,$$

where $\mathcal{U}_k\stackrel{\rm def}{=}\{0,\ldots,k\}\setminus\mathcal{S}_k$. Thus we deduce inductively that $\sigma_0\gamma_1^{|\mathcal{S}_k|}\gamma_2^{|\mathcal{U}_k|}\le\sigma_k$. We therefore obtain, using (2.23), that

$$|\mathcal{S}_k|\log\gamma_1+|\mathcal{U}_k|\log\gamma_2\le\log\left(\frac{\sigma_{\max}}{\sigma_0}\right),$$

which then implies that

$$|\mathcal{U}_k|\le-|\mathcal{S}_k|\frac{\log\gamma_1}{\log\gamma_2}+\frac{1}{\log\gamma_2}\log\left(\frac{\sigma_{\max}}{\sigma_0}\right),$$

since $\gamma_2>1$. The desired result (2.24) then follows from the equality $k+1=|\mathcal{S}_k|+|\mathcal{U}_k|$ and the inequality $\gamma_1<1$ given by (2.17). □

Proof of Lemma 2.4. We first observe that $\nabla_s^j\big(\|s\|^{p+\beta}\big)$ is a j-th order tensor, whose norm is defined using (1.1). Moreover, using the relationships

$$\nabla_s\big(\|s\|^\tau\big)=\tau\,\|s\|^{\tau-2}s\quad\text{and}\quad\nabla_s\big(s^{\tau\otimes}\big)=\tau\,s^{(\tau-1)\otimes}\otimes I,\quad(\tau\in\mathbb{R}),\tag{A.4}$$

defining

$$\nu_0\stackrel{\rm def}{=}1,\quad\text{and}\quad\nu_i\stackrel{\rm def}{=}\prod_{\ell=1}^{i}(p+2-2\ell),\tag{A.5}$$

and proceeding by induction, we obtain that, for some $\mu_{j,i} \geq 0$ with $\mu_{1,1} = 1$,

$$\begin{aligned}
&\nabla_s \left[\nabla_s^{j-1}\big(\|s\|^{p+\beta}\big)\right] \\
&\quad = \nabla_s \left[\sum_{i=2}^{j} \mu_{j-1,i-1}\nu_{i-1}\|s\|^{p+\beta-2(i-1)}\ s^{(2(i-1)-(j-1))\otimes} \otimes I^{((j-1)-(i-1))\otimes}\right] \\
&\quad = \sum_{i=2}^{j} \mu_{j-1,i-1}\nu_{i-1}\Big[(p+\beta-2(i-1))\|s\|^{p+\beta-2(i-1)-2}\ s^{(2(i-1)-(j-1)+1)\otimes} \otimes I^{(j-i)\otimes} \\
&\qquad\qquad + ((2(i-1)-(j-1))\|s\|^{p+\beta-2(i-1)}\ s^{(2(i-1)-(j-1)-1)\otimes} \otimes I^{(j-1)-(i-1)+1)\otimes}\Big] \\
&\quad = \sum_{i=2}^{j} \mu_{j-1,i-1}\nu_{i-1}\Big[(p+\beta+2-2i)\|s\|^{p+\beta-2i}\ s^{(2i-j)\otimes} \otimes I^{(j-i)\otimes} \\
&\qquad\qquad + (2(i-1)-j+1)\|s\|^{p+\beta-2(i-1)}\ s^{(2(i-1)-j)\otimes} \otimes I^{(j-(i-1))\otimes}\Big] \\
&\quad = \sum_{i=2}^{j} \mu_{j-1,i-1}\nu_{i-1}(p+\beta+2-2i)\|s\|^{p+\beta-2i}\ s^{(2i-j)\otimes} \otimes I^{(j-i)\otimes} \\
&\qquad\qquad + \sum_{i=1}^{j-1}(2i-j+1)\mu_{j-1,i}\nu_i\|s\|^{p+\beta-2i}\ s^{(2i-j)\otimes} \otimes I^{(j-i)\otimes}\Big] \\
&\quad = \sum_{i=1}^{j} \big((p+\beta+2-2i)\mu_{j-1,i-1}\nu_{i-1} + (2i-j+1)\mu_{j-1,i}\nu_i\big)\|s\|^{p+\beta-2i}\ s^{(2i-j)\otimes} \otimes I^{(j-i)\otimes}.
\end{aligned}$$

where the last equation uses the convention that $\mu_{j,0} = 0$ for all j. Thus we may write

$$\nabla_s^j\big(\|s\|^{p+\beta}\big) = \nabla_s\left[\nabla_s^{j-1}\big(\|s\|^{p+\beta}\big)\right] = \sum_{i=1}^{j} \mu_{j,i}\nu_i\, \|s\|^{p+\beta-2i}\, s^{(2i-j)\otimes} \otimes I^{(j-i)\otimes} \tag{A.6}$$

with

$$\begin{aligned}
\mu_{j,i}\nu_i &= (p+\beta+2-2i)\mu_{j-1,i-1}\nu_{i-1} + (2i-j+1)\mu_{j-1,i}\nu_i \\
&= \big[\mu_{j-1,i-1} + (2i-j+1)\mu_{j-1,i}\big]\nu_i,
\end{aligned} \tag{A.7}$$

where we used the identity

$$\nu_i = (p+\beta+2-2i)\nu_{i-1} \quad \text{for} \quad i = 1,\ldots,j \tag{A.8}$$

to deduce the second equality. Now (A.6) gives that

$$\nabla_s^j\big(\|s\|^{p+\beta}\big)[v]^j = \sum_{i=1}^{j} \mu_{j,i}\nu_i\|s\|^{p+\beta-j}\left(\frac{s^Tv}{\|s\|}\right)^{2i-j}(v^Tv)^{j-i}.$$

It is then easy to see that the maximum in (1.1) is achieved for $v = s/\|s\|$, so that

$$\|\,\nabla_s^j\big(\|s\|^{p+\beta}\big)\,\|_{[j]} = \left(\sum_{i=1}^{j}\mu_{j,i}\nu_i\right)\|s\|^{p+\beta-j} = \pi_j\|s\|^{p+\beta-j}. \tag{A.9}$$

with

$$\pi_j \stackrel{\text{def}}{=} \sum_{i=1}^{j} \mu_{j,i}\,\nu_i. \tag{A.10}$$

Successively using this definition, (A.7), (A.8) (twice), the identity $\mu_{j-1,j} = 0$ and (A.10) again, we then deduce that

$$\begin{aligned}
\pi_j &= \sum_{i=1}^{j} \mu_{j-1,i-1}\nu_i + \sum_{i=1}^{j}(2i-j+1)\mu_{j-1,i}\big]\nu_i \\
&= \sum_{i=1}^{j-1} \mu_{j-1,i}\nu_{i+1} + \sum_{i=1}^{j}(2i-j+1)\mu_{j-1,i}\big]\nu_i \\
&= \sum_{i=1}^{j-1} \mu_{j-1,i}\big[\nu_{i+1} + (2i-j+1)\nu_i\big] \\
&= \sum_{i=1}^{j-1} \mu_{j-1,i}\big[(p+\beta+2-2(i+1))\nu_i + (2i-j+1)\nu_i\big] \\
&= (p+\beta+1-j)\sum_{i=1}^{j-1} \mu_{j-1,i}\,\nu_i \\
&= (p+\beta+1-j)\pi_{j-1},
\end{aligned} \tag{A.11}$$

Since $\pi_1 = p+\beta$ from the first part of (A.4), we obtain that $\pi_j = (p+\beta)!/(p-j+\beta)!$, which, combined with (A.9) and (A.10), gives (2.25). We obtain (2.26) from (A.9) and (A.10), the observation that $\pi_p = (p+\beta)!$ and (A.11) for $j = p+1$. □

A.2 Proof of Lemmas in Section 3

Proof of Lemma 3.1. (See [2, Lemma 2.1]) Observe that, because of (2.18) and (2.16),

$$0 \le m_k(0) - m_k(s_k) = T_p(x_k, 0) - T_p(x_k, s_k) - \frac{\sigma_k}{p+1}\|s_k\|^{p+\beta}$$

which implies the desired bound. Note that $s_k \neq 0$ as long as we can satisfy condition (2.18), and so (3.1) implies (2.21) is well defined. □

Proof of Lemma 3.2. (See [2, Lemma 2.2]) Assume that

$$\sigma_k \ge \frac{L}{1-\eta_2}. \tag{A.12}$$

Using (2.4) and (3.1), we may then deduce that

$$|\rho_k - 1| \le \frac{|f(x_k+s_k) - T_p(x_k, s_k)|}{|T_p(x_k, 0) - T_p(x_k, s_k)|} \le \frac{L}{\sigma_k} \le 1 - \eta_2$$

and thus that $\rho_k \ge \eta_2$. Then iteration k is very successful in that $\rho_k \ge \eta_2$ and $\sigma_{k+1} \le \sigma_k$. As a consequence, the mechanism of the algorithm ensures that (3.2) holds. □