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WORST-CASE EVALUATION COMPLEXITY AND OPTIMALITY OF SECOND-ORDER METHODS FOR NONCONVEX SMOOTH OPTIMIZATION

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Abstract

We establish or refute the optimality of inexact second-order methods for unconstrained nonconvex optimization from the point of view of worst-case evaluation complexity, improving and generalizing our previous results. To this aim, we consider a new general class of inexact second-order algorithms for unconstrained optimization that includes regularization and trust-region variations of Newton's method as well as of their linesearch variants. For each method in this class and arbitrary accuracy threshold $\epsilon \in (0,1)$, we exhibit a smooth objective function with bounded range, whose gradient is globally Lipschitz continuous and whose Hessian is $\alpha-$Hölder continuous (for given $\alpha \in [0,1]$), for which the method in question takes at least $\lfloor \epsilon^{-(2+\alpha)/(1+\alpha)} \rfloor$ function evaluations to generate a first iterate whose gradient is smaller than ϵ in norm. Moreover, we also construct another function on which Newton's takes $\lfloor \epsilon^{-2} \rfloor$ evaluations, but whose Hessian is Lipschitz continuous on the path of iterates. These examples provide lower bounds on the worst-case evaluation complexity of methods in our class when applied to smooth problems satisfying the relevant assumptions. Furthermore, for $\alpha = 1$, this lower bound is of the same order in ϵ as the upper bound on the worst-case evaluation complexity of the cubic regularization method and other algorithms in a class of methods recently proposed by Curtis, Robinson and Samadi or by Royer and Wright, thus implying that these methods have optimal worst-case evaluation complexity within a wider class of second-order methods, and that Newton's method is suboptimal.

1 Introduction

Newton's method has long represented a benchmark for rapid asymptotic convergence when minimizing smooth, unconstrained objective functions Dennis and Schnabel [1983]. It has also been efficiently safeguarded to ensure its global convergence to first- and even second-order critical points, in the presence of local nonconvexity of the objective using linesearch Nocedal and Wright [1999], trust-region Conn, N. I. M. Gould, and P. L. Toint [2000] or other regularization techniques Griewank [1981], Nesterov

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and Polyak [2006], and Cartis, N. I. M. Gould, and P. L. Toint [2011a]. Many variants of these globalization techniques have been proposed. These generally retain fast local convergence under non-degeneracy assumptions, are often suitable when solving large-scale problems and sometimes allow approximate rather than true Hessians to be employed. We attempt to capture the common features of these methods in the description of a general class of second-order methods, which we denote by $\mathfrak{M}.\alpha$ in what follows.

In this paper, we are concerned with establishing *lower bounds* on the worst-case evaluation complexity of the $\mathfrak{M}.\alpha$ methods[1] when applied to "sufficiently smooth" nonconvex minimization problems, in the sense that we exhibit objective functions on which these methods take a large number of function evaluations to obtain an approximate first-order point.

There is a growing literature on the global worst-case evaluation complexity of first- and second-order methods for nonconvex smooth optimization problems (for which we provide a partial bibliography with this paper). In particular, it is known Vavasis [1993], Nesterov [2004, p. 29] that steepest-descent method with either exact or inexact linesearches takes at most[2] $\mathcal{O}\left(\epsilon^{-2}\right)$ iterations/function-evaluations to generate a gradient whose norm is at most ϵ when started from an arbitrary initial point and applied to nonconvex smooth objectives with gradients that are globally Lipschitz continuous within some open convex set containing the iterates generated. Furthermore, this bound is essentially sharp (for inexact Cartis, N. I. M. Gould, and P. L. Toint [2010] and exact Cartis, N. Gould, and P. L. Toint [2012] linesearches). Similarly, trust-region methods that ensure at least a Cauchy (steepest-descent-like) decrease on each iteration satisfy a worst-case evaluation complexity bound of the same order under identical conditions Gratton, Sartenaer, and P. L. Toint [2008]. It follows that Newton's method globalized by trust-region regularization has the same $\mathcal{O}\left(\epsilon^{-2}\right)$ worst-case evaluation upper bound; such a bound has also been shown to be essentially sharp Cartis, N. I. M. Gould, and P. L. Toint [2010].

From a worst-case complexity point of view, one can do better when a cubic regularization/perturbation of the Newton direction is used Griewank [1981], Nesterov and Polyak [2006], Cartis, N. I. M. Gould, and P. L. Toint [2011a], and Curtis, Robinson, and Samadi [2017b]—such a method iteratively calculates step corrections by (exactly or approximately) minimizing a cubic model formed of a quadratic approximation of the objective and the cube of a weighted norm of the step. For such a method, the worst-case global complexity improves to be $\mathcal{O}\left(\epsilon^{-3/2}\right)$ Nesterov and Polyak [2006] and Cartis, N. I. M. Gould, and P. L. Toint [2011a], for problems whose gradients and Hessians are Lipschitz continuous as above; this bound is also essentially sharp Cartis, N. I. M. Gould, and P. L. Toint [2010]. If instead powers between two and three are used in the regularization, then an "intermediate" worst-case complexity of $\mathcal{O}\left(\epsilon^{-(2+\alpha)/(1+\alpha)}\right)$

[1] And, as an aside, on that of the steepest-descent method.

[2] When $\{a_k\}$ and $\{b_k\}$ are two sequences of real numbers, we say that $a_k = \mathcal{O}(b_k)$ if the ratio a_k/b_k is bounded.

is obtained for such variants when applied to functions with globally $\alpha-$Hölder continuous Hessian on the path of iterates, where $\alpha \in (0, 1]$ Cartis, N. Gould, and P. L. Toint [2011]. It is finally possible, as proposed in C. W. Royer and Wright [2017], to obtain the desired $\mathcal{O}\left(\epsilon^{-3/2}\right)$ order of worst-case evaluation complexity using a purely quadratic regularization, at the price of mixing iterations using the regularized and unregularized Hessian with iterations requiring the computation of its left-most eigenpair.

These (essentially tight) upper bounds on the worst-case evaluation complexity of such second-order methods naturally raise the question as to whether other second-order methods might have better worst-case complexity than cubic (or similar) regularization over certain classes of sufficiently smooth functions. To attempt to answer this question, we define a general, parametrized class of methods that includes Newton's method, and that attempts to capture the essential features of globalized Newton variants we have mentioned. Our class includes for example, the algorithms discussed above as well as multiplier-adjusting types such as the Goldfeld-Quandt-Trotter approach Goldfeld, Quandt, and Trotter [1966]. The methods of interest take a potentially-perturbed Newton step at each iteration so long as the perturbation is "not too large" and the subproblem is solved "sufficiently accurately". The size of the perturbation allowed is simultaneously related to the parameter α defining the class of methods and the rate of the asymptotic convergence of the method. For each method in each α-parametrized class and each $\epsilon \in (0, 1)$, we construct a function with globally $\alpha-$Hölder-continuous Hessian and Lipschitz continuous gradient for which the method takes precisely $\lceil \epsilon^{-(2+\alpha)/(1+\alpha)} \rceil$ function evaluations to drive the gradient norm below ϵ. As such counts are the same order as the worst-case upper complexity bound of regularization methods, it follows that the latter methods are optimal within their respective α-class of methods. As α approaches zero, the worst-case complexity of these methods approaches that of steepest descent, while for $\alpha = 1$, we recover that of cubic regularization. We also improve the examples proposed in Cartis, N. I. M. Gould, and P. L. Toint [2010] and Cartis, N. Gould, and P. L. Toint [2011] in two ways. The first is that we now employ objective functions with bounded range, which allows refining the associated definition of sharp worst-case evaluation complexity bounds, the second being that the new examples now have finite isolated global minimizers.

The structure of the paper is as follows. Section 2 describes the parameter-dependent class of methods and objectives of interest; Section 2.1 gives properties of the methods such as their connection to fast asymptotic rates of convergence while Section 2.2 reviews some well-known examples of methods covered by our general definition of the class. Section 3 then introduces two examples of inefficiency of these methods and Section 4 discusses the consequences of these examples regarding the sharpness and possible optimality of the associated worst-case evaluation complexity bounds. Further consequences of our results on the new class proposed by Curtis, Robinson, and Samadi [2017b] and C. W. Royer and Wright [2017] are developed in Section 5 and 6, respectively. Section 7 draws our conclusions.

Notation. Throughout the paper, $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{R}^n$, I the $n \times n$ identity matrix, and $\lambda_{\min}(H)$ and $\lambda_{\max}(H)$ the left- and right-most eigenvalue

of any given symmetric matrix H, respectively. The condition number of a symmetric positive definite matrix M is denoted by $\kappa(M) \stackrel{\text{def}}{=} \lambda_{\max}(M)/\lambda_{\min}(M)$. If M is only positive-semidefinite which we denote by $M \succeq 0$, and $\lambda_{\min}(M) = 0$, then $\kappa(0) \stackrel{\text{def}}{=} +\infty$ unless $M = 0$, in which case we set $\kappa(0) \stackrel{\text{def}}{=} 1$. Positive definiteness of M is written as $M \succ 0$.

2 A general parametrized class of methods and objectives

Our aim is to minimize a given C^2 objective function $f(x)$, $x \in \mathbb{R}^n$. We consider methods that generate sequences of iterates $\{x_k\}$ for which $\{f(x_k)\}$ is monotonically decreasing, we let

$$f_k \stackrel{\text{def}}{=} f(x_k), \quad g_k \stackrel{\text{def}}{=} g(x_k) \text{ and } H_k \stackrel{\text{def}}{=} H(x_k).$$

where $g(x) = \nabla_x f(x)$ and $H(x) = \nabla_{xx} f(x)$.

Let $\alpha \in [0,1]$ be a fixed parameter and consider iterative methods whose iterations are defined as follows. Given some $x_0 \in \mathbb{R}^n$, let

$$x_{k+1} = x_k + s_k, \quad k \geq 0, \tag{2.1}$$

where s_k satisfies

$$(H_k + M_k)s_k = -g_k + r_k \quad \text{with} \quad \|r_k\| \leq \min\left[\kappa_{rg}\|g_k\|, \kappa_{rs}\|M_k s_k\|\right] \tag{2.2}$$

for some residual r_k and constants $\kappa_{rg} \in [0,1)$ and $\kappa_{rs} > 0$, and for some symmetric matrix M_k such that

$$M_k \succeq 0, \quad H_k + M_k \succeq 0 \tag{2.3}$$

and

$$\lambda_{\min}(H_k) + \lambda_{\min}(M_k) \leq \kappa_\lambda \max\left\{|\lambda_{\min}(H_k)|, \|g_k\|^{\frac{\alpha}{1+\alpha}}\right\} \tag{2.4}$$

for some $\kappa_\lambda > 1$ independent of k. Without loss of generality, we assume that $s_k \neq 0$. Furthermore, we require that no infinite steps are taken, namely

$$\|s_k\| \leq \kappa_s \tag{2.5}$$

for some $\kappa_s > 0$ independent of k. *The $\mathfrak{M}.\alpha$ class of second-order methods consists of all methods whose iterations satisfy (2.1)–(2.5).* The particular choices $M_k = \lambda_k I$ and $M_k = \lambda_k N_k$ (with N_k symmetric, positive definite and with bounded condition number) will be of particular interest in what follows[3]. Note that the definition of $\mathfrak{M}.\alpha$ just introduced generalizes that of M.α in Cartis, N. Gould, and P. L. Toint [2011].

[3]Note that (2.4) is slightly more general than a maybe more natural condition involving $\lambda_{\min}(H_k + M_k)$ instead of $\lambda_{\min}(H_k) + \lambda_{\min}(M_k)$.

Typically, the expression (2.2) for s_k is derived by minimizing (possibly approximately) the second-order model

(2.6)
$$m_k(s) = f_k + g_k^T s + \tfrac{1}{2} s^T (H_k + \beta_k M_k) s, \quad \text{with} \quad \beta_k \stackrel{\text{def}}{=} \beta_k(s) \geq 0 \quad \text{and} \quad \beta_k \leq 1$$

of $f(x_k+s)$—possibly with an explicit regularizing constraint—with the aim of obtaining a sufficient decrease of f at the new iterate $x_{k+1} = x_k + s_k$ compared to $f(x_k)$. In the definition of an $\mathfrak{M}.\alpha$ method however, the issue of (sufficient) objective-function decrease is not explicitly addressed/required. There is no loss of generality in doing so here since although local refinement of the model may be required to ensure function decrease, the number of function evaluations to do so (at least for known methods) does not increase the overall worst-case evaluation complexity by more than a constant multiple and thus does not affect quantitatively the worst-case bounds derived; see for example, Cartis, N. I. M. Gould, and P. L. Toint [2010], Cartis, N. I. M. Gould, and P. L. Toint [2011b], and Gratton, Sartenaer, and P. L. Toint [2008] and also Section 2.2. Furthermore, the examples of inefficiency proposed in Section 3 are constructed in such a way that each iteration of the method automatically provides sufficient decrease of f.

Having defined the classes of methods we shall be concerned with, we now specify the problem classes that we shall apply the methods in each class to, in order to demonstrate slow convergence. Given a method in $\mathfrak{M}.\alpha$, we are interested in minimizing functions f that satisfy

A.α $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable and bounded below, with gradient g being globally Lipschitz continuous on $\mathbb{R}^n$ with constant L_g, namely,

$$\|g(x) - g(y)\| \leq L_g \|x - y\|, \quad \text{for all } x,\ y \in \mathbb{R}^n; \tag{2.7}$$

and the Hessian H being globally $\alpha-$Hölder continuous on $\mathbb{R}^n$ with constant $L_{H,\alpha}$, i.e.,

$$\|H(x) - H(y)\| \leq L_{H,\alpha} \|x - y\|^\alpha, \quad \text{for all } x, y \in \mathbb{R}^n. \tag{2.8}$$

□

The case when $\alpha = 1$ in A.α corresponds to the Hessian of f being globally Lipschitz continuous. Moreover, (2.7) implies (2.8) when $\alpha = 0$, so that the A.0 class is that of twice continuously differentiable functions with globally Lipschitz continuous gradient. Note also that (2.7) and the existence of $H(x)$ imply that

$$\|H(x)\| \leq L_g \tag{2.9}$$

for all $x \in \mathbb{R}^n$ Nesterov [2004, Lemma 1.2.2], and that every function f satisfying A.α with $\alpha > 1$ must be quadratic. As we will see below, it turns out that we could weaken the conditions defining A.α by only requiring (2.7) and (2.8) to hold in an open set containing all the segments $[x_k, x_k + s_k]$ (the "path of iterates"), but these segments of course depend themselves on f and the method applied.

The next subsection provides some background and justification for the technical condition (2.4) by relating it to fast rates of asymptotic convergence, which is a defining feature of second-order algorithms. In Section 2.2, we then review some methods belonging to $\mathfrak{M}.\alpha$.

2.1 Properties of the methods in $\mathfrak{M}.\alpha$. We first state inclusions properties for $\mathfrak{M}.\alpha$ and A.α.

Lemma 2.1. *1. Consider a method of $\mathfrak{M}.\alpha_1$ for $\alpha_1 \in [0,1]$ and assume that it generates bounded gradients. Then it belongs to $\mathfrak{M}.\alpha_2$ for $\alpha_2 \in [0,\alpha_1]$.*

2. A.α_1 implies A.α_2 for $\alpha_2 \in [0,\alpha_1]$, with $L_{H,\alpha_2} = \max[L_{H,\alpha_1}, 2L_g]$.

Proof. By assumption, $\|g_k\| \leq \kappa_g$ for some $\kappa_g \geq 1$. Hence, if $\|g_k\| \geq 1$,

$$\|g_k\|^{\frac{\alpha_1}{1+\alpha_1}} \leq \kappa_g^{\frac{\alpha_1}{1+\alpha_1}} \leq \kappa_g \leq \kappa_g \|g_k\|^{\frac{\alpha_2}{1+\alpha_2}} \tag{2.10}$$

for any $\alpha_2 \in [0,\alpha_1]$. Moreover, (2.10) also holds if $\|g_k\| \leq 1$, proving the first statement of the lemma. Now we obtain from (2.9), that, if $\|x-y\| > 1$, then

$$\|H(x)-H(y)\| \leq \|H(x)\| + \|H(y)\| \leq 2L_g \leq 2L_g\|x-y\|^\alpha$$

for any $\alpha \in [0,1]$. When $\|x-y\| \leq 1$, we may deduce from (2.8) that, if $\alpha_1 \geq \alpha_2$, then (2.8) with $\alpha = \alpha_1$ implies (2.8) with $\alpha = \alpha_2$. This proves the second statement. □

Observe if a method is known to be globally convergent in the sense that $\|g_k\| \to 0$ when $k \to \infty$, then it obviously generates bounded gradients and thus the globally convergent methods of $\mathfrak{M}.\alpha_1$ are included in $\mathfrak{M}.\alpha_2$ ($\alpha_2 \in [0,\alpha_1]$).

We next give a sufficient, more concise, condition on the algorithm-generated matrices M_k that implies the bound (2.4).

Lemma 2.2. *Let (2.2) and (2.3) hold. Assume also that the algorithm-generated matrices M_k satisfies*

$$\lambda_{\min}(M_k) \leq \overline{\kappa}_\lambda \|s_k\|^\alpha, \quad \text{for some } \overline{\kappa}_\lambda > 1 \text{ and } \alpha \in [0,1] \text{ independent of } k. \tag{2.11}$$

Then (2.4) holds with $\kappa_\lambda \stackrel{\text{def}}{=} 2\overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})$.

Proof. Clearly, (2.4) holds when $\lambda_{\min}(H_k+M_k) = 0$. When $\lambda_{\min}(H_k+M_k) > 0$ and hence $H_k + M_k \succ 0$, (2.2) implies that

$$\|s_k\| \leq \frac{\|g_k\| + \|r_k\|}{\lambda_{\min}(H_k+M_k)} \leq \frac{(1+\kappa_{rg})\|g_k\|}{\lambda_{\min}(H_k)+\lambda_{\min}(M_k)}. \tag{2.12}$$

This and (2.11) give the inequality

$$\psi(\lambda_{\min}(M_k)) \leq 0 \quad \text{with} \quad \psi(\lambda) \stackrel{\text{def}}{=} \lambda^{\frac{1}{\alpha}}(\lambda + \lambda_{\min}(H_k)) - \overline{\kappa}_\lambda^{\frac{1}{\alpha}}(1+\kappa_{rg})\|g_k\|. \tag{2.13}$$

Now note that $\psi(0) = \psi(-\lambda_{\min}(H_k)) = -\overline{\kappa}_\lambda^{\frac{1}{\alpha}}(1+\kappa_{rg})\|g_k\|$ and thus

$$\psi(\lambda_{1,k}) < 0 \quad \text{with} \quad \lambda_{1,k} = \max\{0, -\lambda_{\min}(H_k)\}. \tag{2.14}$$

Moreover, the form of $\psi(\lambda)$ implies that $\psi(\lambda)$ is strictly increasing for $\lambda \geq \lambda_{1,k}$. Define now

$$\lambda_{2,k} \stackrel{\text{def}}{=} -\lambda_{\min}(H_k) + 2\max\left\{|\lambda_{\min}(H_k)|, \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\|^{\frac{\alpha}{1+\alpha}}\right\} > \lambda_{1,k}. \tag{2.15}$$

Suppose first that $\lambda_{\min}(H_k) < 0$ and $|\lambda_{\min}(H_k)| \geq \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\|^{\frac{\alpha}{1+\alpha}}$. Then one verifies that $\lambda_{2,k} = 3|\lambda_{\min}(H_k)|$ and

$$\begin{aligned}\psi(\lambda_{2,k}) &= (3|\lambda_{\min}(H_k)|)^{\frac{1+\alpha}{\alpha}} - (3|\lambda_{\min}(H_k)|)^{\frac{1}{\alpha}}|\lambda_{\min}(H_k)| - \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\| \\ &= 2\cdot 3^{\frac{1}{\alpha}}|\lambda_{\min}(H_k)|^{\frac{1+\alpha}{\alpha}} - \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\| > 0\end{aligned}$$

Suppose now that $\lambda_{\min}(H_k) \geq 0$ and $|\lambda_{\min}(H_k)| \geq \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\|^{\frac{\alpha}{1+\alpha}}$. Then $\lambda_{2,k} = \lambda_{\min}(H_k)$ and

$$\psi(\lambda_{2,k}) = (\lambda_{\min}(H_k))^{\frac{1+\alpha}{\alpha}} + (\lambda_{\min}(H_k))^{\frac{1}{\alpha}}|\lambda_{\min}(H_k)| - \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\| > 0.$$

Thus we deduce that $\psi(\lambda_{2,k}) > 0$ whenever $|\lambda_{\min}(H_k)| \geq \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\|^{\frac{\alpha}{1+\alpha}}$. Moreover the same inequality obviously holds if $|\lambda_{\min}(H_k)| < \overline{\kappa}_\lambda^{\frac{1}{1+\alpha}}(1+\kappa_{rg})^{\frac{\alpha}{1+\alpha}}\|g_k\|^{\frac{\alpha}{1+\alpha}}$ because $\psi(\lambda)$ is increasing with λ. As a consequence, $\psi(\lambda_{2,k}) > 0$ in all cases. We now combine this inequality, (2.14) and the monotonicity of $\psi(\lambda)$ for $\lambda \geq \lambda_{1,k}$ to obtain that either $\lambda_{\min}(M_k) \leq \lambda_{1,k} < \lambda_{2,k}$ or $\lambda_{\min}(M_k) \in [\lambda_{1,k}, \lambda_{2,k})$ because of of (2.13). Thus $\lambda_{\min}(M_k) \leq \lambda_{2,k}$, which, due to (2.15) and $\overline{\kappa}_\lambda > 1$, implies (2.4). □

Thus a method satisfying (2.1)–(2.5) and (2.11) belongs to $\mathfrak{M}.\alpha$, but not every method in $\mathfrak{M}.\alpha$ needs to satisfy (2.11). This latter requirement implies the following property regarding the length of the step generated by methods in $\mathfrak{M}.\alpha$ satisfying (2.11) when applied to functions satisfying A.α.

Lemma 2.3. *Assume that an objective function f satisfying A.α is minimized by a method satisfying (2.1), (2.2), (2.11) and such that the conditioning of M_k is bounded in that $\kappa(M_k) \leq \kappa_\kappa$ for some $\kappa_\kappa \geq 1$. Then there exists $\overline{\kappa}_{s,\alpha} > 0$ independent of k such that, for $k \geq 0$,*

$$\|s_k\| \geq \overline{\kappa}_{s,\alpha}\|g_{k+1}\|^{\frac{1}{1+\alpha}}. \tag{2.16}$$

Proof. The triangle inequality provides

$$\|g_{k+1}\| \leq \|g_{k+1} - (g_k + H_k s_k)\| + \|g_k + H_k s_k\|. \tag{2.17}$$

From (2.1), $g_{k+1} = g(x_k+s_k)$ and Taylor expansion provides $g_{k+1} = g_k + \int_0^1 H(x_k+\tau s_k)s_k\,d\tau$. This and (2.8) now imply

$$\|g_{k+1}-(g_k+H_k s_k)\| \le \left\|\int_0^1 [H(x_k+\tau s_k)-H(x_k)]d\tau\right\|\cdot\|s_k\| \le L_{H,\alpha}(1+\alpha)^{-1}\|s_k\|^{1+\alpha},$$

so that (2.17) and (2.2) together give that

$$\|g_{k+1}\| \;\le\; L_{H,\alpha}(1+\alpha)^{-1}\|s_k\|^{1+\alpha} + (1+\kappa_{rs})\|M_k\|\,\|s_k\|.$$

If $M_k \neq 0$, this inequality and the fact that $\kappa(M_k)$ is bounded then imply that

$$\|g_{k+1}\| \le L_{H,\alpha}(1+\alpha)^{-1}\|s_k\|^{1+\alpha} + \kappa(M_k)(1+\kappa_{rs})\lambda_{\min}(M_k)\,\|s_k\|,$$

while we may ignore the last term on the right-hand side if $M_k = 0$. Hence, in all cases,

$$\|g_{k+1}\| \le L_{H,\alpha}(1+\alpha)^{-1}\|s_k\|^{1+\alpha} + \kappa_\kappa(1+\kappa_{rs})\lambda_{\min}(M_k)\,\|s_k\|,$$

where we used that $\kappa(M_k) \le \kappa_\kappa$ by assumption. This bound and (2.11) then imply (2.16) with $\overline{\kappa}_{s,\alpha} \stackrel{\rm def}{=} [L_{H,\alpha}(1+\alpha)^{-1} + \kappa_\kappa(1+\kappa_{rs})\overline{\kappa}_\lambda]^{-\frac{1}{1+\alpha}}$. □

Property (2.16) will be central for proving (in Appendix A2) desirable properties of a class of methods belonging to $\mathfrak{M}.\alpha$. In addition, we now show that (2.16) is a necessary condition for fast local convergence of methods of type (2.2), under reasonable assumptions; fast local rate of convergence in a neighbourhood of well-behaved minimizers is a "trademark" of what is commonly regarded as second-order methods.

Lemma 2.4. *Let f satisfy assumptions A.α. Apply an algorithm to minimizing f that satisfies (2.1) and (2.2) and for which*

$$\|M_k\| \le \overline{\kappa}_\lambda, \quad k \ge 0, \quad \text{for some } \overline{\kappa}_\lambda > 0 \text{ independent of } k. \tag{2.18}$$

Assume also that convergence at linear or faster than linear rate occurs, namely,

$$\|g_{k+1}\| \le \kappa_c\|g_k\|^{1+\alpha}, \quad k \ge 0, \tag{2.19}$$

for some $\kappa_c > 0$ independent of k, with $\kappa_c \in (0,1)$ when $\alpha = 0$. Then (2.16) holds.

Proof. Let

$$0 \le \alpha_k \stackrel{\rm def}{=} \frac{\|s_k\|}{\|g_{k+1}\|^{\frac{1}{1+\alpha}}}, \quad k \ge 0. \tag{2.20}$$

From (2.19) and the definition of α_k in (2.20), we have that, for $k \ge 0$,

$$\begin{aligned}(1-\kappa_{rg})\tfrac{\|s_k\|}{\alpha_k} \;&\le\; \kappa_{c,\alpha}(1-\kappa_{rg})\|g_k\| \;\le\; \kappa_{c,\alpha}\|g_k + r_k\| \\ &=\; \kappa_{c,\alpha}\|(H_k+M_k)s_k\| \;\le\; \kappa_{c,\alpha}\|H_k+M_k\|\cdot\|s_k\|,\end{aligned}$$

where $\kappa_{c,\alpha} \stackrel{\text{def}}{=} \kappa_c^{\frac{1}{1+\alpha}}$ and where we used (2.2) to obtain the first equality. It follows that

$$\|H_k + M_k\| \geq \frac{(1-\kappa_{rg})}{\alpha_k \kappa_{c,\alpha}}, \quad k \geq 0. \tag{2.21}$$

The bounds (2.9) and (2.18) imply that $\{H_k + M_k\}$ is uniformly bounded above for all k, namely,

$$\|H_k + M_k\| \leq \kappa_{hl}, \quad k \geq 0, \tag{2.22}$$

where $\kappa_{hl} \stackrel{\text{def}}{=} L_g + \overline{\kappa}_\lambda$. Now (2.21) and (2.22) give that $\alpha_k \geq 1/(\kappa_{hl}\kappa_{c,\alpha}) > 0$, for all $k \geq 0$, and so it follows from (2.20), that (2.16) holds with $\overline{\kappa}_{s,\alpha} \stackrel{\text{def}}{=} (1-\kappa_{rg})/(\kappa_{c_1}\kappa_{c,\alpha})$. □

It is clear from the proof of Lemma 2.4 that (2.19) is only needed asymptotically, that is for all k sufficiently large; for simplicity, we have assumed it holds globally.

Note that letting $\alpha = 1$ in Lemma 2.4 provides a necessary condition for quadratically convergent methods satisfying (2.1), (2.2) and (2.18). Also, similarly to the above proof, one can show that if superlinear convergence of $\{g_k\}$ to zero occurs, then (2.16) holds with $\alpha = 0$ for all $\overline{\kappa}_{s,\alpha} > 0$, or equivalently, $\|g_{k+1}\|/\|s_k\| \to 0$, as $k \to \infty$.

Summarizing, we have shown that (2.16) holds for a method in $\mathfrak{M}.\alpha$ if (2.11) holds and $\kappa(M_k)$ is bounded, or if linear of faster asymptotic convergence takes place for unit steps.

2.2 Some examples of methods that belong to the class $\mathfrak{M}.\alpha$. Let us now illustrate some of the methods that either by construction or under certain conditions belong to $\mathfrak{M}.\alpha$. This list of methods does not attempt to be exhaustive and other practical methods may be found to belong to $\mathfrak{M}.\alpha$.

Newton's method Dennis and Schnabel [1983]. Newton's method for convex optimization is characterised by finding a correction s_k that satisfies $H_k s_k = -g_k$ for nonzero $g_k \in \text{Range}(H_k)$. Letting

$$M_k = 0, \quad r_k = 0 \text{ and } \beta_k = 0 \tag{2.23}$$

in (2.2) and (2.6), respectively, yields Newton's method. Provided additionally that both $g_k \in \text{Range}(H_k)$ and H_k is positive semi-definite, s_k is a descent direction and (2.3) holds. Since (2.4) is trivially satisfied in this case, it follows that Newton's method belongs to the class $\mathfrak{M}.\alpha$, for any $\alpha \in [0,1]$, provided it does not generate infinite steps to violate (2.5). As Newton's method is commonly embedded within trust-region or regularization frameworks when applied to nonconvex functions, (2.5) will in fact, hold as it is generally enforced for the latter methods. Note that allowing $\|r_k\| > 0$ subject to the second part of (2.2) then covers inexact variants of Newton's method.

Regularization algorithms Griewank [1981], Nesterov [2004], and Cartis, N. I. M. Gould, and P. L. Toint [2011b]. In these methods, the step s_k from the current iterate

x_k is computed by (possibly approximately) globally minimizing the model

$$m_k(s) = f_k + g_k^T s + \tfrac{1}{2} s^T H_k s + \frac{\sigma_k}{2+\alpha}\|s\|^{2+\alpha}, \tag{2.24}$$

where the regularization weight σ_k is adjusted to ensure sufficient decrease of f at $x_k + s_k$. We assume here that the minimization of (2.24) is carried accurately enough to ensure that $\nabla^2_{ss} m_k - (s) = H_k + \sigma_k \|s\| I$ is positive semidefinite, which is always possible because of Cartis, N. I. M. Gould, and P. L. Toint [2011a, Theorem 3.1]. The scalar α is the same fixed parameter as in the definition of A.α and $\mathfrak{M}.\alpha$, so that for each $\alpha \in [0,1]$, we have a different regularization term and hence what we shall call an $(2+\alpha)$-regularization method. For $\alpha = 1$, we recover the cubic regularization (ARC) approach Griewank [1981], Weiser, Deuflhard, and Erdmann [2007], Nesterov and Polyak [2006], and Cartis, N. I. M. Gould, and P. L. Toint [2011a,b]. For $\alpha = 0$, we obtain a quadratic regularization scheme, reminiscent of the Levenberg-Morrison-Marquardt method Nocedal and Wright [1999]. For these $(2+\alpha)$-regularization methods, we have

$$\alpha \in [0,1], \quad M_k = \sigma_k \|s_k\|^\alpha I, \quad \text{and} \quad \beta_k = \frac{2}{2+\alpha} \tag{2.25}$$

in (2.2) and (2.6). If scaling the regularization term is considered, then the second of these relation is replaced by $M_k = \sigma_k \|s_k\|^\alpha N_k$ for some fixed scaling symmetric positive definite matrix having a bounded condition number. Note that, by construction, $\kappa(M_k) = 1$. Since $\alpha \geq 0$, we have $0 \leq \beta_k \leq 1$ which is required in (2.6). A mechanism of successful and unsuccessful iterations and σ_k adjustments can be devised similarly to ARC Cartis, N. I. M. Gould, and P. L. Toint [2011a, Alg. 2.1] in order to deal with steps s_k that do not give sufficient decrease in the objective. An upper bound on the number of unsuccessful iterations which is constant multiple of successful ones can be given under mild assumptions on f Cartis, N. I. M. Gould, and P. L. Toint [2011b, Theorem 2.1]. Note that each (successful or unsuccessful) iteration requires one function- and at most one gradient evaluation.

We now show that for each $\alpha \in [0,1]$, the $(2+\alpha)-$regularization method based on the model (2.24) satisfies (2.5) and (2.4) when applied to f in A.α, and so it belongs to $\mathfrak{M}.\alpha$.

Lemma 2.5. *Let f satisfy A.α with $\alpha \in (0,1]$. Consider minimizing f by applying an $(2+\alpha)$-regularization method based on the model (2.24), where the step s_k is chosen as the global minimizer of the local $\alpha-$model, namely of $m_k(s)$ in (2.6) with the choice (2.25), and where the regularization parameter σ_k is chosen to ensure that*

$$\sigma_k \geq \sigma_{\min}, \quad k \geq 0, \tag{2.26}$$

for some $\sigma_{\min} > 0$ independent of k. Then (2.5) and (2.11) hold, and so the $(2+\alpha)$-regularization method belongs to $\mathfrak{M}.\alpha$.

(see Appendix A2 for details). The same argument that is used in Cartis, N. I. M. Gould, and P. L. Toint [2011a, Lem.2.2] for the $\alpha = 1$ case (see also Appendix A2) provides

$$\|s_k\| \leq \max\left\{\left(\frac{3(2+\alpha)L_g}{4\sigma_k}\right)^{\frac{1}{\alpha}}, \left(\frac{3(2+\alpha)\|g_k\|}{\sigma_k}\right)^{\frac{1}{1+\alpha}}\right\}, \quad k \geq 0, \tag{2.27}$$

so long as A.α holds, which together with (2.26), implies

$$\|s_k\| \leq \max\left\{\left(\frac{3(2+\alpha)L_g}{4\sigma_{\min}}\right)^{\frac{1}{\alpha}}, \left(\frac{3(2+\alpha)\|g_k\|}{\sigma_{\min}}\right)^{\frac{1}{1+\alpha}}\right\}, \quad k \geq 0. \tag{2.28}$$

The assumptions A.α, that the model is minimized globally imply that the $\alpha \leq 1$ analog of Cartis, N. I. M. Gould, and P. L. Toint [ibid., Corollary 2.6] holds, which gives $\|g_k\| \to 0$ as $k \to \infty$, and so $\{\|g_k\|\}$, $k \geq 0$, is bounded above. The bound (2.5) now follows from (2.28).

Using the same techniques as in Cartis, N. I. M. Gould, and P. L. Toint [ibid., Lemma 5.2] that applies when f satisfies A.1, it is easy to show for the more general A.α case that $\sigma_k \leq c_\sigma \max(\sigma_0, L_{H,\alpha})$ for all k, where c_σ is a constant depending solely on α and algorithm parameters. It then follows from (2.25) that (2.11) holds and therefore that the $(2+\alpha)$-regularization method belongs to $\mathfrak{M}.\alpha$ for $\alpha \in (0, 1]$. □

We cannot extend this result to the $\alpha = 0$ case unless we also assume that H_k is positive semi-definite. If this is the case, further examination of the proof of Cartis, N. I. M. Gould, and P. L. Toint [ibid., Lem.2.2] allows us to remove the first term in the max in (2.28), and the remainder of the proof is valid.

We note that bounding the regularization parameter σ_k away from zero in (2.26) appears crucial when establishing the bounds (2.5) and (2.4). Requiring (2.26) implies that the Newton step is always perturbed, but does not prevent local quadratic convergence of ARC Cartis, N. I. M. Gould, and P. L. Toint [2011b].

Goldfeld-Quandt-Trotter-type (GQT) methods Goldfeld, Quandt, and Trotter [1966]. Let $\alpha \in (0, 1]$. These algorithms set $M_k = \lambda_k I$, where

$$\lambda_k = \begin{cases} 0, & \text{when } \lambda_{\min}(H_k) \geq \omega_k \|g_k\|^{\frac{\alpha}{1+\alpha}}; \\ -\lambda_{\min}(H_k) + \omega_k \|g_k\|^{\frac{\alpha}{1+\alpha}}, & \text{otherwise,} \end{cases} \tag{2.29}$$

in (2.2), where $\omega_k > 0$ is a parameter that is adjusted so as to ensure sufficient objective decrease. (Observe that replacing $\frac{\alpha}{1+\alpha}$ by 1 in the exponent of $\|g_k\|$ in (2.29) recovers the original method of Goldfeld et al. Goldfeld, Quandt, and Trotter [ibid.].) It is straightforward to check that (2.3) holds for the choice (2.29). Thus the GQT approach takes the pure Newton step whenever the Hessian is locally sufficiently positive definite, and a suitable regularization of this step otherwise. The parameter ω_k is increased by a factor, say $\gamma_1 > 1$, and x_{k+1} left as x_k whenever the step s_k does not give sufficient decrease in f (i.e., iteration k is unsuccessful), namely when

$$\rho_k \stackrel{\text{def}}{=} \frac{f_k - f(x_k + s_k)}{f_k - m_k(s_k)} \leq \eta_1, \tag{2.30}$$

where $\eta_1 \in (0,1)$ and

$$m_k(s) = f_k + g_k^T s + \tfrac{1}{2} s^T H_k s \tag{2.31}$$

is the model (2.6) with $\beta_k = 0$. If $\rho_k > \eta_1$, then $\omega_{k+1} \leq \omega_k$ and x_{k+1} is constructed as in (2.1). Note that the choice (2.29) implies that (2.4) holds, provided ω_k is uniformly bounded above. We show that the latter, as well as (2.5), hold for functions in A.α.

Lemma 2.6. *Let f satisfy A.α with $\alpha \in (0,1]$. Consider minimizing f by applying a GQT method that sets λ_k in (2.2) according to (2.29), measures progress according to (2.30), and chooses the parameter ω_k and the residual r_k to satisfy, for $k \geq 0$,*

$$\omega_k \geq \omega_{\min} \quad k \geq 0. \quad \textit{and} \quad r_k^T s_k \leq 0. \tag{2.32}$$

Then (2.5) and (2.4) hold, and so the GQT method belongs to $\mathfrak{M}.\alpha$.

Note that the second part of (2.32) merely requires that s_k is not longer that the line minimum of the regularized model along the direction s_k, that is $1 \leq \arg\min_{\tau \geq 0} m_k(\tau s_k)$.

Proof. Let us first show (2.5). Since $\omega_k > 0$, and $g_k + r_k \neq 0$ until termination, the choice of λ_k in (2.29) implies that $\lambda_k + \lambda_{\min}(H_k) > 0$, for all k, and so (2.2) provides

$$s_k = -(H_k + \lambda_k I)^{-1}(g_k + r_k), \tag{2.33}$$

and hence,

$$\|s_k\| \leq \|(H_k + \lambda_k I)^{-1}\| \cdot \|g_k + r_k\| = \frac{(1+\kappa_{rg})\|g_k\|}{\lambda_k + \lambda_{\min}(H_k)}, \quad k \geq 0. \tag{2.34}$$

It follows from (2.29) and the first part of (2.32) that, for all $k \geq 0$,

$$\lambda_k + \lambda_{\min}(H_k) \geq \omega_k \|g_k\|^{\frac{\alpha}{1+\alpha}} \geq \omega_{\min} \|g_k\|^{\frac{\alpha}{1+\alpha}}, \tag{2.35}$$

This and (2.34) further give

$$\|s_k\| \leq \frac{(1+\kappa_{rg})\|g_k\|^{\frac{1}{1+\alpha}}}{\omega_{\min}}, \quad k \geq 0. \tag{2.36}$$

As global convergence assumptions are satisfied when f in A.α Conn, N. I. M. Gould, and P. L. Toint [2000] and Goldfeld, Quandt, and Trotter [1966], we have $\|g_k\| \to 0$ as $k \to \infty$ (in fact, we only need the gradients $\{g_k\}$ to be bounded). Thus (2.36) implies (2.5).

Due to (2.29), (2.4) holds if we show that $\{\omega_k\}$ is uniformly bounded above. For this, we first need to estimate the model decrease. Taking the inner product of (2.2) with s_k, we obtain that

$$-g_k^T s_k = s_k^T H_k s_k + \lambda_k \|s_k\|^2 - r_k^T s_k.$$

Substituting this into the model decrease, we deduce also from (2.6) with $\beta_k = 0$ that

$$f_k - m_k(s_k) = -g_k^T s_k - \tfrac{1}{2} s_k^T H_k s_k = \tfrac{1}{2} s_k^T H_k s_k + \lambda_k \|s_k\|^2 - r_k^T s_k \geq \left(\tfrac{1}{2}\lambda_{\min}(H_k) + \lambda_k\right) \|s_k\|^2.$$

where we used the second part of (2.32) to obtain the last inequality. It is straightforward to check that this and (2.35) now imply

$$f_k - m_k(s_k) \geq \tfrac{1}{2}\omega_k \|g_k\|^{\frac{\alpha}{1+\alpha}} \cdot \|s_k\|^2. \tag{2.37}$$

We show next that iteration k is successful for ω_k sufficiently large. From (2.30) and second-order Taylor expansion of $f(x_k + s_k)$, we deduce

$$|\rho_k - 1| = \left| \frac{f(x_k + s_k) - m_k(s_k)}{f_k - m_k(s_k)} \right| \leq \frac{|H_k - H(\xi_k)| \cdot \|s_k\|^2}{2(f_k - m_k(s_k))} \leq \frac{L_{H,\alpha} \|s_k\|^{2+\alpha}}{2(f_k - m_k(s_k))}.$$

This and (2.37) now give

$$|\rho_k - 1| \leq \frac{L_{H,\alpha} \|s_k\|^{\alpha}}{\omega_k \|g_k\|^{\frac{\alpha}{1+\alpha}}} \leq \frac{L_{H,\alpha}}{\omega_{\min}^{\alpha} \omega_k}, \tag{2.38}$$

where to obtain the last inequality, we used (2.36). Due to (2.30), iteration k is successful when $|\rho_k - 1| \leq 1 - \eta_1$, which from (2.38) is guaranteed to hold whenever $\omega_k \geq \frac{L_{H,\alpha}}{\omega_{\min}^{\alpha}(1-\eta_1)}$. As on each successful iteration we set $\omega_{k+1} \leq \omega_k$, it follows that

$$\omega_k \leq \overline{\omega} \stackrel{\text{def}}{=} \max\left\{\omega_0, \frac{\gamma_1 L_{H,\alpha}}{\omega_{\min}^{\alpha}(1-\eta_1)}\right\}, \quad k \geq 0, \tag{2.39}$$

where the max term addresses the situation at the starting point and the γ_1 factor is included in case an iteration was unsuccessful and close to the bound. This concludes proving (2.4). □

Trust-region algorithms Conn, N. I. M. Gould, and P. L. Toint [2000]. These methods compute the correction s_k as the global solution of the subproblem

$$\text{minimize} \;\; f_k + g_k^T s + \tfrac{1}{2} s^T H_k s \;\; \text{subject to} \;\; \|s\| \leq \Delta_k, \tag{2.40}$$

where Δ_k is an evolving trust-region radius that is chosen to ensure sufficient decrease of f at $x_k + s_k$. The resulting global minimizer satisfies (2.2)–(2.3) Conn, N. I. M. Gould, and P. L. Toint [ibid., Corollary 7.2.2] with $M_k = \lambda_k I$ (or $M_k = \lambda_k N_k$ if scaling is considered) and $r_k = 0$. The scalar λ_k is the Lagrange multiplier of the trust-region constraint, satisfies

$$\lambda_k \geq \max\{0, -\lambda_{\min}(H_k)\} \tag{2.41}$$

and is such that $\lambda_k = 0$ whenever $\|s_k\| < \Delta_k$ (and then, s_k is the Newton step) or calculated using (2.2) to ensure that $\|s_k\| = \Delta_k$. The scalar $\beta_k = 0$ in (2.6). The iterates are defined by (2.1) whenever sufficient progress can be made in some relative

function decrease (so-called *successful iterations*), and they remain unchanged otherwise (*unsuccessful iterations*) while Δ_k is adjusted to improve the model (decreased on unsuccessful iterations, possibly increased on successful ones). The total number of unsuccessful iterations is bounded above by a constant multiple of the successful ones plus a (negligible) term in $\log \epsilon$ Gratton, Sartenaer, and P. L. Toint [2008, page 23] provided Δ_k is not increased too fast on successful iterations. One successful iteration requires one gradient and one function evaluation while an unsuccessful one only evaluates the objective.

The property (2.5) of $\mathfrak{M}.\alpha$ methods can be easily shown for trust-region methods, see Lemma 2.7. It is unclear however, whether conditions (2.4) or (2.11) can be guaranteed in general for functions in A.α. The next lemma gives conditions ensuring a uniform upper bound on the multiplier λ_k, which still falls short of (2.4) in general.

Lemma 2.7. *Let f satisfy assumptions A.0. Consider minimizing f by applying a trust-region method as described in Conn, N. I. M. Gould, and P. L. Toint [2000, Algorithm 6.1.1], where the trust-region subproblem is minimized globally to compute s_k and where the trust-region radius is chosen to ensure that*

$$\Delta_k \leq \Delta_{\max}, \quad k \geq 0, \tag{2.42}$$

for some $\Delta_{\max} > 0$. Then (2.5) holds. Additionally, if

$$\|g_{k+1}\| \leq \|g_k\|, \text{ for all } k \text{ sufficiently large,} \tag{2.43}$$

then $\lambda_k \leq \lambda_{\max}$ for all k and some $\lambda_{\max} > 0$, and $\lambda_{\min}(M_k)$ is bounded.

Proof. Consider the basic trust-region algorithm as described in Conn, N. I. M. Gould, and P. L. Toint [ibid., Algorithm 6.1.1], using the same notation. Since the global minimizer s_k of the trust-region subproblem is feasible with respect to the trust-region constraint, we have $\|s_k\| \leq \Delta_k$, and so (2.5) follows trivially from (2.42).

Clearly, the upper bound on λ_k holds whenever $\lambda_k = 0$ or $\lambda_k = -\lambda_{\min}(H_k) \leq L_g$. Thus it is sufficient to consider the case when $\lambda_k > 0$ and $H_k + \lambda_k I \succ 0$. The first condition implies that the trust-region constraint is active, namely $\|s_k\| = \Delta_k$ Conn, N. I. M. Gould, and P. L. Toint [ibid., Corollary 7.2.2]. The second condition together with (2.2) implies, as in the proof of Lemma 2.2, that (2.12) holds. Thus we deduce

$$\Delta_k \leq \frac{\|g_k\|}{\lambda_k + \lambda_{\min}(H_k)},$$

or equivalently,

$$\lambda_k \leq \frac{\|g_k\|}{\Delta_k} - \lambda_{\min}(H_k) \leq \frac{\|g_k\|}{\Delta_k} + L_g, \quad k \geq 0. \tag{2.44}$$

It remains to show that

$$\{\|g_k\|/\Delta_k\} \text{ is bounded above independently of } k. \tag{2.45}$$

By Conn, N. I. M. Gould, and P. L. Toint [ibid., Theorem 6.4.2], we have that there exists $c \in (0,1)$ such that the implication holds

$$\Delta_k \leq c\|g_k\| \quad \Longrightarrow \quad \Delta_{k+1} \geq \Delta_k, \text{ i.e., } k \text{ is successful.} \tag{2.46}$$

(Observe that the Cauchy model decrease condition Conn, N. I. M. Gould, and P. L. Toint [ibid., Theorem 6.3.3] is sufficient to obtain the above implication.) Let $\gamma_1 \in (0,1)$ denote the largest factor we allow Δ_k to be decreased by (during unsuccessful iterations). Using a similar argument to that of Conn, N. I. M. Gould, and P. L. Toint [ibid., Theorem 6.4.3], we let $k \geq k_0$ be the first iterate such that

$$\Delta_{k+1} < c\gamma_1\|g_{k+1}\|, \tag{2.47}$$

where k_0 is the iteration from which onwards (2.43) holds. Then since $\Delta_{k+1} \geq \gamma_1\Delta_k$ and from (2.43) we have that $\Delta_k < c\|g_k\|$. This and (2.46) give

$$\Delta_{k+1} \geq \Delta_k \geq c\gamma_1\|g_k\| \geq c\gamma_1\|g_{k+1}\|,$$

where to obtain the second and third inequalities, we used the hypothesis and (2.43), respectively. We have reached a contradiction with our assumption that $k+1$ is the first iteration greater than k_0 such that (2.47) holds. Hence there is no such k and we deduce that

$$\Delta_k \geq \min\left\{\Delta_{k_0}, c\gamma_1\|g_k\|\right\} \quad \text{for all } k \geq k_0. \tag{2.48}$$

Note that since g_k remains unchanged on unsuccessful iterations, (2.43) trivially holds on such iterations. Since the assumptions of Conn, N. I. M. Gould, and P. L. Toint [ibid., Theorem 6.4.6] are satisfied, we have that $\|g_k\| \to 0$, as $k \to \infty$. This and (2.48) imply (2.45). The desired conclusion then follows from (2.44). □

Note that if (2.19) holds for some $\alpha \in [0,1]$, then (2.43) is satisfied, and so Lemma 2.7 shows that if (2.19) holds, then (2.18) is satisfied. It follows from Lemma 2.4 that fast convergence of trust-region methods for functions in A.α alone is sufficient to ensure (2.16), which in turn is connected to our definition of the class $\mathfrak{M}.\alpha$. However, the properties of the multipliers (in the sense of (2.4) for any $\alpha \in [0,1]$ or even (2.16)) remain unclear in the absence of fast convergence of the method. Based on our experience, we are inclined to believe that generally, the multipliers λ_k are at best guaranteed to be uniformly bounded above, even for specialized, potentially computationally expensive, rules of choosing the trust-region radius.

As the Newton step is taken in the trust-region framework satisfying (2.2) whenever it is within the trust region and gives sufficient decrease in the presence of local convexity, the A.1- (hence A.α-) example of inefficient behaviour for Newton's method of worst-case evaluation complexity precisely ϵ^{-2} can be shown to apply also to trust-region methods Cartis, N. I. M. Gould, and P. L. Toint [2010] (see also Gratton, Sartenaer, and P. L. Toint [2008]).

Linesearch methods Dennis and Schnabel [1983] and Nocedal and Wright [1999]. We finally consider methods using a linesearch to control improvement in the objective at each step. Such methods compute $x_{k+1} = x_k + s_k$, $k \geq 0$, where s_k is defined

via (2.2) in which M_k is chosen so that $H_k + M_k$, the Hessian of the selected quadratic model $m_k(s)$, is "sufficiently" positive definite, and $r_k = (1-\mu_k)g_k$, yielding a step-size $\mu_k \in [1-\kappa_{rg}, 1]$ which is calculated so as to decrease f (the *linesearch*); this is always possible for sufficiently small μ_k (and hence sufficiently small κ_{rg}.) The precise definition of "sufficient decrease" depends on the particular linesearch scheme being considered, but we assume here that

$$\mu_k = 1 \quad \text{is acceptable whenever} \quad m_k(s_k) = f(x_k + s_k).$$

In other words, we require the unit step to be acceptable when the model and the true objective function match at the trial point. Because the minimization of the quadratic model along the step always ensure that $m_k(s_k) = f(x_k) + \frac{1}{2} g_k s_k$, the above condition says that s_k must be acceptable with $\mu_k = 1$ whenever $f(x_k + s_k) = f(x_k) + \frac{1}{2} g_k s_k$. This is for instance the case for the Armijo and Goldstein linesearch conditions[(4)], two standard linesearch techniques. As a consequence, the corresponding linesearch variants of Newton's method and of the $(2+\alpha)$-regularization methods also belong to $\mathfrak{M}.\alpha$ (with $\beta_k = 1$ for all k), and the list is not exhaustive. Note that linesearch methods where the search direction is computed inexactly are also covered by setting $r_k = g_k - \mu_k(g_k + w_k)$ for some "error vector" w_k, provided the second part of (2.2) still holds.

3 Examples of inefficient behaviour

After reviewing the methods in $\mathfrak{M}.\alpha$, we now turn to showing they can converge slowly when applied to specific functions with fixed range[(5)] and the relevant degree of smoothness.

3.1 General methods in $\mathfrak{M}.\alpha$. Let $\alpha \in [0,1]$ and $\epsilon \in (0,1)$ be given and consider an arbitrary method in $\mathfrak{M}.\alpha$. Our intent is now to construct a univariate function $f_\epsilon^{\mathfrak{M}.\alpha}(x)$ satisfying A.α such that

$$f_\epsilon^{\mathfrak{M}.\alpha}(0) = 1, \quad f_\epsilon^{\mathfrak{M}.\alpha}(x) \in [a,b] \ \text{ for } \ x \geq 0, \tag{3.1}$$

for some constants $a \leq b$ independent of ϵ and α, and such that the method will terminate in exactly

$$k_{\epsilon,\alpha} = \left\lceil \epsilon^{-\frac{2+\alpha}{1+\alpha}} \right\rceil \tag{3.2}$$

iterations (and evaluations of f, g and H).

We start by defining the sequences f_k, g_k and H_k for $k = 0, \ldots, k_{\epsilon,\alpha}$ by

$$f_k = 1 - \tfrac{1}{2} k \epsilon^{\frac{2+\alpha}{1+\alpha}}, \quad g_k = -2\,\epsilon\, f_k \ \text{ and } \ H_k = 4\,\epsilon^{\frac{\alpha}{1+\alpha}}\, f_k^2. \tag{3.3}$$

(4) With reasonable algorithmic constants, see Appendix A1.

(5) At variancewith the examples proposed in Cartis, N. I. M. Gould, and P. L. Toint [2010] and Cartis, N. Gould, and P. L. Toint [2011].

They are intended to specify the objective function, gradient and Hessian values at successive iterates generated by the chosen method in $\mathfrak{M}.\alpha$, according to (2.1) and (2.2) for some choice of multipliers $\{\lambda_k\} = \{M_k\} = \{\lambda_{\min}(M_k)\}$ satisfying (2.3) and (2.4). In other words, we impose that $f_k = f_\epsilon^{\mathfrak{M}.\alpha}(x_k)$, $g_k = \nabla f_\epsilon^{\mathfrak{M}.\alpha}(x_k)$ and $H_k = \nabla^2 f_\epsilon^{\mathfrak{M}.\alpha}(x_k)$ for $k \in \mathcal{K} \stackrel{\text{def}}{=} \{0, \ldots, k_{\epsilon,\alpha}\}$. Note that f_k, $|g_k|$ and H_k are monotonically decreasing and that, using (3.2),

$$f_k \in [\tfrac{1}{2}, 1] \quad \text{for} \quad k \in \mathcal{K}. \tag{3.4}$$

In addition, (2.3) and (2.4) impose that, for $k \in \mathcal{K}$,

$$0 \le \lambda_k + 4\epsilon^{\frac{\alpha}{1+\alpha}} f_k^2 \le \kappa_\lambda \max[4\epsilon^{\frac{\alpha}{1+\alpha}} f_k^2, (2\epsilon f_k)^{\frac{\alpha}{1+\alpha}}] = 4\kappa_\lambda \epsilon^{\frac{\alpha}{1+\alpha}} f_k^2.$$

yielding that

$$\lambda_k \in \left[0, 4(\kappa_\lambda - 1)\epsilon^{\frac{\alpha}{1+\alpha}} f_k^2\right], \tag{3.5}$$

As a consequence, we obtain, using both parts of (2.2), that, for $k \in \mathcal{K}$,

$$s_k = \theta_k \frac{\epsilon^{\frac{1}{1+\alpha}}}{2 f_k} \quad \text{for some} \quad \theta_k \in \left[\frac{1-\kappa_{rg}}{\kappa_\lambda}, 1+\kappa_{rg}\right]. \tag{3.6}$$

Note that our construction imposes that

$$\begin{aligned} m_k(s_k) &= f_k + g_k s_k + \tfrac{1}{2} g_k s_k + \tfrac{1}{2} s_k (H_k + \beta_k \lambda_k) s_k \\ &= f_k + g_k s_k + \tfrac{1}{2} s_k [-g_k + r_k + (\beta_k - 1)\lambda_k s_k] \\ &\ge f_k - \tfrac{1}{2}|g_k| s_k - \tfrac{1}{2}\kappa_{rg}|g_k| s_k + \tfrac{1}{2}\theta_k^2(\kappa_\lambda - 1)(\beta_k - 1)\epsilon^{\frac{2+\alpha}{1+\alpha}} \\ &\ge f_k - \tfrac{1}{2}\theta_k \epsilon^{\frac{2+\alpha}{1+\alpha}}[1 + \kappa_{rg} + \theta_k(1-\beta_k)(\kappa_\lambda - 1)] \\ &\ge f_k - \tfrac{1}{2}\epsilon^{\frac{2+\alpha}{1+\alpha}}(1+\kappa_{rg})^2[1 + (1-\beta_k)(\kappa_\lambda - 1)] \\ &\ge f_k - \tfrac{1}{2}\epsilon^{\frac{2+\alpha}{1+\alpha}}(1+\kappa_{rg})^2 \kappa_\lambda \end{aligned} \tag{3.7}$$

where we have used (2.2), (3.3), (3.6), (3.5) and $\beta_k \le 1$. Hence, again taking (3.3) into account,

$$\frac{f_k - f_{k+1}}{f_k - m_k(s_k)} \ge \frac{\frac{1}{2}\epsilon^{\frac{2+\alpha}{1+\alpha}}}{\frac{1}{2}\epsilon^{\frac{2+\alpha}{1+\alpha}}\kappa_\lambda(1+\kappa_{rg})^2} = \frac{1}{(1+\kappa_{rg})^2\kappa_\lambda} \in (0,1), \tag{3.8}$$

and sufficient decrease of the objective function automatically follows. Moreover, given (3.4), we deduce from (3.6) that $|s_k| \le 1$ for $k \in \mathcal{K}$ and (2.5) holds with $\kappa_s = 1$, as requested for a method in $\mathfrak{M}.\alpha$. It also follows from (2.1) and (3.6) that, if $x_0 = 0$,

$$s_k > 0 \ \text{ and } \ x_k = \sum_{i=0}^{k-1} s_i, \quad k = 0, \ldots, k_{\epsilon,\alpha}. \tag{3.9}$$

We therefore conclude that the sequences $\{f_k\}_{k=0}^{k_{\epsilon,\alpha}}$, $\{g_k\}_{k=0}^{k_{\epsilon,\alpha}}$, $\{H_k\}_{k=0}^{k_{\epsilon,\alpha}}$, $\{\lambda_k\}_{k=0}^{k_{\epsilon,\alpha}-1}$ and $\{s_k\}_{k=0}^{k_{\epsilon,\alpha}-1}$ can be viewed as produced by our chosen method in $\mathfrak{M}.\alpha$, and, from (3.3), that termination occurs precisely for $k = k_{\epsilon,\alpha}$, as desired.

We now construct the function $f_\epsilon^{\mathfrak{M},\alpha}(x)$ for $x \in [0, x_{k_{\epsilon,\alpha}}]$ using Hermite interpolation. We set

$$f_\epsilon^{\mathfrak{M},\alpha}(x) = p_k(x-x_k)+f_{k+1} \quad \text{for } x \in [x_k, x_{k+1}] \text{ and } k = 0, \ldots, k_{\epsilon,\alpha}-1, \tag{3.10}$$

where p_k is the polynomial

$$p_k(s) = c_{0,k} + c_{1,k}s + c_{2,k}s^2 + c_{3,k}s^3 + c_{4,k}s^4 + c_{5,k}s^5,$$

with coefficients defined by the interpolation conditions

$$\begin{aligned} &p_k(0) = f_k - f_{k+1}, \quad p_k(s_k) = 0; \\ &p_k'(0) = g_k, \quad p_k'(s_k) = g_{k+1}; \\ &p_k''(0) = H_k, \quad p_k''(s_k) = H_{k+1}, \end{aligned} \tag{3.11}$$

where s_k is defined in (3.6). These conditions yield the following values for the coefficients

$$c_{0,k} = f_k - f_{k+1}, \quad c_{1,k} = g_k, \quad c_{2,k} = \tfrac{1}{2}H_k; \tag{3.12}$$

with the remaining coefficients satisfying

$$\begin{pmatrix} s_k^3 & s_k^4 & s_k^5 \\ 3s_k^2 & 4s_k^3 & 5s_k^4 \\ 6s_k & 12s_k^2 & 20s_k^3 \end{pmatrix} \begin{pmatrix} c_{3,k} \\ c_{4,k} \\ c_{5,k} \end{pmatrix} = \begin{pmatrix} \Delta f_k - g_k s_k - \frac{1}{2}s_k^T H_k s_k \\ \Delta g_k - H_k s_k \\ \Delta H_k \end{pmatrix},$$

where

$$\Delta f_k = f_{k+1} - f_k, \quad \Delta g_k = g_{k+1} - g_k \text{ and } \Delta H_k = H_{k+1} - H_k.$$

Hence we obtain after elementary calculations that

$$\begin{aligned} c_{3,k} &= 10\frac{\Delta f_k}{s_k^3} - 4\frac{\Delta g_k}{s_k^2} + \frac{\Delta H_k}{2s_k} - 10\frac{g_k}{s_k^2} - \frac{H_k}{s_k}; \\ c_{4,k} &= -15\frac{\Delta f_k}{s_k^4} + 7\frac{\Delta g_k}{s_k^3} - \frac{\Delta H_k}{s_k^2} + 15\frac{g_k}{s_k^3} + \frac{H_k}{2s_k^2}; \\ c_{5,k} &= 6\frac{\Delta f_k}{s_k^5} - 3\frac{\Delta g_k}{s_k^4} + \frac{\Delta H_k}{2s_k^3} - 6\frac{g_k}{s_k^4}; \end{aligned} \tag{3.13}$$

The top three graphs of Figure 3.1 illustrate the global behaviour of the resulting function $f_\epsilon^{\mathfrak{M},\alpha}(x)$ and of its first and second derivatives for $x \in [0, x_{k_{\epsilon,\alpha}}]$, while the bottom ones show more detail of the first 10 iterations. The figure is constructed using $\epsilon = 5.10^{-2}$ and $\alpha = \frac{1}{2}$, which then yields that $k_{\epsilon,\alpha} = 148$. In addition, we set $\lambda_k = \frac{1}{10}|g_k|^{\frac{\alpha}{1+\alpha}}$ for $k = 0, \ldots, k_{\epsilon,\alpha}$. The nonconvexity of $f_\epsilon^{\mathfrak{M},\alpha}(x)$ is clear from the bottom graphs.

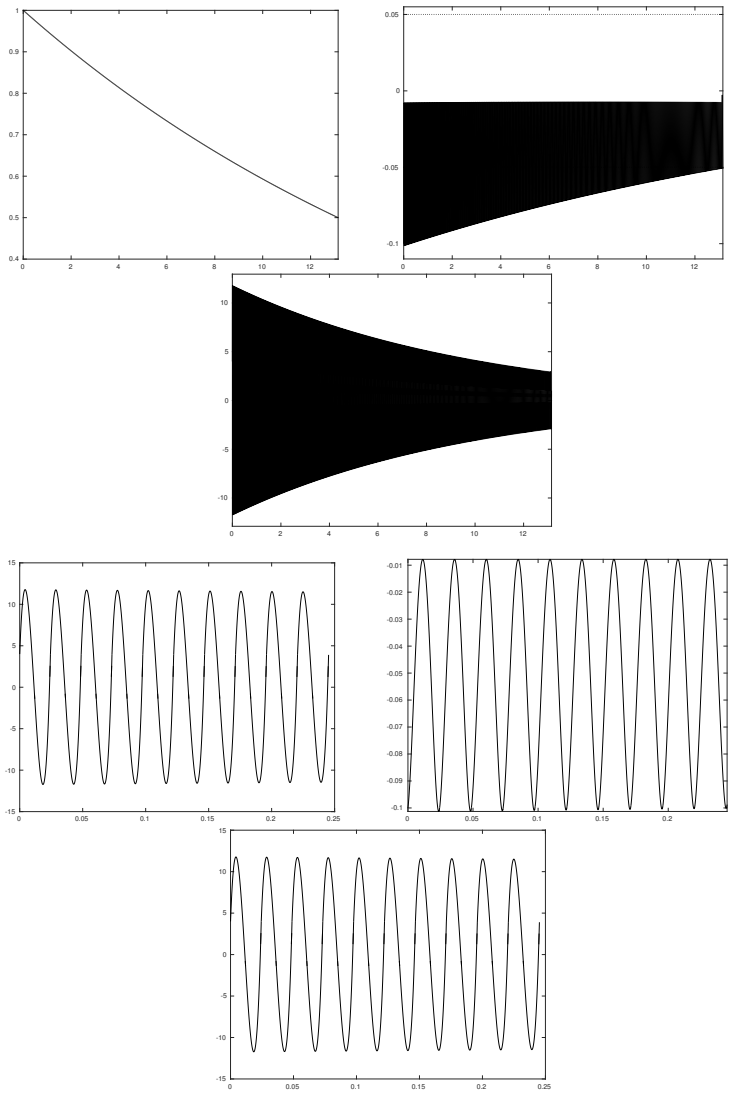

Figure 3.1: $f_\epsilon^{\mathfrak{M},\alpha}(x)$ (left) and its first (center) and second (right) derivatives as a function of x for $\alpha = \frac{1}{2}$ and $\epsilon = 5.10^{-2}$ (top: $x \in [0, x_{k_{\epsilon,\alpha}}]$; bottom: $x \in [0, x_{10}]$). Horizontal dotted lines indicate values of $-\epsilon$ and ϵ in the central top graph.

Lemma 3.1. *The function $f_\epsilon^{\mathfrak{M}.\alpha}$ defined above on the interval $[0, x_{k_{\epsilon,\alpha}}]$ can be extended to a function from $\mathbb{R}$ to $\mathbb{R}$ satifying A.α and whose range is bounded independently of α and ϵ.*

Proof. We start by showing that, on

$$[0, x_{k_{\epsilon,\alpha}}] = \bigcup_{k\in\mathcal{K}} [x_k, x_k + s_k],$$

$f_\epsilon^{\mathfrak{M}.\alpha}$ is bounded in absolute value independently of ϵ and α, twice continuously differentiable with Lipschitz continuous gradient and α-Hölder continous Hessian. Recall first (3.10) provide that $f_\epsilon^{\mathfrak{M}.\alpha}$ is twice continuously differentiable by construction on $[0, x_{k_{\epsilon,\alpha}}]$. It thus remains to investigate the gradient's Lipschitz continuity and Hessian's $\alpha-$Hölder continuity, as well as whether $|f_\epsilon^{\mathfrak{M}.\alpha}(x)|$ is bounded on this interval.

Defining now

$$\pi_k \stackrel{\rm def}{=} \frac{\theta_k}{2}\frac{2f_k - 1}{f_k} \in [0, \tfrac{1}{2}\theta_k] \quad \text{and} \quad \phi(\theta) \stackrel{\rm def}{=} 2 - \frac{1}{\theta} \in [2 - \frac{\kappa_\lambda}{1-\kappa_{rg}}, 1 + \kappa_{rg}] \tag{3.14}$$

(where we used (3.4) and (3.6)), we obtain from (3.2), (3.3), (3.6) and (3.13), that, for $k \in \mathcal{K}$,

(3.15)

$$\begin{aligned}
|c_{3,k}|s_k^2 &= \epsilon f_k\left(20 - \frac{10}{\theta_k} - 2\theta_k\right) - \epsilon^{\frac{3+2\alpha}{1+\alpha}}(4+\pi_k) &&\le \epsilon\left[10|\phi(\theta)| + 2\theta + \tfrac{9}{2}\epsilon^{\frac{2+\alpha}{1+\alpha}}\right] &&= \mathcal{O}(\epsilon),\\
|c_{4,k}|s_k^3 &= \epsilon f_k\left(\frac{15}{\theta_k} - 30 + \theta_k\right) + \epsilon^{\frac{3+2\alpha}{1+\alpha}}(7+2\pi_k) &&\le \epsilon\left[15|\phi(\theta)| + \theta + 8\epsilon^{\frac{2+\alpha}{1+\alpha}}\right] &&= \mathcal{O}(\epsilon),\\
|c_{5,k}|s_k^4 &= \epsilon f_k\left(12 - \frac{6}{\theta_k}\right) - \epsilon^{\frac{3+2\alpha}{1+\alpha}}(3+\pi_k) &&\le \epsilon\left[6|\phi(\theta)| + \tfrac{7}{2}\epsilon^{\frac{2+\alpha}{1+\alpha}}\right] &&= \mathcal{O}(\epsilon),
\end{aligned}$$

where we also used $\epsilon \le 1$ and (3.4). To show that the Hessian of $f_\epsilon^{\mathfrak{M}.\alpha}$ is globally $\alpha-$Hölder continuous on $[0, x_{k_{\epsilon,\alpha}}]$, we need to verify that (2.8) holds for all x, y in this interval. From (3.10), this is implied by

$$|p'''(s)| \le c|s|^{-1+\alpha}, \quad \text{for all } s \in [0, s_k] \text{ and } k \in \mathcal{K}, \tag{3.16}$$

for some $c > 0$ independent of ϵ, s and k. We have from the expression of p_k and $s \in [0, s_k]$ that

$$\begin{aligned}
|p_k'''(s)| \cdot |s|^{1-\alpha} &\le (6|c_{3,k}| + 24|c_{4,k}|s_k + 60|c_{5,k}|s_k^2)s_k^{1-\alpha}\\
&= (6|c_{3,k}|s_k^2 + 24|c_{4,k}|s_k^3 + 60|c_{5,k}|s_k^4)s_k^{-(1+\alpha)}.
\end{aligned} \tag{3.17}$$

The boundedness of this last right-hand side on $[0, x_{k_{\epsilon,\alpha}}]$, and thus the α-Hölder continuity of the Hessian of f^M, then follow from (3.15), (3.6) and (3.4).

Similarly, to show that the gradient of f^M is globally Lipschitz continuous in $[0, x_{k_{\epsilon,\alpha}}]$ is equivalent to proving that $p_k''(s)$ is uniformly bounded above on the interval $[0, s_k]$ for $k \in \mathcal{K}$. Since $s_k > 0$, we have

$$\begin{aligned}
|p_k''(s)| &\le 2|c_{2,k}| + 6|c_{3,k}|s_k + 12|c_{4,k}|s_k^2 + 20|c_{5,k}|s_k^3\\
&= 2|c_{2,k}| + (6|c_{3,k}|s_k^2 + 12|c_{4,k}|s_k^3 + 20|c_{5,k}|s_k^4)s_k^{-1}.
\end{aligned} \tag{3.18}$$

Then the third part of (3.3) and the bounds $\epsilon \leq 1$, (3.15), (3.12), (3.6) and (3.4) again imply the boundedness of the last right-hand side on $[0, x_{k_{\epsilon,\alpha}}]$, as requested. Finally, the fact that $|f_\epsilon^{\mathfrak{M}.\alpha}|$ is bounded on $[0, x_{k_{\epsilon,\alpha}}]$ results from the observation that, on the interval $[0, s_k]$ with $k \in \mathcal{K}$,

$$|p_k(s)| \leq f_k + |g_k||s_k| + \tfrac{1}{2}|H_k|\,|s_k|^2 + (|c_{3,k}|s_k^2 + |c_{4,k}|s_k^3 + |c_{5,k}|s_k^4)s_k$$

from which a finite bound a independent from α and ϵ again follows from $\epsilon \leq 1$, (3.3), (3.10), (3.15), (3.12), (3.6) and (3.4). We have thus proved that $f_\epsilon^{\mathfrak{M}.\alpha}$ satisfies the desired properties on $[0, x_{k_{\epsilon,\alpha}}]$.

We may then smoothly prolongate $f_\epsilon^{\mathfrak{M}.\alpha}$ for $x \in \mathbb{R}$, for instance by defining two additional interpolation intervals $[x_{-1}, x_0] = [-1, 0]$ and $[x_{k_{\epsilon,\alpha}}, x_{k_{\epsilon,\alpha}} + 1]$ with end conditions

$$f_{-1} = 1, \quad f_{k_{\epsilon,\alpha}+1} = f_{k_{\epsilon,\alpha}} \text{ and } g_{-1} = H_{-1} = g_{k_{\epsilon,\alpha}+1} = H_{k_{\epsilon,\alpha}+1} = 0,$$

and setting

$$f_\epsilon^{\mathfrak{M}.\alpha}(x) = \begin{cases} 1 & \text{for } x \leq -1, \\ p_k(x - x_k) + f_{k+1} & \text{for } x \in [x_k, x_{k+1}] \text{ and } k \in \{-1, \ldots, k_{\epsilon,\alpha}\}, \\ f_\epsilon^{\mathfrak{M}.\alpha}(x_{k_{\epsilon,\alpha}}) & \text{for } x \geq x_{k_{\epsilon,\alpha}} + 1, \end{cases}$$

which subsumes (3.10). Using arguments similar to those used above, it is easy to verify from (3.12), (3.13) and $s_{-1} = s_{k_{\epsilon,\alpha}} = 1$ that all desired properties are maintained. □

We formulate the results of this development in the following theorem.

Theorem 3.2. *For every $\epsilon \in (0, 1)$, every $\alpha \in [0, 1]$ and every method in $\mathfrak{M}.\alpha$, a function $f_\epsilon^{\mathfrak{M}.\alpha}$ satisfying A.α with values in a bounded interval independent of ϵ and α can be constructed, such, when applied to $f_\epsilon^{\mathfrak{M}.\alpha}$, the considered method terminates exactly at iteration*

$$k_{\epsilon,\alpha} = \left\lceil \epsilon^{-\frac{2+\alpha}{1+\alpha}} \right\rceil.$$

with the first iterate $x_{k_{\epsilon,\alpha}}$ such that $\|\nabla_x f_\epsilon^{\mathfrak{M}.\alpha}(x_{k_{\epsilon,\alpha}})\| \leq \epsilon$.

Note that the prolongation of $f_\epsilon^{\mathfrak{M}.\alpha}(x)$ to $x \geq 0$ suggested as an example in the proof of Lemma 3.1 admits an isolated finite global minimizer. Indeed, since the $g_{k_{\epsilon,\alpha}} < 0$, there must be a value lower than $f(x_{k_{\epsilon,\alpha}})$ in $(x_{k_{\epsilon,\alpha}}, x_{k_{\epsilon,\alpha}} + 1)$, and thus the global minimizer must lie in one of the constructed sub-intervals in $(-1, x_{k_{\epsilon,\alpha}+1})$; since $f_\epsilon^{\mathfrak{M}.\alpha}(x)$ is quintic (and not constant) in each of these, the global minimizer must therefore be isolated.

3.2 The inexact Newton's method. It is interesting that the technique developed in the previous subsection can also be used to derive an $\mathcal{O}\left(\epsilon^{-2}\right)$ lower bound on worst-case evaluation complexity for an inexact Newton's method applied to a function having Lipschitz continuous Hessians on the path of iterates. This is stronger than using Theorem 3.2 above for $\alpha = 1$, as it would result in a weaker $\mathcal{O}\left(\epsilon^{-3/2}\right)$ lower bound, or

for $\alpha = 0$ as it would then only guarantee bounded Hessians. In the spirit of Cartis, N. I. M. Gould, and P. L. Toint [2010], this new function is constructed by extending to $\mathbb{R}^2$ the unidimensional $f_\epsilon^{\mathfrak{M}.0}(x)$ obtained in the previous section for the specific choice $M_k = 0$, which then ensures that $\theta_k \in [1-\kappa_{rg}, 1+\kappa_{rg}]$ for all k (see (3.5) and (3.6)). The proposed extension is of the form

$$h_\epsilon^N(x,y) \stackrel{\text{def}}{=} f_\epsilon^{\mathfrak{M}.0}(x) + u_\epsilon(y), \tag{3.19}$$

where we still have to specify the univariate function u_ϵ such that Newton's method applied to u_ϵ converges with large steps. In order to define it, we start by redefining

$$k_\epsilon = k_{\epsilon,0} = \lceil \epsilon^{-2} \rceil \quad \text{and} \quad \mathcal{K} = \{0, \ldots, k_\epsilon\}.$$

Then we set, for $k \in \mathcal{K}$,

$$u_k = 1 - \tfrac{1}{2}k\epsilon^2, \quad g_k^u = -2\epsilon^2 u_k, \quad H_k^u = 2|g_k^u|u_k > 0, \tag{3.20}$$

and

$$s_k^u = \frac{v_k}{2u_k} \ \text{ with } \ v_k \in [1-\kappa_{rg}, 1+\kappa_{rg}] \ \text{ and } \ u_k \in [\tfrac{1}{2}, 1], \tag{3.21}$$

this definition allowing for

$$H_k^u s_k^u = -g_k^u + r_k^u \quad \text{with} \quad |r_k^u| \le \kappa_{rg}|g_k^u|.$$

(Remember that $M_k = 0$ because we are considering Newton's method.) Note that sufficient decrease is obtained in manner similar to (3.7)-(3.8), because of (3.20), (3.21) and $\lambda_k = 0$, yielding that $u_k - u_{k+1} \ge -(g_k^u s_k^u + \frac{1}{2}H_k^u(s_k^u)^2)/(1+\kappa_{rg})$. Setting now $y_0 = 0$ and $y_{k+1} = y_k + s_k^u$ for $k \in \{1, \ldots, k_\epsilon\}$, we may then, as in Section 3.1, define

$$u_\epsilon(y) = p_k^u(y - y_k) + u_{k+1} \ \text{ for } y \in [y_k, y_{k+1}] \text{ and } k = 0, \ldots, k_\epsilon - 1, \tag{3.22}$$

where p_k^u is a fifth degree polynomial interpolating the values and derivatives given by (3.20) on the interval $[0, s_k^u]$. We then obtain the following result.

Theorem 3.3. *For every $\epsilon \in (0,1)$, there exists a function h_ϵ^N with Lipschitz continuous gradient and Lipschitz continuous Hessian along the path of iterates $\cup_{k=0}^{k_\epsilon-1}[x_j, x_{j+1}]$, and with values in a bounded interval independent of ϵ, such that, when applied to h_ϵ^N, Newton's terminates exactly at iteration*

$$k_\epsilon = \lceil \epsilon^{-2} \rceil$$

with the first iterate x_{k_ϵ} such that $\|\nabla_x f_\epsilon^{\mathfrak{M}.\alpha}(x_{k_\epsilon})\| \le \epsilon\sqrt{1+\epsilon^2}$.

Proof. One easily verifies from (3.20), (3.21) and (3.13) that the interpolation coefficients, now denoted by $|d_{i,k}|$, are bounded for all $k \in \{0, \ldots, k_\epsilon - 1\}$ and $i \in \{0, \ldots, 5\}$. This observation and (3.21) in turn guarantee that u_ϵ and all its derivatives (including the third) remain bounded on each interval $[0, s_k^u]$ by constants independent of ϵ.

As in Lemma 3.1, we next extend u_ϵ to the whole of $\mathbb{R}$ while preserving this property. We then construct h^N using (3.19). From the properties of $f_\epsilon^{\mathfrak{M}.0}$ and u_ϵ, we deduce that h_ϵ^N is twice continuously differentiable and has a range bounded independently of ϵ. Moreover, it satisfies A.0. When applied on $h_\epsilon^N(x,y)$, Newton's generates the iterates (x_k, y_k) and its gradient at the k_ϵ-th iterate is (ϵ, ϵ^2) so that $\|\nabla h^N(x_{k_\epsilon}, y_{k_\epsilon})\| = \epsilon\sqrt{1+\epsilon^2}$, prompting termination. Before that, the algorithm generates the steps (s_k, s_k^u), where, because both f_k and u_k belong to $[\frac{1}{2}, 1]$ and because of (3.6) with $\alpha = 0$,

$$s_k \in [\epsilon(1-\kappa_{rg}), 2\epsilon(1+\kappa_{rg})] \quad \text{and} \quad s_k^u \in [1-\kappa_{rg}, 2(1+\kappa_{rg})]. \tag{3.23}$$

Thus the absolute value of the third derivative of $h_\epsilon^N(x,y)$ is given, for (x,y) in the k-th segment of the path of iterates, by

$$\begin{aligned}
&\frac{1}{\|(s_k, s_k^u)\|}\left|p_k'''(x-x_k)s_k^3 + (p_k^u)'''(y-y_k)(s_k^u)^3\right| \\
&\quad\le \frac{1}{1-\kappa_{rg}}\left[|p_k'''(x-x_k)|s_k^3 + |(p_k^u)'''(y-y_k)|(s_k^u)^3\right] \\
&\quad= \frac{1}{1-\kappa_{rg}}\Big[\Big(6|c_{3,k}| + 24|c_{4,k}|s_k + 60|c_{5,k}|s_k^2\Big)s_k^3 \\
&\qquad\qquad +\Big(6|d_{3,k}| + 24|d_{4,k}|s_k^u + 60|d_{5,k}|(s_k^u)^2\Big)(s_k^u)^3\Big] \\
&\quad= \frac{1}{1-\kappa_{rg}}\Big[\Big(6|c_{3,k}|s_k^2 + 24|c_{4,k}|s_k^3 + 60|c_{5,k}|s_k^4\Big)s_k \\
&\qquad\qquad +6|d_{3,k}|(s_k^u)^3 + 24|d_{4,k}|(s_k^u)^4 + 60|d_{5,k}|(s_k^u)^5\Big],
\end{aligned} \tag{3.24}$$

where we used the fact that $\|(s_k, s_k^u)\| \ge \|s_k^u\|$. and (3.23). But, in view of (3.15), (3.14) with $\theta_k \in [1-\kappa_{rg}, 1+\kappa_{rg}]$, (3.23), $\epsilon \le 1$ and the boundedness of the $d_{i,k}$, the last right-hand side of (3.24) is bounded by a constant independent of ϵ. Thus the third derivative of $h_\epsilon^N(x,y)$ is bounded on every segment by the same constant, and, as a consequence, the Hessian of $h_\epsilon^N(x,y)$ is Lipschitz continuous of each segment, as desired. □

Note that the same result also holds for any method in $\mathfrak{M}.0$ with M_k small enough to guarantee that s_k is bounded away from zero for all k.

4 Complexity and optimality for methods in $\mathfrak{M}.\alpha$

We now consider the consequences of the examples derived in Section 3 on the evaluation complexity analysis of the various methods identified in Section 2 as belonging to $\mathfrak{M}.\alpha$.

4.1 Newton's method. First note that the third part of (3.3) ensures that $H_k > 0$ so that the Newton iteration is well-defined for the choice (2.23). This choice corresponds to setting $\theta_k = 1$ for all $k \ge 0$ in the example of Section 3. So we first conclude from Theorem 3.2 that Newton's method may require $\epsilon^{-(2+\alpha)/(1+\alpha)}$ evaluations when applied on the resulting objective function $f_\epsilon^{\mathfrak{M}.\alpha}$ satisfying A.α to generate $|g_k| \le \epsilon$.

However, Theorem 3.3 provides the stronger result that it may in fact require ϵ^{-2} evaluations (as a method in $\mathfrak{M}.0$) for nearly the same task (we traded Lipschitz continuity of the Hessian on the whole space for that along the path of iterates). As a consequence we obtain that *Newton's method is not optimal in $\mathfrak{M}.\alpha$ as far as worst-case evaluation complexity is concerned*.

The present results also improves on the similar bound given in Cartis, N. Gould, and P. L. Toint [2011], in that the objective function on Sections 3.1 and 3.2 ensure the existence of a lower bound $f_{\rm low}$ on $f_\epsilon^{\mathfrak{M}.\alpha}(x)$ such that $f_\epsilon^{\mathfrak{M}.\alpha}(x_0) - f_{\rm low}$ is bounded, while the latter difference is unbounded in Cartis, N. Gould, and P. L. Toint [ibid.] (for $\alpha \in \{0,1\}$) as the number of iterations approaches ϵ^{-2}. We will return to the significance of this observation when discussing regularization methods.

Since the steepest-descent method is known to have a worst-case evaluation complexity of $\mathcal{O}\left(\epsilon^{-2}\right)$ when applied on functions having Lipschitz continuous gradients Nesterov [2004, p. 29] , Theorem 3.3 shows that Newton's method may, in the worst case, converge as slowly as steepest descent in the worst case. Moreover, we show in Appendix A1 that the quoted worst-case evaluation complexity bound for steepest descent is sharp, which means that steepest-descent and Newton's method are undistinguishable from the point of view of worst-case complexity orders.

Note also that if the Hessian of the objective is unbounded, and hence, we are outside of the class A.0, the worst-case evaluation complexity of Newton's method worsens, and in fact, it may be arbitrarily bad Cartis, N. I. M. Gould, and P. L. Toint [2010].

4.2 Cubic and other regularizations. Recalling our discussion of the $(2+\alpha)$-regularization method in Section 2.2, we first note, in the example of Section 3.1, that, because of (2.2) and (2.3), s_k is a minimizer of the model (2.6) with $\beta_k = \lambda_k$ at iteration k, in that

$$m_k(s_k) = f_\epsilon^{\mathfrak{M}.\alpha}(x_k + s_k) = f_{k+1} \tag{4.1}$$

for $k \in \mathcal{K}$. Thus every iteration is successful as the objective function decrease exactly matches decrease in the model. Hence the choice $\sigma_k = \sigma > 0$ for all k is allowed by the method, and thus $\lambda_k = \sigma\|s_k\|^{2+\alpha}$ satisfies (2.3) and (2.4). Theorem 3.2 then shows that this method may require at least $\epsilon^{-(2+\alpha)/(1+\alpha)}$ iterations to generate an iterate with $|g_k| \le \epsilon$. This is important as the *upper* bound on this number of iterations was proved[(6)] in Cartis, N. I. M. Gould, and P. L. Toint [2011b] to be

$$O\Big(\left[f(x_0) - f_{\rm low}\right]\epsilon^{-\frac{2+\alpha}{1+\alpha}}\Big) \tag{4.2}$$

where $f_{\rm low}$ is any lower bound of $f(x)$. Since we have that $f(x_0) - f_{\rm low}$ is a fixed number independent of ϵ for the example of Section 3.1, this shows that the ratio

$$\rho_{\rm comp} \stackrel{\rm def}{=} \frac{\text{upper bound on the worst-case evaluation complexity}}{\text{lower bound on the worst-case evaluation complexity}} \tag{4.3}$$

[(6)] As a matter of fact, Cartis, N. I. M. Gould, and P. L. Toint [2011b] contains a detailed proof of the result for $\alpha = 1$, as well as the statement that it generalizes for $\alpha \in (0,1]$. Because of the central role of this result in the present paper, a more detailed proof of the worst-case evaluation complexity bound for $\alpha \in (0,1]$ in provided as Appendix A2.

for the $(2+\alpha)$-regularization method is bounded independently of ϵ and α. Given that (4.2) involves an unspecified constant, this is the best that can be obtained as far as the order in ϵ is concerned, and yields the following important result on worst-case evaluation complexity.

Theorem 4.1. *When applied to a function satisfying A.α, the $(2+\alpha)$-regularization method may require at most (4.2) function and derivatives evaluations. Moreover this bound is sharp (in the sense that ρ_{comp} is bounded independently of ϵ and α) and the $(2+\alpha)$-regularization method is optimal in $\mathfrak{M}.\alpha$.*

Proof. The optimality of the $(2+\alpha)$-regularization method within $\mathfrak{M}.\alpha$ results from the observation that the example of Section 3 implies that no method in $\mathfrak{M}.\alpha$ can have a worst-case evaluation complexity of a better order. □

In particular, the cubic regularization method is optimal for smooth optimization problems with Lipschitz continuous second derivatives. As we have seen above, this is in contrast with Newton's method.

Note that Theorem 4.1 as stated does *not* result from the statement in Cartis, N. Gould, and P. L. Toint [2011] that the bound (4.2) is "essentially sharp". Indeed this latter statement expresses the fact that, for any $\tau > 0$, there exists a function independent of ϵ, on which the relevant method may need at least $\epsilon^{-3/2+\tau}$ evaluations to terminate with $|g_k| \leq \epsilon$. But, for any fixed ϵ, the value of $f(x_0) - f_{\text{low}}$ tends to infinity when, in the example of that paper, the number of iterations to termination approaches $\epsilon^{-3/2}$ as τ goes to zero. As a consequence, the numerator of the ratio (4.3), that is (4.2), and ρ_{comp} itself are unbounded for that example. Theorem 4.1 thus brings a formal improvement on the conclusions of Cartis, N. Gould, and P. L. Toint [ibid.].

4.3 Goldfeld-Quandt-Trotter. Recalling (2.29), we can set $\omega_k = \omega$ in the algorithm as every iteration is successful due to (4.1) which, with (3.3) and $f_k \in [\frac{1}{2}, 1]$ gives that $\lambda_k + \lambda_{\min}(H_k) \leq \omega |g_k|^{\frac{\alpha}{1+\alpha}}$, which is in agreement with (2.5) and (2.4). Thus the lower bound of $\epsilon^{-(2+\alpha)/(1+\alpha)}$ iterations for termination also applies to this method.

An upper bound on the worst-case evaluation complexity for the GQT method can be obtained by the following argument. We first note that, similarly to regularization methods, we can bound the total number of unsuccessful iterations as a constant multiple of the successful ones, provided ω_k is chosen such that (2.32) holds. Moreover, since f satisfies A.α, its Hessian is bounded above by (2.9). In addition, we have noted in Section 2.2 that $\|g_k\|$ is also bounded above. In view of (2.29) and (2.39), this in turn implies that $\|H_k + \lambda_k I\|$ is also bounded above. Hence we obtain from (2.33) that $\|s_k\| \geq \kappa_{GQT} \|g_k\| \geq \kappa_{GQT}\, \epsilon$ for some $\kappa_{QGT} > 0$, as along as termination has not occurred. This last bound and (2.37) then give that GQT takes at most $\mathcal{O}\left((f(x_0) - f_{\text{low}}) \epsilon^{-\frac{\alpha}{1+\alpha}-2}\right)$ iterations, which is worse than (4.2) for $\alpha > 0$. Note that this bound improves if only Newton steps are taken (i.e. $\lambda_k = 0$ is chosen for all $k \geq 0$), to be of the order of (4.2); however, this cannot be assumed in the worst-case for nonconvex functions. In any case, it implies that the GQT method is not optimal in $\mathfrak{M}.\alpha$.

4.4 Trust-region methods. Recall the choices (2.41) we make in this case. If $\lambda_k = 0$, the trust-region constraint $\|s\| \leq \Delta_k$ is inactive at s_k, in which case, s_k is the Newton step. If we make precisely the choices we made for Newton's method above, choosing Δ_0 such that $\Delta_0 > |s_0|$ implies that the Newton step will be taken in the first and in all subsequent iterations since each iteration is successful and then Δ_k remains unchanged or increases while the choice (3.6) implies that s_k decreases. Thus the trust-region approach, through the Newton step, has a worst-case evaluation complexity when applied to $f_\epsilon^{\mathfrak{M}.\alpha}$ which is at least that of the Newton's method, namely ϵ^{-2}.

4.5 Linesearch methods. Because the examples of Sections 3.1 and 3.2 are valid for $r_k = 0$ which corresponds to $\mu_k = 1$ for all k, and because this stepsize is acceptable since $f(x_{k+1}) = m_k(s_k)$, we deduce that at least $\epsilon^{-\frac{2+\alpha}{1+\alpha}}$ iterations and evaluations may be needed for the linesearch variants of any method in $\mathfrak{M}.\alpha$ applied to a function satisfying A.α, and that ϵ^{-2} evaluations may be needed for the linesearch variant of Newton's method applied on a function satisfying A.0. Thus the conclusions drawn regarding their (sub-)optimality in terms of worst-case evaluation complexity are not affected by the use of a linesearch.

5 The Curtis-Robinson-Samadi class

We finally consider a class of methods recently introduced in Curtis, Robinson, and Samadi [2017b], which we call the CRS class. This class depends on the parameters $0 < \underline{\sigma} \leq \bar{\sigma}$, $\eta \in (0,1)$ and two non-negative accuracy thresholds κ_1 and κ_2. It is defined as follows. At the start, adaptive regularization thresholds are set according to

$$\sigma_0^L = 0 \text{ and } \sigma_0^U = \bar{\sigma}. \tag{5.1}$$

Then for each iteration $k \geq 0$, a step s_k from the current iterate x_k and a regularization parameter $\lambda_k \geq 0$ are chosen to satisfy[(7)]

$$(H_k + \lambda_k I)s_k = -g_k + r_k, \tag{5.2}$$

$$\sigma_k^L \|s_k\| \leq \lambda_k \leq \sigma_k^U \|s_k\|, \tag{5.3}$$

$$s_k^T r_k \leq \tfrac{1}{2} s_k^T (H_k + \lambda_k I)s_k + \tfrac{1}{2}\kappa_1 \|s_k\|^3, \tag{5.4}$$

and

$$\|r_k\| \leq \lambda_k \|s_k\| + \kappa_2 \|s_k\|^2. \tag{5.5}$$

[(7)] In Curtis, Robinson, and Samadi [2017b], further restrictions on the step are imposed in order to obtain global convergence under A.0 and bounded gradients, but are irrelevant for the worst-case complexity analysis under A.1. We thus ignore them here, but note that this analysis also ensures global convergence to first-order stationary points.

The step is then accepted, setting $x_{k+1} = x_k + s_k$, if

$$\rho_{CRS} = \frac{f(x_k) - f(x_k + s_k)}{\|s_k\|^3} \geq \eta \tag{5.6}$$

or rejected otherwise. In the first case, the regularization thresholds are reset according to (5.1). If s_k is rejected, σ_k^L and σ_k^U are updated by a simple mechanism (using $\underline{\sigma}$) which is irrelevant for our purpose here. The algorithm is terminated as soon as an iterate is found such that $\|g_k\| \leq \epsilon$.

Observe that (5.2) corresponds to inexactly minimizing the regularized model (2.6) and that (5.5) is very similar to the subproblem termination rule of E. G. Birgin, Gardenghi, Martínez, Santos, and P. L. Toint [2017].

An upper bound of $\mathcal{O}\left(\epsilon^{-3/2}\right)$ is proved in Curtis, Robinson, and Samadi [2017b, Theorem 17] for the worst-case evaluation complexity of the methods belonging to the CRS class. It is stated in Curtis, Robinson, and Samadi [ibid.] that both ARC Griewank [1981], Weiser, Deuflhard, and Erdmann [2007], Nesterov and Polyak [2006], and Cartis, N. I. M. Gould, and P. L. Toint [2011a,b] and TRACE Curtis, Robinson, and Samadi [2017a] belong to the class, although the details are not given.

Clearly, the CRS class is close to $\mathfrak{M}.1$, but yet differs from it. In particular, no requirement is made that $H_k + \lambda_k I$ be positive semi-definite but (5.4) is required instead, there is no formal need for the step to be bounded and (5.5) combined with (5.3) is slightly more permissive than the second part of (2.2). We now define CRS$_a$, a sub-class of the CRS class of methods, as the set of CRS methods for which (5.5) is strengthened[8] to become

$$\|r_k\| \leq \min\left[\kappa_{rg}\|g_k\|, \lambda_k\|s_k\| + \kappa_2\|s_k\|^2\right] \quad \text{with} \quad \kappa_{rg} < 1. \tag{5.7}$$

(in a manner reminiscent of the second part of (2.2)) and such that

$$2\eta(1 + \kappa_{rg})^3 \leq 1 \tag{5.8}$$

(a mild technical condition[9] whose need will become apparent below). We claim that, for any choice of method in the CRS$_a$ class and termination threshold ϵ, we can construct a function satisfying A.1 such that the considered CRS$_a$ method terminates in exactly $\lceil \epsilon^{-3/2} \rceil$ iterations and evaluations. This achieved simply by showing that the generated sequences of iterates, function, gradient and Hessian values belong to those detailed in the example of Section 3.1.

We now apply a method of the CRS$_a$ class for a given $\epsilon > 0$, and first consider an iterate x_k with associated values f_k, g_k and H_k given by (3.3) for $\alpha = 1$, that is

$$f_0 = 1, \quad f_k = f_0 - \tfrac{1}{2}k\epsilon^{3/2}, \quad g_k = -2\epsilon f_k \text{ and } H_k = 4\epsilon^{1/2} f_k^2; \tag{5.9}$$

Suppose that

$$\sigma_k^L = 0 \quad \text{and} \quad \sigma_k^U = \bar{\sigma} \tag{5.10}$$

[8] Hence the subscript a, for "accurate".

[9] Due to the lack of scaling invariance of (5.6), at variance with (2.30).

(as is the case by definition for $k = 0$), and let

$$s_k = \theta_k \frac{\epsilon^{1/2}}{2 f_k} \quad (\theta_k > 0) \tag{5.11}$$

be an acceptable step for an arbitrary method in the CRS$_a$ class. Now, because of (5.10), (5.3) reduces to

$$\lambda_k \in [0, \bar{\sigma}|s_k|] = \left[0, \bar{\sigma}\theta_k \frac{\epsilon^{1/2}}{2 f_k}\right] \tag{5.12}$$

and, given that $H_k > 0$ because of (5.9), this in turn implies that $H_k + \lambda_k > 0$. Condition (5.7) requires that

$$|g_k + (H_k + \lambda_k)s_k| = |r_k| \leq \kappa_{rg}|g_k| = 2\kappa_{rg}\epsilon f_k < 2\epsilon, \tag{5.13}$$

where we used the fact that $f_k \leq 1$ because of (5.9) and $\kappa_{rg} < 1$ because of (5.7). Moreover, (5.13) and (5.12) imply that

$$\frac{2(1-\kappa_{rg})\epsilon f_k}{4\epsilon^{1/2} f_k^2 + \bar{\sigma} s_k} \leq \frac{|g_k|(1-\kappa_{rg})}{H_k + \lambda_k} \leq s_k \leq \frac{|g_k|(1+\kappa_{rg})}{H_k + \lambda_k} \leq \frac{(1+\kappa_{rg})\epsilon^{1/2}}{2 f_k}. \tag{5.14}$$

Thus, using (5.11) and the right-most part of these inequalities, we obtain that $\theta_k \leq 1 + \kappa_{rg}$, which in turn ensures that $s_k \leq (1+\kappa_{rg})\epsilon^{1/2}/(2 f_k)$. Substituting this latter bound in the denominator of the left-most part of (5.14) and using (5.11) again with the fact that $f_k \geq \frac{1}{2}$ before termination, we obtain that

$$\theta_k \in \left[\frac{1-\kappa_{rg}}{1+\bar{\sigma}(1+\kappa_{rg})}, 1+\kappa_{rg}\right] \tag{5.15}$$

(note that this is (3.6) with $\kappa_\lambda = 1 + \bar{\sigma}(1+\kappa_{rg})$). We immediately note that π_k and $\phi(\theta_k)$ are then both guaranteed to be bounded above and below as in (3.14). (Since this is enough for our purpose, we ignore the additional restriction on θ_k which might result from (5.4).) Using the definitions (5.9) for $k+1$, we may then construct the objective function f_ϵ^{CRS} on the interval $[x_k, x_k + s_k]$ by Hermite interpolation, as in Section 3.1. Moreover, using (5.6), (5.9), (5.11), (5.15), $f_k \in [\frac{1}{2}, 1]$ and the condition (5.8), we obtain that

$$\rho_k = \frac{\epsilon^{3/2}}{2}\left(\frac{2 f_k}{\theta_k \epsilon^{1/2}}\right)^3 = \frac{4 f_k^3}{\theta_k^3} \geq \frac{1}{2(1+\kappa_{rg})^3} \geq \eta.$$

Thus iteration k is successful, $x_{k+1} = x_k + s_k$, $\sigma_{k+1}^L = \sigma_k^L = 0$, $\sigma_{k+1}^U = \sigma_k^U = \bar{\sigma}$, and all subsequent iterations of the CRS$_a$ method up to termination follow the same pattern in accordance with (5.9). As in Section 3.1, we may construct f_ϵ^{CRS} on the whole of $\mathbb{R}$ which satisfies A.1 and such that, the considered CRS$_a$ method applied to f_ϵ^{CRS} will terminate in exactly $\lceil \epsilon^{-3/2} \rceil$ iterations and evaluations. This and the $\mathcal{O}\left(\epsilon^{-3/2}\right)$ upper bound on the worst-case evaluation complexity of CRS methods allow stating the following theorem.

Theorem 5.1. *For every $\epsilon \in (0,1)$ and every method in the CRS$_a$ class, a function f_ϵ^{CRS} satisfying A.1 with values in a bounded interval independent of ϵ can be constructed, such that the considered method terminates exactly at iteration*

$$k_\epsilon = \left\lceil \epsilon^{-3/2} \right\rceil$$

with the first iterate x_{k_ϵ} such that $\|\nabla_x f_\epsilon^{CRS}(x_{k_\epsilon})\| \leq \epsilon$. As a consequence, methods in CRS$_a$ are optimal within the CRS class and their worst-case evaluation complexity is, in order, also optimal with respect to that of methods in $\mathfrak{M}$.1.

CRS$_a$ then constitutes a kernel of optimal methods (from the worst-case evaluation complexity point of view) within CRS and $\mathfrak{M}$.1. Methods in CRS but not in CRS$_a$ correspond to very inaccurate minimization of the regularized model, which makes it unlikely that their worst-case evaluation complexity surpasses that of methods in CRS$_a$. Finally note that, since we did not use (5.4) to construct our example, it effectively applies to a class larger than CRS$_a$ where this condition is not imposed.

6 The algorithm of Royer and Wright

We finally consider the linesearch algorithm proposed in C. W. Royer and Wright [2017, Algorithm 1], which is reminiscent of the double linesearch algorithm of N. I. M. Gould, Lucidi, Roma, and P. L. Toint [1998] and Conn, N. I. M. Gould, and P. L. Toint [2000, Section 10.3.1]. From a given iterate x_k, this algorithm computes a search direction d_k whose nature depends on the curvature of the (unregularized) quadratic model along the negative gradient, and possibly computes the left-most eigenpair of the Hessian if this curvature is negative or if the gradient's norm is small enough to declare first-order stationarity. A linesearch along d_k is then performed by reducing the steplength α_k from $\alpha_k = 1$ until

$$f(x_k + \alpha_k d_k) \leq f(x_k) - \frac{\eta}{6}\alpha_k^3 \|d_k\|^3 \tag{6.1}$$

for some $\eta > 0$. The algorithm uses ϵ_g and ϵ_H, two different accuracy thresholds for first- and second-order approximate criticality, respectively.

Our objective is now to show that, when applied to the function $f_{\epsilon_g}^{\mathfrak{M}.1}$ of Section 3.1 with $\epsilon = \epsilon_g$, this algorithm, which we call the RW algorithm, takes exactly $k_{\epsilon_g,1} = \lceil \epsilon_g^{-3/2} \rceil$ iterations and evaluations to terminate with $\|g_k\| \leq \epsilon_g$.

We first note that (3.3) guarantees that H_k is positive definite and, using (3.4), that

$$\frac{g_k^T H_k g_k}{\|g_k\|^2} = 4\epsilon_g^{1/2} f_k^2 > \epsilon_g$$

for $k \in \{0, \ldots, k_{\epsilon_g,1}\}$. Then, provided

$$\epsilon_H \leq \sqrt{\epsilon_g}, \tag{6.2}$$

and because $\lambda_{\min}(H_k) = 4\epsilon_g^{1/2} f_k^2 > \epsilon_H$ (using (3.4) again), the RW algorithm defines the search direction from Newton's equation $H_k d_k = -g_k$ (which corresponds, as we have already seen, to taking $M_k = 0 = r_k$ and thus $\theta_k = 1$ in the example of Section 3.1). The RW algorithm is therefore, on that example, identical to a linesearch variant of Newton's method with the specific linesearch condition (6.1). Moreover, using (3.4) once more,

$$f(x_k) - f(x_k + d_k) = \frac{1}{2}\epsilon_g^{3/2} \geq \frac{\eta}{6}\left(\frac{\epsilon_g^{1/2}}{2f_k}\right)^3 \geq \frac{\eta}{6}\epsilon_g^{3/2}$$

whenever $\eta \leq 3$, an extremely weak condition[10]. Thus (6.1) holds[11] with $\alpha_k = 1$. We have thus proved that the RW algorithm generates the same sequence of iterates as Newton's method when applied to $f_{\epsilon_g}^{\mathfrak{M}.1}$. The fact that an upper bound of $\mathcal{O}\left(\epsilon_g^{-3/2}\right)$ iterations and evaluations was proved to hold in C. W. Royer and Wright [2017, Theorem 5] then leads us to stating the following result.

Theorem 6.1. *Assume that $\eta \in (0, 3]$. Then, for every $\epsilon_g \in (0, 1)$ and ϵ_H satisfying (6.2), a function $f_{\epsilon_g}^{\mathfrak{M}.1}$ satisfying A.1 with values in a bounded interval (independent of ϵ_g and ϵ_H) can be constructed, such that the Royer-Wright algorithm terminates exactly at iteration*

$$k_{\epsilon_g} = \left\lceil \epsilon_g^{-3/2} \right\rceil$$

with the first iterate $x_{k_{\epsilon_g}}$ such that $\|\nabla_x f_{\epsilon_g}^{\mathfrak{M}.1}(x_{k_{\epsilon_g}})\| \leq \epsilon_g$. As a consequence and under assumption (6.2), the first-order worst-case evaluation complexity order of $\mathcal{O}\left(\epsilon_g^{-3/2}\right)$ for this algorithm is sharp and it is (in order of ϵ_g), also optimal with respect to that of algorithms in the $\mathfrak{M}.1$ and CRS classes.

7 Conclusions

We have provided lower bounds on the worst-case evaluation complexity of a wide class of second-order methods for reaching approximate first-order critical points of nonconvex, adequately smooth unconstrained optimization problems. This has been achieved by providing improved examples of slow convergence on functions with bounded range independent of ϵ. We have found that regularization algorithms, methods belonging to a subclass of that proposed in Curtis, Robinson, and Samadi [2017b] and the linesearch algorithm of C. W. Royer and Wright [2017] are optimal from a worst-case complexity point of view within a very wide class of second-order methods, in that their upper complexity bounds match in order the lower bound we have shown for relevant, sufficiently smooth objectives satisfying A.α. At this point, the question of whether all known optimal second-order methods share enough design concepts to be made members of a single class remains open.

[10] In practice, η is most likely to belong to $(0, 1)$ and even be reasonably close to zero.
[11] But fails for the example of Section 3.2 as $\|s_k\| = 1$.

Note that every iteration complexity bound discussed above is of the order ϵ^{-p} (for various values of $p > 0$) for driving the objective's gradient below ϵ; thus the methods we have addressed may require an exponential number of iterations $10^{p \cdot k}$ to generate k correct digits in the solution. Also, as our examples are one-dimensional, they fail to capture the problem-dimension dependence of the upper complexity bounds. Indeed, besides the accuracy tolerance ϵ, existing upper bounds depend on the distance to the solution set, that is $f(x_0) - f_{\text{low}}$, and the gradient's and Hessian's Lipschitz or Hölder constants, all of which may dependent on the problem dimension. Some recent developments in this respect can be found in Jarre [2013], Agarwal, Allen-Zhu, Bullins, Hazan, and T. Ma [2016], B. Jiang, Lin, S. Ma, and S. Zhang [2016], and C. W. Royer and Wright [2017].

Here we have solely addressed the evaluation complexity of generating first-order critical points, but it is common to require second-order methods for nonconvex problems to achieve second-order criticality. Indeed, upper worst-case complexity bounds are known in this case for cubic regularization and trust-region methods Nesterov and Polyak [2006], Cartis, N. I. M. Gould, and P. L. Toint [2011b], and Cartis, N. I. M. Gould, and P. L. Toint [2012b], which are essentially sharp in some cases Cartis, N. I. M. Gould, and P. L. Toint [2012b]. A lower bound on the whole class of second order methods for achieving second-order optimality remains to be established, especially when different accuracy is requested in the first- and second-order criticality conditions.

Regarding the worst-case evaluation complexity of constrained optimization problems, we have shown Cartis, N. I. M. Gould, and P. L. Toint [2012a] and Cartis, N. I. M. Gould, and P. L. Toint [2011c, 2014] that the presence of constraints does not change the order of the bound, so that the unconstrained upper bound for some first- or second-order methods carries over to the constrained case; note that this does not include the cost of solving the constrained subproblems as the latter does not require additional problem evaluations. Since constrained problems are at least as difficult as unconstrained ones, these bounds are also sharp. It remains an open question whether a unified treatment such as the one given here can be provided for the worst-case evaluation complexity of methods for constrained problems.

A1. An example of slow convergence of the steepest-descent method

We show in this paragraph that the steepest-descent method may need at least ϵ^{-2} iteration to terminate on a function whose range is fixed and independent of ϵ.

We once again follow the methodology used in Section 3.1 and build a unidimensional function f_ϵ^{SD} by Hermite interpolation, such that the steepest-descent method applied to this function takes exactly $k_\epsilon = \lceil \epsilon^{-2} \rceil$ iterations and function evaluations to terminate with an iterate x_k such that $|g(x_k)| \leq \epsilon$. Note that, for the sequence of function values to be interpretable as the result of applying the steepest-descent method (using a Goldstein linesearch), we require that, for all k,

(A.1)

$$f(x_k) + \mu_1 g_k^T s_k \leq f(x_k - \mu_k g_k) \leq f(x_k) + \mu_2 g_k^T s_k \quad \text{for constants} \quad 0 < \mu_2 < \mu_1 < 1$$

where, as above, $s_k = x_{k+1} - x_k$. Keeping this in mind, we define the sequences f_k, g_k, H_k and s_k for $k \in \{0, \ldots, k_\epsilon - 1\}$ by

$$f_k = 1 - \tfrac{1}{2}k\epsilon^2 \quad g_k = -2\epsilon f_k, \quad H_k = 0, \quad r_k = 0 \text{ and } \mu_k = \frac{1}{4f_k^2} \in [\tfrac{1}{4}, 1].$$

Note that this last definition ensures that (A.1) holds provided $0 < \mu_2 < \frac{1}{2} < \mu_1 < 1$. It also gives that $s_k = \epsilon/(2f_k) \leq \epsilon < 1$. Using these values, it can also be verified that termination occurs for $k = k_\epsilon$, that f_ϵ^{SD} defined by (3.10) and Hermite interpolation is twice continuously differentiable on $[0, x_{k_\epsilon}]$ and that (3.12) again holds. Since $|g_k| \leq \epsilon$, we also obtain that, for $k \in \{0, \ldots, k_\epsilon - 1\}$,

$$\left|\frac{\Delta f_k}{s_k^2}\right| = 2f_k^2 \leq 1, \quad \left|\frac{\Delta g_k}{s_k}\right| = 2\epsilon^2 f_k \leq 2 \text{ and } \left|\frac{g_k}{s_k}\right| = 4f_k^2 \leq 4.$$

These bounds, $H_k = \Delta H_k = 0$, the first equality of (3.18) and (3.13) then imply that the Hessian of f_ϵ^{SD} is bounded above by a constant independent of ϵ. f_ϵ^{SD} thus satisfies A.0 and therefore has Lipchitz continuous gradient. Moreover, since $s_k \leq 1$, we also obtain, as in Section 3.1 and 3.2, that $|f_\epsilon^{SD}|$ is bounded by a constant independent of ϵ on $[0, x_{k_\epsilon}]$. As above we then extend f_ϵ^{SD} to the whole of $\mathbb{R}$ while preserving A.0.

Theorem A.1. *For every $\epsilon \in (0, 1)$, a function f_ϵ^{SD} satisfying A.0 (and thus having Lipschitz continuous gradient) with values in a bounded interval independent of ϵ can be constructed, such that the steepest-descent method terminates exactly at iteration*

$$k_\epsilon = \lceil \epsilon^{-2} \rceil$$

with the first iterate x_{k_ϵ} such that $\|\nabla_x f_\epsilon^{SD}(x_{k_\epsilon})| \leq \epsilon$.

As a consequence, the $\mathcal{O}\left(\epsilon^{-2}\right)$ order of worst-case evaluation complexity is sharp for the steepest-descent method in the sense that the complexity ratio ρ_{comp} is bounded above independently of of ϵ, which improves on the conclusion proposed in Cartis, N. I. M. Gould, and P. L. Toint [2010] for the steepest-descent method.

The top three graphs of Figure A.2 illustrate the global behaviour of the resulting function $f_\epsilon^N(x)$ and of its first and second derivatives for $x \in [0, x_{k_\epsilon}]$, while the bottom ones show more detail of the first 10 iterations. The figure is once more constructed using $\epsilon = 5.10^{-2}$ ($k_\epsilon = 400$).

A2. Upper complexity bound for the $(2 + \alpha)$-regularization method

The purpose of this paragraph is to to provide some of the missing details in the proof of Lemma 2.5, as well as making explicit the statement made at the end of Section 5.1 in Cartis, N. I. M. Gould, and P. L. Toint [2011b] that the $(2+\alpha)$-regularization method needs at most (4.2) iterations (and function/derivatives evaluations) to obtain and iterate x_k such that $|g_k| \leq \epsilon$.

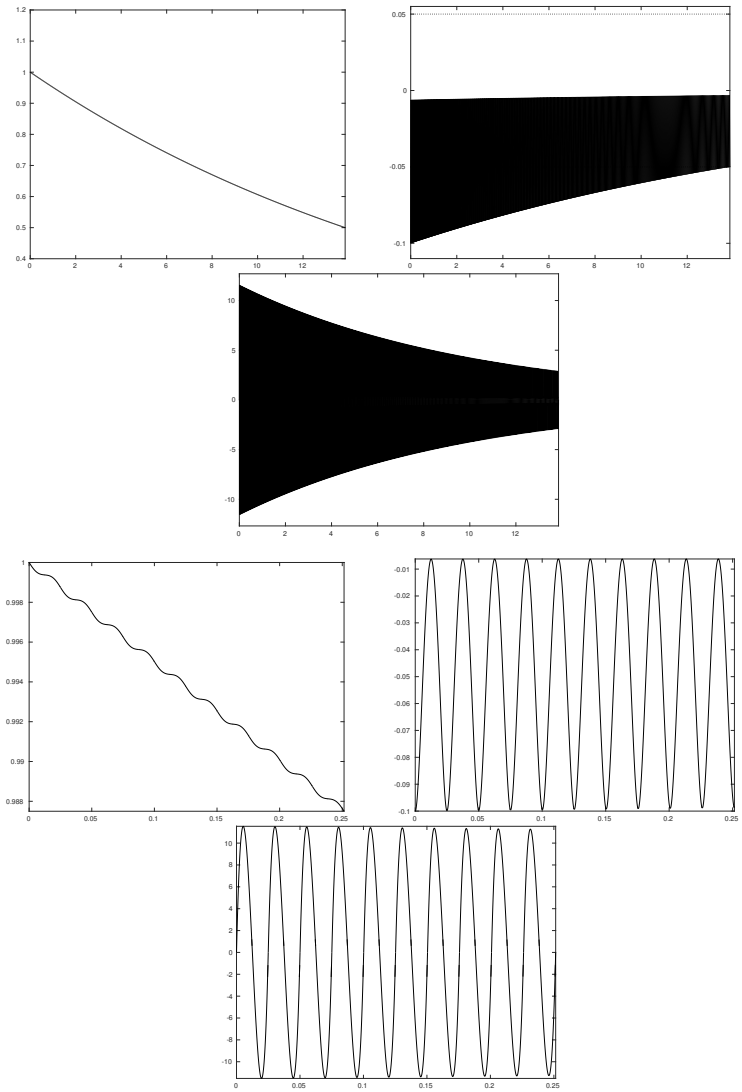

Figure A.2: $f_\epsilon^{SD}(x)$ (left) and its first (center) and second (right) derivatives as a function of x for $\epsilon = 5.10^{-2}$ (top: $x \in [0, x_{k_{\epsilon,\alpha}}]$; bottom: $x \in [0, x_{10}]$). Horizontal dotted lines indicate values of $-\epsilon$ and ϵ in the central top graph.

We start by proving (2.27) following the reasoning of Cartis, N. I. M. Gould, and P. L. Toint [2011a, Lem.2.2]. Consider

$$\begin{aligned} m_k(s) - f(x_k) &= g_k^T s + \tfrac{1}{2} s^T H_k s + \tfrac{1}{2+\alpha}\sigma_k \|s\|^{2+\alpha} \\ &\geq -\|g_k\|\,\|s\| - \tfrac{1}{2}\|s\|^2\,\|H_k\| + \tfrac{1}{2+\alpha}\sigma_k\|s\|^{2+\alpha} \\ &\geq \left(\tfrac{1}{3(2+\alpha)}\sigma_k\|s\|^{2+\alpha} - \|g_k\|\,\|s\|\right) + \left(\tfrac{2}{3(2+\alpha)}\sigma_k\|s\|^{2+\alpha} - \tfrac{1}{2}\|s\|^2\|H_k\|\right) \end{aligned}$$

But then $\frac{2}{3(2+\alpha)}\sigma_k\|s\|^{2+\alpha} - \|H_k\|\,\|s\|^2 > 0$ if $\|s_k\| < (3(2+\alpha)\|H_k\|/(4\sigma_k))^{\frac{1}{\alpha}}$ while $\frac{1}{3(2+\alpha)}\sigma_k\|s\|^{2+\alpha} - \|g_k\|\,\|s\| > 0$ if $\|s_k\| < (3(2+\alpha)\|g_k\|/\sigma_k)^{\frac{1}{1+\alpha}}$. Hence, since $m_k(s_k) < f(x_k)$, we have that

$$\|s_k\| \leq \max\left[\left(\frac{3(2+\alpha)\|H_k\|}{4\sigma_k}\right)^{\frac{1}{\alpha}}, \left(\frac{3(2+\alpha)\|g_k\|}{\sigma_k}\right)^{\frac{1}{1+\alpha}}\right]$$

which yields (2.27) because $\|H_k\| \leq L_g$.

We next explicit the worst-case evaluation complexity bounf of Section 5.1 in Cartis, N. I. M. Gould, and P. L. Toint [2011b]. Following Cartis, N. I. M. Gould, and P. L. Toint [2011a, Lemma 5.2], we start by proving that

$$\sigma_{\max} \stackrel{\text{def}}{=} c_\sigma \max(\sigma_0, L_{H,\alpha}) \tag{A.1}$$

for some constant c_σ only dependent on α and algorithm's parameters. To show this inequality, we deduce from Taylor's theorem that, for each $k \geq 0$ and some ξ_k belonging the the segment $[x_k, x_k + s_k]$,

$$f(x_k+s_k)-m_k(s_k) \leq \frac{1}{2}\|H(\xi_k)-H(x_k)\|\cdot\|s_k\|^2 - \frac{\sigma_k}{2+\alpha}\|s_k\|^{2+\alpha} \leq \left(\frac{L_{H,\alpha}}{2} - \frac{\sigma_k}{2+\alpha}\right)\|s_k\|^{2+\alpha},$$

where, to obtain the second inequality, we employed (2.8) in A.α and $\|\xi_k - x_k\| \leq \|s_k\|$. Thus $f(x_k+s_k) < m_k(s_k)$ whenever $\sigma_k > \frac{1}{2}(2+\alpha)L_{H,\alpha}$, providing sufficient descent and ensuring that $\sigma_{k+1} \leq \sigma_k$. Taking into account the (possibly large) choice of the regularization parameter at startup then yields (A.1).

We next note that, because of (2.25) and (A.1), (2.11) holds. Moreover, $\kappa(M_k) = \kappa\left(\sigma_k\|s_k\|^\alpha I\right) = 1$. Lemma 2.3 then ensures that (2.16) also holds.

We finally follow Cartis, N. I. M. Gould, and P. L. Toint [ibid., Corollary 5.3] to prove the final upper bound on the number of successful iterations (and hence on the number of function and derivatives evaluations). Let $\mathcal{S}_k^\epsilon$ index the subset of the first k iterations that are successful and such that $\min[\|g_k\|, \|g_{k+1}\|] > \epsilon$, and let $|\mathcal{S}_k^\epsilon|$ denote its cardinality. It follows from this definition, (2.11), (2.26) and the fact that sufficient decrease is obtained at successful iterations that, for all k before termination,

$$f(x_j) - m_k(s_j) \geq \alpha_S \epsilon^{\frac{2+\alpha}{1+\alpha}}, \quad \text{for all } j \in \mathcal{S}_k^\epsilon, \tag{A.2}$$

for some positive constant α_S independent of ϵ. Now, if $f_{\text{low}} > -\infty$ is a lower bound on $f(x)$, we have, using the monotonically decreasing nature of $\{f(x_k)\}$, that

$$\begin{aligned} f(x_0) - f_{\text{low}} \;\geq\; & f(x_0) - f(x_{k+1}) \;=\; \sum_{j \in \mathcal{S}_k^\epsilon} [f(x_j) - f(x_{j+1})] \\ \geq\; & \eta_1 \sum_{j \in \mathcal{S}_k^\epsilon} [f(x_j) - m_k(s_j)] \;\geq\; |\mathcal{S}_k^\epsilon|\, \eta_1 \alpha_S\, \epsilon^{\frac{2+\alpha}{1+\alpha}}, \end{aligned}$$

where the constant $\eta_1 \in (0,1)$ defines sufficient decrease. Hence, for all $k \geq 0$,

$$|\mathcal{S}_k^\epsilon| \leq \frac{f(x_0) - f_{\text{low}}}{\eta_1 \alpha_S}\, \epsilon^{-\frac{2+\alpha}{1+\alpha}}.$$

As a consequence, the $(2+\alpha)$-regularization method needs at most (4.2) successful iterations to terminate. Since it known that, for regularization methods, $k \leq \kappa_{\mathcal{S}} |\mathcal{S}_k^\epsilon|$ for some constant $\kappa_{\mathcal{S}}$ Cartis, N. I. M. Gould, and P. L. Toint [2011b, Theorem 2.1] and because every iteration involves a single evaluation, we conclude that the $(2+\alpha)$-regularization method needs at most (4.2) function and derivatives evaluations to produce an iterate x_k such that $\|g_k\| \leq \epsilon$ when applied to an objective function satisfying A.α.

We finally oserve that the statement (made in the proof of Lemma 2.5) that $\|g_k\|$ is bounded above immediately follows from this worst-case evaluation complexity bound.

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