OFFO minimization algorithms for second-order optimality and their complexity

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Abstract

An Adagrad-inspired class of algorithms for smooth unconstrained optimization is presented in which the objective function is never evaluated and yet the gradient norms decrease at least as fast as $\mathcal{O}(1/\sqrt{k+1})$ while second-order optimality measures converge to zero at least as fast as $\mathcal{O}(1/(k+1)^{1/3})$. This latter rate of convergence is shown to be essentially sharp and is identical to that known for more standard algorithms (like trust-region or adaptive-regularization methods) using both function and derivatives' evaluations. A related "divergent stepsize" method is also described, whose essentially sharp rate of convergence is slighly inferior. It is finally discussed how to obtain weaker second-order optimality guarantees at a (much) reduced computional cost.

Keywords: Second-order optimality, objective-function-free optimization (OFFO), Adagrad, global rate of convergence, evaluation complexity.

1 Introduction

This paper considers an *a priori* unexpected but fundamental and challenging question: is evaluating the value of the objective function necessary for obtaining (complexity-wise) efficient minimization algorithms which find second-order approximate minimizers? This question arose as a natural consequence of the somewhat surprising results of [14], where it was shown that OFFO (i.e. Objective-Function Free Optimization) algorithms[(1)] exist which converge to first-order points at a global rate which in order identical to that to well-known methods using both gradient and objective function evaluations. That these algorithms include the deterministic version of Adagrad [10], a very popular method for deep learning applications, was an added bonus and a good motivation.

We show here that, *from the point of view of evaluation complexity alone, evaluating the value of the objective function during optimization is also unnecessary*[(2)] *for finding approximate second-order minimizers* at a (worst-case) cost entirely comparable to that incurred by

[(1)]For which the only source of information on the problem at hand is the value of the gradient.

[(2)]The authors are well aware that this is a theoretical statement, as it may be impractical to evaluate derivatives without first evaluating the function itself.

familiar and reliable techniques such as second-order trust-region or adaptive regularization methods. This conclusion is coherent with that of [14] for first-order points and is obtained by exhibiting an OFFO algorithm whose global rate of convergence is proved to be $\mathcal{O}(1/\sqrt{k+1})$ for the gradients'norm and $\mathcal{O}(1/(k+1)^{1/3})$ for second-order measures. The new ASTR2 algorithm is of the adaptively scaled trust-region type, as those studied in [14]. The key difference is that it now hinges on a scaling technique which depends on second-order information, when relevant.

The paper is organized as follows. Section 2 presents the new ASTR2 class of algorithms and discusses some of its scaling-independent properties. The complexity analysis of a first, Adagrad-like, subclass of ASTR2 is then presented in Section 3. Another subclass of interest is also considered and analyzed in Section 4. Section 5 discusses how weaker optimality conditions may be guaranteed by the ASTR2 algorithms at significantly reduced computational cost. Conclusions and perspectives are finally presented in Section 6

2 The ASTR2 class of minimization methods

2.1 Approximate first- and second-order optimality

We consider the nonlinear unconstrained optimization problem

$$\min_{x\in\mathbb{R}^n} f(x) \tag{2.1}$$

where f is a function from $\mathbb{R}^n$ to $\mathbb{R}$. More precisely, we assume that

AS.1: the objective function $f(x)$ is twice continuously differentiable;

AS.2: its gradient $g(x) \stackrel{\text{def}}{=} \nabla_x^1 f(x)$ and Hessian $H(x) \stackrel{\text{def}}{=} \nabla_x^2 f(x)$ are Lipschitz continuous with Lipschitz constant L_1 and L_2, respectively, that is

$$\|g(x) - g(y)\| \le L_1\|x - y\| \quad \text{and} \quad \|H(x) - H(y)\| \le L_2\|x - y\|$$

for all $x, y \in \mathbb{R}^n$;

AS.3: there exists a constant f_{low} such that $f(x) \ge f_{\text{low}}$ for all $x \in \mathbb{R}^n$.

As our purpose is to find approximate first- and second-order minimizers, we need to clarify these concepts. In this paper we choose to follow the " strong ϕ" concept of optimality discussed in [4, 6] or [5, Chapters 12–14]. It is based on the quantity

$$\phi_{f,2}^{\delta}(x) = f(x) - \min_{\|d\| \le \delta} T_{f,2}(x, d), \tag{2.2}$$

where $T_{f,2}(x, d)$ is the second-order Taylor expansion of f at x, that is

$$T_{f,1}(x, d) = f(x) + g(x)^T d \quad \text{and} \quad T_{f,2}(x, d) = f(x) + g(x)^T d + \tfrac{1}{2} d^T H(x) d.$$

Observe that $\phi_{f,j}^{\delta}(x)$ is interpreted as the maximum decrease of the local j-th order Taylor model of the objective function f at x, within a ball of radius δ. Importantly for our present

purposes, the evaluation of $\phi_{f,2}^{\delta}(x)$ *does not require the evaluation of* $f(x)$, as it can be rewritten as

$$\phi_{f,2}^{\delta}(x) = \max_{\|d\| \le \delta} -\left(g(x)^T d + \tfrac{1}{2} d^T H(x) d\right). \tag{2.3}$$

The next result recalls the link between the ϕ optimality measure and the more standard ones.

Lemma 2.1 [5, Theorems 12.1.4 and 12.1.6] Suppose that f is twice continuously differentiable. Then

(i) for any $\delta > 0$ and any $x \in \mathbb{R}^n$, we have that

$$\|g(x)\| = \frac{\phi_{f,1}^{\delta}(x)}{\delta}, \tag{2.4}$$

and so $\phi_{f,1}^{\delta}(x) = 0$ if and only if $g(x) = 0$;

(ii) we have that

$$\phi_{f,2}^{\delta}(x) = 0 \text{ for some } \delta > 0, \text{ then } g(x) = 0 \text{ and } \lambda_{\min}[H(x)] \ge 0,$$

and so any such x is a first- and second-order minimizer;

(iii) if $\phi_{f,1}^{\delta_1}(x) \le \epsilon_1 \, \delta_1$ (and so (2.5) holds with $j = 1$), then $\|g(x)\| \le \epsilon_1$;

(iv) if $\phi_{f,2}^{\delta}(x) \le \tfrac{1}{2}\epsilon_2 \delta^2$, then $\lambda_{\min}[H(x)] \ge -\epsilon_2$ (and so (2.5) holds for $j = 2$) and $\|g(x)\| \le \delta\kappa(x)\sqrt{\epsilon_2}$, where $\kappa(x)$ depends on (the eigenvalues of) $H(x)$.

Note also that computing $\phi_{f,1}^{\delta}(x)$ simply results from (2.4) and that, in particular, $\phi_{f,1}^{1}(x) = \|g(x)\|$. Computing $\phi_{f,2}^{\delta}(x)$ is a standard Euclidean trust-region step calculation (see [7, Chapter 7], for instance).

For $j \in \{1, 2\}$, we then say that an iterate x_k is an ϵ-approximate minimizer if

$$\phi_{f,j}^{\delta}(x_k) \le \epsilon_j \frac{\delta^j}{j} \quad \text{for some} \quad \delta \in (0, 1] \quad \text{and all} \quad 1 \le i \le j, \tag{2.5}$$

where $\epsilon = (\epsilon_1, \ldots, \epsilon_j)$. There are two ways to express how fast an algorithm tends to such points in the worst case. The first (the "ϵ-orders") is to assume ϵ is given and then give a bound on the maximum number of iterations and evaluations that are needed to satisfy (2.5). In this paper we focus on the second (the "k-orders"), where one instead gives an upper bound[3] on $\phi_{f,j}^{\delta}(x_k)$ as a function of k (for specified j and δ).

2.2 The ASTR2 class

After these preliminaries, we now introduce the new ASTR2 class of algorithms. Methods in this class are of "adaptively scaled trust-region" type, a term we now briefly explain. Classical

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[3] Converging to zero.

trust-region algorithms (see [7] for an in-depth coverage or [20] for a more recent survey) are iterative. At each iteration, they define a local model of the objective function which is deemed trustable within the "trust region", a ball of given radius centered at the current iterate. A step and corresponding trial point are then computed by (possibly approximately) minimizing this model in the trust region. The objective function value is then computed at the trial point, and this point is accepted as the new iterate if the ratio of the achieved reduction in the objective function to that predicted by the model is sufficiently large. The radius of the trust region is then updated using the value of this ratio. As is clear from this description, these methods are intrinsically dependent of the evaluation of the objective function, and therefore not suited to our Objective-Function Free Optimization (OFFO) context. Here we follow [14] in interpreting the mechanism designed for the Adagrad methods [10] as an alternative trust-region design not using function evaluations. In this interpretation, the trial point is always accepted and the trust-region radius is determined by the gradient sizes, in a manner reminiscent also of [11]. In this approach, one uses *scaling factors* to determine the radius (hence the name of Adaptively Scaled Trust Region). Given these factors, we may then state the ASTR2 class of algorithms as shown on the following page. This algorithm involves requirements on the step which are standard (and practical) for trust-region methods.

A few additional comments on this algorithm are now in order.

1. The algorithms in the ASTR2 class belong to the OFFO framework: the objective function is never evaluated (remember that $\phi_{f,j}^1(x)$ can be computed without any such evaluation, the same being obviously true for Δq_k, Δq_k^C and Δq_k^E).

2. Given our focus on k-orders of convergence, the algorithm does not include a termination criterion. It is however easy, should one be interested in ϵ-orders instead, to test (2.5) for $\delta = 1$ and the considered ϵ_1 and ϵ_2 at the end of Step 1, and then terminate if this condition holds.

3. Despite their somewhat daunting statements, conditions (2.9)–(2.12) are relatively mild and have been extensively used for standard trust-region algorithms, both in theory and practice. Condition (2.10) defines the so-called "Cauchy decrease", which is the decrease achievable on the quadratic model $T_{f,2}(x_k, s)$ in the steepest descent direction [7, Section 6.3.2]. Conditions (2.11) and (2.12) define the "eigen-point decrease", which is that achievable along u_k, a (χ-approximate) eigenvector associated with the smallest Hessian eigenvalue [7, Section 6.6]. We discuss in Section 5 how they can be ensured in practice, possibly approximately, for instance by the GLTR algorithm [13].

4. The computation of ϕ_k can be reused to compute s_k^Q, should it be necessary. If $\Delta_k > 1$, the model minimization may be pursued beyond the boundary of the unit ball. If $\Delta_k < 1$, backtracking is also possible [7, Section 10.3.2].

5. Note that *two* scaling factors are updated from iteration to iteration: one for first-order models and one for second-order ones. It does indeed make sense to trust these two types of models in region of different sizes, as Taylor's theory suggests second-order models may be reasonably accurate in larger neighbourhoods.

Algorithm 2.1: ASTR2

Step 0: Initialization. A starting point x_0 is given. The constants $\tau, \chi \in (0, 1]$ and $\xi \geq 1$ are also given. Set $k = 0$.

Step 1: Compute derivatives. Compute $g_k = g(x_k)$ and $H_k = H(x_k)$, as well as $\phi_k \stackrel{\text{def}}{=} \phi_{f,2}^1(x_k)$ and $\widehat{\phi}_k \stackrel{\text{def}}{=} \min[\phi_k, \xi]$.

Step 2: Define the trust-region radii. Set

$$\Delta_k^L = \frac{\|g_k\|}{w_k^L} \quad \text{and} \quad \Delta_k^Q = \frac{\widehat{\phi}_k}{w_k^Q} \tag{2.6}$$

where $w_k^L = w^L(x_0, \ldots, x_k)$ and $w_k^Q = w^Q(x_0, \ldots, x_k)$.

Step 3: Step computation. If

$$\|g_k\|^2 \geq \widehat{\phi}_k^3, \tag{2.7}$$

then set

$$s_k = s_k^L = -\frac{g_k}{w_k^L}. \tag{2.8}$$

Otherwise, set $s_k = s_k^Q$, where s_k^Q is such that

$$\|s_k^Q\| \leq \Delta_k^Q \quad \text{and} \quad \Delta q_k \geq \tau \max\left[\Delta q_k^C, \Delta q_k^E\right] \tag{2.9}$$

where

$$\Delta q_k^C = \max_{\substack{\alpha \geq 0 \\ \alpha\|g_k\| \leq \Delta_k^Q}} \left[f(x_k) - T_{f,2}(x_k, -\alpha g_k)\right] \tag{2.10}$$

and

$$\Delta q_k^E = \max_{\substack{\alpha \geq 0 \\ \alpha \leq \Delta_k^Q}} \left[f(x_k) - T_{f,2}(x_k, \alpha u_k)\right] \tag{2.11}$$

with u_k satisfying

$$u_k^T H_k u_k \leq \chi \lambda_{\min}[H_k], \quad u_k^T g_k \leq 0 \quad \text{and} \quad \|u_k\| = 1. \tag{2.12}$$

Step 4: New iterate. Define

$$x_{k+1} = x_k + s_k, \tag{2.13}$$

increment k by one and return to Step 1.

6. A "componentwise" version where the trust region is defined in the $\| \cdot \|_\infty$ norm is possible with

$$\phi_{i,k} = \max \left[\phi_k, - \min_{|\alpha| \leq 1} \left(\alpha g_{i,k} + \tfrac{1}{2}\alpha^2 [H_k]_{i,i} \right) \right]$$

and

$$\Delta_{i,k}^L = \frac{|g_{i,k}|}{w_{i,k}^L} \quad \text{and} \quad \Delta_{i,k}^Q = \frac{\min[\xi, \phi_{i,k}]}{w_{i,k}^Q}.$$

We will not explicitly consider this variant to keep our notations reasonably simple.

Our assumption that the gradient and Hessian are Lipschitz continuous (AS.2) ensures the following standard result.

Lemma 2.2 [1] or [5, Theorem A.8.3] Suppose that AS.1 and AS.2 hold. Then

$$f(x_k + s_k^L) - f(x_k) \leq \langle g_k, s_k^L \rangle + \frac{L_1}{2}\|s_k^L\|^2 \tag{2.14}$$

and

$$f(x_k + s_k^Q) - f(x_k) \leq -\Delta q_k + \frac{L_2}{6}\|s_k^Q\|^3. \tag{2.15}$$

The first step in analyzing the convergence of the ASTR2 algorithm is to derive bounds on the objective function's change from iteration to iteration, depending on which step (linear with $s_k = s_k^L$, or quadratic with $s_k = s_k^Q$) is chosen. We start by a few auxiliary results on the relations between first- and second-order optimality measures.

Lemma 2.3 Suppose that H is an $n \times n$ symmetric positive semi-definite matrix and $g \in \mathbb{R}^n$, and consider the (convex) quadratic $q(d) = \langle g, d \rangle + \frac{1}{2}\langle d, Hd \rangle$. Then

$$\phi_{q,2}^1(0) = \left| \min_{\|d\| \leq 1} q(d) \right| \leq \|g\|. \tag{2.16}$$

Proof. From the definition of the gradient, we have that

$$\|g\| = \left| \min_{\|d\| \leq 1} \langle g, d \rangle \right|.$$

But $\langle g, d \rangle$ defines the supporting hyperplane of $q(d)$ at $d = 0$ and thus the convexity of q implies that $q(d) \geq \langle g, d \rangle$ for all d. Hence

$$\left| \min_{\|d\| \leq 1} q(d) \right| \leq \left| \min_{\|d\| \leq 1} \langle g, d \rangle \right|$$

and (2.16) follows. $\qquad\qquad\square$

Lemma 2.4 Suppose that

$$0 < \eta_k \le \tfrac{1}{2}\phi_k \tag{2.17}$$

where

$$\eta_k \stackrel{\text{def}}{=} \min\left(0, -\lambda_{\min}[H_k]\right). \tag{2.18}$$

Then

$$\tfrac{1}{2}\phi_k \le \|g_k\|. \tag{2.19}$$

Proof. Observe first that (2.17) implies that $\lambda_{\min}[H_k] < 0$ and $\eta_k = |\lambda_{\min}[H_k]|$. Let d_k be a solution of the optimization problem defining ϕ_k, i.e.,

$$d_k = \arg\min_{\|d\| \le 1} T_{f,2}(x_k, d),$$

so that $\phi_k = f_k - T_{f,2}(x_k, d_k)$. Since $\lambda_{\min}[H_k] < 0$, it is known from trust-region theory [7, Corollary.2.2] that d_k may be chosen such that $\|d_k\| = 1$. Now define

$$q_0(d) \stackrel{\text{def}}{=} \langle g_k, d \rangle + \tfrac{1}{2}\langle d, (H_k - \lambda_{\min}[H_k]I)d \rangle = T_{f,2}(x_k, d) - f_k + \eta_k \|d\|^2$$

and note that $q_0(d)$ is convex by construction. Then, at d_k,

$$q_0(d_k) = -\phi_k + \eta_k$$

and (2.17) implies that $q_0(d_k) < 0$. Moreover,

$$\tfrac{1}{2}\phi_k \le -q_0(d_k) \le -\langle g_k, d_k \rangle \le \|g_k\|,$$

where we used the convexity of q_0 to deduce the the first inequality, and Cauchy-Schwarz with $\|d_k\| \le 1$ to derive the second. This proves (2.19). □

Using these results, we may now prove a crucial property on objective function change. For this purpose, we partition the iterations in two sets, depending which type of step is chosen, that is

$$\mathcal{K}^L = \{k \ge 0 \mid s_k = s_k^L\} \quad \text{and} \quad \mathcal{K}^Q = \{k \ge 0 \mid s_k = s_k^Q\}.$$

Lemma 2.5 Suppose that AS.1 and AS.2 hold. Then

$$f_{k+1} - f_k \le -\frac{\|g_k\|^2}{w_k^L} + \frac{L_1}{2}\frac{\|g_k\|^2}{(w_k^L)^2} \quad \text{for} \quad k \in \mathcal{K}^L \tag{2.20}$$

and

$$f_{k+1} - f_k \le -\frac{\tau}{4\xi}\min\left[\frac{1}{2(1+L_1)}, \frac{1}{w_k^Q}, \frac{1}{(w_k^Q)^2}\right]\widehat{\phi}_k^3 + \frac{L_2}{6}\frac{\widehat{\phi}_k^3}{(w_k^Q)^3} \quad \text{for} \quad k \in \mathcal{K}^Q. \tag{2.21}$$

Proof. Suppose first that $s_k = s_k^L$. Then (2.14), (2.8) and (2.6) ensure that

$$f_{k+1} - f_k \leq -\frac{\|g_k\|^2}{w_k^L} + \frac{L_1}{2}(\Delta_k^L)^2 = -\frac{\|g_k\|^2}{w_k^L} + \frac{L_1}{2}\frac{\|g_k\|^2}{(w_k^L)^2}, \tag{2.22}$$

giving (2.20).

Suppose now that $s_k = s_k^Q$, i.e. $k \in \mathcal{K}^Q$. Then, because of (2.9)–(2.12), the decrease Δq_k in the quadratic model $T_{f,2}(x_k, s)$ at s_k is at least a fraction τ of the maximum of the Cauchy and eigen-point decreases given by (2.10) and (2.11). Standard trust-region theory (see [7, Lemmas 6.3.2 and 6.6.1] for instance) then ensures that, for possibly non-convex $T_{f,2}(x_k, s)$,

$$\begin{aligned} \Delta q_k &\geq \tau \max\left[\frac{1}{2}\min\left(\frac{\|g_k\|^2}{1+\|H_k\|}, \|g_k\|\Delta_k^Q\right), \frac{\eta_k}{2}(\Delta_k^Q)^2\right] \\ &\geq \frac{\tau}{2}\max\left[\min\left(\frac{\|g_k\|^2}{1+L_1}, \frac{\|g_k\|\widehat{\phi}_k}{w_k^Q}\right), \frac{\eta_k\widehat{\phi}_k^2}{(w_k^Q)^2}\right] \end{aligned}$$

where we used the bound $\|H_k\| \leq L_1$ and (2.6) to derive the last inequality. If $\eta_k \leq \frac{1}{2}\phi_k$, then, using Lemma 2.4 and the inequality $\phi_k \geq \widehat{\phi}_k$,

$$\Delta q_k \geq \frac{\tau}{2}\min\left(\frac{\|g_k\|^2}{1+L_1}, \frac{\|g_k\|\widehat{\phi}_k}{w_k^Q}\right) \geq \frac{\tau}{2}\min\left(\frac{(\frac{1}{2}\widehat{\phi}_k)^2}{1+L_1}, \frac{(\frac{1}{2}\widehat{\phi}_k)\widehat{\phi}_k}{w_k^Q}\right).$$

Now $\widehat{\phi}_k^3 \leq \xi\widehat{\phi}_k^2$ and thus

$$\Delta q_k \geq \frac{\tau}{2}\min\left(\frac{\widehat{\phi}_k^3}{4\xi(1+L_1)}, \frac{\widehat{\phi}_k^3}{2\xi w_k^Q}\right). \tag{2.23}$$

If instead $\eta_k > \frac{1}{2}\phi_k \geq \frac{1}{2}\widehat{\phi}_k$, then

$$\Delta q_k \geq \frac{\tau}{2}\frac{\eta_k\widehat{\phi}_k^2}{(w_k^Q)^2} \geq \frac{\tau}{2}\frac{(\frac{1}{2}\widehat{\phi}_k)\widehat{\phi}_k^2}{(w_k^Q)^2}. \tag{2.24}$$

Given that, if $k \in \mathcal{K}^Q$, $\|s_k\| \leq \Delta_k^Q = \widehat{\phi}_k/w_k^Q$, we deduce (2.21) from (2.15), (2.23) and (2.24). □

Observe that neither (2.20) nor (2.21) guarantees that the objective function values are monotonically decreasing.

3   An Adagrad-like algorithm for second-order optimality

We first consider a choice of scaling factors directly inspired by the Adagrad algorithm [10] and assume that, for some $\varsigma > 0$, $\mu, \nu \in (0,1)$, $\vartheta_L, \vartheta_Q \in (0,1]$ and all $k \geq 0$,

$$w_k^L \in [\vartheta_L\hat{w}_k^L, \hat{w}_k^L] \quad \text{where} \quad \hat{w}_k^L = \left(\varsigma + \sum_{\substack{\ell=0 \\ \ell\in\mathcal{K}^L}}^{k} \|g_k\|^2\right)^{\mu} \tag{3.1}$$

and

$$w_k^Q \in [\vartheta_Q \hat{w}_k^Q, \hat{w}_k^Q] \quad \text{where} \quad \hat{w}_k^Q = \left(\varsigma + \sum_{\substack{\ell=0 \\ \ell \in \mathcal{K}^Q}}^{k} \widehat{\phi}_k^3 \right)^\nu. \tag{3.2}$$

Note that selecting the parameters ϑ_L and ϑ_Q strictly less than one allows the scaling factors w_k^L and w_k^Q to be chosen in an interval at each iteration without any monotonicity.

We now present a two technical lemmas which will be necessary in our analysis. The first states useful results for a specific class of inequalities.

Lemma 3.1 Let $a \geq \frac{1}{2}\varsigma$ and $b \geq \frac{1}{2}\varsigma$. Suppose that, for some $\theta_a \geq 1$, $\theta_b \geq 1$, $\theta \geq 0$, $\mu \in (0,1)$, and $\nu \in (0, \frac{1}{3})$

$$a^{1-\mu} + b^{1-2\nu} \leq \theta_a A(a) + \theta_b B(b) + \theta \tag{3.3}$$

where $A(a)$ and $B(b)$ are given, as a function of μ and ν, by

	$\mu < \frac{1}{2}$	$\mu = \frac{1}{2}$	$\mu > \frac{1}{2}$
$A(a)$	$a^{1-2\mu}$	$\log(2a)$	0

and

	$\nu < \frac{1}{3}$	$\nu = \frac{1}{3}$	$\nu > \frac{1}{3}$
$B(k)$	$b^{1-3\nu}$	$\log(2b)$	0

.

Then there exists positive constants κ_a and κ_b only depending on θ_a, θ_b, θ, μ and ν such that

$$a \leq \kappa_a \quad \text{and} \quad b \leq \kappa_b. \tag{3.4}$$

Proof.   This result is proved by comparing the value of the left- and right-hand sides for possibly large a and b. The details are given in Lemmas A.2–A.8 in appendix, whose results are then combined as shown in Table 1. The details of the constants κ_a and κ_b for

	$\mu < \frac{1}{2}$	$\mu = \frac{1}{2}$	$\mu > \frac{1}{2}$
$\nu < \frac{1}{3}$	Lemma A.4	Lemma A.7	Lemma A.5
$\nu = \frac{1}{3}$	Lemma A.7	Lemma A.8	Lemma A.7
$\nu > \frac{1}{3}$	Lemma A.5	Lemma A.7	Lemma A.2

Table 1: Lemmas for combinations of μ and ν

the various cases are explicitly given in the statements of the relevant lemmas.   □

The second auxiliary result is a bound extracted from [14] (see also [9, 19] for the case $\alpha = 1$).

Lemma 3.2 Let $\{c_k\}$ be a non-negative sequence, $\varsigma > 0$, $\alpha > 0$, $\nu \geq 0$ and define, for each $k \geq 0$, $d_k = \sum_{j=0}^{k} c_j$. If $\alpha \neq 1$, then

$$\sum_{j=0}^{k} \frac{c_j}{(\varsigma + d_j)^\alpha} \leq \frac{1}{(1 - \alpha)}((\varsigma + d_k)^{1-\alpha} - \varsigma^{1-\alpha}). \tag{3.5}$$

Otherwise,

$$\sum_{j=0}^{k} \frac{c_j}{(\varsigma + d_j)} \leq \log\left(\frac{\varsigma + d_k}{\varsigma}\right). \tag{3.6}$$

Note that, if $\alpha > 1$, then the bound (3.5) can be rewritten as

$$\sum_{j=0}^{k} \frac{c_j}{(\varsigma + d_j)^\alpha} \leq \frac{1}{\alpha - 1}\left(\varsigma^{1-\alpha} - (\varsigma + d_k)^{1-\alpha}\right),$$

whose right-hand side is positive.

Armed with the above results, we are now in position to specify particular choices of the scaling factors w_k and derive the convergence properties of the resulting variants of ASTR2.

Theorem 3.3 Suppose that AS.1–AS.3 hold and that the ASTR2 algorithm is applied to problem (2.1), where w_k^L and w_k^Q are given by (3.1) and (3.2), respectively. Then there exists a positive constant κ_{ASTR2} only depending on the problem-related quantities x_0, f_{low}, L_1 and L_2 and on the algorithmic parameters ς, τ, ξ, μ and ν such that

$$\underset{j\in\{0,\ldots,k\}}{\text{average}} \|g_j\|^2 \leq \frac{\kappa_{\text{ASTR2}}}{k+1} \quad \text{and} \quad \underset{j\in\{0,\ldots,k\}}{\text{average}} \widehat{\phi}_j^3 \leq \frac{\kappa_{\text{ASTR2}}}{k+1}, \tag{3.7}$$

and therefore that

$$\min_{j\in\{0,\ldots,k\}} \|g_j\| \leq \frac{\kappa_{\text{ASTR2}}}{(k+1)^{\frac{1}{2}}} \quad \text{and} \quad \min_{j\in\{0,\ldots,k\}} \widehat{\phi}_j \leq \frac{\kappa_{\text{ASTR2}}}{(k+1)^{\frac{1}{3}}}. \tag{3.8}$$

Proof. To simplify notations in the proof, define

$$a_k = 2 \sum_{\substack{j=0 \\ j\in\mathcal{K}^L}}^{k} \|g_j\|^2 \quad \text{and} \quad b_k = 2 \sum_{\substack{j=0 \\ j\in\mathcal{K}^Q}}^{k} \widehat{\phi}_k^3. \tag{3.9}$$

Consider first an iteration index $j \in \mathcal{K}^L$ Then (2.20) (expressed for for $j \geq 0$), (3.1) and the inequality $\tau \leq 1$ give that

$$f(x_{j+1}) - f(x_j) \leq -\frac{\tau}{2} \frac{\|g_j\|^2}{w_j^L} + \frac{L_1}{2\vartheta_L^2} \frac{\|g_j\|^2}{(w_j^L)^2} \leq -\frac{\tau}{2} \frac{\|g_j\|^2}{(\varsigma + \frac{1}{2}a_j)^\mu} + \frac{L_1}{2\vartheta_L^2} \frac{\|g_j\|^2}{(\varsigma + \frac{1}{2}a_j)^{2\mu}}. \tag{3.10}$$

Suppose now that $j \in \mathcal{K}^Q$. Then (2.21) and (3.2) imply that

$$f_{j+1} - f_j \le -\frac{\tau}{4\xi} \min\left[\frac{\widehat{\phi}_j^3}{2(1+L_1)}, \frac{\widehat{\phi}_j^3}{(\varsigma + \frac{1}{2}b_j)^\nu} \frac{\widehat{\phi}_j^3}{(\varsigma + \frac{1}{2}b_j)^{2\nu}}\right] + \frac{L_2}{6\vartheta_Q^3} \frac{\widehat{\phi}_j^3}{(\varsigma + \frac{1}{2}b_j)^{3\nu}}, \quad (3.11)$$

Suppose now that

$$a_j > 2\varsigma \quad \text{and} \quad b_j > \max\left[1, 2\varsigma, \left(2(1+L_1)\right)^{\frac{1}{\nu}}\right], \quad (3.12)$$

which implies that

$$w_j^L \le a_j^\mu, \quad w_j^Q \le b_j^\nu \quad \text{and} \quad 2(1+L_1) \le b_j^\nu.$$

Then combining (3.10) and (3.11), the inequality $\xi \ge 1$ and AS.3, we deduce that, for all $k \ge 0$,

$$f(x_0) - f_{\text{low}} \ge \frac{\tau}{4\xi}\left[\sum_{\substack{j=0 \\ j\in\mathcal{K}^L}}^{k} \frac{\|g_j\|^2}{a_j^\mu} + \sum_{\substack{j=0 \\ j\in\mathcal{K}^q}}^{k} \frac{\widehat{\phi}_j^3}{b_j^{2\nu}}\right] - \frac{L_1}{2\vartheta_L^2} \sum_{\substack{j=0 \\ j\in\mathcal{K}^L}}^{k} \frac{\|g_j\|^2}{(w_k^L)^2} - \frac{L_2}{6\vartheta_Q^3} \sum_{\substack{j=0 \\ j\in\mathcal{K}^Q}}^{k} \frac{\widehat{\phi}_j^3}{(w_k^Q)^3}.$$

But, by definition, $a_j \le a_k$ and $b_j \le b_k$ for $j \le k$, and thus, for all $k \ge 0$,

$$a_k^{1-\mu} + b_k^{1-2\nu} \le \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau} + \frac{2\xi L_1}{\tau\vartheta_L^2} \sum_{\substack{j=0 \\ j\in\mathcal{K}^L}}^{k} \frac{\|g_j\|^2}{(w_k^L)^2} + \frac{2\xi L_2}{3\tau\vartheta_Q^3} \sum_{\substack{j=0 \\ j\in\mathcal{K}^Q}}^{k} \frac{\widehat{\phi}_j^3}{(w_k^Q)^3}. \quad (3.13)$$

We now have to bound the last two terms on the right-hand side of (3.13). Using (3.1) and Lemma 3.2 with $\{c_k\} = \{\|g_k\|^2\}_{k\in\mathcal{K}^L}$ and $\alpha = 2\mu$, gives that

$$\sum_{\substack{j=0 \\ k\in\mathcal{K}^L}}^{k} \frac{\|g_j\|^2}{(w_k^L)^2} \le \frac{1}{\vartheta_L^2(1-2\mu)}\left(\left(\varsigma + \sum_{\substack{j=0 \\ k\in\mathcal{K}^L}}^{k} \|g_k\|^2\right)^{1-2\mu} - \varsigma^{1-2\mu}\right) \le \frac{a_k^{1-2\mu}}{\vartheta_L^2(1-2\mu)} \quad (3.14)$$

if $\mu < \frac{1}{2}$, and

$$\sum_{\substack{j=0 \\ k\in\mathcal{K}^L}}^{k} \frac{\|g_j\|^2}{(w_j^L)^2} \le \frac{1}{\vartheta_L^2} \log\left(\frac{\varsigma + \sum_{j=0,k\in\mathcal{K}^L}^{k} \|g_k\|^2}{\varsigma}\right) \le \frac{1}{\vartheta_L^2} \log\left(\frac{\varsigma + a_k}{\varsigma}\right) \quad (3.15)$$

if $\mu = \frac{1}{2}$ and

$$\sum_{\substack{j=0 \\ k\in\mathcal{K}^L}}^{k} \frac{\|g_j\|^2}{(w_k^L)^2} \le \frac{1}{\vartheta_L^2(2\mu-1)}\left(\varsigma^{1-2\mu} - \left(\varsigma + \sum_{\substack{j=0 \\ k\in\mathcal{K}^L}}^{k} \|g_k\|^2\right)^{1-2\mu}\right) \le \frac{\varsigma^{1-2\mu}}{\vartheta_L^2(2\mu-1)} \quad (3.16)$$

if $\mu > \frac{1}{2}$. Similarly, using (3.2) and Lemma 3.2 with $\{c_k\} = \{\widehat{\phi}_k^3\}_{k \in \mathcal{K}^Q}$ and $\alpha = 3\nu$ yields that

$$\sum_{\substack{j=0 \\ k \in \mathcal{K}^Q}}^{k} \frac{\phi_j^3}{(w_k^Q)^3} \leq \frac{1}{\vartheta_Q^3(1-3\nu)} \left(\left(\varsigma + \sum_{\substack{j=0 \\ k \in \mathcal{K}^Q}}^{k} \widehat{\phi}_k^3 \right)^{1-3\nu} - \varsigma^{1-3\nu} \right) \leq \frac{b_k^{1-3\nu}}{\vartheta_Q^3(1-3\nu)}; \tag{3.17}$$

if $\nu < \frac{1}{3}$,

$$\sum_{\substack{j=0 \\ k \in \mathcal{K}^Q}}^{k} \frac{\widehat{\phi}_j^3}{(w_j^Q)^3} \leq \frac{1}{\vartheta_Q^3} \log \left(\frac{\varsigma + \sum_{j=0, k \in \mathcal{K}^Q}^{k} \widehat{\phi}_k^3}{\varsigma} \right) \leq \frac{1}{\vartheta_Q^3} \log \left(\frac{\varsigma + b_k}{\varsigma} \right) \tag{3.18}$$

if $\nu = \frac{1}{3}$, and

$$\sum_{\substack{j=0 \\ k \in \mathcal{K}^Q}}^{k} \frac{\widehat{\phi}_j^3}{(w_k^Q)^3} \leq \frac{1}{\vartheta_Q^3(3\nu-1)} \left(\varsigma^{1-3\nu} - \left(\varsigma + \sum_{\substack{j=0 \\ k \in \mathcal{K}^Q}}^{k} \widehat{\phi}_j^3 \right) \right) \leq \frac{\varsigma^{1-3\nu}}{\vartheta_Q^3(3\nu-1)} \tag{3.19}$$

if $\nu > \frac{1}{3}$. Moreover, unless $a_k < 1$, the argument of the logarithm in the right-hand side of (3.15) satisfies

$$1 \leq \frac{\varsigma + a_k}{\varsigma} \leq 1 + a_k \leq 2a_k. \tag{3.20}$$

Similarly, unless $b_k < 1$, the argument of the logarithm in the right-hand side of (3.18) satisfies

$$1 \leq \frac{\varsigma + b_k}{\varsigma} \leq 1 + b_k \leq 2b_k. \tag{3.21}$$

Moreover, we may assume, without loss of generality, that L_1 and L_2 are large enough to ensure that

$$2\xi L_1 \geq \tau \vartheta_L^2 \quad \text{and} \quad 2\xi L_2 \geq 3\tau \vartheta_Q^3.$$

Because of these observations and since (3.13) together with one of (3.14)–(3.16) and one of (3.17)-(3.19) has the form of condition (3.3), we may then apply Lemma 3.1 for each $k \geq 0$ with $a = a_k$, $b = b_k$ and the following associations:

• for $\mu \in (0, \frac{1}{2})$, $\nu \in (0, \frac{1}{3})$:

$$\theta_a = \frac{2\xi L_1}{\tau \vartheta_L^2}(1-2\mu), \quad \theta_b = \frac{2\xi L_2}{3\tau \vartheta_Q^3(1-3\nu)}, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau};$$

• for $\mu = \frac{1}{2}$, $\nu \in (0, \frac{1}{3})$:

$$\theta_a = \frac{2\xi L_1}{\tau \vartheta_L^2}, \quad \theta_b = \frac{2\xi L_2}{3\vartheta_Q^3 \tau(1-3\nu)}, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau};$$

• for $\mu \in (\frac{1}{2}, 1)$, $\nu \in (0, \frac{1}{3})$:

$$\theta_a = 1, \quad \theta_b = \frac{2\xi L_2}{3\tau \vartheta_Q^3(1-3\nu)}, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau} + \frac{2\xi L_1}{\tau \vartheta_L^2} \cdot \frac{\varsigma^{1-2\mu}}{2\mu-1};$$

- for $\mu \in (0, \frac{1}{2})$, $\nu = \frac{1}{3}$:

$$\theta_a = \frac{2\xi L_1}{\tau \vartheta_L^2 (1 - 2\mu)}, \quad \theta_b = \frac{2\xi L_2}{3\tau \vartheta_Q^3}, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau};$$

- for $\mu = \frac{1}{2}$, $\nu = \frac{1}{3}$:

$$\theta_a = \frac{2\xi L_1}{\tau \vartheta_L^2}, \quad \theta_b = \frac{2\xi L_2}{3\tau \vartheta_Q^3}, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau};$$

- for $\mu \in (\frac{1}{2}, 1)$, $\nu = \frac{1}{3}$:

$$\theta_a = \frac{2\xi L_1}{\tau \vartheta_L^2}, \quad \theta_b = \frac{2\xi L_2}{3\vartheta_Q^3 \tau}; \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau} + \frac{2\xi L_1}{\tau \vartheta_L^2} \cdot \frac{\varsigma^{1-2\mu}}{2\mu - 1};$$

- for $\mu \in (0, \frac{1}{2})$, $\nu \in (\frac{1}{3}, 1)$:

$$\theta_a = \frac{2\xi L_1}{\tau \vartheta_L^2 (1 - 2\mu)}, \quad \theta_b = 1, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau} + \frac{2\xi L_2}{3\tau \vartheta_Q^3} \cdot \frac{\varsigma^{1-3\nu}}{3\nu - 1};$$

- for $\mu = \frac{1}{2}$, $\nu \in (\frac{1}{3}, 1)$:

$$\theta_a = \frac{2\xi L_1}{\tau \vartheta_L^2}, \quad \theta_b = 1, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau} + \frac{2\xi L_2}{3\tau \vartheta_Q^3} \cdot \frac{\varsigma^{1-3\nu}}{3\nu - 1};$$

- for $\mu \in (\frac{1}{2}, 1)$, $\nu \in (\frac{1}{3}, 1)$:

$$\theta_a = 1, \quad \theta_b = 1, \quad \theta = \frac{4\xi(f(x_0) - f_{\text{low}})}{\tau} + \frac{2\xi L_1}{\tau \vartheta_L^2} \cdot \frac{\varsigma^{1-2\mu}}{2\mu - 1} + \frac{2\xi L_2}{3\tau \vartheta_Q^3} \cdot \frac{\varsigma^{1-3\nu}}{3\nu - 1}.$$

As a consequence of applying Lemma 3.1, we obtain that there exists positive constants[4] $\kappa_{\text{1rst}} \geq 1$ and $\kappa_{\text{2nd}} \geq 1$ only depending on problem-related quantities and on ς, ξ, μ and ν such that, for all $k \geq 0$,

$$a_k \leq \kappa_{\text{1rst}} \quad \text{and} \quad b_k \leq \kappa_{\text{2nd}}. \tag{3.22}$$

We also have, from the mechanism of Step 3 of the algorithm (see (2.7)) and (3.9), that

$$\sum_{j=0}^{k} \|g_j\|^2 = \sum_{\substack{j=0 \\ j \in \mathcal{K}^L}}^{k} \|g_j\|^2 + \sum_{\substack{j=0 \\ j \in \mathcal{K}^Q}}^{k} \|g_j\|^2 \leq \sum_{\substack{j=0 \\ j \in \mathcal{K}^L}}^{k} \|g_j\|^2 + \sum_{\substack{j=0 \\ j \in \mathcal{K}^Q}}^{k} \widehat{\phi}_j^3 \leq \tfrac{1}{2}(a_k + b_k) \leq \tfrac{1}{2}(\kappa_{\text{1rst}} + \kappa_{\text{2nd}})$$

and

$$\sum_{j=0}^{k} \widehat{\phi}_j^3 = \sum_{\substack{j=0 \\ j \in \mathcal{K}^L}}^{k} \widehat{\phi}_j^3 + \sum_{\substack{j=0 \\ j \in \mathcal{K}^Q}}^{k} \widehat{\phi}_j^3 \leq \sum_{\substack{j=0 \\ j \in \mathcal{K}^L}}^{k} \|g_j\|^2 + \sum_{\substack{j=0 \\ j \in \mathcal{K}^Q}}^{k} \widehat{\phi}_j^3 \leq \tfrac{1}{2}(a_k + b_k) \leq \tfrac{1}{2}(\kappa_{\text{1rst}} + \kappa_{\text{2nd}}).$$

These two inequalities in turn imply that, for all $k \geq 0$,

$$(k+1) \operatorname*{average}_{j \in \{0,\ldots,k\}} \|g_j\|^2 \leq \tfrac{1}{2}(\kappa_{\text{1rst}} + \kappa_{\text{2nd}}) \quad \text{and} \quad (k+1) \operatorname*{average}_{j \in \{0,\ldots,k\}} \widehat{\phi}_j^3 \leq \tfrac{1}{2}(\kappa_{\text{1rst}} + \kappa_{\text{2nd}}),$$

and the desired results follow with $\kappa_{\text{ASTR2}} = \tfrac{1}{2}(\kappa_{\text{1rst}} + \kappa_{\text{2nd}})$. □

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[4]We choose them to be at least one, in order to cover the cases where $a_k \leq 1$ or $b_k \leq 1$ mentioned before (3.20) and (3.21).

Comments:

1. Note that $\widehat{\phi}_k < \phi_k$ only when $\phi_k > \xi$. Thus, if ϕ_k is bounded[5], one can choose ξ large enough to ensure that $\phi_k = \widehat{\phi}_k$ for all k, and therefore that $\min_{j\{0,...,k\}} \phi_j \leq \kappa_{\text{ASTR2}}/(k+1)^{\frac{1}{3}}$. In practice, ξ can be used to tune the algorithm's sensitivity to second-order information.

2. If the k-orders of convergence specified by (3.8) are translated in ϵ-orders, that is numbers of iterations/evaluations to achieve $\|g(x_k\| \leq \epsilon_1$ and $\phi_k = \widehat{\phi}_k \leq \epsilon_2$, where ϵ_1 and ϵ_2 are precribed accuracies, we verify that at most $\mathcal{O}(\epsilon_1^{-2})$ of them are needed to achieve the first of these conditions, while at most $\mathcal{O}(\epsilon_2^{-3})$ are needed to achieve the second. As a consequence, at most $\mathcal{O}(\max[\epsilon_1^{-2}, \epsilon_2^{-3}])$ iterations/evaluations are needed to satisfy both conditions. These orders are identical to the sharp bounds known for the familiar trust-region methods (see [16, 2] or [5, Theorems 2.3.7 and 3.2.6][6]), or, for second-order optimality[7], for the Adaptive Regularization method (see [18], [5, Theorem 3.3.2]). This is quite remarkable because function values are essential in these two latter classes of algorithms to enforce descent, itself a crucial ingredient of existing convergence proofs.

3. While (3.8) is adequate to allow a meaningful comparison of the global convergence rates with standard algorithms, as we just discussed, we note that (3.7) is stronger, because the average is of course a majorant of the minimum. One is then led to the question of whether such bounds in average can be proved for trust-region or adaptive regularization methods. As long as they haven't, *the result presented here for second-order optimality can be viewed as one of the strongest available across all known methods using first and second derivatives.*

4. The expression of the constants is very intricate. However it is remarkable that they do not explicitly depend on the problem dimension. However, and although a good sign, this does not tell the whole story and caution remains advisable, because the Lipschitz constants L_1 and L_2 may themselves hide this (potentially severe) dependence.

5. It is also remarkable that the bounds (3.7) and (3.8) specify the same order of global convergence irrespective of the values of μ and ν in $(0, 1)$, although these values do affect the constants involved.

6. The condition (2.7) determining the choice of a linear (in $\mathcal{K}^L$) or quadratic (in $\mathcal{K}^Q$) step is only used at the very end of the theorem's proof, after (3.22) has already been obtained. This means that other choice mechanisms are possible without affecting this last conclusion, which is enough to derive bounds on $\|g_j\|^2$ and $\widehat{\phi}_j^3$ averaged on iterations in $\mathcal{K}^L$ and $\mathcal{K}^Q$, respectively (rather than on all iterations).

We now show that the bound (3.8) is essentially sharp (in the sense of [3], meaning that a lower bound on evaluation complexity exists which is arbitrarily close to its upper bound)

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[5] Which is the case if $\|g_k\| \leq \kappa_g$ (as we will require in Section 4) since then $\phi_k \leq \|g_k\| + \frac{1}{2}\|H_k\| \leq \kappa_g + \frac{1}{2}L_1$.

[6] This second of these theorems quotes an $\mathcal{O}(\max[\epsilon_1^{-2}\epsilon_2^{-1}, \epsilon_2^{-3}])$ order bound known for standard trust-region methods using first and second derivatives.

[7] Adaptive Regularization algorithms are faster for finding first-order points, as they find such points in $\mathcal{O}(\epsilon_1^{-3/2})$ evaluations of the objective function and its gradient [18], [5, Theorem 3.3.9].

by following ideas of [5, Theorem 2.2.3] in an argument parallel to that used in [14] for the first-order bound.

Theorem 3.4 The bound (3.8) is essentially sharp in that, for each $\mu, \nu \in (0, 1)$, $\vartheta_L = \vartheta_Q = 1$ and each $\varepsilon \in (0, \frac{2}{3})$, there exists a univariate function $f_{\mu,\nu,\varepsilon}$ satisfying AS.1–AS.3 such that, when applied to minimize $f_{\mu,\nu,\varepsilon}$ from the origin, the ASTR2 algorithm with new(3.1)-(3.2) produces second-order optimality measures given by

$$\phi_k = \widehat{\phi}_k = \min_{j \in \{0,...,k\}} \widehat{\phi}_j = \frac{1}{(k+1)^{\frac{1}{3}+\varepsilon}}. \tag{3.23}$$

Proof. We start by constructing $\{x_k\}$ for which $f_{\mu,\nu,\varepsilon}(x_k) = f_k$, $\nabla^1_x f_{\mu,\nu,\varepsilon}(x_k) = g_k$ and $\nabla^2_x f_{\mu,\nu,\varepsilon}(x_k) = H_k$ for associated sequences of function, gradient and Hessian values $\{f_k\}$, $\{g_k\}$ and $\{H_k\}$, and then apply Hermite interpolation to exhibit the function $f_{\mu,\nu,\varepsilon}$ itself. We select an arbitrary $\varsigma > 0$ and define, for $k \geq 0$,

$$g_k \overset{\text{def}}{=} 0, \quad \text{and} \quad H_k = -\frac{2}{(k+1)^{\frac{1}{3}+\varepsilon}}, \tag{3.24}$$

from which we deduce, using (2.2), that, for $k > 0$,

$$\phi_k = \widehat{\phi}_k = \frac{1}{(k+1)^{\frac{1}{3}+\varepsilon}}.$$

Since $\phi_k^3 > 0 = \|g_k\|^2$, we set

$$s_k = s_k^Q \overset{\text{def}}{=} \frac{1}{(k+1)^{\frac{1}{3}+\varepsilon}[\varsigma + \sum_{j=0}^k \widehat{\phi}_j^3]^\nu}, \tag{3.25}$$

which is the exact minimizer of the quadratic model within the trust region, yielding that, for $k \geq 0$,

$$\Delta q_k \overset{\text{def}}{=} \left| g_k s_k + \tfrac{1}{2} H_k s_k^2 \right| = \frac{1}{(k+1)^{1+3\varepsilon}\left[\varsigma + \sum_{j=0}^k \widehat{\phi}_j^3\right]^{2\nu}} \leq \frac{1}{(k+1)^{1+3\varepsilon}}, \tag{3.26}$$

where we used the fact that $\varsigma + \sum_{j=0}^k \widehat{\phi}_j^3 > \varsigma + \widehat{\phi}_0 > 1$ to deduce the last inequality. We then define, for all $k \geq 0$,

$$x_0 = 0, \quad x_{k+1} = x_k + s_k \quad (k \geq 0) \tag{3.27}$$

and

$$f_0 = \zeta(1 + 3\varepsilon), \quad f_{k+1} = f_k - \Delta q_k \quad (k \geq 0), \tag{3.28}$$

where $\zeta(\cdot)$ is the Riemann zeta function. Observe that the sequence $\{f_k\}$ is decreasing and that, for all $k \geq 0$,

$$f_{k+1} = f_0 - \sum_{k=0}^k \Delta q_k \geq f_0 - \sum_{k=0}^k \frac{1}{(k+1)^{1+3\varepsilon}} \geq f_0 - \zeta(1 + 3\varepsilon), \tag{3.29}$$

where we used (3.28) and (3.26). Hence (3.28) implies that

$$f_k \in [0, f_0] \quad \text{for all} \quad k \geq 0. \tag{3.30}$$

Also note that, using (3.28),

$$|f_{k+1} - f_k + \Delta q_k| = 0, \tag{3.31}$$

while, using (3.24),

$$|g_{k+1} - g_k| = 0 \quad (k \geq 0). \tag{3.32}$$

Moreover, using the fact that $1/x^{\frac{1}{3}+\nu}$ is a convex function of x over $[1, +\infty)$, and that from (3.25) $s_k \geq \dfrac{1}{(k+1)^{\frac{1}{3}+\nu}(\varsigma+k+1)^\nu}$, we derive that, for $k \geq 0$,

$$
\begin{aligned}
|H_{k+1} - H_k| &= 2 \left| \frac{1}{(k+2)^{\frac{1}{3}+\nu}} - \frac{1}{(k+1)^{\frac{1}{3}+\nu}} \right| \\
&\leq 2 \left(\frac{1}{3} + \nu \right) \frac{1}{(k+1)^{\frac{4}{3}+\nu}} \\
&\leq \frac{8}{3} \frac{(\varsigma+k+1)^\nu}{(k+1)(k+1)^{\frac{1}{3}+\nu}(\varsigma+k+1)^\nu} \\
&\leq \frac{8}{3} \frac{(\varsigma+k+1)^\nu}{k+1} s_k \\
&\leq \frac{8}{3} (\varsigma+2)^\nu s_k.
\end{aligned}
$$

These last bounds with (3.30), (3.31) and (3.32) allow us to use standard Hermite interpolation on the data given by $\{f_k\}$, $\{g_k\}$ and $\{H_k\}$: see, for instance, Theorem A.9.1 in [5] with $p = 2$ and

$$\kappa_f = \max \left[\frac{8}{3}(\varsigma+2)^\nu, f_0, 2 \right]$$

(the second term in the max bounding $|f_k|$ because of (3.30) and the third bounding $|g_k|$ and $|H_k|$ because of (3.24)). We then deduce that there exists a twice continuously differentiable function $f_{\mu,\nu,\varepsilon}$ from $\mathbb{R}$ to $\mathbb{R}$ with Lipschitz continuous gradient and Hessian (i.e. satisfying AS.1 and AS.2) such that, for $k \geq 0$,

$$f_{\mu,\nu,\varepsilon}(x_k) = f_k, \quad \nabla_x^1 f_{\mu,\nu,\varepsilon}(x_k) = g_k \quad \text{and} \quad \nabla_x^2 f_{\mu,\nu,\varepsilon}(x_k) = H_k.$$

Moreover, the range of $f_{\mu,\nu,\varepsilon}$ is constant independent of ε, hence guaranteeing AS.3. The definitions (3.24), (3.25), (3.27) and (3.28) imply that the sequences $\{x_k\}$, $\{f_k\}$, $\{g_k\}$ and $\{H_k\}$ can be seen as generated by the ASTR2 algorithm applied to $f_{\mu,\nu,\varepsilon}$, starting from $x_0 = 0$. $\qquad \square$

Figure 1 shows the behaviour of $f_{\mu,\nu,\varepsilon}(x)$ for $\mu = \frac{1}{2}$, $\nu = \frac{1}{3}$, $\vartheta_L = \vartheta_Q = 1$ and $\varepsilon = \varsigma = \frac{1}{100}$, its gradient and Hessian, as resulting from the first 10 iterations of the ASTR2 algorithm with (3.1)-(3.2). (We have chosen to shift f_0 to 100 in order to avoid large numbers on the vertical axis of the left panel.) Due to the slow convergence of the series $\sum_j 1/j^{\frac{1}{1+3/100}}$, illustrating the boundeness of $f_0 - f_{k+1}$ would require many more iterations. One also notes that the gradient is not monotonically increasing, which implies that $f_{\mu,\nu,\varepsilon}(x)$ is nonconvex, as can be verified
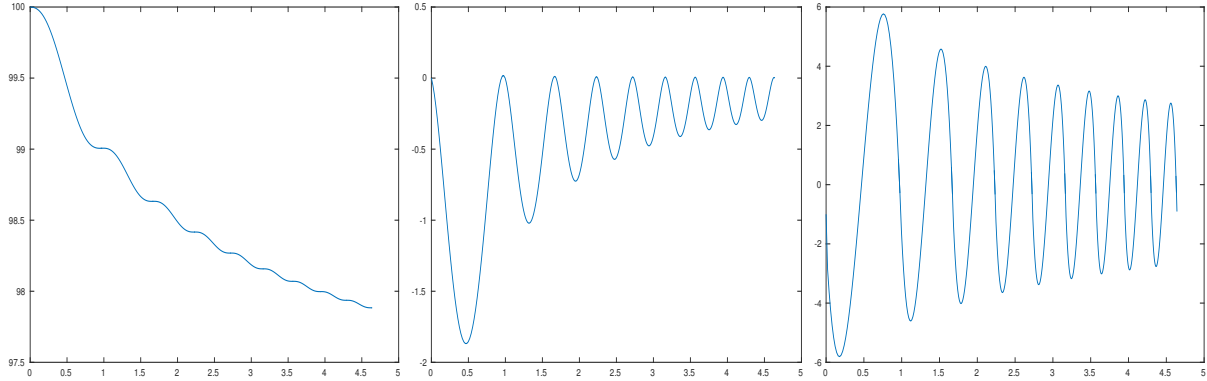
Figure 1: The function $f_{\mu,\nu,\varepsilon}(x)$ (left), its gradient $\nabla^1_x f_{\mu,\nu,\varepsilon}(x)$ (middle) and its Hessian $\nabla^2_x f_{\mu,\nu,\varepsilon}(x)$ (right) plotted as a function of x, for the first 10 iterations of the ASTR2 algorithm with (3.1)-(3.2) ($\mu = \frac{1}{2}$, $\nu = \frac{1}{3}$, $\varepsilon = \varsigma = \frac{1}{100}$, $\vartheta_L = \vartheta_Q = 1$)

in the left panel. Note that the unidimensional nature of the example is not restrictive, since it is always possible to make the value of its objective function and gradient independent of all dimensions but one. Also note that, as was the case in [14], the argument of Theorem 3.4 fails for $\varepsilon = 0$ since then the sums in (3.29) diverge when k tends to infinity.

Note that, because

$$\sum_{j=0}^{k} \frac{1}{(j+1)^{\frac{1}{3}+\varepsilon}} \geq \int_0^k \frac{dj}{(j+2)^{\frac{1}{3}+\varepsilon}}$$

$$= \frac{3}{2+3\varepsilon} \left[\frac{k+2}{(k+2)^{\frac{1}{3}+\varepsilon}} - 2 \right]$$

$$\geq \frac{3}{2(2+3\varepsilon)} \left[\frac{k+1}{(k+1)^{\frac{1}{3}+\varepsilon}} - 2 \right],$$

one deduces that

$$\operatorname*{average}_{j \in \{0,\dots,k\}} \widehat{\phi}_j \geq \frac{3}{2(2+3\varepsilon)} \left[\frac{1}{(k+1)^{\frac{1}{3}+\varepsilon}} - \frac{2}{k+1} \right],$$

which, when compared to (3.8), reflects the (slight) difference in strength between (3.7) and (3.8).

4 A "divergent stepsize" ASTR2 subclass

A "divergent stepsize" first-order method was analyzed in [14], motivated by its good practical behaviour in the stochastic context [15]. For coherence, we now present and analyze a similar variant, this time for second-order optimality. This requires the following additional assumption.

AS.4: there exists a constant $\kappa_g > 0$ such that, for all x, $\|g(x)\|_\infty \leq \kappa_g$.

Theorem 4.1 Suppose that AS.1–AS.3 and AS.4 hold and that the ASTR2 algorithm is applied to problem (2.1), where, the scaling factors $w_{i,k}$ are chosen such that, for some power parameters $0 < \nu_1 \leq \mu_1 < 1$ and $0 < \nu_2 \leq \mu_2 < \frac{1}{2}$, some constants $\varsigma \in (0,1]$ and $\kappa_w \geq \max[1,\varsigma]$, all $i \in \{1,\ldots,n\}$ and all $k \geq 0$,

$$0 < \varsigma\,(k+1)^{\nu_1} \leq w_k^L \leq \kappa_w\,(k+1)^{\mu_1} \quad \text{and} \quad 0 < \varsigma\,(k+1)^{\nu_2} \leq w_k^Q \leq \kappa_w\,(k+1)^{\mu_2}. \quad (4.1)$$

Let $\psi_k \stackrel{\text{def}}{=} \min[1, \max[\|g_k\|^2, \phi_k^3]]$. Then, for any $\theta \in (0, \frac{1}{4}\tau)$ and $k > j_\theta$,

$$\min_{j \in \{j_\theta,\ldots,k\}} \psi_k \leq \kappa_\diamond(\theta)\frac{(k+1)^{\max[\mu_1,2\mu_2]}}{k - j_\theta} \leq \frac{\kappa_\diamond(\theta)(j_\theta+1)}{(k+1)^{1-\max[\mu_1,2\mu_2]}}, \quad (4.2)$$

where

$$j_\theta \stackrel{\text{def}}{=} \max\left[\left(\frac{L_1}{2\varsigma(1-\theta)}\right)^{\frac{1}{\nu_1}}, \left(\frac{2(1+L_1)}{\varsigma}\right)^{\frac{1}{\nu_2}}, \left(\frac{L_2}{3\varsigma(\frac{1}{4}\tau - \theta)}\right)^{\frac{1}{\nu_2}}, \left(\frac{L_2\xi}{3\varsigma^2(\frac{1}{4}\tau - \theta)}\right)^{\frac{1}{2\nu_2}}\right] \quad (4.3)$$

and

$$\kappa_\diamond(\theta) \stackrel{\text{def}}{=} \left\{\frac{\kappa_w^2}{\theta}\left(f(x_0) - f_{\text{low}} + (j_\theta+1)\max\left[\frac{L_1\kappa_g^2}{2\varsigma^2}, \frac{L_2\xi^3}{3\varsigma^3}\right]\right)\right\}^{\frac{1}{3}}.$$

Proof. Consider an arbitrary $\theta \in (0, \frac{1}{4}\tau)$ and note that AS.4, (4.1) and the definition of $\widehat{\phi}_k$ imply that

$$w_k^L \in [\varsigma^\mu, \kappa_w(k+1)^{\mu_1}] \quad \text{and} \quad w_k^Q \in [\varsigma^\nu, \kappa_w(k+1)^{\mu_2}]. \quad (4.4)$$

If we define j_θ by (4.3), we immediately obtain from AS.4 and Lemma 2.5 (where we neglect the first term in the right-hand sides of (2.20) and (2.21)) that

$$f(x_{j_\theta+1}) \leq f(x_0) + (j_\theta+1)\kappa_{\text{over}} \quad \text{where} \quad \kappa_{\text{over}} = \max\left[\frac{L_1\kappa_g^2}{2\varsigma^2}, \frac{L_2\xi^3}{3\varsigma^3}\right]. \quad (4.5)$$

If we choose $j > j_\theta$, one then verifies that the definition of j_θ in (4.3), the bounds (2.20) and (2.21) and the definition (4.1) together ensure that

$$f(x_{j+1}) - f(x_j) \leq \begin{cases} -\theta\dfrac{\|g_k\|^2}{w_k^L} & \text{if } j \in \mathcal{K}^L, \\[2ex] -\theta\dfrac{\phi_k^3}{(w_k^Q)^2} & \text{if } j \in \mathcal{K}^Q. \end{cases}$$

Using now the mechanism of Step 3, the definition of ψ_k, (4.1) and the inequality $\kappa_w \geq 1$, we obtain that, for $j > j_\theta$

$$f(x_j) - f(x_{j+1}) \geq \theta\psi_j \min\left[\frac{1}{w_k^L}, \frac{1}{(w_k^Q)^2}\right] \geq \frac{\theta\psi_j}{\kappa_w^2(j+1)^{\max[\mu_1,2\mu_2]}}. \quad (4.6)$$

As a consequence, we obtain from (4.5) and the summation of (4.6) for $j \in \{j_\theta + 1, \ldots, k\}$ that, for $k > j_\theta$,

$$f(x_0) - f(x_{j+1}) \geq -(j_\theta + 1)\kappa_{\text{over}} + \sum_{j=j_\theta+1}^{k} \frac{\theta \psi_j}{\kappa_w^2 (j+1)^{\max[\mu_1, 2\mu_2]}}.$$

We therefore deduce, using AS.3, that

$$(k - j_\theta) \min_{j_{\theta,\max}+1,\ldots,k} \psi_j \leq \sum_{j=j_\theta+1}^{k} \psi_j \leq \frac{\kappa_w^2 (k+1)^{\max[\mu_1, 2\mu_2]}}{\theta} \Big[f(x_0) - f_{\text{low}} + (j_\theta + 1)\kappa_{\text{over}} \Big],$$

and (4.2) follows. □

This theorem gives a bound on the rate at which the combined optimality measure ψ_k tends to zero, and this bound is slightly worse than but close to what we obtained in the previous section whenever $\max[\mu_1, 2\mu_2]$ approaches zero.

Using the methodology of Theorem 3.4, we now show that the bound (4.2) is also essentially sharp.

Theorem 4.2 The bound (4.2) is essentially sharp in that, for each $\mu = (\mu_1, \mu_2)$, each $\nu = (\nu_1, \nu_2)$ with $0 < \nu_1 \leq \mu_1 < 1$ and $0 < \nu_2 \leq \mu_2 < \frac{1}{2}$ and each $\varepsilon \in (0, 1 - \frac{1}{3}(1 - 2\mu_2))$, there exists a univariate function $h_{\mu,\nu,\varepsilon}$ satisfying AS.1–AS.4 such that, when applied to minimize $h_{\mu,\nu,\varepsilon}$ from the origin, the ASTR2 algorithm with (4.1) produces second-order optimality measures given by

$$\phi_k = \widehat{\phi}_k = \psi_k = \min_{j \in \{0,\ldots,k\}} \psi_j = \frac{1}{(k+1)^{\frac{1}{3}(1-2\mu_2)+\varepsilon}}. \tag{4.7}$$

Proof. As above, we start by defining, for $k \geq 0$, $\gamma = \frac{1}{3}(1 - 2\mu_2) + \varepsilon$, $w_k = \kappa_w(k+1)^{\mu_2}$, and, for $k \geq 0$,

$$g_k \overset{\text{def}}{=} 0, \quad \text{and} \quad H_k = -\frac{2}{(k+1)^\gamma}, \tag{4.8}$$

which then implies, using (2.2) that, for $k > 0$,

$$\phi_k = \widehat{\phi}_k = \frac{1}{(k+1)^\gamma}. \tag{4.9}$$

Given these definitions and because $\widehat{\phi}_k^3 > 0 = \|g_k\|^2$, we set

$$s_k = s_k^Q \overset{\text{def}}{=} \frac{1}{(k+1)^\gamma [\kappa_w(k+1)^{\mu_2}]} = \frac{1}{\kappa_w(k+1)^{\gamma+\mu_2}}, \tag{4.10}$$

yielding that, for $k > 0$,

$$\Delta q_0 \overset{\text{def}}{=} \frac{1}{(\varsigma+1)^{2\nu}} \quad \text{and} \quad \Delta q_k \overset{\text{def}}{=} \left| g_k s_k + \tfrac{1}{2} H_k s_k^2 \right| = \frac{1}{\kappa_w^2 (k+1)^{3\gamma+2\mu_2}} \leq \frac{1}{(k+1)^{3\gamma+2\mu_2}}, \tag{4.11}$$

where we used the fact that $\kappa_w \geq 1$ to deduce the last inequality. We then define, for all $k \geq 0$,

$$x_0 = 0, \quad x_{k+1} = x_k + s_k \quad (k > 0) \tag{4.12}$$

and

$$h_0 = \zeta(3\gamma + 2\mu_2) \quad \text{and} \quad h_{k+1} = h_k - \Delta q_k \quad (k \geq 0), \tag{4.13}$$

where $\zeta(\cdot)$ is the Riemann zeta function. Note that, since $\gamma > 1 - 2\mu_2$, the argument $3\gamma + 2\mu_2$ of ζ is strictly larger than one and $\zeta(3\gamma + 2\mu_2)$ is finite. Observe also that the sequence $\{h_k\}$ is decreasing and that, for all $k \geq 0$,

$$h_{k+1} = h_0 - \sum_{k=0}^{k} \Delta q_k \geq h_0 - \sum_{k=0}^{k} \frac{1}{(k+1)^{3\gamma+2\mu_2}} \geq h_0 - \zeta(3\gamma + 2\mu_2), \tag{4.14}$$

where we used (3.28) and (3.26). Hence (3.28) implies that

$$h_k \in [0, h_0] \quad \text{for all} \ \ k \geq 0. \tag{4.15}$$

Also note that, using (3.28),

$$|h_{k+1} - h_k + \Delta q_k| = 0, \tag{4.16}$$

while, using (3.24),

$$|g_{k+1} - g_k| = 0 \quad (k \geq 0). \tag{4.17}$$

Moreover, using the fact that $1/x^\gamma$ is a convex function of x over $[1, +\infty)$ and (4.10), we derive that, for $k \geq 0$,

$$|H_{k+1} - H_k| = 2 \left| \frac{1}{(k+2)^\gamma} - \frac{1}{(k+1)^\gamma} \right| \leq \frac{2\gamma}{(k+1)^{1+\gamma}} \leq \frac{2\gamma\kappa_w(k+1)^{\mu_2}}{k+1} s_k \leq 2\gamma\kappa_w s_k.$$

This bound with (4.15), (4.16) and (4.17) once more allow us to use standard Hermite interpolation on the data given by $\{h_k\}$, $\{g_k\}$ and $\{H_k\}$, as stated in [5, Theorem A.9.1] with $p = 2$ and

$$\kappa_f = \max\left[2\gamma\kappa_w, h_0, 2\right]$$

(the second term in the max bounds $|h_k|$ because of (4.15) and the third bounds both $|g_k|$ and $|H_k|$ because of (4.8)). As a consequence, there exists a twice continuously differentiable function $h_{\mu,\nu,\varepsilon}$ from $\mathbb{R}$ to $\mathbb{R}$ with Lipschitz continuous gradient and Hessian (i.e. satisfying AS.1 and AS.2) such that, for $k \geq 0$,

$$h_{\mu,\nu,\varepsilon}(x_k) = h_k, \quad \nabla_x^1 h_{\mu,\nu,\varepsilon}(x_k) = g_k \quad \text{and} \quad \nabla_x^2 h_{\mu,\nu,\varepsilon}(x_k) = H_k.$$

Moreover, the ranges of $h_{\mu,\nu,\varepsilon}$ and its derivatives is constant independent of γ, hence guaranteeing AS.3 and AS.4. Thus (4.8), (4.10), (4.12) and (4.13) imply that the sequences $\{x_k\}$, $\{h_k\}$, $\{g_k\}$ and $\{H_k\}$ can be seen as generated by the ASTR2 algorithm applied to $h_{\mu,\nu,\varepsilon}$, starting from $x_0 = 0$. The first bound of (4.7) then results from (4.9) and the definition of γ. □
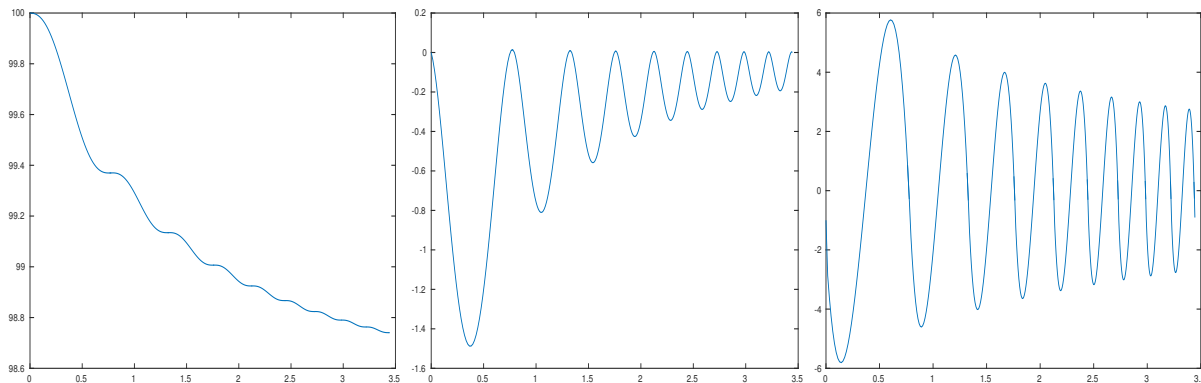
Figure 2: The function $h_{\mu,\nu,\varepsilon}(x)$ (left), its gradient $\nabla_x^1 h_{\mu,\nu,\varepsilon}(x)$ (middle) and its Hessian $\nabla_x^2 h_{\mu,\nu,\varepsilon}(x)$ (right) plotted as a function of x, for the first 10 iterations of the ASTR2 algorithm with (4.2) ($\mu = \nu = (\frac{1}{2}, \frac{1}{3})$)

The behaviour of $h_{\mu,\nu,\varepsilon}$ is illustrated in Figure 2. It is qualitatively similar to that of $f_{\mu,\nu,\varepsilon}$ shown in Figure 1, although the decrease in objective-value is somewhat slower, as expected. As in Section 3, note that the inequality

$$\sum_{j=0}^{k} \frac{1}{(j+1)^\gamma} \geq \int_0^k \frac{dj}{(j+2)^\gamma} = \frac{1}{1-\gamma} \left[\frac{k+2}{(k+2)^\gamma} - 1 \right] \geq \frac{1}{2(1-\gamma)} \left[\frac{k+1}{(k+1)^\gamma} - 2 \right]$$

implies that

$$\operatorname*{average}_{j \in \{0,\ldots,k\}} \psi_j \geq \frac{1}{2(1-\gamma)} \left[\frac{1}{(k+1)^{\frac{1}{3}(1-2\mu_2)+\varepsilon}} - \frac{2}{k+1} \right],$$

which has the same flavour as the second bound of (3.23).

5 Second-order optimality in a subspace

While the ASTR2 algorithms guarantee second-order optimality conditions, they come at a computational price. The key of this guarantee is of course that significant negative curvature in any direction of $\mathbb{R}^n$ must be exploited, which requires evaluating the Hessian. In addition, the optimality measure ϕ_k and the step s_k must also be computed. However, these computational costs may be judged excessive, so the question arises whether a potentially cheaper algorithm is able to ensure a "degraded" or weaker form of second-order optimality. Fortunately, the answer is positive: one can guarantee second-order optimality in subspaces of $\mathbb{R}^n$ at lower cost.

The first step is to assume that a subspace $\mathcal{S}_k$ is of interest at iteration k. Then, instead of computing ϕ_k from (2.3), one can choose to calculate

$$\phi_k^{\mathcal{S}_k} = \max_{\substack{\|d\| \leq 1 \\ d \in \overline{\mathcal{S}}_k}} -\left(g(x)^T d + \tfrac{1}{2} d^T H(x) d \right).$$

Because the dimension of $\mathcal{S}_k$ may be much smaller than n, the cost of this computation may be significantly smaller than that of computing ϕ_k. The measure $\phi_k^{\mathcal{S}_k}$ may for instance be

obtained using a Krylov-based method, as conjugate gradients [17], GLRT [13] or variants thereof, where the minimum of the model $T_{f,2}(x,d)$ within the trust region is derived iteratively in a sequence of nested Krylov subspaces of increasing dimension, which tend to contain vector along which curvature is extreme [12, Chapter 9], thereby improving the quality of the second-order guarantee compared to random subspaces. This process may then be terminated before the subspaces fill $\mathbb{R}^n$, should the calculation become too expensive or a desired accuracy be reached. In addition, there is no need for n_k, the dimension of the final Krylov space at iteration k to be constant: it is often kept very small when far from optimality. This technique has the added benefit that the full Hessian is not evaluated, but only n_k Hessian-times-vector products are needed, again significantly reducing the computational burden. Calculating the step s_k^Q for $k \in \mathcal{K}^Q$ once $\phi_k^{\mathcal{S}_k}$ is known is also cheaper in a space of dimension n_k much less than n, especially since only a τ-approximation is needed (see the comments after the algorithm).

Importantly, the theory developed in the previous sections is not affected by the transition from $\mathbb{R}^n$ to $\mathcal{S}_k$, except that now the complexity bounds (3.7)-(3.8) and (4.2) are no longer expressed using $\widehat{\phi}_k$ but now involve $\widehat{\phi}_k^{\mathcal{S}_k} = \min[1, \phi_k^{\mathcal{S}_k}]$ instead. While clearly not as powerful as the complete second-order guarantee in $\mathbb{R}^n$, weaker guarantees based on (Krylov) subspaces are often sufficient in practice and make the ASTR2 algorithm more affordable. Note that, in the limit, one can even choose $\mathcal{S}_k = \{0\}$ for all k, in which case we can set $H_k = 0$ for all k and we do not obtain any second-order guarantee (but the first-order complexity bounds remain valid, recovering results of [14]).

6   Conclusions

We have introduced an OFFO algorithm whose global rate of convergence to first-order minimizers is $\mathcal{O}((k+1)^{-\frac{1}{2}})$ while it converges to second-order ones as $\mathcal{O}((k+1)^{-\frac{1}{3}})$. These bounds are equivalent to the best known bounds for second-order optimality for algorithms using objective-function evaluations, despite the latter exploiting significantly more information. Thus we conclude that, from the point of view of evaluation complexity at least, evaluating values of the objective function is an unnecessary effort for efficiently finding second-order minimizers. We have also discussed another closely related algorithm, whose global rates of convergence can be nearly as good. We have finally considered how weaker second-order guarantees may be obtained at a much reduced computational cost.

We expect that extending our proposal to convexly constrained cases (for instance to problems involving bounds on the variables) should be possible. As in [7, Chapter 12], the idea would be to restrict the model minimization at each iteration to the intersection of the trust region with the feasible domain, but this should of course be verified.

It is of course too early to assess whether the new algorithms will turn out to be of practical interest. The appraisal of their numerical behaviour is the object of ongoing research.

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Appendix: technical lemmas

Lemma A.1 Let $w > 0$ and suppose that

$$w^\alpha \leq \beta \log(2w). \tag{A.1}$$

for some $\alpha \in (0, 1)$ and β such that

$$\beta > \frac{3\alpha}{2^\alpha}. \tag{A.2}$$

Then

$$w \leq \sigma(\alpha, \beta) \overset{\text{def}}{=} \left[-\frac{\beta}{\alpha} W_{-1}\left(-\frac{\alpha}{\beta\,2^\alpha} \right) \right]^{\frac{1}{\alpha}} \tag{A.3}$$

where $W_{-1}(\cdot)$ is the second branch of the Lambert function [8].

Proof. First note that (A.1) is equivalent to

$$\frac{1}{2^\alpha}(2w)^\alpha \leq \frac{\beta}{\alpha} \log\left((2w)^\alpha \right)$$

Setting now $u = (2w)^\alpha$, one obtains that

$$\omega(u) \overset{\text{def}}{=} \frac{1}{2^\alpha} u - \frac{\beta}{\alpha} \log(u) \leq 0. \tag{A.4}$$

But $\omega(u)$ is convex for $u > 0$ and tends to infinity if u tends to zero or to infinity. Moreover, it achieves its minimum at $u_{\min} = \beta 2^\alpha/\alpha$, at which it takes the value

$$\omega(u_{\min}) = \frac{\beta}{\alpha}\left(1 - \log\left(\frac{\beta\,2^\alpha}{\alpha} \right) \right) < 0,$$

where the inequality results from (A.2). Hence $\omega(u)$ has two real roots $u_1 \leq u_2$ and the set of u for which (A.4) holds is bounded above by u_2. By definition,

$$\log(u_2) - \frac{\alpha}{\beta\,2^\alpha}\, u_2 = 0,$$

which is

$$u_2 e^{-\frac{\alpha}{\beta\,2^\alpha} u_2} = 1.$$

Defining now $z = -\frac{\alpha}{\beta\,2^\alpha}\, u_2$, we obtain that

$$ze^z = -\frac{\alpha}{\beta\,2^\alpha}.$$

By definition of the Lambert function, this gives that

$$u_2 = -\frac{\beta\,2^\alpha}{\alpha} z = -\frac{\beta 2^\alpha}{\alpha} W_{-1}\left(-\frac{\alpha}{\beta\,2^\alpha} \right) > 0$$

which is well-defined because (A.2) implies that $-\frac{\alpha}{\beta \, 2^{\alpha}} \in [-\frac{1}{e}, 0)$. Since $w = u^{\frac{1}{\alpha}}/2$, this implies (A.3). □

Lemma A.2 Let $a \geq 0$ and $b \geq 0$. Suppose that, for some $\mu \in (0, \frac{1}{2})$, $\nu \in (0, \frac{1}{3})$ and some $\theta_{a,0}, \theta_{b,0}$ and $\theta_0 \geq 0$,

$$\theta_{a,0} a^{1-\mu} + \theta_{b,0} b^{1-2\nu} \leq \theta_0. \tag{A.5}$$

Then

$$a \leq \left(\frac{\theta_0}{\theta_{a,0}} \right)^{\frac{1}{1-\mu}} \quad \text{and} \quad b \leq \left(\frac{\theta_0}{\theta_{b,0}} \right)^{\frac{1}{1-2\nu}}.$$

Proof. Obvious from the inequalities $\theta_{a,0} a^{1-\mu} \leq \theta_{a,0} a^{1-\mu} + \theta_{b,0} b^{1-2\nu}$ and $\theta_{b,0} b^{1-2\nu} \leq \theta_{a,0} a^{1-\mu} + \theta_{b,0} b^{1-2\nu}$. □

Lemma A.3 Let $a \geq 0$ and $b \geq 0$. Suppose that, for some $\mu \in (0, \frac{1}{2})$, some $\theta_{a,1} > 0$ and some $\theta_1 \geq 0$,

$$a^{1-\mu} \leq \theta_{a,1} a^{1-2\mu} + \theta_1. \tag{A.6}$$

Then

$$a \leq \max \left[(2\theta_1)^{\frac{1}{1-\mu}}, (2\theta_{a,1})^{\frac{1}{\mu}} \right].$$

Symmetrically, if $\nu \in (0, \frac{1}{3})$, $\theta_{b,1} > 0$ and

$$b^{1-2\nu} \leq \theta_{b,1} b^{1-3\nu} + \theta_1. \tag{A.7}$$

Then

$$b \leq \max \left[(\theta_1)^{\frac{1}{1-2\nu}}, (2\theta_{b,1})^{\frac{1}{\nu}} \right].$$

Proof. Suppose first that $\theta_{a,1} a^{1-2\mu} \leq \theta_1$. Then $a^{1-\mu} \leq 2\theta_1$ and thus $a \leq (2\theta_1)^{\frac{1}{1-\mu}}$ Suppose now that $\theta_{a,1} a^{1-2\mu} > \theta_1$. Then $a^{1-\mu} \leq 2\theta_{a,1} a^{1-2\mu}$, that is $a \leq (2\theta_a)^{\frac{1}{\mu}}$. The proof of the second part is similar. □

Lemma A.4 Let $a \geq 0$ and $b \geq 0$. Suppose that, for some $\mu \in (0, \frac{1}{2})$, $\nu \in (0, \frac{1}{3})$ and some $\theta_a, \theta_b > 0$ and $\theta_2 \geq 0$,

$$a^{1-\mu} + b^{1-2\nu} \leq \theta_{a,2} a^{1-2\mu} + \theta_{b,2} b^{1-3\nu} + \theta_2. \tag{A.8}$$

Then

$$a \leq \max \left[\left(\frac{\theta_2}{\theta_{a,2}} \right)^{\frac{1}{1-2\mu}}, 2^{\frac{1}{1-\mu}} (2\theta_{b,2})^{\frac{1-2\nu}{\nu(1-\mu)}}, (4\theta_{a,2})^{\frac{1}{\mu}} \right]$$

and

$$b \leq \max \left[\left(\frac{\theta_2}{\theta_{b,2}} \right)^{\frac{1}{1-3\nu}}, 2^{\frac{1}{1-2\nu}} (2\theta_{a,2})^{\frac{1-\mu}{\mu(1-2\nu)}}, (4\theta_{b,2})^{\frac{1}{\nu}} \right].$$

Proof. Suppose first that

$$\theta_{a,2} a^{1-2\mu} + \theta_{b,2} b^{1-3\nu} \leq \theta_2. \tag{A.9}$$

Then, from Lemma A.2,

$$a \leq \left(\frac{\theta_2}{\theta_{a,2}} \right)^{\frac{1}{1-2\mu}} \quad \text{and} \quad b \leq \left(\frac{\theta_2}{\theta_{b,2}} \right)^{\frac{1}{1-3\nu}}. \tag{A.10}$$

Suppose now that (A.9) fails, and thus that

$$\theta_{a,2} a^{1-2\mu} + \theta_{b,2} b^{1-3\nu} + \theta_2 \leq 2\theta_{a,2} a^{1-2\mu} + 2\theta_{b,2} b^{1-3\nu}. \tag{A.11}$$

Assume also that

$$a > (2\theta_{a,2})^{\frac{1}{\mu}} \quad \text{and} \quad b > (2\theta_{b,2})^{\frac{1}{\nu}} \tag{A.12}$$

Then,

$$2\theta_{a,2} a^{1-2\mu} + 2\theta_{b,2} b^{1-3\nu} < a^{1-\mu} + b^{1-2\nu}$$

and so, using (A.8) and (A.11),

$$a^{1-\mu} + b^{1-2\nu} \leq \theta_{a,2} a^{1-2\mu} + \theta_{b,2} b^{1-3\nu} + \theta_2 < a^{1-\mu} + b^{1-2\nu},$$

which is impossible. Hence (A.12) cannot hold, and at least one of its inequalities must fail. Suppose that it is the first, that is

$$a \leq (2\theta_{a,2})^{\frac{1}{\mu}} \overset{\text{def}}{=} \kappa_1. \tag{A.13}$$

Then (A.8) and (A.11) give that

$$b^{1-2\nu} \leq a^{1-\mu} + b^{1-2\nu} \leq 2\theta_{a,2} \kappa_1^{1-2\mu} + 2\theta_{b,2} b^{1-3\nu}$$

and we may apply Lemma A.3 with $\theta_{b,1} = 2\theta_{b,2}$ and $\theta_1 = 2\theta_{a,2} \kappa_1^{1-2\mu}$ to deduce that

$$b \leq \max \left[\left(4\theta_{a,2} \kappa_1^{1-2\mu} \right)^{\frac{1}{1-2\nu}}, (4\theta_{b,2})^{\frac{1}{\nu}} \right].$$

Symmetrically, we deduce that if the second inequality of (A.12) fails, that is if

$$b \leq (2\theta_{b,2})^{\frac{1}{\nu}} \stackrel{\text{def}}{=} \kappa_2,$$

then, applying Lemma A.3 with $\theta_{a,1} = 2\theta_{a,2}$ and $\theta_1 = 2\theta_{b,2}\kappa_2^{1-3\nu}$,

$$a \leq \max\left[\left(4\theta_{b,2}\kappa_2^{1-3\nu}\right)^{\frac{1}{1-\mu}}, (4\theta_{a,2})^{\frac{1}{\mu}}\right].$$

Combining the two cases yields the desired result. □

Lemma A.5 Let $a \geq 0$ and $b \geq 0$. Suppose that, for some $\mu \in (0, \frac{1}{2})$, $\nu \in (\frac{1}{3}, 1)$ and some $\theta_{a,3} > 0$, $\theta_3 \geq 0$,

$$a^{1-\mu} + b^{1-2\nu} \leq \theta_{a,3} a^{1-2\mu} + \theta_3. \tag{A.14}$$

Then

$$a \leq \max\left[(2\theta_3)^{\frac{1}{1-\mu}}, (2\theta_{a,3})^{\frac{1}{\mu}}\right] = \kappa_{a,3} \quad \text{and} \quad b \leq \left(\theta_{a,3}\kappa_{a,3}^{1-2\mu} + \theta_3\right)^{\frac{1}{1-2\nu}}.$$

Symmetrically, if $\theta_{b,3} > 0$ and

$$a^{1-\mu} + b^{1-2\nu} \leq \theta_{b,3} b^{1-3\nu} + \theta_3,$$

then

$$b \leq \max\left[(2\theta_3)^{\frac{1}{1-2\nu}}, (2\theta_{b,3})^{\frac{1}{\nu}}\right] = \kappa_{b,3} \quad \text{and} \quad a \leq \left(\theta_{b,3}\kappa_{b,3}^{1-3\nu} + \theta_3\right)^{\frac{1}{1-\mu}}.$$

Proof. From (A.14), we have that

$$a^{1-\mu} \leq a^{1-\mu} + b^{1-2\nu} \leq \theta_{a,3} a^{1-2\mu} + \theta_2$$

and we may apply Lemma A.3 with $\theta_{a,1} = \theta_{a,3}$ and $\theta_1 = \theta_3$ to deduce that

$$a \leq \max\left[(2\theta_3)^{\frac{1}{1-\mu}}, (2\theta_{a,3})^{\frac{1}{\mu}}\right] \stackrel{\text{def}}{=} \kappa_a$$

From the inequality $b^{1-2\nu} \leq a^{1-\mu} + b^{1-2\nu}$ and (A.14), we also obtain that

$$b \leq \left(\theta_{a,3}\kappa_a^{1-2\mu} + \theta_3\right)^{\frac{1}{1-2\nu}}.$$

□

Lemma A.6 Let $a > 0$ and $b > 0$. Suppose that, for some $\nu \in (0, \frac{1}{3}]$, some $\theta_{a,4} \geq 1$ and some $\theta_4 \geq 0$,

$$a^{\frac{1}{2}} + b^{1-2\nu} \leq \theta_{a,4} \log(2a) + \theta_4. \tag{A.15}$$

Then

$$a \leq \max \left[\frac{1}{2} e^{\frac{\theta_4}{\theta_{a,4}}}, \sigma\left(\tfrac{1}{2}, 2\theta_{a,4}\right) \right] = \kappa_{a,4} \quad \text{and} \quad b \leq \left(\theta_{a,4} \log(2\kappa_{a,4}) + \theta_4 \right)^{\frac{1}{1-2\nu}}.$$

Symmetrically, if $\theta_{b,4} \geq 1$, $\mu \in (0, \frac{1}{2}]$ and

$$a^{1-\mu} + b^{\frac{1}{3}} \leq \theta_{b,4} \log(2b) + \theta_4,$$

then

$$b \leq \max \left[\frac{1}{2} e^{\frac{\theta_4}{\theta_{b,4}}}, \sigma\left(\tfrac{1}{2}, 2\theta_{b,4}\right) \right] = \kappa_{b,4} \quad \text{and} \quad a \leq \left(\theta_{b,4} \log(2\kappa_{b,4}) + \theta_4 \right)^{\frac{1}{1-\mu}}.$$

Proof. Suppose first that $\theta_{a,4} \log(2a) \leq \theta_4$. Then

$$a \leq \frac{1}{2} e^{\frac{\theta_4}{\theta_{a,4}}}. \tag{A.16}$$

Otherwise, (A.15) gives that

$$a^{\frac{1}{2}} \leq a^{\frac{1}{2}} + b^{1-2\nu} \leq 2\theta_{a,4} \log(2a)$$

from which one deduces using Lemma A.1 with $\alpha = \frac{1}{2}$ and $\beta = 2\theta_{a,4}$ (which is allowed since $2\theta_{a,4} \geq 2 > 3/2^{\frac{5}{2}}$ implies (A.2)) that

$$a \leq \sigma\left(\tfrac{1}{2}, 2\theta_{a,4}\right),$$

where $\sigma(\cdot, \cdot)$ is defined in (A.3). This inequality and (A.16) give the desired bound on a. Substituting this in (A.15) gives the bound on b. The proof of the symmetric statement is similar, in which the use of Lemma A.1 is now allowed because $\theta_{b,4} \geq 1 > 1/2^{\frac{4}{3}}$ again implies (A.2). $\square$

Lemma A.7 Let $a > 0$ and $b \geq 0$. Suppose that, for some $\nu \in (0, \frac{1}{3})$, some $\theta_{a,5} \geq 1$, $\theta_{b,5} > 0$ and some $\theta_5 \geq 0$,

$$a^{\frac{1}{2}} + b^{1-2\nu} \leq \theta_{a,5} \log(2a) + \theta_{b,5} b^{1-3\nu} + \theta_5, \tag{A.17}$$

Then

$$a \leq \max\left[\frac{1}{2} e^{\frac{\theta_5}{\theta_{a,5}}}, \sigma(\tfrac{1}{2}, 4\theta_{a,5}) \frac{1}{2} e^{\frac{\theta_{b,5}(2\theta_{b,5})^{\frac{1-3\nu}{\nu}}}{\theta_{a,5}}} \right]$$

and

$$b \leq \max\left[\left(\frac{\theta_5}{\theta_{b,5}} \right)^{\frac{1}{1-3\nu}}, (2\theta_{a,5} \log(2\sigma_a))^{\frac{1}{1-2\nu}}, \left(4\theta_{b,5} \right)^{\frac{1}{\nu}}, (2\theta_{b,5})^{\frac{1}{\nu}} \right].$$

with $\sigma_a = \sigma\left(\frac{1}{2}, 2\theta_{a,5}\right)$. Symmetrically, if $\theta_{a,5} \geq 1$, $\mu \in (0, \frac{1}{2})$, $b > 0$ and

$$a^{1-\mu} + b^{\frac{1}{3}} \leq \theta_{a,5} a^{1-2\mu} + \theta_{b,5} \log(2b) + \theta_5,$$

then

$$a \leq \max\left[\left(\frac{\theta_5}{\theta_{a,5}} \right)^{\frac{1}{1-2\mu}}, (2\theta_{b,5} \log(2\sigma_b))^{\frac{1}{1-\mu}}, \left(4\theta_{a,5} \right)^{\frac{1}{\mu}}, (2\theta_{a,5})^{\frac{1}{\mu}} \right]$$

and

$$b \leq \max\left[\frac{1}{2} e^{\frac{\theta_5}{\theta_{b,5}}}, \sigma(\tfrac{1}{2}, 4\theta_{b,5}) \frac{1}{2} e^{\frac{\theta_{a,5}(2\theta_{a,5})^{\frac{1-2\mu}{\mu}}}{\theta_{b,5}}} \right]$$

with $\sigma_b = \sigma\left(\frac{1}{2}, 2\theta_{b,5}\right)$.

Proof. Suppose first that,

$$\theta_{a,5} \log(2a) + \theta_{b,5} b^{1-3\nu} \leq \theta_5. \tag{A.18}$$

Then

$$a \leq \frac{1}{2} e^{\frac{\theta_5}{\theta_{a,5}}} \quad \text{and} \quad b \leq \left(\frac{\theta_5}{\theta_{b,5}} \right)^{\frac{1}{1-3\nu}}. \tag{A.19}$$

Suppose now that (A.18) fails. Then, from (A.17),

$$a^{\frac{1}{2}} + b^{1-2\nu} \leq 2\theta_{a,5} \log(2a) + 2\theta_{b,5} b^{1-3\nu}. \tag{A.20}$$

If

$$a > \sigma\left(\tfrac{1}{2}, 2\theta_{a,5}\right) \quad \text{and} \quad b > (2\theta_{b,5})^{\frac{1}{\nu}}, \tag{A.21}$$

we obtain, using Lemma A.1 (which we may apply because $\theta_{a,5} \geq 1 > 3/2^{\frac{5}{2}}$), (A.20) and (A.17) that

$$a^{\frac{1}{2}} + b^{1-2\nu} \leq 2\theta_{a,5} \log(2a) + 2\theta_{b,5} b^{1-3\nu} < a^{\frac{1}{2}} + b^{1-2\nu},$$

which is impossible. Hence one of the inequalities of (A.21) must be violated. Suppose that

$$a \le \sigma\left(\tfrac{1}{2}, 2\theta_{a,5}\right) \stackrel{\text{def}}{=} \sigma_a.$$

Using Lemma A.1 again and (A.20), this implies that

$$b^{1-2\nu} \le a^{\frac{1}{2}} + b^{1-2\nu} \le 2\theta_{a,5}\log(2\sigma_a) + 2\theta_{b,5}b^{1-3\nu}$$

and we deduce from Lemma A.3 with $\theta_{b,1} = 2\theta_{b,5}$ and $\theta_1 = 2\theta_{a,5}\log(2\sigma_a)$ that

$$b \le \max\left[(2\theta_{a,5}\log(2\sigma_a))^{\frac{1}{1-2\nu}}, \left(4\theta_{b,5}\right)^{\frac{1}{\nu}}\right].$$

If we now suppose that $b \le (2\theta_{b,5})^{\frac{1}{\nu}}$, then (A.20) ensures that

$$a^{\frac{1}{2}} \le a^{\frac{1}{2}} + b^{1-2\nu} \le 2\theta_{a,5}\log(2a) + 2\theta_{b,5}(2\theta_{b,5})^{\frac{1-3\nu}{\nu}},$$

and we now obtain from Lemma A.6 with $\theta_{a,4} = 2\theta_{a,5}$ and $\theta_4 = 2\theta_{b,5}(2\theta_{b,5})^{\frac{1-3\nu}{\nu}}$ that

$$a \le \max\left[\frac{1}{2}e^{\frac{\theta_{b,5}(2\theta_{b,5})^{\frac{1-3\nu}{\nu}}}{\theta_{a,5}}}, \sigma\left(\tfrac{1}{2}, 4\theta_{a,5}\right)\right].$$

$\square$

Lemma A.8 Let $a > 0$ and $b > 0$. Suppose that, for some $\theta_{a,6} \ge 1$, $\theta_{b,6} \ge 1$ and some $\theta_6 \ge 0$,

$$a^{\frac{1}{2}} + b^{\frac{1}{3}} \le \theta_{a,6}\log(2a) + \theta_{b,6}\log(2b) + \theta_6, \tag{A.22}$$

where $2a \ge \varsigma$ and $2b \ge \varsigma$. Then

$$a \le \max\left[\frac{1}{2}e^{\frac{\theta_6 + |\log(\varsigma)|}{\theta_{a,6}}}, \sigma\left(\tfrac{1}{2}, 2\theta_{a,6}\right), \sigma\left(\tfrac{1}{3}, 2\theta_{b,6}\right)e^{\frac{\theta_{b,6}}{2\theta_{a,6}}}, \sigma\left(\tfrac{1}{3}, 4\theta_{a,6}\right)\right]$$

and

$$b \le \max\left[\frac{1}{2}e^{\frac{\theta_6 + |\log(\varsigma)|}{\theta_{b,6}}}, \sigma\left(\tfrac{1}{2}, 2\theta_{b,6}\right), \sigma\left(\tfrac{1}{3}, 2\theta_{ba6}\right)e^{\frac{\theta_{a,6}}{2\theta_{b,6}}}, \sigma\left(\tfrac{1}{3}, 4\theta_{b,6}\right)\right].$$

Proof. Suppose first that

$$\theta_{a,6}\log(2a) + \theta_{b,6}\log(2b) \le \theta_6. \tag{A.23}$$

Then

$$\theta_{a,6}\log(2a) \le \theta_6 + |\log(\varsigma)| \quad \text{and} \quad \theta_{b,6}\log(2b) \le \theta_6 + |\log(\varsigma)|$$

and hence

$$a \le \frac{1}{2}e^{\frac{\theta_6 + |\log(\varsigma)|}{\theta_{a,6}}} \quad \text{and} \quad b \le \frac{1}{2}e^{\frac{\theta_6 + |\log(\varsigma)|}{\theta_{b,6}}}. \tag{A.24}$$

Suppose now that (A.23) fails, and thus (A.22) implies that

$$a^{\frac{1}{2}} + b^{\frac{1}{3}} \leq 2\theta_{a,6}\log(2a) + 2\theta_{b,6}\log(2b). \tag{A.25}$$

Assume also that

$$a > \sigma\left(\tfrac{1}{2}, 2\theta_{a,6}\right) \quad \text{and} \quad b > \sigma\left(\tfrac{1}{3}, 2\theta_{b,6}\right). \tag{A.26}$$

Then, using (A.22) and (A.25),

$$a^{\frac{1}{2}} + b^{\frac{1}{3}} \leq 2\theta_{a,6}\log(2a) + 2\theta_{b,6}\log(2b) < a^{\frac{1}{2}} + b^{\frac{1}{3}},$$

which is impossible. Hence one of the inequalities of (A.26) must fail. If

$$a \leq \sigma\left(\tfrac{1}{2}, 2\theta_{a,6}\right),$$

then (A.22) gives that

$$b^{\frac{1}{3}} \leq a^{\frac{1}{2}} + b^{\frac{1}{3}} \leq \theta_{a,6}\log\left(2\sigma\left(\tfrac{1}{2}, 2\theta_{a,6}\right)\right) + 2\theta_{b,6}\log(2b).$$

and Lemma A.6 with $\theta_{b,4} = 2\theta_{b,6}$ and $\theta_4 = \theta_{a,6}\log\left(2\sigma\left(\tfrac{1}{2}, 2\theta_{a,6}\right)\right)$ then implies that

$$b \leq \max\left[\frac{1}{2}e^{\frac{\theta_{a,6}\log(2\sigma(\frac{1}{2},2\theta_{a,6}))}{2\theta_{b,6}}}, \sigma\left(\tfrac{1}{2}, 4\theta_{b,6}\right)\right] = \max\left[\sigma\left(\tfrac{1}{2}, 2\theta_{a,6}\right)e^{\frac{\theta_{a,6}}{2\theta_{b,6}}}, \sigma\left(\tfrac{1}{2}, 4\theta_{b,6}\right)\right].$$

Symmetrically, if

$$b < \sigma\left(\tfrac{1}{3}, 2\theta_{b,6}\right),$$

then

$$a \leq \max\left[\sigma\left(\tfrac{1}{3}, 2\theta_{b,6}\right)e^{\frac{\theta_{b,6}}{2\theta_{a,6}}}, \sigma\left(\tfrac{1}{3}, 4\theta_{a,6}\right)\right].$$

□