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Abstract

A parametric class of trust-region algorithms for unconstrained nonconvex optimization is considered where the value of the objective function is never computed. The class contains a deterministic version of the first-order Adagrad method typically used for minimization of noisy function, but also allows the use of (possibly approximate) second-order information when available. The rate of convergence of methods in the class is analyzed and is shown to be identical to that known for first-order optimization methods using both function and gradients values, recovering existing results for purely-first order variants and improving the explicit dependence on problem dimension. This rate is shown to be essentially sharp. A new class of methods is also presented, for which a slightly worse and essentially sharp complexity result holds. Limited numerical experiments show that the new methods' performance may be comparable to that of standard steepest descent, despite using significantly less information, and that this performance is relatively insensitive to noise.

Keywords: First-order methods, objective-function-free optimization (OFFO), Adagrad, convergence bounds, evaluation complexity, second-order models.

1 Introduction

This paper is concerned with Objective-Function-Free Optimization (OFFO) algorithms, which we define as numerical optimization methods in which *the value of the problem's objective function is never calculated*, although we obviously assume that it exists. This is clearly at variance with the large majority of available numerical optimization algorithms, where the objective function is typically evaluated at every iteration, and its value then used to assess progress towards a minimizer and (often) to enforce descent. Dispensing with this information is therefore challenging. As it turns out, first-order OFFO methods (i.e. OFFO methods using gradients only) already exist for some time and have proved popular and useful in fields such as machine learning or sparse optimization, thereby justifying our interest. Many algorithms have been proposed, regrouped under the denomination of adaptive gradient methods, such

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as Adagrad [38, 19], RMSprop [47], ADADELTA [54], Adam [35], SC-Adagrad [41], WNGrad [51] or AMSgrad [45] to cite a few.

Adagrad was originally proposed for online learning [38, 19], where strong convergence guarantee were derived using current and past gradient information for a class of problems where the objective function changes at every iteration. The component-wise weighting of the gradient descent direction described in [19] has proved to be remarkably successful in practice and has prompted the proposal of many variants. Among those, RMSprop [47], ADADELTA [54], Adam [35] use an exponentially decreasing moving average when updating the weights instead of the non-decreasing technique proposed in [19]. In particular, Adam [19] has exhibited excellent performance in deep learning applications, as illustrated in recent numerical survey [46]. Closely related variants were also shown to be practically competitive in [13]. However, its potential divergence was shown in [45] where AMSGrad, a non-decreasing convergent scheme, was proposed as an alternative. The original theoretical analysis of Adagrad [19, 38] was subsequently refined for strongly convex functions [41] with a slight modification of the update rule, extended for minmax problems [52], further adapted for online use [43], modified to ensure privacy [1], enhanced with a linesearch for specific machine learning problems [49], or with an accelerated-gradient-like update [34]. Of special interest is WNGrad [51] which uses a mechanism to adapt the learning rate (or stepsize) using gradient information. Their update rule is very close to Adagrad-Norm [50], where a global (rather than componentwise) weight is used for all components. However, and despite its excellent performance, an analysis of Adagrad in the nonconvex setting appeared only relatively recently in [36] and [50]. [36] requires the *a-priori* knowledge of the Lipschitz constant (a serious theoretical drawback) whereas [50] is parameter agnostic. Both assume boundedness of the gradients for stochastic problems and obtain the conclusion that Adagrad's global rate of convergence is comparable to that of well-tuned stochastic gradient methods [25] up to logarithmic factors. Other proofs, still requiring a uniform bound on the sampled gradient, were subsequently developed using simpler arguments [17], yielding improved convergence rates under 'gradient sparsity' [55]. The assumption of bounded stochastic gradients was finally removed, see [24, 23, 2] and the references therein. A complexity analysis of Adagrad-Norm for deterministic nonconvex optimization was established in [50], showing a global rate of convergence equal to that of standard exact first order methods, without assuming bounded gradients. Inspired by this reference, [48] proposed a new analysis of a (componentwise) Adagrad for the convex case, which features an explicit[(1)] dependence on the problem's size which does not appear in the analysis of [50].

In this paper, we consider the deterministic Adagrad algorithm [19] using a trust-region point [14] of view. Although this approach has not been used much in the machine learning context, trust region techniques have been investigated in the framework of noisy optimization problems. The method proposed in [22] uses function values but updates the radius bounding the steplength as a function of the gradient norm, which is also the case of [16]. The algorithm of [7] and [5] also uses the (noisy) objective function's value while also allowing noise in the derivatives. In contrast, the algorithms described in [28] and [21] do not evaluate the objective function. They differ from the proposal we are about to describe both in the technique of proof and the fact that they do not subsume Adagrad or many of its variants. Moreover, the analysis of [21] requires the explicit knowledge of the problem's Lipschitz constant in the algorithm for obtaining the best complexity estimate.

[(1)] That is ignoring the potential dependence of the problem Lipschitz constant on dimension.

The purpose of the present paper is to bridge the gap between standard first-order OFFO methods such as Adagrad and OFFO trust-region algorithms by considering a unified framework. More specifically,

1. we re-interpret the deterministic Adagrad as a particular member of a fairly general parametric class of trust-region methods (Sections 2 and 3). This class not only contains purely first-order algorithms such as Adagrad, but also allows the use of (possibly approximate) second-order information, should it be available using a Barzilai-Borwein approach [3], a limited-memory BFGS technique [37] or even exact second derivatives.

2. We then provide, for our proposed class, an essentially sharp global[(2)] bound on the gradient's norm as a function of the iteration counter, which is identical to that known for first-order optimization methods using both function and gradients values. This complexity result does not assume bounded gradients and extends that of [50] only valid for Adagrad-Norm to the complete class. It also uses one of the available parameters of the class to mitigate the explicit dependence of that bound on the problem's dimension.

3. We next exploit the proposed OFFO trust-region framework of Section 2 to propose (in Section 4) a new class class of such methods, for which an essentially sharp complexity result is also provided.

4. We finally illustrate our proposals by discussing some numerical experiments in Section 5, suggesting that the considered OFFO methods may indeed be competitive with steepest descent in efficiency and reliability while being much less sensitive to noise.

Notations. In what follows, the superscript T denotes the transpose and $w_{i,k}$ denotes the i-th component of a vector $w_k \in \mathbb{R}^n$. Unless specified otherwise, $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^n$. We also say, for non-negative quantities α and β, that α is $\mathcal{O}(\beta)$ is there exists a finite constant κ such that $\alpha \leq \kappa\beta$.

2 A class of first-order minimization methods

We consider the problem

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

where f is a smooth function from $\mathbb{R}^n$ to $\mathbb{R}$. In particular, we will assume in what follows that

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

AS.2: its gradient $g(x) \stackrel{\rm def}{=} \nabla^1_x f(x)$ is Lipschitz continuous with Lipschitz constant $L \geq 0$, that is

$$\|g(x) - g(y)\| \leq L\|x - y\|$$

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

AS.3: there exists a constant $f_{\rm low}$ such that, for all x, $f(x) \geq f_{\rm low}$.

[(2)] I.e., valid at every iteration.

AS.1, AS.2 and AS.3 are standard for the complexity analysis of optimization methods seeking first-order critical points, AS.3 guaranteeing in particular that the problem is well-posed. We stress once more that we do not assume that the gradient are uniformly bounded, at variance with [51, 17, 55, 30].

The class of methods of interest here are iterative and generate a sequence of iterates $\{x_k\}_{k\geq 0}$. The move from an iterate to the next directly depends on the gradient at x_k and algorithm-dependent *scaling factors* $\{w_k = w(x_0, \ldots, x_k)\}$ whose main purpose is to control the move's magnitude. In our analysis, we will assume that

AS.4: for each $i \in \{1, \ldots, n\}$ there exists a constant $\varsigma_i \in (0, 1]$ such that, $w_{i,k} \geq \varsigma_i$ for all $k \geq 0$,

Since scaling factors are designed to control the length of the step, they are strongly reminiscent of the standard mechanism of the much studied trust-region optimization methods (see [14] for an extensive coverage and [53] for a more recent survey). In trust-region algorithms, a model of the objective function at an iterate x_k is built, typically using a truncated Taylor series, and a step s_k is chosen that minimizes this model with a *trust-region*, that is a region where the model is assumed to represent the true objective function sufficiently well. This region is a ball around the current iterate, whose radius is updated adaptively from iteration to iteration, based on the quality of the prediction of the objective function value at the trial point $x_k + s_k$. For methods using gradient only, the model is then chosen as the first two terms of the Taylor's expansion of f at the iterate x_k. Although, we are interested here in methods where the objective function's value is not evaluated, and therefore cannot be used to accept/reject iterates and update the trust-region radius, a similar mechanism may be designed, this time involving the weights $\{w_k\}$, the choice of which will detailed in the following two sections for two algorithmic subclasses of interest. The resulting algorithm, which we call ASTR1 (for Adaptively Scaled Trust Region using 1rst order information) is stated on the following page.

The algorithm description calls for some comments.

1. Observe that we allow the use of second-order information by effectively defining a quadratic model
$$g_k^T s + \tfrac{1}{2} s^T B_k s \tag{2.10}$$
where B_k can of course be chosen as the true second-derivative matrix of f at x_k (provided it remains bounded to satisfy (2.3)) or any approximation thereof. Choosing $B_k = 0$ results in a purely first-order algorithm.

   The condition (2.3) on the Hessian approximations is quite weak, and allows in particular for a variety of quasi-Newton approaches, limited-memory or otherwise. In a finite-sum context, sampling bounded Hessians is also possible.

2. Conditions (2.5)–(2.8) define a "generalized Cauchy point" (GCP), much in the spirit of standard trust-region methodology (see [14, Section 6.3] for instance), where the quadratic model (2.10) is minimized in (2.8) along a good first-order direction (s_k^L) to obtain a "Cauchy step" s_k^Q. Any step s_k can then be accepted provided it remains in the trust region (see (2.4)) and enforces a decrease in the quadratic model which is a least a fraction τ of that achieved at the Cauchy step (see (2.5)).

Algorithm 2.1: ASTR1

Step 0: Initialization. A starting point x_0 is given. Constants $\kappa_{\rm B} \geq 1$ and $\tau \in (0, 1]$ are also given. Set $k = 0$.

Step 1: Define the TR. Compute $g_k = g(x_k)$ and define

$$\Delta_{i,k} = \frac{|g_{i,k}|}{w_{i,k}} \tag{2.2}$$

where $w_k = w(x_0, \ldots, x_k)$.

Step 2: Hessian approximation. Select a symmetric Hessian approximation B_k such that

$$\|B_k\| \leq \kappa_{\rm B}. \tag{2.3}$$

Step 3: GCP. Compute a step s_k such that

$$|s_{i,k}| \leq \Delta_{i,k} \quad (i \in \{1, \ldots, n\}), \tag{2.4}$$

and

$$g_k^T s_k + \tfrac{1}{2} s_k^T B_k s_k \leq \tau \left(g_k^T s_k^Q + \tfrac{1}{2} (s_k^Q)^T B_k s_k^Q \right), \tag{2.5}$$

where

$$s_{i,k}^L = -\mathrm{sign}(g_{i,k}) \Delta_{i,k}, \tag{2.6}$$

$$s_k^Q = \gamma_k s_k^L, \tag{2.7}$$

with

$$\gamma_k = \begin{cases} \min \left[1, \dfrac{|g_k^T s_k^L|}{(s_k^L)^T B_k s_k^L} \right] & \text{if} \quad (s_k^L)^T B_k s_k^L > 0, \\ 1 & \text{otherwise.} \end{cases} \tag{2.8}$$

Step 4: New iterate. Define

$$x_{k+1} = x_k + s_k, \tag{2.9}$$

increment k by one and return to Step 1.

3. At variance with many existing trust-region algorithms, the radius Δ_k of the trust-region (2.2) is not recurred adaptively from iteration to iteration depending on how well the quadratic model predicts function values, but is directly defined as a scaled version of the local gradient. This is not without similarities with the trust-region methods proposed by [22], which corresponds to a scaling factor equal to $\|g_k\|^{-1}$, or [21] where the trust-region radius depends on $\|g_k\|$.

4. As stated, the ASTR1 algorithm does not include a termination rule, but such a rule can easily be introduced by terminating the algorithm in Step 1 if $\|g_k\| \leq \epsilon$, where $\epsilon > 0$ is a user-defined first-order accuracy threshold.

5. It may seem to the reader that we have introduced two algorithmic parameters typically not present in existing OFFO methods. As it turns out, this is standard practice for trust-region methods and it is widely acknowledged that the behaviour of the algorithm is relatively insensitive to the choice made. Typically value are

$$\tau = \tfrac{1}{10} \quad \text{and} \quad \kappa_{\rm B} = 10^5,$$

the last one being possibly adapted to reflect the problem scaling. Note that these values are constant throughout the execution of the algorithm. At variance, γ_k is the iteration dependent stepsize, a quantity present in every first-order minimization method. Observe that we do not impose restrictions of the stepsize (beyond being positive), thereby covering most standard choices. Note that $\gamma_k = 1$ and $s_k^Q = s_k^L$ whenever $B_k = 0$.

The algorithm being defined, the first step of our analysis is to derive a fundamental property of objective-function decrease, valid for all choices of the scaling factors satisfying AS.4.

Lemma 2.1 Suppose that AS.1, AS.2 and AS.4 hold. Then we have that, for all $k \geq 0$,

$$f(x_{j+1}) \leq f(x_j) - \sum_{i=1}^{n} \frac{\tau \varsigma_{\min} g_{i,j}^2}{2\kappa_{\rm B} w_{i,j}} + \tfrac{1}{2}(\kappa_{\rm B} + L) \sum_{i=1}^{n} \frac{g_{i,j}^2}{w_{i,j}^2} \tag{2.11}$$

and

$$f(x_0) - f(x_{k+1}) \geq \sum_{j=0}^{k} \sum_{i=1}^{n} \frac{g_{i,j}^2}{2\kappa_{\rm B} w_{i,j}} \left[\tau \varsigma_{\min} - \frac{\kappa_{\rm BBL}}{w_{i,j}} \right] \tag{2.12}$$

where $\varsigma_{\min} \stackrel{\rm def}{=} \min_{i \in \{1,\ldots,n\}} \varsigma_i$ and $\kappa_{\rm BBL} \stackrel{\rm def}{=} \kappa_{\rm B}(\kappa_{\rm B} + L)$.

Proof. Using (2.6) and AS.4, we deduce that, for every $j \geq 0$,

$$|g_j^T s_j^L| = \sum_{i=1}^{n} \frac{g_{i,j}^2}{w_{i,j}} = \sum_{i=1}^{n} \frac{w_{i,j} g_{i,j}^2}{w_{i,j}^2} \geq \sum_{i=1}^{n} \frac{\varsigma_i g_{i,j}^2}{w_{i,j}^2} \geq \varsigma_{\min} \|s_j^L\|^2. \tag{2.13}$$

Suppose first that $(s_j^L)^T B_j s_j^L > 0$ and $\gamma_j < 1$. Then, in view of (2.7), (2.8), (2.13) and

(2.3),

$$g_j^T s_j^Q + \tfrac{1}{2}(s_j^Q)^T B_j s_j^Q = \gamma_j g_j^T s_j^L + \tfrac{1}{2}\gamma_j^2 (s_j^L)^T B_j s_j^L = -\frac{(g_j^T s_j^L)^2}{2(s_j^L)^T B_j s_j^L} \leq -\frac{\varsigma_{\min}|g_j^T s_j^L|}{2\kappa_{\rm B}}.$$

Combining this inequality with the first equality in (2.13) then gives that

$$g_j^T s_j^Q + \tfrac{1}{2}(s_j^Q)^T B_j s_j^Q \leq -\frac{\varsigma_{\min}}{2\kappa_{\rm B}} \sum_{i=1}^{n} \frac{g_{i,j}^2}{w_{i,j}}. \tag{2.14}$$

Suppose now that $(s_j^L)^T B_j s_j^L \leq 0$ or $\gamma_j = 1$. Then, using (2.7), (2.14) and (2.6),

$$g_j^T s_j^Q + \tfrac{1}{2}(s_j^Q)^T B_j s_j^Q = g_j^T s_j^L + \tfrac{1}{2}(s_j^L)^T B_j s_j^L \leq \tfrac{1}{2} g_j^T s_j^L < 0$$

and (2.14) then again follows from the bound $\kappa_{\rm B} \geq 1$. Successively using AS.1–AS.2, (2.5), (2.14), (2.3) and (2.2) then gives that, for $j \geq 0$,

$$\begin{aligned} f(x_{j+1}) &\leq f(x_j) + g_j^T s_j + \tfrac{1}{2} s_j^T B_j s_j - \tfrac{1}{2} s_j^T B_j s_j + \tfrac{1}{2} L \|s_j\|^2 \\ &\leq f(x_j) + \tau \left(g_j^T s_j^Q + \tfrac{1}{2}(s_j^Q)^T B_j s_j^Q \right) + \tfrac{1}{2}(\kappa_{\rm B} + L)\|s_j\|^2 \\ &\leq f(x_j) - \sum_{i=1}^{n} \frac{\tau \varsigma_{\min} g_{i,j}^2}{2\kappa_{\rm B} w_{i,j}} + \tfrac{1}{2}(\kappa_{\rm B} + L) \sum_{i=1}^{n} \Delta_{i,j}^2 \\ &\leq f(x_j) - \sum_{i=1}^{n} \frac{\tau \varsigma_{\min} g_{i,j}^2}{2\kappa_{\rm B} w_{i,j}} + \tfrac{1}{2}(\kappa_{\rm B} + L) \sum_{i=1}^{n} \frac{g_{i,j}^2}{w_{i,j}^2} \end{aligned}$$

This is (2.11). Summing up this inequality for $j \in \{0, \ldots, k\}$ then yields (2.12). □

Armed with Lemma 2.1, we are now in position to specify particular choices of the scaling factors $w_{i,k}$ and derive the convergence properties of the resulting variants of ASTR1.

3 An Adagrad-like variant of ASTR1 using second-order models

We first consider a choice of scaling factors directly derived from the definition of the Adagrad algorithm [19]. For given $\varsigma \in (0, 1]$, $\vartheta \in (0, 1]$, $\theta > 0$ and $\mu \in (0, 1)$, define, for all $i \in \{1, \ldots, n\}$ and for all $k \geq 0$,

$$w_{i,k} \in \left[\sqrt{\vartheta}\, v_{i,k}, v_{i,k} \right] \quad \text{where} \quad v_{i,k} \stackrel{\rm def}{=} \theta \left(\varsigma + \sum_{\ell=0}^{k} g_{i,\ell}^2 \right)^{\mu}. \tag{3.1}$$

The Adagrad scaling factors are recovered by $\mu = \frac{1}{2}$, $\theta = 1$ and $\vartheta = 1$, and ASTR1 with (3.1) and $B_k = 0$ is then the standard (deterministic) Adagrad method. The formulation (3.1) allows a parametric analysis of methods "in the neighbourhood" of Adagrad, using not only first-order but also second-order information. The ϑ parameter is introduced for flexibility, in particular allowing non-monotone scaling factors[3] The additional scaling parameter[4]

[3] Typical values are $\varsigma_i = \frac{1}{100}$ and $\vartheta = \frac{1}{1000}$.

[4] Which can be viewed as a stepsize/learning rate parameter when $B_k = 0$.

θ is introduced as a technique to improve the convergence rate of the resulting algorithm. Such a scaling may be useful when the gradient is sparse [20] or when designing a private Adagrad version [1] in order to improve the complexity bound with respect to the problem's parameters. The above parametrization with $\theta = 1$ has also been considered in [11] in the context of a continuous Ordinary Differential Equations analysis and, with θ depending on problem's constants, in [36] where the sum on ℓ in (3.1) is terminated at $\ell = k - 1$ and μ is restricted to the interval $[\frac{1}{2}, 1)$ in the stochastic regime. In what follows, we consider the discrete deterministic case for the interval $(0, 1)$.

Before stating the global rate of convergence of the variant of ASTR1 using (3.1), we first prove a lemma, partly inspired by [50, 17].

Lemma 3.1 Let $\{a_k\}_{k\geq 0}$ be a non-negative sequence, $\alpha > 0$, $\xi > 0$ and define, for each $k \geq 0$, $b_k = \sum_{j=0}^{k} a_j$. Then if $\alpha \neq 1$,

$$\sum_{j=0}^{k} \frac{a_j}{(\xi + b_j)^\alpha} \leq \frac{1}{(1-\alpha)}((\xi + b_k)^{1-\alpha} - \xi^{1-\alpha}). \tag{3.2}$$

Otherwise (i.e. if $\alpha = 1$),

$$\sum_{j=0}^{k} \frac{a_j}{(\xi + b_j)} \leq \log\left(\frac{\xi + b_k}{\xi}\right). \tag{3.3}$$

Proof. Consider first the case where $\alpha \neq 1$ and note that $\frac{1}{(1-\alpha)}x^{1-\alpha}$ is then a non-decreasing and concave function on $(0, +\infty)$. Setting $b_{-1} = 0$ and using these properties, we obtain that, for $j \geq 0$,

$$\begin{aligned}\frac{a_j}{(\xi + b_j)^\alpha} &\leq \frac{1}{1-\alpha}\left((\xi + b_j)^{1-\alpha} - (\xi + b_j - a_j)^{1-\alpha}\right) \\ &= \frac{1}{1-\alpha}\left((\xi + b_j)^{1-\alpha} - (\xi + b_{j-1})^{1-\alpha}\right).\end{aligned}$$

We then obtain (3.2) by summing this inequality for $j \in \{0, \ldots, k\}$.

Suppose now that $\alpha = 1$, we then use the concavity and non-decreasing character of the logarithm to derive that

$$\frac{a_j}{(\xi + b_j)^\alpha} = \frac{a_j}{(\xi + b_j)} \leq \log(\xi + b_j) - \log(\xi + b_j - a_j) = \log(\xi + b_j) - \log(\xi + b_{j-1}).$$

The inequality (3.3) then again follows by summing for $j \in \{0, \ldots, k\}$. □

From (3.2), we also obtain that, for $\alpha < 1$,

$$\sum_{j=0}^{k} \frac{a_j}{(\xi + b_j)^\alpha} \leq \frac{1}{(1-\alpha)}(\xi + b_k)^{1-\alpha} \tag{3.4}$$

while, for $\alpha > 1$,

$$\sum_{j=0}^{k} \frac{a_j}{(\xi + b_j)^\alpha} \leq \frac{\xi^{1-\alpha}}{(\alpha - 1)}. \tag{3.5}$$

Note that both the numerator and the denominator of the right-hand side of (3.2) tend to zero when α tends to one. Applying l'Hospital rule, we then see that this right-hand side tends to the right-hand side of (3.3) and the bounds on $\sum_{j=0}^{k} a_j/(\xi + b_j)^\alpha$ are therefore continuous at $\alpha = 1$.

Lemma 3.1 is crucial in the proof of our main complexity result, which we now state.

Theorem 3.2 Suppose that AS.1–AS.3 hold and that the ASTR1 algorithm is applied to problem (2.1) with its scaling given by (3.1). If we define

$$\Gamma_0 \stackrel{\rm def}{=} f(x_0) - f_{\rm low},$$

then,

(i) if $0 < \mu < \frac{1}{2}$,

$$\operatorname*{average}_{j \in \{0,\ldots,k\}} \|g_j\|^2 \leq \frac{\kappa_1}{k+1}, \tag{3.6}$$

with

$$\kappa_1 = \max\left\{\varsigma, \left[\frac{2^{2\mu}\vartheta(1-2\mu)\theta^2\Gamma_0}{n(\kappa_{\rm B}+L)}\right]^{\frac{1}{1-2\mu}}, \left[\frac{4\,n\,\kappa_{\rm BBL}}{(1-2\mu)\tau\theta\varsigma^\mu\vartheta^{\frac{3}{2}}}\right]^{\frac{1}{\mu}}\right\}; \tag{3.7}$$

(ii) if $\mu = \frac{1}{2}$,

$$\operatorname*{average}_{j \in \{0,\ldots,k\}} \|g_j\|^2 \leq \frac{\kappa_2}{k+1}, \tag{3.8}$$

with

$$\kappa_2 = \max\left\{\varsigma, \frac{1}{2}e^{\frac{2\Gamma_0\vartheta\theta^2}{n(\kappa_B+L)}}, \frac{1}{2\varsigma}\left(\frac{8n\kappa_{\rm B}(\kappa_{\rm B}+L)}{\tau\vartheta^{\frac{3}{2}}\theta}\right)^2 \left|W_{-1}\left(-\frac{\tau\varsigma\theta\vartheta^{\frac{3}{2}}}{8n\kappa_{\rm B}(\kappa_{\rm B}+L)}\right)\right|^2\right\}, \tag{3.9}$$

where W_{-1} is the second branch of the Lambert function [15];

(iii) if $\frac{1}{2} < \mu < 1$,

$$\operatorname*{average}_{j \in \{0,\ldots,k\}} \|g_j\|^2 \leq \frac{\kappa_3}{k+1} \tag{3.10}$$

with

$$\kappa_3 \stackrel{\rm def}{=}= \max\left\{\varsigma, \left[\frac{2^{1+\mu}\kappa_{\rm B}}{\tau\varsigma^\mu\sqrt{\vartheta}}\left(\Gamma_0\theta + \frac{n(\kappa_{\rm B}+L)\varsigma^{1-2\mu}}{2\vartheta\theta(2\mu-1)}\right)\right]^{\frac{1}{1-\mu}}\right\} \tag{3.11}$$

Proof. We see from (3.1) that $w_{i,k}$ verifies **AS.4**. We may thus use Lemma 2.1.

Moreover, (3.1) also implies that

$$\varsigma^{\mu}\sqrt{\vartheta}\theta \leq w_{i,j} \leq \theta\left(\varsigma + \sum_{\ell=0}^{j} \|g_\ell\|^2\right)^{\mu} \tag{3.12}$$

for all $j \geq 0$ and all $i \in \{1,\ldots,n\}$. We now deduce from (2.2) and (2.12) that, for $k \geq 0$,

$$f(x_{k+1}) \;\leq\; f(x_0) - \sum_{j=0}^{k} \frac{\tau\varsigma^{\mu}\sqrt{\vartheta}\,\|g_j\|^2}{2\kappa_{\rm B} \max\limits_{i\in\{1,\ldots,n\}} w_{i,k}} + \tfrac{1}{2}(\kappa_{\rm B}+L)\sum_{i=1}^{n}\sum_{j=0}^{k}\Delta_{i,j}^2. \tag{3.13}$$

For each $i \in \{1,\ldots,n\}$, we then apply Lemma 3.1 with $a_\ell = g_{i,\ell}^2$, $\xi = \varsigma$ and $\alpha = 2\mu < 1$, and obtain from (2.2) and (3.1) that,

$$\sum_{j=0}^{k}\Delta_{i,j}^2 \leq \frac{1}{\theta^2\vartheta(1-2\mu)}\left[\left(\varsigma + \sum_{\ell=0}^{k} g_{i,\ell}^2\right)^{1-2\mu} - \varsigma^{1-2\mu}\right] \leq \frac{1}{\theta^2\vartheta(1-2\mu)}\left(\varsigma + \sum_{\ell=0}^{k} g_{i,\ell}^2\right)^{1-2\mu}. \tag{3.14}$$

Now

$$\sum_{i=1}^{n}\sum_{j=0}^{k}\Delta_{i,j}^2 \leq \sum_{i=1}^{n}\frac{1}{\theta^2\vartheta(1-2\mu)}\left(\varsigma + \sum_{i=1}^{n}\sum_{\ell=0}^{k} g_{i,\ell}^2\right)^{1-2\mu} \leq \frac{n}{\theta^2\vartheta(1-2\mu)}\left(\varsigma + \sum_{\ell=0}^{k}\|g_\ell\|^2\right)^{1-2\mu} \tag{3.15}$$

and thus substituting this bound in (3.13) and using AS.3 gives that

$$\sum_{j=0}^{k}\frac{\tau\varsigma^{\mu}\sqrt{\vartheta}\|g_j\|^2}{2\kappa_{\rm B}\max\limits_{i\in\{1,\ldots,n\}} w_{i,k}} \leq \Gamma_0 + \frac{n(\kappa_{\rm B}+L)}{2\theta^2\vartheta}(1-2\mu)\left(\varsigma + \sum_{j=0}^{k}\|g_j\|^2\right)^{1-2\mu}. \tag{3.16}$$

Suppose now that

$$\sum_{j=0}^{k}\|g_j\|^2 \geq \max\left\{\varsigma, \left[\frac{2^{2\mu}\theta^2\vartheta(1-2\mu)\Gamma_0}{n(\kappa_{\rm B}+L)}\right]^{\frac{1}{1-2\mu}}\right\}, \tag{3.17}$$

implying

$$\varsigma + \sum_{j=0}^{k}\|g_j\|^2 \leq 2\sum_{j=0}^{k}\|g_j\|^2 \;\text{ and }\; \Gamma_0 \leq \frac{n(\kappa_{\rm B}+L)}{2\theta^2\vartheta(1-2\mu)}\left(2\sum_{j=0}^{k}\|g_j\|^2\right)^{1-2\mu}.$$

Then, using (3.16) and (3.12),

$$\frac{\tau\varsigma^{\mu}\sqrt{\vartheta}}{2^{1+\mu}\,\kappa_{\rm B}\theta\left[\sum_{\ell=0}^{k}\|g_\ell\|^2\right]^{\mu}}\sum_{j=0}^{k}\|g_j\|^2 \leq \frac{2^{1-2\mu}\,n\,(\kappa_{\rm B}+L)}{\vartheta\theta^2(1-2\mu)}\left(\sum_{j=0}^{k}\|g_j\|^2\right)^{1-2\mu}.$$

Solving this inequality for $\sum_{j=0}^{k}\|g_j\|^2$ gives that

$$\sum_{j=0}^{k}\|g_j\|^2 \leq \left[\frac{4\,n\;\kappa_{\rm BBL}}{(1-2\mu)\theta\tau\varsigma^{\mu}\vartheta^{\frac{3}{2}}}\right]^{\frac{1}{\mu}}$$

and therefore

$$\underset{j\in\{0,\ldots,k\}}{\text{average}} \|g_j\|^2 \leq \left[\frac{4\,n\,\kappa_{\rm BBL}}{(1-2\mu)\theta\tau\varsigma^\mu\vartheta^{\frac{3}{2}}}\right]^{\frac{1}{\mu}} \cdot \frac{1}{k+1}. \tag{3.18}$$

Alternatively, if (3.17) fails, then

$$\underset{j\in\{0,\ldots,k\}}{\text{average}} \|g_j\|^2 < \max\left\{\varsigma, \left[\frac{2^{2\mu}\vartheta(1-2\mu)\theta^2\Gamma_0}{2^{1-2\mu}n(\kappa_{\rm B}+L)}\right]^{\frac{1}{1-2\mu}}\right\} \cdot \frac{1}{k+1}. \tag{3.19}$$

Combining (3.18) and (3.19) gives (3.6).

Let us now consider the case where $\mu = \frac{1}{2}$. For each $i \in \{1,\ldots,n\}$, we apply Lemma 3.1 with $a_k = g_{i,k}^2$, $\xi = \varsigma$ and $\alpha = 2\mu = 1$ and obtain that,

$$\sum_{i=1}^{n}\sum_{j=0}^{k}\Delta_{i,j}^2 \leq \frac{1}{\vartheta\theta^2}\sum_{i=1}^{n}\log\left(\frac{1}{\varsigma}\left(\varsigma+\sum_{\ell=0}^{k}g_{i,\ell}^2\right)\right) \leq \frac{n}{\vartheta\theta^2}\log\left(1+\frac{1}{\varsigma}\sum_{\ell=0}^{k}\|g_\ell\|^2\right).$$

and substituting this bound in (3.13) then gives that

$$\sum_{j=0}^{k}\frac{\tau\sqrt{\varsigma\vartheta}\|g_j\|^2}{2\kappa_{\rm B}\max\limits_{i\in\{1,\ldots,n\}}w_{i,k}} \leq \Gamma_0 + \frac{n(\kappa_{\rm B}+L)}{2\vartheta\theta^2}\log\left(1+\frac{1}{\varsigma}\sum_{j=0}^{k}\|g_j\|^2\right).$$

Suppose now that

$$\sum_{j=0}^{k}\|g_j\|^2 \geq \max\left[\varsigma, \frac{1}{2}e^{\frac{2\vartheta\theta^2\Gamma_0}{n(\kappa_B+L)}}\right], \tag{3.20}$$

implying that

$$1+\frac{1}{\varsigma}\sum_{j=0}^{k}\|g_j\|^2 \leq \frac{2}{\varsigma}\sum_{j=0}^{k}\|g_j\|^2 \;\text{ and }\; \Gamma_0 \leq \frac{n(\kappa_{\rm B}+L)}{2\vartheta\theta^2}\log\left(\frac{2}{\varsigma}\sum_{j=0}^{k}\|g_j\|^2\right).$$

Using (3.12) for $\mu = \frac{1}{2}$, we obtain then that

$$\frac{\tau\sqrt{\varsigma\vartheta}}{2\sqrt{2}\,\theta\,\kappa_{\rm B}\sqrt{\sum_{\ell=0}^{k}\|g_\ell\|^2}}\sum_{j=0}^{k}\|g_j\|^2 \leq \frac{n(\kappa_{\rm B}+L)}{\vartheta\theta^2}\log\left(\frac{2}{\varsigma}\sum_{j=0}^{k}\|g_j\|^2\right),$$

that is

$$\frac{\tau\sqrt{2\varsigma}\vartheta^{\frac{3}{2}}\theta}{4\kappa_{\rm B}}\sqrt{\sum_{j=0}^{k}\|g_j\|^2} \leq 2n(\kappa_{\rm B}+L)\log\left(\sqrt{\frac{2}{\varsigma}\sum_{j=0}^{k}\|g_j\|^2}\right). \tag{3.21}$$

Now define

$$\gamma_1 \stackrel{\rm def}{=} \frac{\tau\varsigma\vartheta^{\frac{3}{2}}\theta}{4\kappa_{\rm B}}, \quad \gamma_2 \stackrel{\rm def}{=} 2n(\kappa_{\rm B}+L) \quad\text{and}\quad u \stackrel{\rm def}{=} \sqrt{\frac{2}{\varsigma}\sum_{j=0}^{k}\|g_j\|^2} \tag{3.22}$$

and observe that that $\gamma_2 > 3\gamma_1$ because $\tau\sqrt{\varsigma}\vartheta^{\frac{3}{2}} \leq 1$ and $\kappa_{\rm B} \geq 1$. The inequality (3.21) can then be rewritten as

$$\gamma_1 u \leq \gamma_2 \log(u). \tag{3.23}$$

Let us denote by $\psi(u) \stackrel{\rm def}{=} \gamma_1 u - \gamma_2 \log(u)$. Since $\gamma_2 > 3\gamma_1$, the equation $\psi(u) = 0$ admits two roots $u_1 \leq u_2$ and (3.23) holds for $u \in [u_1, u_2]$. The definition of u_2 then gives that

$$\log(u_2) - \frac{\gamma_1}{\gamma_2} u_2 = 0$$

which is

$$u_2 e^{-\frac{\gamma_1}{\gamma_2} u_2} = 1.$$

Setting $z = -\frac{\gamma_1}{\gamma_2} u_2$, we obtain that

$$z e^z = -\frac{\gamma_1}{\gamma_2}$$

Thus $z = W_{-1}(-\frac{\gamma_1}{\gamma_2}) < 0$, where W_{-1} is the second branch of the Lambert function defined over $[-\frac{1}{e}, 0)$. As $-\frac{\gamma_1}{\gamma_2} \geq -\frac{1}{3}$, z is well defined and thus

$$u_2 = -\frac{\gamma_2}{\gamma_1} z = -\frac{\gamma_2}{\gamma_1} W_{-1}\left(-\frac{\gamma_1}{\gamma_2}\right) > 0.$$

As a consequence, we deduce from (3.23) and (3.22) that

$$\sum_{j=0}^{k} \|g_j\|^2 = \frac{\varsigma}{2} u_2^2 = \frac{1}{2\varsigma} \left(\frac{8n\kappa_{\rm B}(\kappa_{\rm B}+L)}{\tau\vartheta^{\frac{3}{2}}\theta}\right)^2 \left| W_{-1}\left(-\frac{\tau\varsigma\vartheta^{\frac{3}{2}}\theta}{8n\kappa_{\rm B}(\kappa_{\rm B}+L)}\right)\right|^2.$$

and

$$\underset{j\in\{0,\ldots,k\}}{\rm average}\ \|g_j\|^2 \leq \frac{1}{2\varsigma} \left(\frac{8n\kappa_{\rm B}(\kappa_{\rm B}+L)}{\tau\vartheta^{\frac{3}{2}}\theta}\right)^2 \left| W_{-1}\left(-\frac{\tau\varsigma\vartheta^{\frac{3}{2}}\theta}{8n\kappa_{\rm B}(\kappa_{\rm B}+L)}\right)\right|^2 \cdot \frac{1}{k+1}. \tag{3.24}$$

If (3.20) does not hold, we have that

$$\underset{j\in\{0,\ldots,k\}}{\rm average}\ \|g_j\|^2 < \max\left\{\varsigma, \frac{1}{2} e^{\frac{2\Gamma_0\vartheta\theta^2}{n(\kappa_B+L)}}\right\} \cdot \frac{1}{k+1}. \tag{3.25}$$

Combining (3.24) and (3.25) gives (3.8).

Finally, suppose that $\frac{1}{2} < \mu < 1$. Once more, we apply Lemma 3.1 for each $i \in \{1, \ldots, n\}$ with $a_\ell = g_{i,\ell}^2$, $\xi = \varsigma$ and $\alpha = 2\mu > 1$ and obtain that

$$\sum_{j=1}^{k} \Delta_{k,j}^2 \leq \frac{1}{\theta^2\vartheta(1-2\mu)} \left(\left(\varsigma + \sum_{\ell=0}^{k} g_{i,\ell}^2\right)^{1-2\mu} - \varsigma^{1-2\mu}\right) \leq \frac{\varsigma^{1-2\mu}}{\vartheta\theta^2(2\mu-1)}. \tag{3.26}$$

Substituting the bound (3.26) in (3.13) and using (3.12) and AS.3 gives that

$$\sum_{j=0}^{k} \frac{1}{(\varsigma + \sum_{j=0}^{k} \|g_j\|^2)^{\mu}} \frac{\tau\varsigma^{\mu}\sqrt{\vartheta}\|g_j\|^2}{2\kappa_{\rm B}\theta} \leq \Gamma_0 + \frac{n(\kappa_{\rm B}+L)\varsigma^{1-2\mu}}{2\theta^2\vartheta(2\mu-1)}.$$

If we now suppose that

$$\sum_{j=0}^{k} \|g_j\|^2 \geq \varsigma, \tag{3.27}$$

then

$$\operatorname*{average}_{j\in\{0,\ldots,k\}} \|g_j\|^2 \leq \left[\frac{2^{1+\mu}\kappa_{\rm B}}{\tau\varsigma^{\mu}\sqrt{\vartheta}}\left(\Gamma_0\theta + \frac{n(\kappa_{\rm B}+L)\varsigma^{1-2\mu}}{2\vartheta(2\mu-1)\theta}\right)\right]^{\frac{1}{1-\mu}} \cdot \frac{1}{k+1}. \tag{3.28}$$

If (3.27) does not hold, we derive that

$$\operatorname*{average}_{j\in\{0,\ldots,k\}} \|g_j\|^2 \leq \frac{\varsigma}{(k+1)}. \tag{3.29}$$

Thus, (3.28) and(3.29) finally imply (3.10). □

These result suggest additional remarks.

1. That the bounds given are not continuous as a function μ at $\mu = \frac{1}{2}$ is a result of our bounding process within the proof of Theorem 3.2 (for instance in the last inequality of (3.14)). Continuous bounds have been proved (see[29]) if one is ready to assume that the objective functions' gradients remain uniformly bounded.

2. If the algorithm is terminated as soon as $\|g_k\| \leq \epsilon$ (which is customary for deterministic algorithms searching for first-order points), it must stop at the latest at iteration

$$k = \kappa_\star^2 \epsilon^{-2}, \tag{3.30}$$

where $\kappa_\star = \kappa_1$ for $\mu \in (0, \frac{1}{2})$, $\kappa_\star = \kappa_2$ for $\mu = \frac{1}{2}$ and $\kappa_\star = \kappa_3$ for $\mu \in (\frac{1}{2}, 1)$. It is truly remarkable that there exist first-order OFFO methods whose global complexity order is identical to that of standard first-order methods using function evaluations (see [42, 32, 8] or [10, Chapter 2]), despite the fact that the latter exploit significantly more information. As mentionned in the introduction, this complexity rate was also derived for the analysis of Adagrad-Norm in [50].

3. It is possible to give a weaker but more explicit bound on κ_2 by finding an upper bound on the value of the involved Lambert function. This can be obtained by using [12, Theorem 1] which states that, for $x > 0$,

$$\left|W_{-1}(-e^{-x-1})\right| \leq 1 + \sqrt{2x} + x. \tag{3.31}$$

Remembering that, for γ_1 and γ_2 given by (3.22), $\log\left(\frac{\gamma_2}{\gamma_1}\right) \geq \log(3) > 1$ and taking $x = \log\left(\frac{\gamma_2}{\gamma_1}\right) - 1 > 0$ in (3.31) then gives that

$$\left|W_{-1}\left(-\frac{\gamma_1}{\gamma_2}\right)\right| \leq \log\left(\frac{\gamma_2}{\gamma_1}\right) + \sqrt{2\left(\log\left(\frac{\gamma_2}{\gamma_1}\right) - 1\right)}.$$

4. It is also possible to extend the definition of s_k^L in (2.6) by premultiplying it by a stepsize $\alpha_k \in [\alpha_{\min}, 1]$ for some $\alpha_{\min} \in (0, 1]$. Our results again remain valid (with modified

constants). Covering a deterministic momentum-less Adam would require extending the results to allow for (3.1) to be replaced by

$$w_{i,k} = \varsigma + \sum_{j=0}^{k} \beta_2^{k-j} g_{i,j}^2 \quad (i \in \{1, \ldots, n\}) \tag{3.32}$$

for some $\beta_2 < 1$. This can be done by following the argument of Theorem 2 in [17]. However, as in this reference, the final bound on the squared gradient norms does not tend to zero when k grows[(5)], illustrating the (known) lack of convergence of Adam. We therefore do not investigate this option in detail.

5. Focusing on the choice of the parameter μ independently of ϑ and θ, we verify that the choice $\mu = \frac{1}{2}$ is best, yielding an upper complexity bound for the deterministic Adagrad algorithm and recovering a similar result obtained in [50] for the Adagrad-Norm algorithm.

   The choice $\mu = 1$ is not covered by our theory but has been considered in [41], where a specific choice of the constant θ with $\mu = 1$ is used to derive a first order method with optimal regret for strongly convex problems. Unfortunately, the proposed SC(Strong Convex)-Adagrad algorithm requires the knowledge of the problem's Lipschitz constant and noise characteristics.

We now discuss the dependence of the bounds given by Theorem 3.2 as a function of the problem's constants L, n and Γ_0 and recall that if n is known *a priori*, this is generally not the case for the Lispchitz constant L, while the gap Γ_0 may be available for some classes of problems (such as nonlinear regressions where $\Gamma_0 \leq f(x_0)$). We are mostly interested in the explicit dependence of the bounds on n, taking into account that the unknown L often varies little with dimension –such as in problems arising from discretizations– but admittedly ignoring the fact it may also depend on n, sometimes severely [10, p. 14]. As we are allowed to do so, we would like to choose the scaling parameter θ in order to offset this dependence as much as possible. In view of (3.7), (3.9) and (3.11), and noting that (3.31) indicates that the $|W_{-1}|^2$ term in (3.9) can be summarized as $\mathcal{O}\left(\log(nL)^2\right)$, we attempt to balance the impact of the various terms involving both θ and n and, in the absence of additional information on the problem, select

$$\theta_\star = \begin{cases} \sqrt{n/\Gamma_0} & \text{when } \Gamma_0 \text{ is known,} \\ \sqrt{n} & \text{otherwise.} \end{cases} \tag{3.33}$$

We may then compare the bounds obtained by reinjecting this value in (3.9) ($\mu = \frac{1}{2}$) with the results for deterministic Adagrad-Norm [50] and Adagrad [48]. This comparison is summarized in the following table.

Regime	Algorithm	Constant dependence
Non-Convex [50]	$w_{i,k} = \sqrt{\varsigma + \sum_{j=0}^{k} \|g_j\|^2}$	$\mathcal{O}\left(L^2 \log(L)^2\right)$
Convex [48]	(3.1) with ($\theta = 1$, $\vartheta = 1$)	$\mathcal{O}\left(n^2 L^2 \log(L)^2\right)$
Non-convex (3.9)	(3.1) with ($\theta = \sqrt{n}$, $\vartheta = 1$)	$\mathcal{O}\left(nL^2 \log(\sqrt{n}L)^2\right)$

[(5)] A constant term in $-\log(\beta_2)$ refuses to vanish.

Are the (good) upper bound given Theorem 3.2 sharp?

Theorem 3.3 The bounds (3.6), (3.8) and (3.10) are essentially sharp in that, for each $\mu \in (0,1)$ and each $\eta \in (0,1]$, there exists a univariate function $f_{\mu,\eta}$ satisfying AS.1-AS.3 such that, when applied to minimize $f_{\mu,\eta}$ from the origin, the ASTR1 algorithm with (3.1), $B_k = 0$ and $\vartheta = \theta = 1$ produces a sequence of gradient norms given by $\|g_k\| = \frac{1}{k^{\frac{1}{2}+\eta}}$.

Proof. Following ideas of [10, Theorem 2.2.3], we first construct a sequence of iterates $\{x_k\}$ for which $f_{\mu,\eta}(x_k) = f_k$ and $\nabla_x^1 f_{\mu,\eta}(x_k) = g_k$ for associated sequences of function and gradient values $\{f_k\}$ and $\{g_k\}$, and then apply Hermite interpolation to exhibit the function $f_{\mu,\eta}$ itself. We start by defining

$$g_0 \stackrel{\rm def}{=} -2, \quad g_k \stackrel{\rm def}{=} -\frac{1}{k^{\frac{1}{2}+\eta}} \quad (k>0), \tag{3.34}$$

$$s_0 \stackrel{\rm def}{=} \frac{2}{(\varsigma+4)^{\mu}}, \quad s_k \stackrel{\rm def}{=} \frac{1}{k^{\frac{1}{2}+\eta}(\varsigma+\sum_{j=0}^{k} g_j^2)^{\mu}} \quad (k>0) \tag{3.35}$$

yielding that

$$|g_0 s_0| = \frac{4}{(\varsigma+4)^{\mu}}, \quad |g_k s_k| = \frac{1}{k^{1+2\eta}(\varsigma+\sum_{j=0}^{k} g_j^2)^{\mu}} \leq \frac{1}{k^{1+2\eta}} \quad (k>0) \tag{3.36}$$

(remember that $g_0^2 = 4$). We then define $B_k \stackrel{\rm def}{=} 0$ for all $k \geq 0$,

$$x_0 = 0, \quad x_{k+1} = x_k + s_k \quad (k>0) \tag{3.37}$$

and

$$f_0 = \frac{4}{(\varsigma+4)^{\mu}} + \zeta(1+2\eta) \quad \text{and} \quad f_{k+1} = f_k + g_k s_k \quad (k \geq 0), \tag{3.38}$$

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

$$f_{k+1} = f_0 - \sum_{k=0}^{k} |g_k s_k| \geq f_0 - \frac{4}{(\varsigma+4)^{\mu}} - \sum_{k=1}^{k} \frac{1}{k^{1+2\eta}} \geq f_0 - \frac{4}{(\varsigma+4)^{\mu}} - \zeta(1+2\eta)$$

where we used (3.38) and (3.36). Hence (3.38) implies that

$$f_k \in [0, f_0] \ \text{ for all } \ k \geq 0. \tag{3.39}$$

Also note that, using (3.38),

$$|f_{k+1} - f_k - g_k s_k| = 0, \tag{3.40}$$

while, using (3.35),

$$|g_0 - g_1| = 1 \leq \frac{1}{2}(\varsigma+4)^{\mu}\, s_0.$$

Moreover, using the fact that $1/x^{\frac{1}{2}+\eta}$ is a convex function of x over $[1,+\infty)$, and that from (3.35) $s_k \geq \frac{1}{k^{\frac{1}{2}+\eta}(\varsigma+4+k)^\mu}$, we derive that, for $k>0$,

$$\begin{aligned}
|g_{k+1}-g_k| &= \left| \frac{1}{(k+1)^{\frac{1}{2}+\eta}} - \frac{1}{k^{\frac{1}{2}+\eta}} \right| \\
&\leq \left(\frac{1}{2}+\eta\right) \frac{1}{k^{\frac{3}{2}+\eta}} \\
&\leq \frac{3}{2} \frac{(\varsigma+4+k)^\mu}{k k^{\frac{1}{2}+\eta}(\varsigma+4+k)^\mu} \\
&\leq \frac{3}{2} \frac{(\varsigma+4+k)^\mu}{k} s_k \\
&\leq \frac{3}{2} (\varsigma+5)^\mu s_k.
\end{aligned}$$

These last bounds and (3.39) allow us to use standard Hermite interpolation on the data given by $\{f_k\}$ and $\{g_k\}$: see, for instance, Theorem A.9.1 in [10] with $p=1$ and

$$\kappa_f = \max\left[\frac{3}{2}(\varsigma+5)^\mu, f_0, 2\right] \tag{3.41}$$

(the second term in the max bounding $|f_k|$ because of (3.39) and the third bounding $|g_k|$ because of (3.34)). We then deduce that there exists a continuously differentiable function $f_{\mu,\eta}$ from $\mathbb{R}$ to $\mathbb{R}$ with Lipschitz continuous gradient (i.e. satisfying AS.1 and AS.2) such that, for $k \geq 0$,

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

Moreover, the range of $f_{\mu,\eta}$ and $\nabla_x^1 f_{\mu,\eta}$ are constant independent of η, hence guaranteeing AS.3 and AS.3. The definitions (3.34), (3.35), (3.37) and (3.38) imply that the sequences $\{x_k\}$, $\{f_k\}$ and $\{g_k\}$ can be seen as generated by the ASTR1 algorithm (with (3.1), $B_k=0$ and $\vartheta=\theta=1$) applied to $f_{\mu,\eta}$, starting from $x_0=0$ and the desired conclusion follows. □

The bounds (3.6), (3.8) and (3.10) are therefore *essentially sharp* (in the sense of [9]) for the ASTR1 algorithm with (3.1) and $\vartheta=\theta=1$, which is to say that the lower complexity bound for the algorithm is arbitrarily close to its upper bound. Interestingly, the argument in the proof of the above theorem fails for $\eta=0$, as this choice yields that

$$\sum_{j=0}^{k} g_j^T s_j \geq \sum_{j=0}^{k} \frac{1}{k(\varsigma+\log(k+1))^\mu}.$$

Since

$$\int_1^k \frac{dt}{t(\log(t+1))^\mu} > \int_1^k \frac{dt}{(t+1)(\log(t+1))^\mu} = \frac{(\log(k+1))^{1-\mu}}{1-\mu} - \frac{\log(2)^{1-\mu}}{1-\mu}$$

tends to infinity as k grows, this indicates (in view (3.38)) that AS.3 cannot hold. Also note that (3.34) implies that the gradients remain uniformly bounded.

4 A further "diminishing stepsizes" variation on this theme

We now use a different proof technique to design new variants of ASTR1 with a fast global k-order. This is achieved by modifying the definition of the scaling factors $w_{i,k}$, requiring them to satisfy a fairly general growth condition explicitly depending on k, the iteration index. More specifically, we will assume, in this section, that the scaling factors $w_{i,k}$ are chosen such that, for some power parameter $0 < \nu \leq \mu < 1$, all $i \in \{1, \ldots, n\}$ and some constants $\varsigma_i \in (0, 1]$ and $\theta > 0$,

$$\theta \max[\varsigma_i, v_{i,k}] \, (k+1)^{\nu} \leq w_{i,k} \leq \theta \max[\varsigma_i, v_{i,k}] \, (k+1)^{\mu} \quad (k \geq 0), \tag{4.1}$$

where, for each i, the $v_{i,k}$ satisfy the properties that

$$v_{i,k+1} > v_{i,k} \quad \text{implies that} \quad v_{i,k+1} \leq |g_{i,k+1}| \tag{4.2}$$

and

$$v_{i,k} \geq |g_{i,k}|/h(k) \tag{4.3}$$

for some positive function $h(k)$ only depending on k. The motivation for introducing these new variants is the remarkable numerical performance [30] of particular choices where

$$v_{i,k} = \max_{j \in \{0,\ldots,k\}} |g_{i,j}| \quad \text{and} \quad v_{i,k} = \frac{1}{k+1} \sum_{j \in \{0,\ldots,k\}} |g_{i,j}|$$

which both satisfy (4.2) and (4.3) (with $h(k) = 1$ for the first and $h(k) = k+1$ for the second). We further illustrate this in Section 5.

We start by proving a useful technical result.

Lemma 4.1 Consider and arbitrary $i \in \{1, \ldots, n\}$ and suppose that there exists a j_ς such that

$$\min \left[\frac{g_{i,j}^2}{\varsigma_i}, \frac{g_{i,j}^2}{v_{i,j}} \right] \leq \varsigma_i \quad \text{for} \quad j \geq j_\varsigma. \tag{4.4}$$

Then

$$\min \left[\frac{g_{i,j}^2}{\varsigma_i}, \frac{g_{i,j}^2}{v_{i,j}} \right] \geq \frac{g_{i,j}^2}{2\varsigma_i} \quad \text{for} \quad j \geq j_\varsigma. \tag{4.5}$$

Proof. Suppose that there exists a $j > j_\varsigma$ such that $v_{i,j} > 2\varsigma_i$. Assume, without loss of generality that j is the smallest such index. Then $v_{i,j} > v_{i,j-1}$ and (4.2) implies that $|g_{i,j}| \geq v_{i,j} \geq 2\varsigma_i$. As a consequence,

$$\min \left[\frac{g_{i,j}^2}{\varsigma_i}, \frac{g_{i,j}^2}{v_{i,j}} \right] \geq \min[4\varsigma_i, 2\varsigma_i] > \varsigma_i,$$

which contradicts (4.4). Thus no such j can exists and $v_{i,j} \leq 2\varsigma_i$ for all $j > j_*$ and (4.5) follows. □

We are now in position to state our complexity result for the ASTR1 algorithm using weight defined by (4.1), (4.2) and (4.3).

Theorem 4.2 Suppose that AS.1, AS.2 and AS.3 hold and that the ASTR1 algorithm is applied to problem (2.1), where the scaling factors $w_{i,k}$ are chosen in accordance with (4.1), (4.2) and (4.3). Then, for any $\eta \in (0, \tau\varsigma_{\min})$ and

$$j_\eta \stackrel{\rm def}{=} \left(\frac{\kappa_{\rm B}(\kappa_{\rm B}+L)}{\theta\varsigma_{\min}(\tau\varsigma_{\min}-\eta)} \right)^{\frac{1}{\nu}}, \tag{4.6}$$

there exist a constant $\kappa_\diamond$, a subsequence $\{k_\ell\} \subseteq \{k\}_{j_\eta+1}^{\infty}$ and an index k_ς (where $\kappa_\diamond$ and k_ς only depend on the problem and the algorithmic constants) such that, for all $k_\ell \geq k_\varsigma$,

$$\min_{j\in\{0,\ldots,k_\ell\}} \|g_j\|^2 \leq \kappa_\diamond \frac{(k_\ell+1)^\mu}{k_\ell - j_\eta} \leq \frac{2\kappa_\diamond(j_\eta+1)}{k_\ell^{1-\mu}}. \tag{4.7}$$

Proof. From (2.12) and AS.3, using $w_{\min,j} \stackrel{\rm def}{=} \min_{i\in\{1,\ldots,n\}} w_{i,k}$ ensures that

$$\Gamma_0 \geq f(x_0) - f(x_{k+1}) \geq \sum_{j=0}^{k}\sum_{i=1}^{n} \frac{g_{i,j}^2}{2\kappa_{\rm B} w_{i,j}} \left[\tau\varsigma_{\min} - \frac{\kappa_{\rm BBL}}{w_{\min,j}} \right]. \tag{4.8}$$

Consider now an arbitrary $\eta \in (0, \tau\varsigma_{\min})$ and suppose first that, for some j,

$$\left[\tau\varsigma_{\min} - \frac{\kappa_{\rm BBL}}{w_{\min,j}} \right] \leq \eta, \tag{4.9}$$

i.e., using (4.1),

$$\theta\varsigma_{\min}\, j^\nu \leq w_{\min,j} \leq \frac{\kappa_{\rm BBL}}{\tau\varsigma_{\min}-\eta}.$$

But this is impossible for $j > j_\eta$ for j_η given by (4.6), and hence (4.9) fails for all $j > j_\eta$. As a consequence, we have that, for $k > j_\eta$,

$$\begin{aligned}
f(x_{j_\eta+1}) - f(x_k) &\geq \eta \sum_{j=j_\eta+1}^{k}\sum_{i=1}^{n} \frac{g_{i,j}^2}{2\kappa_{\rm B} w_{i,j}} \\
&\geq \frac{\eta}{2\kappa_{\rm B}} \sum_{j=j_\eta+1}^{k}\sum_{i=1}^{n} \frac{g_{i,j}^2}{\max[\varsigma_i, v_{i,j}]\,\theta\,(j+1)^\mu} \\
&\geq \frac{\eta}{2\kappa_{\rm B}(k+1)^\mu\theta} \sum_{j=j_\eta+1}^{k}\sum_{i=1}^{n} \min\left[\frac{g_{i,j}^2}{\varsigma_i}, \frac{g_{i,j}^2}{v_{i,j}} \right] \\
&\geq \frac{\eta(k-j_\eta)}{2\kappa_{\rm B}(k+1)^\mu\theta} \min_{j\in\{j_\eta+1,\ldots,k\}} \left(\sum_{i=1}^{n} \min\left[\frac{g_{i,j}^2}{\varsigma_i}, \frac{g_{i,j}^2}{v_{i,j}} \right] \right)
\end{aligned} \tag{4.10}$$

But we also know from (2.11), (4.1) and (4.3) that

$$\begin{aligned} f(x_0) - f(x_{j_\eta+1}) &\geq \sum_{j=0}^{j_\eta}\sum_{i=1}^{n} \frac{\tau\varsigma_{\min} g_{i,j}^2}{2\kappa_{\rm B} w_{i,j}} - \tfrac{1}{2}(\kappa_{\rm B}+L)\sum_{j=0}^{j_\eta}\sum_{i=1}^{n}\frac{g_{i,j}^2}{w_{i,j}^2} \\ &\geq -\tfrac{1}{2}(\kappa_{\rm B}+L)\sum_{j=0}^{j_\eta}\sum_{i=1}^{n}\frac{g_{i,j}^2}{w_{i,j}^2} \\ &\geq -\tfrac{1}{2}(\kappa_{\rm B}+L)\sum_{j=0}^{j_\eta}\sum_{i=1}^{n}\frac{g_{i,j}^2}{\max[\varsigma, v_{i,k}]^2 (j+1)^{2\nu}\theta^2} \\ &\geq -\tfrac{1}{2}\frac{(\kappa_{\rm B}+L)}{\theta^2}\sum_{j=0}^{j_\eta}\sum_{i=1}^{n}\frac{g_{i,j}^2}{v_{i,k}^2 (j+1)^{2\nu}} \\ &\geq -\tfrac{1}{2}\frac{(\kappa_{\rm B}+L)n}{\theta^2}\sum_{j=0}^{j_\eta} h(j)^2. \end{aligned} \tag{4.11}$$

Combining (4.10) and (4.11), we obtain that

$$\Gamma_0 \geq f(x_0)-f(x_{k+1}) \geq -\tfrac{1}{2}\frac{(\kappa_{\rm B}+L)n}{\theta^2}\sum_{j=0}^{j_\eta} h(j)^2 + \frac{\eta(k-j_\eta)}{2\kappa_{\rm B}(k+1)^\mu\theta}\min_{j\in\{j_\theta+1,\ldots,k\}}\left(\sum_{i=1}^{n}\min\left[\frac{g_{i,j}^2}{\varsigma_i}, \frac{g_{i,j}^2}{v_{i,j}}\right]\right)$$

and thus that

$$\min_{j\in\{j_\theta+1,\ldots,k\}}\left(\sum_{i=1}^{n}\min\left[\frac{g_{i,j}^2}{\varsigma_i}, \frac{g_{i,j}^2}{v_{i,j}}\right]\right) \leq \frac{2\kappa_{\rm B}(k+1)^\mu}{\eta(k-j_\eta)}\left[\Gamma_0\theta + \tfrac{1}{2}\frac{n(\kappa_{\rm B}+L)}{\theta}\sum_{j=0}^{j_\eta} h(j)^2\right]$$

and we deduce that there must exist a subsequence $\{k_\ell\} \subseteq \{k\}_{j_\eta+1}^{\infty}$ such that, for each ℓ,

$$\sum_{i=1}^{n}\min\left[\frac{g_{i,k_\ell}^2}{\varsigma_i}, \frac{g_{i,jk_\ell}^2}{v_{i,k_\ell}}\right] \leq \frac{2\kappa_{\rm B}(k_\ell+1)^\mu}{\eta(k_\ell-j_\eta)}\left[\Gamma_0\theta + \tfrac{1}{2}\frac{n(\kappa_{\rm B}+L)}{\theta}\sum_{j=0}^{j_\eta} h(j)^2\right]. \tag{4.12}$$

But

$$\frac{(k_\ell+1)^\mu}{k_\ell-j_\eta} < \frac{2^\mu k_\ell^\mu}{k_\ell-j_\eta} < \frac{2k_\ell^\mu}{k_\ell-j_\eta} = \frac{2k_\ell^\mu k_\ell}{(k_\ell-j_\eta)k_\ell} = \frac{k_\ell}{k_\ell-j_\eta}\cdot\frac{2}{k_\ell^{1-\mu}} \leq \frac{2(j_\eta+1)}{k_\ell^{1-\mu}}, \tag{4.13}$$

where we used the facts that $\mu < 1$ and that $\frac{k_\ell}{k_\ell-j_\theta}$ is a decreasing function for $k_\ell \geq j_\theta+1$. Using this inequality, we thus obtain from (4.12) that, for each ℓ,

$$\sum_{i=1}^{n}\min\left[\frac{g_{i,k_\ell}^2}{\varsigma_i}, \frac{g_{i,jk_\ell}^2}{v_{i,k_\ell}}\right] \leq \frac{4\kappa_{\rm B}(j_\eta+1)}{\eta\, k_\ell^{1-\mu}}\left[\Gamma_0\theta + \tfrac{1}{2}n\frac{(\kappa_{\rm B}+L)}{\theta}\sum_{j=0}^{j_\eta} h(j)^2\right].$$

As a consequence,

$$k_\varsigma \stackrel{\rm def}{=} \left(\frac{4\kappa_{\rm B}(j_\eta+1)\left[\Gamma_0\theta + \frac{1}{2}\frac{n(\kappa_{\rm B}+L)}{\theta}\sum_{j=0}^{j_\eta} h(j)^2\right]}{\eta\varsigma_{\min}}\right)^{\frac{1}{1-\mu}}$$

is such that, for all $k_\ell \geq k_\varsigma$,

$$\min\left[\frac{g_{i,k_\ell}^2}{\varsigma_i,}, \frac{g_{i,\ell}^2}{v_{i,k\ell}}\right] \leq \varsigma_{\min}.$$

Lemma 4.1 then yields that, for all $k_\ell \geq k_\varsigma$,

$$\sum_{i=1}^{n} \frac{g_{i,k_\ell}^2}{2\varsigma_i} \leq \frac{2\kappa_{\rm B}(k_\ell+1)^\mu}{\eta(k_\ell - j_\eta)} \left[\Gamma_0\theta + \tfrac{1}{2}\frac{n(\kappa_{\rm B}+L)}{\theta}\sum_{j=0}^{j_\eta} h(j)^2\right]$$

which, because $\varsigma_i \leq 1$, gives that, for all $k_\ell \geq k_\varsigma$,

$$\|g_{k_\ell}\|^2 \leq \frac{(k_\ell+1)^\mu}{k_\ell - j_\eta}\left(\frac{4\kappa_{\rm B}}{\eta}\right)\left[\Gamma_0\theta + \tfrac{1}{2}n\frac{(\kappa_{\rm B}+L)}{\theta}\sum_{j=0}^{j_\eta} h(j)^2\right], \tag{4.14}$$

finally implying (4.7) because of (4.13). □

We again provide some comments on this last result.

1. The choice (4.1) is of course reminiscent, in a smooth and nonconvex setting, of the "diminishing stepsize" subgradient method for stochastic problems (see [6, Theorem 1.2.4] or [4, Theorems 8.25 and 8.40] and the many references therein), for which a $\mathcal{O}(1/\sqrt{k})$ global rate of convergence is known.

2. Theorem 4.2 provides information on the speed of convergence for iterations that are beyond an *a priori* computable iteration index. Indeed j_θ and k_ς only depends on ν $h(\ell)$ and problem's constants and, in particular do not depend on k. However, the formulation of the theorem is slightly weaker than that of Theorem 3.2. Because (4.7) only holds for iterates along the subsequence $\{k_\ell\}$, there is no guarantee that the bounnd given by the right-hand-side is valid at other iterations. But note that this right-hand side depends on k_ℓ, which is an index in the complete sequence of iterates, rather than on ℓ (the subsequence index).

   This slightly weaker formulation is no longer necessary if one is ready to assume bounded gradients, as can be seen in Theorem 4.1 in [29].

3. As the chosen values of μ and ν approach zero, then the k-order of convergence beyond j_θ tends to $\mathcal{O}(1/\sqrt{k_\ell})$, which the order derived for the methods of the previous section and is the standard k-order for first-order methods using evaluations of the objective function, albeit the value of j_θ might increase.

4. As in Section 3 and considering (4.14), we may choose θ according to (3.33) in an attempt to balance the two terms of the letf-hand side and improve the explicit dependence of the complexity bound on n.

We are now again interested to estimate how sharp the k-order bound (4.7) in $\mathcal{O}(\frac{1}{k^{(1-\mu)/2}})$ is.

Theorem 4.3 The bound (4.7) is essentially sharp in that, for any $\omega > \frac{1}{2}(1-\nu)$, there exists a univariate function $f_\omega(x)$ satisfying AS.1–AS.3 such that the ASTR1 algorithm with (4.1), $B_k = 0$ and $\theta = 1$ applied to this function produces a sequence of gradient norms given by $\|g_k\| = \frac{1}{(k+1)^\omega}$.

Proof. Consider the sequence defined, for some $\omega \in (\frac{1}{2}(1-\nu), 1]$ and all $k \geq 0$, by

$$g_k = -\frac{1}{(k+1)^\omega} \quad w_k = \max\left[\varsigma, \max_{\ell\in\{0,\ldots,k\}} |g_\ell|\right] (k+1)^\nu = (k+1)^\nu, \tag{4.15}$$

$$s_k = \frac{1}{(k+1)^{2\omega-\nu}} < 1 \quad \text{and} \quad f_{k+1} = f_k + g_k s_k, \tag{4.16}$$

where we have chosen $\varsigma \in (0,1)$ and $f_0 = \zeta(2\omega + \frac{1}{2})$ where $\zeta(\cdot)$ is the Riemann zeta function. Immediately note that

$$\lim_{k\to\infty} |g_k| = 0,$$

and $|g_k| \leq= 1 = \kappa_g$ for all k. We now verify that, if

$$x_0 = 0 \quad \text{and} \quad x_k = x_{k-1} + s_{k-1} \ \text{ for } \ k \geq 1,$$

then exists a function $f_\omega(x)$ satisfying AS.1–AS.3 such that, for all $k \geq 0$,

$$f_\omega(x_k) = f_k, \quad \text{and} \quad g_\omega(x_k) = g_k,$$

and such that the sequence defined by (4.15)-(4.16) is generated by applying the ASTR1 algorithm using $B_k = 0$ and $\theta = 1$. The function $f_\omega(x)$ is constructed using Hermite interpolation on each interval $[x_k, x_{k+1}]$ (note that the x_k are monotonically increasing), which known (see [8] or [10, Th. A.9.2]) to exist whenever there exists a constant $\kappa_f \geq 0$ such that, for each k,

$$|f_{k+1} - f_k - g_k s_k| \leq \kappa_f |s_k|^2 \quad \text{and} \quad |g_{k+1} - g_k| \leq \kappa_f |s_k|.$$

The first of these conditions holds by construction of the $\{f_k\}_{k\geq 0}$. To verify the second, we first note that, because $1/(k+1)^\omega$ is a convex function of k and $|1/(k+1)| \leq 1$,

$$\frac{|g_{k+1} - g_k|}{|s_k|} \leq \frac{\omega(k+1)^{2\omega-\nu}}{(k+1)^{1+\omega}} = \frac{\omega}{(k+1)^{\nu-\omega+1}} \leq \omega \quad (k \geq 0), \tag{4.17}$$

where $\nu - \omega + 1 \geq \nu > 0$, so that the desired inequality holds with $\kappa_f = \omega$.

Moreover, Hermite interpolation guarantees that $f_\omega(x)$ is bounded below whenever $|f_k|$ and $|s_k|$ remain bounded. We have already verified the second of these conditions in (4.16). We also have from (4.16) that

$$f_0 - f_{k+1} = \sum_{j=0}^{k} \frac{1}{j+1)^{2\omega}(j+1)^\nu} \tag{4.18}$$

which converges to the finite limit $\zeta(2\omega + \nu)$ because we have chosen $\omega > \frac{1}{2}(1-\nu)$. Thus $f_k \in (0, \zeta(2\omega+\nu)]$ for all k and the first condition is also satisfied and AS.3 holds. This completes our proof. □

The conclusions which can be drawn from this theorem parallel those drawn after Theorem 3.3. The bound (4.7) is essentially sharp (in the sense of [9][(6)]) for the ASTR1 algorithm with (4.1).

5 Numerical illustration

We now provide some numerical illustration on problems which are commonly used for the evaluation of optimization algorithms. For the sake of clarity and conciseness, we needed to keep the list of algorithmic variants reported here reasonably limited, and have taken the following considerations into account for our choice.

1. Both weights' definitions (3.1) and (4.1) are illustrated. Moreover, since the Adam algorithm using (3.32) is so commonly used the stochastic context, we also included it in the comparison.

2. Despite Theorems 3.2 and 4.2 covering a wide choice of the parameters μ and ν, we have chosen to focus here on the most common choice for (3.1) and (3.32) (i.e. $\mu = \frac{1}{2}$ and $\beta_2 = \frac{9}{10}$, corresponding to Adagrad, Adagrad-Norm and Adam). When using (4.1), we have also restricted our comparison to the single choice of μ and ν used (with reasonable success) in [30], namely $\mu = \nu = \frac{1}{10}$. By contrast, we have included results for the variants of the weights' definitions for values of $\theta = 1$ (the standard choice) and $\theta = \sqrt{n}$ suggested in (3.33) for unknown Γ_0.

3. In order to be able to test enough algorithmic variants on enough problems in reasonable computing time, we have decided to focus our experiments on low-dimensional problems in the case where $\vartheta = 1$. We have nevertheless considered a few large-scale instance for the purpose of illustrating the effect of the scaling $\theta = \sqrt{n}$ which is only expected to be significant for such instances.

4. We have chosen to define the step s_k in Step 3 of the ASTR1 algorithm by approximately minimizing the quadratic model (2.10) within the ℓ_∞ trust-region using a projected truncated conjugate-gradient approach [39, 40] which is terminated as soon as

$$\|g_k + B_k s_k\|_2 \leq \max\left[10^{-12}, 10^{-5}\|g_k\|_2\right].$$

   We also considered an alternative, namely that of minimizing the quadratic model in an Euclidean ℓ_2 trust region (with the same accuracy requirement) using a Generalized Lanczos Trust Region (GLTR) technique [26].

5. We thought it would be interesting to compare "purely first-order" variants (that is variants for which $B_k = 0$ for all k) with methods using some kind of Hessian approximation. Among many possibilities, we selected three types of approximations of interest. The first is the diagonal Barzilai-Borwein approximation [3]

$$B_{k+1} = \frac{\|s_k\|_2^2}{y_k^T s_k} I_n \tag{5.1}$$

[(6)] Observe that f_0 now tends to infinity when ω tends to $\frac{1}{2}(\nu - 1)$ and hence that AS.3 fails in the limit. As before, the structure of (4.7) implies that the complexity bound deteriorates when the gap $\Gamma_0 = f(x_0) - f_{\rm low}$ grows.

Name	Norm	$w_{i,k}$ definition ($i \in \{1,\ldots,n\}$)	B_{k+1}	params
`adagnorm`	$\|\cdot\|_2$	$w_{i,k} = \left[\frac{1}{100} + \sum_{j=0}^{k} \|g_j\|_2^2\right]^{\frac{1}{2}}$	0	
`adagrad`	$\|\cdot\|_\infty$	$w_{i,k} = \left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	0	
`adamnorm`	$\|\cdot\|_2$	$w_{i,k} = \left[\frac{1}{100} + \sum_{j=0}^{k} \beta_2^{k-j}\|g_j\|_2^2\right]^{\frac{1}{2}}$	0	$\beta = \frac{9}{10}$
`adam`	$\|\cdot\|_\infty$	$w_{i,k} = \left[\frac{1}{100} + \sum_{j=0}^{k} \beta_2^{k-j} g_{i,j}^2\right]^{\frac{1}{2}}$	0	$\beta = \frac{9}{10}$
`maxgnorm`	$\|\cdot\|_2$	$w_{i,k} = (k+1)^{\frac{1}{10}} \max\left[\frac{1}{100}, \max_{j\in\{0,\ldots,k\}} \|g_j\|_2\right]$	0	
`maxg`	$\|\cdot\|_\infty$	$w_{i,k} = (k+1)^{\frac{1}{10}} \max\left[\frac{1}{100}, \max_{j\in\{0,\ldots,k\}} \|g_{i,j}\|\right]$	0	
`adagbb`	$\|\cdot\|_\infty$	$w_{i,k} = \left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	(5.1)	
`adagbfgs3`	$\|\cdot\|_\infty$	$w_{i,k} = \left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	LBFGS(3)	
`adagH`	$\|\cdot\|_\infty$	$w_{i,k} = \left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	$\nabla_x^2 f(x_{k+1})$	
`adagrads`	$\|\cdot\|_\infty$	$w_{i,k} = \sqrt{n}\left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	0	
`adams`	$\|\cdot\|_\infty$	$w_{i,k} = \sqrt{n}\left[\frac{1}{100} + \sum_{j=0}^{k} \beta_2^{k-j} g_{i,j}^2\right]^{\frac{1}{2}}$	0	$\beta = \frac{9}{10}$
`maxgs`	$\|\cdot\|_\infty$	$w_{i,k} = \sqrt{n}(k+1)^{\frac{1}{10}} \max\left[\frac{1}{100}, \max_{j\in\{0,\ldots,k\}} \|g_{i,j}\|\right]$	0	
`adagbbs`	$\|\cdot\|_\infty$	$w_{i,k} = \sqrt{n}\left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	(5.1)	
`adagbfgs3s`	$\|\cdot\|_\infty$	$w_{i,k} = \sqrt{n}\left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	LBFGS(3)	
`adagHs`	$\|\cdot\|_\infty$	$w_{i,k} = \sqrt{n}\left[\frac{1}{100} + \sum_{j=0}^{k} g_{i,j}^2\right]^{\frac{1}{2}}$	$\nabla_x^2 f(x_{k+1})$	
`sdba`	standard steepest-descent with backtracking (e.g. [10, Algorithm 2.2.1])			

Table 1: The considered algorithmic variants

where I_n is the identity matrix of dimension n, $y_k = g_{k+1} - g_k$ and $y_k^T s_k \geq 10^{-15}\|s_k\|_2^2$. The second is limited-memory BFGS approximations [37], where a small number (3) of BFGS updates are added to the matrix (5.1), each update corresponding to a secant pair (y_k, s_k) with $y_k^T s_k \geq 10^{-15}\|s_k\|_2^2$. The third is not to approximate the Hessian at all, but to use its exact value, that is $B_k = \nabla_x^2 f(x_k)$ for all k.

Given these considerations, we have selected the algorithmic `ASTR1` variants using $\gamma_k = 1$ and detailed in Table 1, where the second column indicates the norm used to define the trust-region.

Note that all variants for which $B_{k+1} = 0$ are "purely first-order" in the sense discussed above. Note also that, under AS.3, `maxgnorm` and `maxg` satisfy (4.1) with $\mu = \nu = \frac{1}{10}$, $\varsigma_i = \varsigma = \frac{1}{100}$ and $\kappa_w = \kappa_g$. All algorithms were run[(7)] on the low dimensional instances

[(7)] In Matlab® running under Ubuntu on a Dell Precision with 16 cores and 64 GB of memory.

of the problems[8] of the OPM collection [33] (April 2023), a subset of widely used CUTEst testing environment [27]. The instances are listed with their dimension in Table 2, until either $\|\nabla_x^1 f(x_k)\|_2 \leq 10^{-6}$, or a maximum of 100000 iterations was reached, or evaluation of the derivatives returned an error.

Problem	n	Problem	n	Problem	n	Problem	n	Problem	n	Problem	n
argauss	3	chebyqad	10	dixmaanl	12	heart8ls	8	msqrtals	16	scosine	10
arglina	10	cliff	2	dixon	10	helix	3	msqrtbls	16	sisser	2
arglinb	10	clplatea	16	dqartic	10	hilbert	10	morebv	12	spmsqrt	10
arglinc	10	clplateb	16	edensch	10	himln3	2	nlminsurf	16	tcontact	49
argtrig	10	clustr	2	eg2	10	himm25	2	nondquar	10	trigger	7
arwhead	10	cosine	10	eg2s	10	himm27	2	nzf1	13	tridia	10
bard	3	crglvy	4	eigfenals	12	himm28	2	osbornea	5	tlminsurfx	16
bdarwhd	10	cube	2	eigenbls	12	himm29	2	osborneb	11	tnlminsurfx	16
beale	2	curly10	10	eigencls	12	himm30	3	penalty1	10	vardim	10
biggs5	5	dixmaana	12	engval1	10	himm32	4	penalty2	10	vibrbeam	8
biggs6	6	dixmaanb	12	engval2	3	himm33	2	penalty3	10	watson	12
brownden	4	dixmaanc	12	expfit	2	hypcir	2	powellbs	2	wmsqrtals	16
booth	2	dixmaand	12	extrosnb	10	indef	10	powellsg	12	wmsqrtbls	16
box3	3	dixmaane	12	fminsurf	16	integreq	10	powellsq	2	woods	12
brkmcc	2	dixmaanf	12	freuroth	4	jensmp	2	powr	10	yfitu	3
brownal	10	dixmaang	12	genhumps	5	kowosb	4	recipe	2	zangwill2	2
brownbs	2	dixmaanh	12	gottfr	2	lminsurg	16	rosenbr	10	zangwill3	3
broyden3d	10	dixmaani	12	gulf	4	macino	10	sensors	10		
broydenbd	10	dixmaanj	12	hairy	2	mexhat	2	schmvett	3		
chandheu	10	dixmaank	12	heart6ls	6	meyer3	3	scurly10	10		

Table 2: The small OPM test problems and their dimension

Before considering the results, we make two additional comments. The first is that very few of the test functions have bounded gradients on the whole of $\mathbb{R}^n$. While this is usually not a problem when testing standard first-order descent methods (because it may then be true in the level set determined by the starting point), this is no longer the case for significantly non-monotone methods like the ones tested here. As a consequence, it may (and does) happen that the gradient evaluation is attempted at a point where its value exceeds the Matlab overflow limit, causing the algorithm to fail on the problem. The second comment is that the (sometimes quite wild) non-monotonicity of the methods considered here has another practical consequence: it happens on several nonconvex problems[9] that convergence of different algorithmic variants occurs to points with gradient norm within termination tolerance (the methods are thus achieving their objective), but these points can be quite far apart and may have very different function values.

We discuss the results of our tests from the efficiency and reliability points of view. Efficiency is measured in number of derivatives' evaluations (or, equivalently, iterations)[10]: the fewer evaluations the more efficient the algorithm. Because the standard performance profiles [18] for our selection of 16 algorithms would be too crowded to read, we follow [44] and consider the derived "global" measure $\pi_{\texttt{algo}}$ to be $\frac{1}{50}$ of the area below the curve corresponding to `algo` in this performance profile, for abscissas in the interval $[1, 50]$. The larger

[8] From their standard starting point.

[9] broyden3d, broydenbd, curly10, gottfr, hairy, indef, jensmp, osborneb, sensors, wmsqrtals, wmsqrtbls, woods.

[10] For `sdba`, gradient and objective-function evaluations.

Method	$\pi_{\texttt{algo}}$	$\rho_{\texttt{algo}}$	algo	$\pi_{\texttt{algo}}$	$\rho_{\texttt{algo}}$
adagbfgs3	0.75	69.75	adagrad	0.69	73.11
sdba	0.73	68.91	adagbfgs3	0.75	69.75
adagH	0.72	69.75	adagH	0.72	69.75
adagrad	0.69	73.11	sdba	0.73	68.91
maxg	0.66	66.39	adagHs	0.63	67.23
adagHs	0.63	67.23	maxg	0.66	66.39
adagbb	0.63	64.71	adagrads	0.60	65.55
adagbfgs3s	0.62	63.87	adagbb	0.63	64.72
maxgs	0.60	62.18	adagbfgs3s	0.62	63.87
adagrads	0.59	65.55	maxgs	0.60	62.18
adagnorm	0.58	61.34	adagnorm	0.58	61.34
maxgnorm	0.56	57.98	adagbbs	0.56	60.50
adagbbs	0.56	60.50	maxgnorm	0.56	57.98
adamnorm	0.55	34.45	adamnorm	0.55	34.45
adam	0.54	30.25	adams	0.52	33.61
adams	0.52	33.61	adam	0.54	30.25

Table 3: Performance and reliability statistics for deterministic OFFO and steepest descent algorithms on small OPM problems ($\epsilon_1 = 10^{-6}$)

this area and closer $\pi_{\texttt{algo}}$ to one, the closer the curve to the right and top borders of the plot and the better the global performance. When reporting reliability, we say that the run of an algorithmic variant on a specific test problem is successful if the gradient norm tolerance has been achieved. In what follows, $\rho_{\texttt{algo}}$ denotes the percentage of successful runs taken on all problems. Table 3 presents the values of these statistics in two columns: for easier reading, the variants are sorted by decreasing global performance ($\pi_{\texttt{algo}}$) in the first, and by decreasing reliability ($\rho_{\texttt{algo}}$) in the second. A total of 18 problems[(11)] could not be successfully solved by any of the above algorithms, we believe mostly because of ill-conditioning.

The authors are of course aware that the very limited experiments presented here do not replace extended numerical practice and could be completed in various ways. They nevertheless suggest the following (very tentative) comments.

1. There often seems to be a definite advantage in using the $\|\cdot\|_\infty$ norm over $\|\cdot\|_2$, as can be seen by comparing `adagnorm` with `adagrad` and `maxgnorm` with `maxg`. While this may be due in part to the fact that the trust region in ℓ_∞ norm is larger than that in ℓ_2 norm (and thus allows larger steps), it is also the case that the disaggregate definition of the scaling factors $w_{i,k}$ ((3.1), (3.32) or (4.1)) used in conjunction with the ℓ_∞ norm may allow a better exploitation of differences of scale between coordinates.

2. Among the "purely first-order" methods, `sdba`, `maxg` and `adagrad` are almost undistinguishable form the performance point of view, with a reliability advantage for `adagrad` (the most reliable method in our tests). This means that, at least in those experiments,

[(11)] biggs5, brownbs, cliff, genhumps, gulf, heart6ls, heart8ls, himm29, mexhat, meyer3, nondquar, osbornea, penalty2, powellbs, powellsg, scurly10, watson, yfitu.

the suggestion resulting from the theory that OFFO methods may perform comparably to standard first-order methods seems vindicated.

3. The Adam variants (`adamnorm` and `adam`) are clearly outperformed in our tests by the Adagrad ones (`adagnorm` and `adagrad`). We recall that analytical examples where Adam fails do exist, while the convergence of Adagrad is guaranteed.

4. The theoretical difference in global rate of convergence between `adagrad` and `maxg` does not seem to have much impact on the relative performance of these two methods.

5. The use of limited memory Hessian approximation (`adagbfgs3`) appears to enhance the performance of `adagrad`, but this is not the case of the Barzilai-Borwein approximation (`adagbb`) or, remarkably, for the use of the exact Hessian (`adagH`). When these methods fail, this is often because the steplength is too small to allow the truncated conjugate-gradient solver to pick up second-order information in other directions than the negative gradient. What favours the limited memory approach remains unclear at this stage.

We also note that the variants scaled with (3.33) (with Γ_0 unknown) did not perform better on small dimensional problems; possibly because the factor n does not dominate the complexity bounds in this case. To illustrate the impact of this scaling in larger cases, we ran a subset of six methods which performed well in Table 3 (namely `adagnorm`, `adagrad`, `adagrads`, `maxgnorm`, `maxg` and `maxgs`) on the broyden3d and nlminsurf problems with increasing problem dimension (we used $\epsilon_1 = 10^{-3}$). The results are reported in Table 4.

Method	broyden3d					nlminsurf				
n	10	100	1000	10000	100000	256	1034	4096	16384	65536
`adagnorm`	37	71	467	4257	43400	166	503	1791	6038	19239
`adagrad`	200	37809	37809	37809	37809	7966	30795	121164	482025	NR
`adagrads`	134	190	1452	13042	125503	138	532	2981	19414	121934
`maxgnorm`	46	76	285	1138	4520	1699	3978	3867	5355	19424
`maxg`	458	410	462	3362	36609	NC	NC	NC	NC	NR
`maxgs`	76	155	567	2048	7370	1142	1155	5049	6407	30661

Table 4: Number of iterations for convergence on the broyden3d and nlminsurf problems as a function of dimension ($\epsilon_1 = 10^{-3}$, NC = more than 10^6 iterations, NR = not run)

Despite the improvement in complexity due to choosing $\theta > 1$ being theoretical (and applies to the worst-case performance), we may still note some positive (if not completely uniform) effect in this table. The interpretation is also blurred somewhat by the fact that `maxg` and `adagrad` converged to local minimas of broyden3d rather than the global one. We nevertheless note the consistently better performance of `adagnorm` compared to `adagrad` and `adagrads`, possibly illustrating the fact that its complexity bound does not explicitly involve n.

Finally, and although this is a slight digression from the paper's main topic, we report in Table 5 how reliability of our selection of OFFO variants is impacted by noise. To obtain these results, we ran the considered methods on all test problems where the evaluations (function[(12)] and derivatives) are contaminated by 5, 15, 25 or 50 % of relative Gaussian noise with unit variance. The reliability percentages in the table result from averaging results obtained for ten independent runs.

[(12)] For `sdba`.

	$\rho_{\texttt{algo}}$/relative noise level				
algo	0%	5%	15%	25%	50%
adagH	83.19	84.96	84.20	84.71	82.18
adagHs	81.51	81.85	81.91	80.50	77.82
adagbfgs3	78.15	80.50	80.50	80.84	80.18
adagrad	77.31	80.50	80.25	80.17	80.17
adagbb	75.69	80.08	80.17	79.58	79.41
adagbfgs3s	78.99	79.50	70.67	79.41	78.66
adagbbs	73.95	78.15	78.40	78.49	77.06
adagrads	78.15	78.07	78.66	78.74	77.23
maxgs	75.63	76.39	75.46	76.05	74.54
adagnorm	75.63	75.21	75.80	75.71	74.03
maxg	74.79	74.37	75.55	78.15	78.07
maxgnorm	69.75	68.74	69.75	70.84	71.01
adams	42.86	37.98	40.25	44.79	50.84
adamnorm	42.02	37.56	44.96	50.84	55.29
adam	40.34	35.55	36.30	44.03	45.80
sdba	81.51	30.92	31.85	34.87	29.58

Table 5: Reliability of OFFO algorithms and steepest descent as a function of the level of relative Gaussian noise ($\epsilon_1 = 10^{-3}$)

As can be seen in the table, the reliability of the `sdba` methods dramatically drops as soon as noise is present, while that of the other OFFO methods is barely affected and remains globally unchanged[(13)] for increasing noise level. This is consistent with widespread experience in the deep learning context, where noise is caused by sampling among the very large number of terms defining the objective function. This observation vindicates the popularity of methods such as Adagrad in the noisy context and suggests that the new OFFO algorithms may have some practical potential.

We conclude by noting that the algorithms' reliability ($\rho_{\texttt{algo}}$ is (expectedly) better for $\epsilon_1 = 10^{-3}$ (first column of Table 5) than for $\epsilon_1 = 10^{-6}$ (Table 3), but that the improvement remains modest, the reliability of Adagrad decreasing marginally slower.

6 Conclusions

We have presented a parametric class of deterministic "trust-region minded" extensions of the Adagrad method, allowing for the use of second-order information, should it be available. We then prove that, for OFFO algorithms in this class, $\min_{j\in\{0,\ldots,k\}} \|g_j\| = \mathcal{O}(1/\sqrt{k+1})$. We have also shown that this bound, which does not require any uniform bound on the gradient, is essentially sharp. It is *identical to the global rate of convergence of standard first-order methods using both objective-function and gradient evaluations*, despite the fact that the latter exploit significantly more information. Thus, *if one considers the order of global convergence only, evaluating the objective-function values is an unnecessary effort.* We have also considered another class of OFFO algorithms inspired by the "diminishing stepsize"

[(13)] It is interesting that reliability is slightly better for the noisy cases and the better OFFO methods.

paradigm in non-smooth convex optimization and have provided an essentially sharp (but slighlty worse) global rate of convergence for this latter class. Limited numerical experiments suggest that the above theoretical conclusions may translate to practice and remain, for OFFO methods, relatively independent of noise.

Although discussed here in the context of unconstrained optimization, adaptation of the above OFFO algorithms to problems involving convex constraints (such as bounds on the variables) is relatively straightforward and practical: one then needs to intersect the trust-region with the feasible set and minimize the quadratic model in this intersection (see [14, Chapter 12]). It will be also of interest to further analyze the possible links between our proposals and those of [28], both from the theoretical and practical perspectives,as well as to extend our investigation to the class of adaptive regularization methods (see [31] for instance).

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