
OPT-AMSGrad: An Optimistic Acceleration of AMSGrad for Nonconvex Optimization

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Abstract

1 In this paper, we propose a new variant of AMSGrad [31], a popular adaptive gra-
2 dent based optimization algorithm widely used in training deep neural networks.
3 Our algorithm adds prior knowledge about the sequence of consecutive mini-batch
4 gradients leveraging an underlying structure which makes the gradients sequen-
5 tially predictable. By exploiting the predictability and ideas from Optimistic On-
6 line Learning, the proposed algorithm can accelerate the convergence and increase
7 sample efficiency. After establishing a tighter upper bound under some convexity
8 conditions on the regret, we offer a complimentary view of our algorithm which
9 generalizes the offline and stochastic versions of nonconvex optimization. In the
10 nonconvex case, we establish a $\mathcal{O}\left(\sqrt{d/T} + d/T\right)$ non-asymptotic bound inde-
11 pendent of the initialization of the method. We illustrate the practical speedup on
12 several deep learning models through numerical experiments.

13 1 Introduction

14 Deep learning models have been successful in several applications, from robotics (e.g. [21]), com-
15 puter vision (e.g. [18, 15]), reinforcement learning (e.g. [25]), to natural language processing (e.g.
16 [16]). With the sheer size of modern data sets and the dimension of neural networks, speeding up
17 training is of utmost importance. To do so, several algorithms have been proposed in recent years,
18 such as AMSGRAD [31], ADAM [19], RMSPROP [35], ADADELTA [41], and NADAM [10].

19 All the prevalent algorithms for training deep networks mentioned above combine two ideas: the
20 idea of adaptivity from ADAGRAD [11, 23] and the idea of momentum from NESTEROV’S METHOD
21 [27] or HEAVY BALL method [28]. ADAGRAD is an online learning algorithm that works well
22 compared to the standard online gradient descent when the gradient is sparse. Its update has a
23 notable feature: it leverages an anisotropic learning rate depending on the magnitude of gradient in
24 each dimension which helps in exploiting the geometry of data. On the other hand, NESTEROV’S
25 METHOD or HEAVY BALL Method [28] is an accelerated optimization algorithm which update not
26 only depends on the current iterate and current gradient but also depends on the past gradients (i.e.
27 momentum). State-of-the-art algorithms like AMSGRAD [31] and ADAM [19] leverage these ideas
28 to accelerate the training of nonconvex objective functions such as deep neural networks losses.

29 In this paper, we propose an algorithm that goes further than the hybrid of the adaptivity and mo-
30 mentum approach. Our algorithm is inspired by OPTIMISTIC ONLINE LEARNING [7, 29, 34, 1, 24],
31 which assumes that a good *predictable process* of the gradient of the loss function in each round of
32 online learning is available, and plays an action by exploiting these predictors. By exploiting this
33 (possibly) arbitrary process, algorithms in OPTIMISTIC ONLINE LEARNING enjoy smaller regret
34 than the ones without. We combine the OPTIMISTIC ONLINE LEARNING idea with the adaptivity
35 and the momentum ideas to design a new algorithm — OPT-AMSGRAD.

A single work along that direction stands out. [8] develops OPTIMISTIC-ADAM in their paper leveraging optimistic online mirror descent [30]. Yet, OPTIMISTIC-ADAM is specifically designed to optimize two-player games (e.g. GANs [15]). GANs is a two-player zero-sum game. There have been some related works in OPTIMISTIC ONLINE LEARNING like [7, 30, 34] showing that if both players use some kinds of OPTIMISTIC-update, then accelerating the convergence to the equilibrium of the game is possible. [8] was inspired by these related works and showed that OPTIMISTIC-MIRROR-DESCENT can avoid the cycle behavior in a bilinear zero-sum game, which accelerates the convergence. In contrast, in this paper, the proposed algorithm is designed to accelerate nonconvex optimization (e.g. empirical risk minimization). To the best of our knowledge, this is the first work exploring towards this direction and bridging the unfilled *theoretical* gap at the crossroads of online learning and stochastic optimization. The contributions of this paper are as follows:

- We derive an optimistic variant of AMSGRAD borrowing techniques from online learning procedures. Our method relies on (I) the addition of *prior knowledge* in the sequence of the model parameter estimations alleviating a predictable process able to provide good guesses of gradients of the loss functions through the iterations and (II) the construction of a *double update* algorithm done sequentially. We interpret this two-projection step as the learning of both an underlying scheme which makes the gradients sequentially predictable and the global parameter learning.
- We focus on the *theoretical* justifications of our method by establishing novel *non-asymptotic* and *global* convergence rates in both the convex and nonconvex case. Based on both *convex regret minimization* and *nonconvex stochastic optimization* views, we prove, respectively, that our algorithm suffers regret of $\mathcal{O}(\sqrt{\sum_{t=1}^T \|g_t - m_t\|_{\psi_{t-1}}^2})$ and achieves a rate of convergence $\mathcal{O}(\sqrt{d/T} + d/T)$.

The proposed algorithm not only adapts to the informative dimensions, exhibits momentum, but also exploits a good guess of the next gradient to facilitate acceleration. Besides the global analysis of OPT-AMSGRAD, we conduct experiments and show that the proposed algorithm not only accelerates convergence of loss function, but also leads to better empirical generalization performance.

Section 2 is devoted to introductory notions on online learning for regret minimization and adaptive learning methods for nonconvex stochastic optimization. We introduce in Section 3 our new algorithm called OPT-AMSGRAD and provide a comprehensive global analysis in both *convex/online* and *nonconvex/offline* settings in Section 4. We illustrate the benefits of our method on several finite-sum nonconvex optimization problem in Section 5. The supplementary material of this paper is devoted to the proofs of our theoretical results.

Notations: We follow the notations in related adaptive optimization papers [19, 31]. For any vector $u, v \in \mathbb{R}^d$, u/v represents element-wise division, u^2 represents element-wise square, \sqrt{u} represents element-wise square-root. We denote $g_{1:T}[i]$ as the sum of the i_{th} element of $g_1, g_2, \dots, g_T \in \mathbb{R}^d$.

2 Preliminaries

Optimistic Online learning. The standard setup of ONLINE LEARNING is that, in each round t , an online learner selects an action $w_t \in \Theta \subseteq \mathbb{R}^d$, then the learner observes $\ell_t(\cdot)$ and suffers loss $\ell_t(w_t)$ after the action is committed. The goal of the learner is to minimize the regret,

$$\mathcal{R}_T(\{w_t\}) := \sum_{t=1}^T \ell_t(w_t) - \sum_{t=1}^T \ell_t(w^*),$$

which is the cumulative loss of the learner minus the cumulative loss of some benchmark $w^* \in \Theta$. The idea of OPTIMISTIC ONLINE LEARNING (e.g. [7, 29, 34, 1]) is as follows. In each round t , the learner exploits a guess $m_t(\cdot)$ of the gradient $\nabla \ell_t(\cdot)$ of the loss function to choose an action w_t ¹. Consider the FOLLOW-THE-REGULARIZED-LEADER (FTRL, [17]) online learning algorithm which update reads

$$w_t = \arg \min_{w \in \Theta} \langle w, L_{t-1} \rangle + \frac{1}{\eta} \mathbf{R}(w), \quad (1)$$

¹Imagine that if the learner would had been known $\nabla \ell_t(\cdot)$ (i.e., exact guess) before committing its action, then it would exploit the knowledge to determine its action and consequently minimizes the regret.

where η is a parameter, $R(\cdot)$ is a 1-strongly convex function with respect to a norm ($\|\cdot\|$) on the constraint set Θ , and $L_{t-1} := \sum_{s=1}^{t-1} g_s$ is the cumulative sum of gradient vectors of the loss functions up to round $t-1$. It has been shown that FTRL has regret at most $O(\sqrt{\sum_{t=1}^T \|g_t\|_*^2})$. The update of its optimistic variant, noted OPTIMISTIC-FTRL and developed in [34] reads

$$w_t = \arg \min_{w \in \Theta} \langle w, L_{t-1} + m_t \rangle + \frac{1}{\eta} R(w), \quad (2)$$

where $\{m_t\}_{t \geq 0}$ is a predictable process incorporating (possibly arbitrarily) knowledge about the sequence of gradients $\{g_t := \nabla \ell_t(w_t)\}_{t \geq 0}$. Under the assumption that loss functions are convex, the regret of OPTIMISTIC-FTRL is at most $O(\sqrt{\sum_{t=1}^T \|g_t - m_t\|_*^2})$.

Remark: Note that the usual worst-case bound is preserved even when the predictors $\{m_t\}_{t \geq 0}$ do not predict well the gradients. Indeed, if we take the example of OPTIMISTIC-FTRL, the bound reads $\sqrt{\sum_{t=1}^T \|g_t - m_t\|_*^2} \leq 2 \max_{w \in \Theta} \|\nabla \ell_t(w)\| \sqrt{T}$ which is equal to the usual bounds up to a factor 2. Yet, when the predictions are well constructed, the regret will be lower. We will have a similar argument when we compare OPT-AMSGRAD and AMSGRAD.

We emphasize in Section 3 the importance of leveraging a good guess m_t for updating w_t in order to get a fast convergence rate (or equivalently, small regret) and present Section 5 a simple, yet effective, predictable process $\{m_t\}_{t \geq 0}$ leading to empirical acceleration.

Adaptive optimization methods. Recently, adaptive optimization has been popular in various deep learning applications due to their superior empirical performance. ADAM [19] is a very popular adaptive algorithm for training deep neural networks. It combines the momentum idea [28] with the idea of ADAGRAD [11], which has different learning rates for different dimensions, adaptive to the learning process. More specifically, the learning rate of ADAGRAD in iteration t for dimension j is proportional to the inverse of $\sqrt{\sum_{s=1}^t g_s[j]^2}$, where $g_s[j]$ is the j -th element of the gradient vector g_s at time s . This adaptive learning rate helps accelerating the convergence when the gradient vector is sparse [11] but, when applying ADAGRAD to train deep networks, it is observed that the learning rate might decay too fast [19]. Therefore, [19] proposes ADAM that uses a moving average of gradients divided by the square root of the second moment of the moving average (element-wise multiplication), for updating the model parameter w . A variant, called AMSGRAD and detailed in Algorithm 1, has been developed in [31] to fix ADAM failures at some online convex optimization problems. The difference between ADAM and AMSGRAD lies in line 7 of Algorithm 1. AMSGRAD [31] adds the max operation to guarantee a non-increasing learning rate, $\frac{\eta_t}{\sqrt{\hat{v}_t}}$, which helps for the convergence (i.e. average regret $\mathcal{R}_T/T \rightarrow 0$).

Algorithm 1 AMSGRAD [31]

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1: Required: parameter  $\beta_1, \beta_2$ , and  $\eta_t$ .
2: Init:  $w_1 \in \Theta \subseteq \mathbb{R}^d$  and  $v_0 = \epsilon \mathbf{1} \in \mathbb{R}^d$ .
3: for  $t = 1$  to  $T$  do
4:   Get mini-batch stochastic gradient  $g_t$  at  $w_t$ .
5:    $\theta_t = \beta_1 \theta_{t-1} + (1 - \beta_1) g_t$ .
6:    $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$ .
7:    $\hat{v}_t = \max(\hat{v}_{t-1}, v_t)$ .
8:    $w_{t+1} = w_t - \eta_t \frac{\theta_t}{\sqrt{\hat{v}_t}}$ . (element-wise division)
9: end for
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3 OPT-AMSGRAD Algorithm

We formulate in this section the proposed optimistic acceleration of AMSGrad, noted OPT-AMSGRAD, and detailed in Algorithm 2. It combines the idea of adaptive optimization with optimistic learning. At each iteration, the learner computes a gradient vector $g_t := \nabla \ell_t(w_t)$ at w_t (line 4), then it maintains an exponential moving average of $\theta_t \in \mathbb{R}^d$ (line 5) and $v_t \in \mathbb{R}^d$ (line 6), which is followed by the max operation to get $\hat{v}_t \in \mathbb{R}^d$ (line 7). The learner first updates an auxiliary variable $\tilde{w}_{t+1} \in \Theta$ (line 8) and then computes the next model parameter (line 9). Observe that the proposed algorithm does not reduce to AMSGRAD when $m_t = 0$, contrary to the optimistic variant of FTRL. Furthermore, combining line 8 and line 9 yields the following single update

$$w_{t+1} = \tilde{w}_t - \eta_t \frac{\theta_t}{\sqrt{\hat{v}_t}} - \eta_t \frac{h_{t+1}}{\sqrt{\hat{v}_t}}.$$

Compared to AMSGRAD, the algorithm is characterized by a *two-level* update that interlinks some *auxiliary state* \tilde{w}_t and the model parameter state, w_t , similarly to the OPTIMISTIC MIRROR DESCENT algorithm developed in [29]. It leverages the auxiliary variable (hidden model) to update

and commit w_{t+1} , which exploits the guess m_{t+1} , see Figure 1 for a schematic illustration. In the following analysis, we show that the interleaving actually leads to some cancellation in the regret bound. Such two-levels method where the guess m_t is equal to the last known gradient g_{t-1} has been exhibited recently in [7]. The gradient prediction plays an important role as discussed Section 5.

Algorithm 2 OPT-AMSGRAD

1: Required: parameter $\beta_1, \beta_2, \epsilon$, and η_t .
2: Init: $w_1 = w_{-1/2} \in \Theta \subseteq \mathbb{R}^d$ and $v_0 = \epsilon \mathbf{1} \in \mathbb{R}^d$.
3: **for** $t = 1$ to T **do**
4: Get mini-batch stochastic gradient g_t at w_t .
5: $\theta_t = \beta_1 \theta_{t-1} + (1 - \beta_1) g_t$.
6: $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$.
7: $\hat{v}_t = \max(\hat{v}_{t-1}, v_t)$.
8: $\tilde{w}_{t+1} = \tilde{w}_t - \eta_t \frac{\theta_t}{\sqrt{\hat{v}_t}}$.
9: $w_{t+1} = \tilde{w}_{t+1} - \eta_t \frac{h_{t+1}}{\sqrt{\hat{v}_t}}$,
 where $h_{t+1} := \beta_1 \theta_{t-1} + (1 - \beta_1) m_{t+1}$ and m_{t+1}
 is the guess of g_{t+1} .
10: **end for**

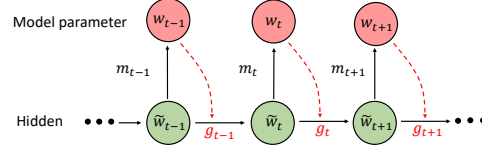


Figure 1: OPT-AMSGRAD UNDERLYING STRUCTURE.

The proposed OPT-AMSGRAD inherits three properties:

- Adaptive learning rate of each dimension as ADAGRAD [11]. (line 6, line 8 and line 9)
- Exponential moving average of the past gradients as NESTEROV'S METHOD [27] and the HEAVY-BALL method [28]. (line 5)
- Optimistic update that exploits *prior knowledge* of the next gradient vector as optimistic online learning algorithms [7, 29, 34]. (line 9)

The first property helps for acceleration when the gradient has a sparse structure. The second one is from the well-recognized idea of momentum which can also help for acceleration. The last one can actually lead to an acceleration when the prediction of the next gradient is good as mentioned above when introducing the regret bound for the OPTIMISTIC-FTRL algorithm. The latter property will be elaborated in the following subsection in which we provide the theoretical analysis of OPT-AMSGRAD. Observe that the proposed algorithm does not reduce to AMSGRAD when $m_t = 0$.

4 Global Convergence of OPT-AMSGRAD

For conciseness, we place all the proofs of the following results in the supplementary material.

Notations. We denote the Mahalanobis norm $\|\cdot\|_H := \sqrt{\langle \cdot, H \cdot \rangle}$ for some positive semidefinite (PSD) matrix H . We let $\psi_t(x) := \langle x, \text{diag}\{\hat{v}_t\}^{1/2} x \rangle$ for a PSD matrix $H_t^{1/2} := \text{diag}\{\hat{v}_t\}^{1/2}$, where $\text{diag}\{\hat{v}_t\}$ represents the diagonal matrix which i_{th} diagonal element is $\hat{v}_t[i]$ defined in Algorithm 2. We define its corresponding Mahalanobis norm $\|\cdot\|_{\psi_t} := \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{1/2} \cdot \rangle}$, where we abuse the notation ψ_t to represent the PSD matrix $H_t^{1/2} := \text{diag}\{\hat{v}_t\}^{1/2}$. Note that $\psi_t(\cdot)$ is 1-strongly convex with respect to the norm $\|\cdot\|_{\psi_t}$. Namely, $\psi_t(\cdot)$ satisfies $\psi_t(u) \geq \psi_t(v) + \langle \psi_t(v), u - v \rangle + \frac{1}{2} \|u - v\|_{\psi_t}^2$ for any point $(u, v) \in \Theta^2$. A consequence of 1-strongly convexity of $\psi_t(\cdot)$ is that $B_{\psi_t}(u, v) \geq \frac{1}{2} \|u - v\|_{\psi_t}^2$, where the Bregman divergence $B_{\psi_t}(u, v)$ is defined as $B_{\psi_t}(u, v) := \psi_t(u) - \psi_t(v) - \langle \psi_t(v), u - v \rangle$ with $\psi_t(\cdot)$ as the distance generating function. We can also define the corresponding dual norm $\|\cdot\|_{\psi_t^*} := \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{-1/2} \cdot \rangle}$.

4.1 Convex Regret Analysis

We prove the following result regarding the regret in the convex optimization setting. That is, we assume that the loss functions $\{\ell_t\}_{t \geq 0}$ are convex. We also assume that Θ has bounded diameter D_∞ , which is a standard assumption in previous works [31, 19] on adaptive methods. It is necessary in regret analysis since if the boundedness assumption is lifted, one might construct a scenario such that the benchmark is $w^* = \infty$ and the learner's regret is infinite.

163 **Theorem 1.** Suppose the learner incurs a sequence of convex loss functions $\{\ell_t(\cdot)\}$. Then, OPT-
 164 AMSGRAD (Algorithm 2) has regret

$$\mathcal{R}_T \leq \frac{B_{\psi_1}(w^*, \tilde{w}_1)}{\eta_1} + \sum_{t=1}^T \frac{\eta_t}{2} \|g_t - \tilde{m}_t\|_{\psi_{t-1}^*}^2 + \frac{D_\infty^2}{\eta_{\min}} \sum_{i=1}^d \hat{v}_T^{1/2}[i] + D_\infty^2 \beta_1^2 \sum_{t=1}^T \|g_t - \theta_{t-1}\|_{\psi_{t-1}^*}, \quad (3)$$

165 where $\tilde{m}_{t+1} = \beta_1 \theta_{t-1} + (1 - \beta_1) m_{t+1}$, $g_t := \nabla \ell_t(w_t)$, $\eta_{\min} := \min_t \eta_t$ and D_∞^2 is the diameter of
 166 the bounded set Θ . The result holds for any benchmark $w^* \in \Theta$ and any step size sequence $\{\eta_t\}_{t>0}$.

167 **Corollary 1.** Suppose $\beta_1 = 0$ and $\{v_t\}_{t>0}$ is an increasing monotone sequence, then we obtain the
 168 following regret bound for any $w^* \in \Theta$ and sequence $\{\eta_t = \eta/\sqrt{t}\}_{t>0}$:

$$\mathcal{R}_T \leq \frac{B_{\psi_1}(w^*, \tilde{w}_1)}{\eta_1} + \frac{\eta\sqrt{1+\log T}}{\sqrt{1-\beta_2}} \sum_{i=1}^d \|(g - m)_{1:T}[i]\|_2 + \frac{D_\infty^2}{\eta_{\min}} \sum_{i=1}^d \left[(1 - \beta_2) \sum_{s=1}^T \beta_2^{T-s} g_s[i]^2 \right]^{1/2},$$

169 where $g_t := \nabla \ell_t(w_t)$ and $\eta_{\min} := \min_t \eta_t$.

170 We can compare the bound of Corollary 1 with that of AMSGRAD [31] with $\eta_t = \eta/\sqrt{t}$:

$$\mathcal{R}_T \leq \frac{\eta\sqrt{1+\log T}}{\sqrt{1-\beta_2}} \sum_{i=1}^d \|g_{1:T}[i]\|_2 + \frac{\sqrt{T}}{2\eta} D_\infty^2 \sum_{i=1}^d \hat{v}_T[i]^2. \quad (4)$$

171 For convex regret minimization, the results above yields that the learner suffers regret of
 172 $\mathcal{O}(\sqrt{\sum_{t=1}^T \|g_t - m_t\|_{\psi_{t-1}}^2})$ with an access to an arbitrary predictable process $\{m_t\}_{t>0}$ of the mini-
 173 batch gradient. The better the predictors, the lower the regret, see the second term in Corollary 1
 174 compared to the first term in (4). The construction of the predictable process $\{m_t\}_{t>0}$ is thus of
 175 utmost importance for achieving optimal acceleration and can be learned through the iterations. We
 176 will not deal with the latter in this paper for the sake of page limit. Though, for implementation pur-
 177 poses, we derive a simple, yet effective, gradient prediction algorithm, see Algorithm 3 in Section 5,
 178 embedded in our OPT-AMSGRAD algorithm.

179 4.2 Nonconvex Analysis (Finite-Time Upper Bound)

180 We discuss the offline and stochastic nonconvex optimization properties of our online framework.
 181 As stated in the Introduction, this paper is about solving optimization problems instead of solving
 182 zero-sum games. Classically, the problem we are tackling reads:

$$\min_{w \in \Theta} f(w) := \mathbb{E}[f(w, \xi)] = n^{-1} \sum_{i=1}^n \mathbb{E}[f(w, \xi_i)], \quad (5)$$

183 for a fixed batch of n samples $\{\xi_i\}_{i=1}^n$. The objective function $f(w)$ is (potentially) nonconvex and
 184 has Lipschitz gradients. Set the terminating number, $T \in \{0, \dots, T_{\max} - 1\}$, as a discrete r.v. with:

$$P(T = \ell) = \frac{\eta_\ell}{\sum_{j=0}^{T_{\max}-1} \eta_j}, \quad (6)$$

185 where T_{\max} is the maximum number of iteration. The random termination number (6) is inspired by
 186 [14] and is widely used for nonconvex optimization. Assume:

187 **H1.** For any $t > 0$, the estimated weight w_t stays within a ℓ_∞ -ball. There exists a constant $W > 0$
 188 such that $\|w_t\| \leq W$ almost surely.

189 **H2.** The function $f(w)$ is L -smooth (has L -Lipschitz gradients) w.r.t. the parameter w . There exist
 190 some constant $L > 0$ such that for $(w, \vartheta) \in \Theta^2$:

$$f(w) - f(\vartheta) - \nabla f(\vartheta)^\top (w - \vartheta) \leq \frac{L}{2} \|w - \vartheta\|^2.$$

191 We assume that the optimistic guess m_t at iteration k and the true gradient g_t are correlated:

192 **H3.** There exists a constant $a \in \mathbb{R}$ such that for any $t > 0$, $\langle m_t | g_t \rangle \leq a \|g_t\|^2$.

193 Classically in nonconvex optimization [14] we make an assumption on the magnitude of the gradient:

194 **H4.** *There exists a constant $M > 0$ such that for any w and ξ , it holds $\|\nabla f(w, \xi)\| < M$.*

195 We first derive several auxiliary Lemmas. The first one ensures bounded norms of various quantities
196 of interests (resulting from the classical stochastic gradient boundedness assumption):

197 **Lemma 1.** *Assume assumption H4, then the quantities defined in Algorithm 2 satisfy for any $w \in \Theta$
198 and $t > 0$, $\|\nabla f(w_t)\| < M$, $\|\theta_t\| < M$ and $\|\hat{v}_t\| < M^2$.*

199 Then, following [39] and their study of the SGD with Momentum we denote for any $t > 0$:

$$\bar{w}_t = w_t + \frac{\beta_1}{1 - \beta_1}(w_t - \bar{w}_{t-1}) = \frac{1}{1 - \beta_1}w_t - \frac{\beta_1}{1 - \beta_1}\bar{w}_{t-1}, \quad (7)$$

200 **Lemma 2.** *Assume a strictly positive and non increasing sequence of stepsizes $\{\eta_t\}_{t>0}$, $\beta_1 < \beta_2 \in$
201 $[0, 1)$, then the following holds:*

$$\bar{w}_{t+1} - \bar{w}_t \leq \frac{\beta_1}{1 - \beta_1}\tilde{\theta}_{t-1} \left[\eta_{t-1}\hat{v}_{t-1}^{-1/2} - \eta_t\hat{v}_t^{-1/2} \right] - \eta_t\hat{v}_t^{-1/2}\tilde{g}_t,$$

202 where $\tilde{\theta}_t = \theta_t + \beta_1\theta_{t-1}$ and $\tilde{g}_t = g_t - \beta_1m_t + \beta_1g_{t-1} + m_{t+1}$.

203 **Lemma 3.** *Assume H4, a strictly positive and a sequence of constant stepsizes $\{\eta_t\}_{t>0}$, $\beta_1 < \beta_2 \in$
204 $[0, 1)$, denote $\gamma = \beta_1/\beta_2$, then the following holds:*

$$\sum_{k=1}^{T_{\max}} \eta_k^2 \mathbb{E} \left[\left\| \hat{v}_k^{-1/2} \theta_k \right\|_2^2 \right] \leq \frac{\eta^2 d T_{\max} (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)}.$$

205 We now formulate the main result of our paper giving a finite-time upper bound of the quantity
206 $\mathbb{E} [\|\nabla f(w_T)\|^2]$ where T is a random termination number distributed according to 6, see [14].

207 **Theorem 2.** *Assume H1-H4, $\beta_1 < \beta_2 \in [0, 1)$ and a sequence of decreasing stepsizes $\{\eta_t\}_{t>0}$, then
208 the following result holds:*

$$\mathbb{E} [\|\nabla f(w_T)\|^2] \leq \tilde{C}_1 \sqrt{\frac{d}{T_{\max}}} + \tilde{C}_2 \frac{1}{T_{\max}}, \quad (8)$$

209 where K is a random termination number distributed according (6). The constants are defined as:

$$\begin{aligned} \tilde{C}_1 &= C_1 + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \left[\frac{a(1 - \beta_1)^2}{1 - \beta_2} + 2L \frac{1}{1 - \beta_2} \right] \\ C_1 &= \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \Delta f + \frac{4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{(1 + \beta_1^2)(1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \\ \tilde{C}_2 &= \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E} \left[\left\| \hat{v}_0^{-1/2} \right\| \right] \end{aligned}$$

210 We remark that the bound for our OPT-AMSGrad method matches the complexity bound of
211 $\mathcal{O} \left(\sqrt{d/T_{\max}} + 1/T_{\max} \right)$ of [14] for SGD and [43] for AMSGrad method.

212 **Checking H1 for a Deep Neural Network:** Boundedness assumption is generally hard to verify.
213 We show here that the weights satisfy assumption H1 and indeed stay in a bounded set when the
214 model being trained, using our method, is a fully connected feed forward neural network. The
215 activation function for this section will be sigmoid function and we use a ℓ_2 regularization. We
216 consider a fully connected feed forward neural network with L layers modeled by the function
217 $\text{MLN}(w, \xi) : \Theta^d \times \mathbb{R}^p \rightarrow \mathbb{R}$:

$$\text{MLN}(w, \xi) = \sigma \left(w^{(L)} \sigma \left(w^{(L-1)} \dots \sigma \left(w^{(1)} \xi \right) \right) \right) \quad (9)$$

218 where $w = [w^{(1)}, w^{(2)}, \dots, w^{(L)}]$ is the vector of parameters, $\xi \in \mathbb{R}^p$ is the input data and σ is the
219 sigmoid activation function. We assume a p dimension input data and a scalar output for simplicity.
220 The stochastic objective function (5) reads:

$$f(w, \xi) = \mathcal{L}(\text{MLN}(w, \xi), y) + \frac{\lambda}{2} \|w\|^2 \quad (10)$$

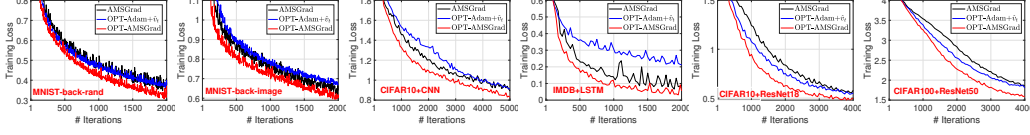


Figure 2: Training loss vs. Number of iterations. The first row are results with fully-connected NN.

where $\mathcal{L}(\cdot, y)$ is the loss function (can be Huber loss or cross entropy), y are the true labels and $\lambda > 0$ is the regularization parameter. For any layer index $\ell \in [1, L]$ we denote the output of layer ℓ by $h^{(\ell)}(w, \xi) = \sigma(w^{(\ell)} \sigma(w^{(\ell-1)} \dots \sigma(w^{(1)} \xi)))$. The following Lemma proves that assumption H1 is satisfied with a feed forward neural net (9):

Lemma 4. *Given the multilayer model (9), assume the boundedness of the input data and of the loss function, i.e., for any $\xi \in \mathbb{R}^p$ and $y \in \mathbb{R}$ there is a constant $T > 0$ such that $\|\xi\| \leq 1$ a.s. and $|\mathcal{L}'(\cdot, y)| \leq T$ where $\mathcal{L}'(\cdot, y)$ denotes its derivative w.r.t. the parameter. Then for each layer $\ell \in [1, L]$, there exist a constant $A_{(\ell)}$ such that $\|w^{(\ell)}\| \leq A_{(\ell)}$*

5 Numerical Experiments

5.1 Gradient Estimation

There are rich literatures on gradient predicting methods, with some classical works including ANDERSON acceleration [37], MINIMAL POLYNOMIAL EXTRAPOLATION [4], REDUCED RANK EXTRAPOLATION [12]. These methods aims at finding a fixed point g^* and assumes that the sequence $\{g_t\} \in \mathbb{R}^d$ has a linear relation as follows:

$$g_t - g^* = A(g_{t-1} - g^*) + e_t, \quad (11)$$

where e_t is a second order term satisfying $\|e_t\|_2 = O(\|g_{t-1} - g^*\|_2^2)$ and $A \in \mathbb{R}^{d \times d}$ is an unknown matrix, see [32] for details and results. In our numerical experiments, we propose to use the extrapolation algorithm of [32] to construct the sequence $\{m_t\}_{t>0}$ based on estimating the limit of a sequence using the last iterates [3].

Algorithm 3 REGULARIZED APPROXIMATE MINIMAL POLYNOMIAL EXTRAPOLATION [32]

- 1: **Input:** sequence $\{g_s \in \mathbb{R}^d\}_{s=0}^{s=r-1}$, parameter $\lambda > 0$.
 - 2: Compute matrix $U = [g_1 - g_0, \dots, g_r - g_{r-1}] \in \mathbb{R}^{d \times r}$.
 - 3: Obtain z by solving $(U^\top U + \lambda I)z = \mathbf{1}$.
 - 4: Get $c = z / (z^\top \mathbf{1})$.
 - 5: **Output:** $\sum_{i=0}^{r-1} c_i g_i$, the approximation of the fixed point g^* .
-

Specifically, at iteration t , m_t is obtained by (a) calling Algorithm 3 with input being a sequence of past r gradients, $\{g_{t-1}, g_{t-2}, \dots, g_{t-r}\}$ and (b) setting $m_t := \sum_{i=0}^{r-1} c_i g_{t-r+i}$ where $c = [c_0, \dots, c_{r-1}]$ is obtained by Algorithm 3. To see why the output from the extrapolation method may be a reasonable estimation, assume that the update converges to a stationary point (i.e. $g^* := \nabla f(w^*) = 0$ for the underlying function f). Then, we might rewrite (11) as $g_t = A g_{t-1} + O(\|g_{t-1}\|_2^2) u_{t-1}$, for some unit vector u_{t-1} . The equation suggests that the next gradient vector g_t is a linear transform of g_{t-1} plus an error vector that may not be in the span of A . If the algorithm is guaranteed to converge to a stationary point, the magnitude of the error component will eventually go to zero.

Computational cost. This extrapolation step consists of: (a) Constructing the linear system $(U^\top U)$ which cost can be optimized to $\mathcal{O}(d)$, since the matrix U only changes one column at a time. (b) Solving the linear system which cost is $\mathcal{O}(r^3)$, and is negligible for a small r used in practice. (c) Outputting a weighted average of previous gradients which cost is $\mathcal{O}(r \times d)$ yielding a computational overhead of $\mathcal{O}((r+1)d + r^3)$. Yet, steps (a) and (c) are parallelizable in the final implementation.

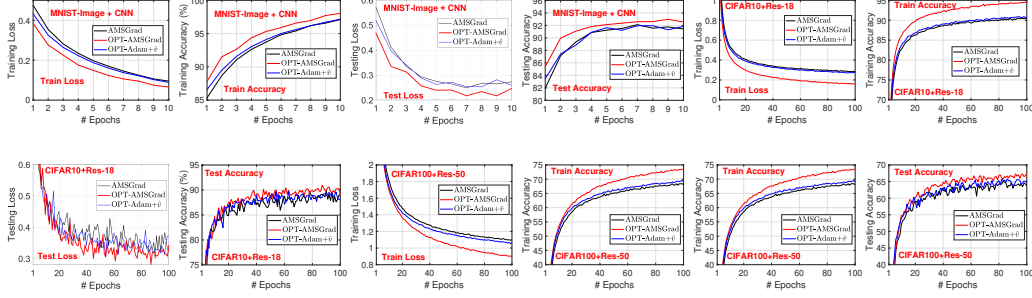


Figure 3: *MNIST-back-image* + CNN, *CIFAR10* + Res-18 and *CIFAR100* + Res-50 . We compare three methods in terms of training (cross-entropy) loss and accuracy, testing loss and accuracy.

5.2 Classification Experiments

Methods. We consider two baselines. The first one is the original AMSGRAD. The hyperparameters are set to be β_1 and β_2 to be 0.9 and 0.999 respectively, as recommended by [31]. We tune the learning rate η over a fine grid and report the best result. The other competing method is the aforementioned OPT-ADAM+ \hat{v}_t method [8], whose details are described in the Supplementary Material. We also report the best result achieved by tuning the step size η for OPT-ADAM+ \hat{v}_t . For OPT-AMSGRAD, we use the same β_1 , β_2 and the best step size η of AMSGRAD for a fair evaluation of the improvement brought by the extra optimistic step. Algorithm 3 has an additional parameter r that controls the number of previous gradients used for gradient prediction. Empirically, we observe similar performance of OPT-AMSGRAD with different values of r . Hence, we report the result for $r = 5$. More details on r will be discussed at the end of this section. In all experiments, the optimization algorithms have same initialization and the results are averaged over 5 repetitions.

Datasets. We compare different algorithms on *MNIST*, *CIFAR10*, *CIFAR100*, and *IMDB* datasets. For *MNIST*, we use two noisy variants named as *MNIST-back-rand* and *MNIST-back-image* from [20]. They both have 12000 training samples and 50000 test samples, where random background is inserted to the original *MNIST* hand written digit images. *CIFAR10* and *CIFAR100* are popular computer-vision datasets, and *IMDB* movie review dataset is a popular dataset for text classification.

Network architecture. We adopt a multi-layer fully-connected ReLU neural network with input layer followed by a hidden layer with 200 nodes, which is connected to another layer with 100 nodes before the output layer. This network is tested on *MNIST* variants. For CIFAR datasets, we adopt ALL-CNN network proposed by [33]. In addition, we also apply residual networks, Resnet-18 and Resnet-50 [18], which have achieved many state-of-the-art results. For the texture *IMDB* dataset, we consider training a Long-Short Term Memory (LSTM) network. The network includes a word embedding layer with 5000 input entries representing most frequent words in the dataset, and each word is embedded into a 32 dimensional space. The output of the embedding layer is passed to 100 LSTM units, which is then connected to 100 fully connected ReLU's before the output layer. A mini-batch size of 128 is used to compute the stochastic gradients for all experiments.

Results. Firstly, to illustrate the acceleration effect of OPT-AMSGRAD at early stage, we provide the training loss against number of iterations in Figure 2. We clearly observe that on all datasets, the proposed OPT-AMSGRAD converges faster than the other competing methods, right after the training begins. In other words, we need fewer iterations (samples) to achieve the same training loss. This validates one of the main advantages of OPT-AMSGRAD, which is a higher sample efficiency. We are also curious about the long-term performance and generalization of the proposed method in test phase. In Figure 3, we plot the corresponding results when the model is trained to the state with stable test accuracy. We observe: 1) In the long term, OPT-AMSGRAD algorithm may converge to a better point with lower loss, and 2) In this three applications, the proposed OPT-AMSGRAD also outperforms the competing methods in terms of test accuracy.

5.3 Choice of parameter r

Figure 4 compares the learning performance with different $r = 3, 5, 10$. We observe that the choice of r does not have significant impact on the training loss. Taking into consideration both quality of gradient prediction and computational cost, we recommend setting $r = 5$ in practice. As shown previously, OPT-AMSGRAD with $r = 5$ outperforms baseline methods on all the datasets.

6 Conclusion

In this paper, we propose OPT-AMSGRAD, which combines optimistic learning and AMSGRAD to improve sampling efficiency and accelerate the process of training, in particular for deep neural networks. With a good gradient prediction, the regret can be smaller than that of standard AMSGRAD. Experiments on various deep learning problems demonstrate the effectiveness of the proposed method in improving the training efficiency.

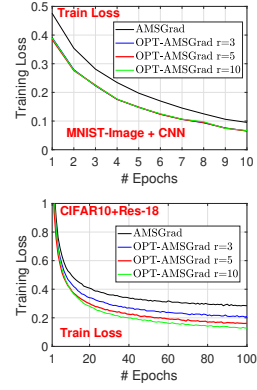


Figure 4: Training loss w.r.t. r .

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385 A Proof of Theorem 1

386 **Theorem.** Suppose the learner incurs a sequence of convex loss functions $\{\ell_t(\cdot)\}$. Then, OPT-
387 AMSGRAD (Algorithm 2) has regret

$$\mathcal{R}_T \leq \frac{B_{\psi_1}(w^*, \tilde{w}_1)}{\eta_1} + \sum_{t=1}^T \frac{\eta_t}{2} \|g_t - \tilde{m}_t\|_{\psi_{t-1}^*}^2 + \frac{D_\infty^2}{\eta_{\min}} \sum_{i=1}^d \hat{v}_T^{1/2}[i] + D_\infty^2 \beta_1^2 \sum_{t=1}^T \|g_t - \theta_{t-1}\|_{\psi_{t-1}^*}, \quad (12)$$

388 where $\tilde{m}_{t+1} = \beta_1 \theta_{t-1} + (1 - \beta_1) m_{t+1}$, $g_t := \nabla \ell_t(w_t)$, $\eta_{\min} := \min_t \eta_t$ and D_∞^2 is the diameter of
389 the bounded set Θ . The result holds for any benchmark $w^* \in \Theta$ and any step size sequence $\{\eta_t\}_{t>0}$.

390 **Proof** Beforehand, note:

$$\begin{aligned} \tilde{g}_t &= \beta_1 \theta_{t-1} + (1 - \beta_1) g_t \\ \tilde{m}_{t+1} &= \beta_1 \theta_{t-1} + (1 - \beta_1) m_{t+1} \end{aligned} \quad (13)$$

391 where we recall that g_t and m_{t+1} are respectively the gradient $\nabla \ell_t(w_t)$ and the predictable guess.
392 By regret decomposition, we have that

$$\begin{aligned} \text{Regret}_T &:= \sum_{t=1}^T \ell_t(w_t) - \min_{w \in \Theta} \sum_{t=1}^T \ell_t(w) \\ &\leq \sum_{t=1}^T \langle w_t - w^*, \nabla \ell_t(w_t) \rangle \\ &= \sum_{t=1}^T \langle w_t - \tilde{w}_{t+1}, g_t - \tilde{m}_t \rangle + \langle w_t - \tilde{w}_{t+1}, \tilde{m}_t \rangle + \langle \tilde{w}_{t+1} - w^*, \tilde{g}_t \rangle + \langle \tilde{w}_{t+1} - w^*, g_t - \tilde{g}_t \rangle. \end{aligned} \quad (14)$$

393 Recall the notation $\psi_t(x)$ and the Bregman divergence $B_{\psi_t}(u, v)$ we defined in the beginning of this
394 section. Now we are going to exploit a useful inequality (which appears in e.g., [36]); for any update
395 of the form $\hat{w} = \arg \min_{w \in \Theta} \langle w, \theta \rangle + B_\psi(w, v)$, it holds that

$$\langle \hat{w} - u, \theta \rangle \leq B_\psi(u, v) - B_\psi(u, \hat{w}) - B_\psi(\hat{w}, v) \quad \text{for any } u \in \Theta. \quad (15)$$

396 For $\beta_1 = 0$, we can rewrite the update on line 8 of (Algorithm 2) as

$$\tilde{w}_{t+1} = \arg \min_{w \in \Theta} \eta_t \langle w, \tilde{g}_t \rangle + B_{\psi_t}(w, \tilde{w}_t), \quad (16)$$

397 By using (15) for (16) with $\hat{w} = \tilde{w}_{t+1}$ (the output of the minimization problem), $u = w^*$ and
398 $v = \tilde{w}_t$, we have

$$\langle \tilde{w}_{t+1} - w^*, \tilde{g}_t \rangle \leq \frac{1}{\eta_t} [B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1}) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t)]. \quad (17)$$

399 We can also rewrite the update on line 9 of (Algorithm 2) at time t as

$$w_{t+1} = \arg \min_{w \in \Theta} \eta_{t+1} \langle w, \tilde{m}_{t+1} \rangle + B_{\psi_t}(w, \tilde{w}_{t+1}). \quad (18)$$

400 and, by using (15) for (18) (written at iteration t), with $\hat{w} = w_t$ (the output of the minimization
401 problem), $u = \tilde{w}_{t+1}$ and $v = \tilde{w}_t$, we have

$$\langle w_t - \tilde{w}_{t+1}, \tilde{m}_t \rangle \leq \frac{1}{\eta_t} [B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_{t-1}}(\tilde{w}_{t+1}, w_t) - B_{\psi_{t-1}}(w_t, \tilde{w}_t)], \quad (19)$$

402 By (14), (17), and (19), we obtain

$$\begin{aligned} \mathcal{R}_T &\stackrel{(14)}{\leq} \sum_{t=1}^T \langle w_t - \tilde{w}_{t+1}, g_t - \tilde{m}_t \rangle + \langle w_t - \tilde{w}_{t+1}, \tilde{m}_t \rangle + \langle \tilde{w}_{t+1} - w^*, \tilde{g}_t \rangle + \langle \tilde{w}_{t+1} - w^*, g_t - \tilde{g}_t \rangle \\ &\stackrel{(17), (19)}{\leq} \sum_{t=1}^T \|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}} \|g_t - \tilde{m}_t\|_{\psi_{t-1}^*} + \|\tilde{w}_{t+1} - w^*\|_{\psi_{t-1}} \|g_t - \tilde{g}_t\|_{\psi_{t-1}^*} \\ &\quad + \frac{1}{\eta_t} [B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_{t-1}}(\tilde{w}_{t+1}, w_t) - B_{\psi_{t-1}}(w_t, \tilde{w}_t) + B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1}) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t)], \end{aligned} \quad (20)$$

403 which is further bounded by

$$\begin{aligned} \mathcal{R}_T \leq & \sum_{t=1}^T \left\{ \frac{1}{2\eta_t} \|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}}^2 + \frac{\eta_t}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2 + \|\tilde{w}_{t+1} - w^*\|_{\psi_{t-1}} \|g_t - \tilde{g}_t\|_{\psi_{t-1}^*} \right. \\ & \left. + \frac{1}{\eta_t} \underbrace{(B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t))}_{A_1} - \frac{1}{2} \|\tilde{w}_{t+1} - w_t\|_{\psi_{t-1}}^2 + \underbrace{(B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1}))}_{A_2} \right\}, \end{aligned} \quad (21)$$

404 where the inequality is due to $\|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}} \|g_t - m_t\|_{\psi_{t-1}^*} = \inf_{\beta > 0} \frac{1}{2\beta} \|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}}^2 +$
 405 $\frac{\beta}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2$ by Young's inequality and the 1-strongly convex of $\psi_{t-1}(\cdot)$ with respect to $\|\cdot\|_{\psi_{t-1}}$
 406 which yields that $B_{\psi_{t-1}}(\tilde{w}_{t+1}, w_t) \geq \frac{1}{2} \|\tilde{w}_{t+1} - w_t\|_{\psi_t}^2 \geq 0$.

407 To proceed, notice that

$$A_1 = B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t) = \langle \tilde{w}_{t+1} - \tilde{w}_t, \text{diag}(\hat{v}_{t-1}^{1/2} - \hat{v}_t^{1/2})(\tilde{w}_{t+1} - \tilde{w}_t) \rangle \leq 0, \quad (22)$$

408 as the sequence $\{\hat{v}_t\}$ is non-decreasing. And that

$$\begin{aligned} A_2 &= B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1}) = \langle w^* - \tilde{w}_{t+1}, \text{diag}(\hat{v}_{t+1}^{1/2} - \hat{v}_t^{1/2})(w^* - \tilde{w}_{t+1}) \rangle \\ &\leq (\max_i (w^*[i] - \tilde{w}_{t+1}[i])^2) \cdot \left(\sum_{i=1}^d \hat{v}_{t+1}^{1/2}[i] - \hat{v}_t^{1/2}[i] \right) \end{aligned} \quad (23)$$

409 Therefore, by (21),(23),(22), we have

$$\begin{aligned} \mathcal{R}_T \leq & \frac{D_\infty^2}{\eta_{\min}} \sum_{i=1}^d \hat{v}_T^{1/2}[i] + \frac{B_{\psi_1}(w^*, \tilde{w}_1)}{\eta_1} + \sum_{t=1}^T \frac{\eta_t}{2} \|g_t - \tilde{m}_t\|_{\psi_{t-1}^*}^2 \\ & + D_\infty^2 \beta_1^2 \sum_{t=1}^T \|g_t - \theta_{t-1}\|_{\psi_{t-1}^*}^2. \end{aligned}$$

410 since $\|g_t - \tilde{g}_t\|_{\psi_{t-1}^*} = \|g_t - \beta_1 \theta_{t-1} - (1 - \beta_1)g_t\|_{\psi_{t-1}^*} = \beta^2 \|g_t - \theta_{t-1}\|_{\psi_{t-1}^*}$. This completes the
 411 proof.

412 □

413 B Proof of Corollary 1

414 **Corollary.** Suppose $\beta_1 = 0$ and $\{v_t\}_{t>0}$ is an increasing monotone sequence, then we obtain the
 415 following regret bound for any $w^* \in \Theta$ and sequence $\{\eta_t = \eta/\sqrt{t}\}_{t>0}$:

$$\mathcal{R}_T \leq \frac{B_{\psi_1}(w^*, \tilde{w}_1)}{\eta_1} + \frac{\eta\sqrt{1+\log T}}{\sqrt{1-\beta_2}} \sum_{i=1}^d \|(g - m)_{1:T}[i]\|_2 + \frac{D_\infty^2}{\eta_{\min}} \sum_{i=1}^d \left[(1 - \beta_2) \sum_{s=1}^T \beta_2^{T-s} g_s[i]^2 \right]^{1/2},$$

416 where $g_t := \nabla \ell_t(w_t)$ and $\eta_{\min} := \min_t \eta_t$.

417 **Proof** Recall the bound in Theorem 1:

$$\mathcal{R}_T \leq \frac{B_{\psi_1}(w^*, \tilde{w}_1)}{\eta_1} + \sum_{t=1}^T \frac{\eta_t}{2} \|g_t - \tilde{m}_t\|_{\psi_{t-1}^*}^2 + \frac{D_\infty^2}{\eta_{\min}} \sum_{i=1}^d \hat{v}_T^{1/2}[i] + D_\infty^2 \beta_1^2 \sum_{t=1}^T \|g_t - \theta_{t-1}\|_{\psi_{t-1}^*}^2,$$

418 The second term reads:

$$\begin{aligned}
\sum_{t=1}^T \frac{\eta_t}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2 &= \sum_{t=1}^{T-1} \frac{\eta_t}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2 + \eta_T \sum_{i=1}^d \frac{(g_T[i] - m_T[i])^2}{\sqrt{v_{T-1}[i]}} \\
&= \sum_{t=1}^{T-1} \frac{\eta_t}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2 + \eta \sum_{i=1}^d \frac{(g_T[i] - m_T[i])^2}{\sqrt{T((1-\beta_2) \sum_{s=1}^{T-1} \beta_2^{T-1-s} (g_s[i] - m_s[i])^2)}} \\
&\leq \eta \sum_{i=1}^d \sum_{t=1}^T \frac{(g_t[i] - m_t[i])^2}{\sqrt{t((1-\beta_2) \sum_{s=1}^{t-1} \beta_2^{t-1-s} (g_s[i] - m_s[i])^2)}}.
\end{aligned}$$

419 To interpret the bound, let us make a rough approximation such that $\sum_{s=1}^{t-1} \beta_2^{t-1-s} (g_s[i] - m_s[i])^2 \simeq$
420 $(g_t[i] - m_t[i])^2$. Then, we can further get an upper-bound as

$$\sum_{t=1}^T \frac{\eta_t}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2 \leq \frac{\eta}{\sqrt{1-\beta_2}} \sum_{i=1}^d \sum_{t=1}^T \frac{|g_t[i] - m_t[i]|}{\sqrt{t}} \leq \frac{\eta \sqrt{1+\log T}}{\sqrt{1-\beta_2}} \sum_{i=1}^d \|(g - m)_{1:T}[i]\|_2,$$

421 where the last inequality is due to Cauchy-Schwarz.

422

□

423 C Proofs of Auxiliary Lemmas

424 C.1 Proof of Lemma 1

Lemma. Assume assumption H4, then the quantities defined in Algorithm 2 satisfy for any $w \in \Theta$ and $t > 0$:

$$\|\nabla f(w_t)\| < M, \quad \|\theta_t\| < M, \quad \|\hat{v}_t\| < M^2.$$

Proof Assume assumption H4 we have:

$$\|\nabla f(w)\| = \|\mathbb{E}[\nabla f(w, \xi)]\| \leq \mathbb{E}[\|\nabla f(w, \xi)\|] \leq M$$

425 By induction reasoning, since $\|\theta_0\| = 0 \leq M$ and suppose that for $\|\theta_t\| \leq M$ then we have

$$\|\theta_{t+1}\| = \|\beta_1 \theta_t + (1 - \beta_1) g_{t+1}\| \leq \beta_1 \|\theta_t\| + (1 - \beta_1) \|g_{t+1}\| \leq M \quad (24)$$

426 Using the same induction reasoning we prove that

$$\|\hat{v}_{t+1}\| = \|\beta_2 \hat{v}_t + (1 - \beta_2) g_{t+1}^2\| \leq \beta_2 \|\hat{v}_t\| + (1 - \beta_1) \|g_{t+1}^2\| \leq M^2 \quad (25)$$

427

□

428 C.2 Proof of Lemma 2

429 **Lemma.** Assume a strictly positive and non increasing sequence of stepsizes $\{\eta_t\}_{t>0}$, $\beta \in [0, 1]$, then
430 the following holds:

$$\bar{w}_{t+1} - \bar{w}_t \leq \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \left[\eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t, \quad (26)$$

431 where $\tilde{\theta}_t = \theta_t + \beta_1 \theta_{t-1}$ and $\tilde{g}_t = g_t - \beta_1 m_t + \beta_1 g_{t-1} + m_{t+1}$.

432 **Proof** By definition (7) and using the Algorithm updates, we have:

$$\begin{aligned} \bar{w}_{t+1} - \bar{w}_t &= \frac{1}{1 - \beta_1} (w_{t+1} - \tilde{w}_t) - \frac{\beta_1}{1 - \beta_1} (w_t - \tilde{w}_{t-1}) \\ &= -\frac{1}{1 - \beta_1} \eta_t \hat{v}_t^{-1/2} (\theta_t + h_{t+1}) + \frac{\beta_1}{1 - \beta_1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + h_t) \\ &= -\frac{1}{1 - \beta_1} \eta_t \hat{v}_t^{-1/2} (\theta_t + \beta_1 \theta_{t-1}) - \frac{1}{1 - \beta_1} \eta_t \hat{v}_t^{-1/2} (1 - \beta_1) m_{t+1} \\ &\quad + \frac{\beta_1}{1 - \beta_1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + \beta_1 \theta_{t-2}) + \frac{\beta_1}{1 - \beta_1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} (1 - \beta_1) m_t \end{aligned} \quad (27)$$

433 Denote $\tilde{\theta}_t = \theta_t + \beta_1 \theta_{t-1}$ and $\tilde{g}_t = g_t - \beta_1 m_t + \beta_1 g_{t-1} + m_{t+1}$. Notice that $\tilde{\theta}_t = \beta_1 \tilde{\theta}_{t-1} + (1 -$
434 $\beta_1)(g_t + \beta_1 g_{t-1})$.

$$\bar{w}_{t+1} - \bar{w}_t \leq \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \left[\eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \quad (28)$$

435

□

436 C.3 Proof of Lemma 3

437 **Lemma.** Assume H4, a strictly positive and a sequence of constant stepsizes $\{\eta_t\}_{t>0}$, $\beta \in [0, 1]$, then
438 the following holds:

$$\sum_{t=1}^{T_{\max}} \eta_t^2 \mathbb{E} \left[\left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] \leq \frac{\eta^2 d T_{\max} (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \quad (29)$$

439 **Proof** We denote by index $p \in [1, d]$ the dimension of each component of vectors of interest. Noting
 440 that for any $t > 0$ and dimension p we have $\hat{v}_{t,p} \geq v_{t,p}$, then:

$$\begin{aligned} \eta_t^2 \mathbb{E} \left[\left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] &= \eta_t^2 \mathbb{E} \left[\sum_{p=1}^d \frac{\theta_{t,p}^2}{\hat{v}_{t,p}} \right] \\ &\leq \eta_t^2 \mathbb{E} \left[\sum_{i=1}^d \frac{\theta_{t,p}^2}{v_{t,p}} \right] \\ &\leq \eta_t^2 \mathbb{E} \left[\sum_{i=1}^d \frac{(\sum_{r=1}^t (1 - \beta_1) \beta_1^{t-r} g_{r,p})^2}{\sum_{r=1}^t (1 - \beta_2) \beta_2^{t-r} g_{r,p}^2} \right] \end{aligned} \quad (30)$$

441 where the last inequality is due to initializations. Denote $\gamma = \frac{\beta_1}{\beta_2}$. Then,

$$\begin{aligned} \eta_t^2 \mathbb{E} \left[\left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] &\leq \frac{\eta_t^2 (1 - \beta_1)^2}{1 - \beta_2} \mathbb{E} \left[\sum_{i=1}^d \frac{(\sum_{r=1}^t \beta_1^{t-r} g_{r,p})^2}{\sum_{r=1}^t \beta_2^{t-r} g_{r,p}^2} \right] \\ &\stackrel{(a)}{\leq} \frac{\eta_t^2 (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[\sum_{i=1}^d \frac{\sum_{r=1}^t \beta_1^{t-r} g_{r,p}^2}{\sum_{r=1}^t \beta_2^{t-r} g_{r,p}^2} \right] \\ &\leq \frac{\eta_t^2 (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[\sum_{i=1}^d \sum_{r=1}^t \gamma^{t-r} \right] = \frac{\eta_t^2 d (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[\sum_{r=1}^t \gamma^{t-r} \right] \end{aligned} \quad (31)$$

442 where (a) is due to $\sum_{r=1}^t \beta_1^{t-r} \leq \frac{1}{1 - \beta_1}$. Summing from $t = 1$ to $t = T_{\max}$ on both sides yields:

$$\begin{aligned} \sum_{t=1}^{T_{\max}} \eta_t^2 \mathbb{E} \left[\left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] &\leq \frac{\eta_t^2 d (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[\sum_{t=1}^{T_{\max}} \sum_{r=1}^t \gamma^{t-r} \right] \\ &\leq \frac{\eta^2 d T (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[\sum_{t=1}^t \gamma^{t-r} \right] \\ &\leq \frac{\eta^2 d T (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \end{aligned} \quad (32)$$

443 where the last inequality is due to $\sum_{r=1}^t \gamma^{t-r} \leq \frac{1}{1 - \gamma}$ by definition of γ . \square

444 **D Proof of Theorem 2**

445 **Theorem.** Assume H2-H4, $(\beta_1, \beta_2) \in [0, 1]$ and a sequence of decreasing stepsizes $\{\eta_t\}_{t \geq 0}$, then
 446 the following result holds:

$$\mathbb{E} [\|\nabla f(w_T)\|^2] \leq \tilde{C}_1 \sqrt{\frac{d}{T_{\max}}} + \tilde{C}_2 \frac{1}{T_{\max}} \quad (33)$$

447 where T is a random termination number distributed according (6) and the constants are defined as
 448 follows:

$$\begin{aligned} \tilde{C}_1 &= C_1 + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \left[\frac{a(1 - \beta_1)^2}{1 - \beta_2} + 2L \frac{1}{1 - \beta_2} \right] \\ C_1 &= \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \Delta f + \frac{4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{(1 + \beta_1^2)(1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \\ \tilde{C}_2 &= \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E} \left[\left\| \hat{v}_0^{-1/2} \right\| \right] \end{aligned} \quad (34)$$

449 **Proof** Using H2 and the iterate \bar{w}_t we have:

$$\begin{aligned} f(\bar{w}_{t+1}) &\leq f(\bar{w}_t) + \nabla f(\bar{w}_t)^\top (\bar{w}_{t+1} - \bar{w}_t) + \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2 \\ &\leq f(\bar{w}_t) + \underbrace{\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t)}_A + \underbrace{(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t)}_B + \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\| \end{aligned} \quad (35)$$

450 **Term A.** Using Lemma 2, we have that:

$$\begin{aligned} \nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) &\leq \nabla f(w_t)^\top \left[\frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \left[\eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right] \\ &\leq \frac{\beta_1}{1 - \beta_1} \|\nabla f(w_t)\| \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right\| \left\| \tilde{\theta}_{t-1} \right\| - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \end{aligned} \quad (36)$$

451 where the inequality is due to trivial inequality for positive diagonal matrix. Using Lemma 1 and
452 assumption H3 we obtain:

$$\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \frac{\beta_1(1 + \beta_1)}{1 - \beta_1} M^2 \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right\| - \left\| \eta_t \hat{v}_t^{-1/2} \right\| \right] - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \quad (37)$$

453 where we have used the fact that $\eta_t \hat{v}_t^{-1/2}$ is a diagonal matrix such that $\eta_{t-1} \hat{v}_{t-1}^{-1/2} \succcurlyeq \eta_t \hat{v}_t^{-1/2} \succcurlyeq 0$
454 (decreasing stepsize and max operator). Also note that:

$$\begin{aligned} -\nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t &= -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t - \nabla f(w_t)^\top \left[\eta_t \hat{v}_t^{-1/2} - \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right] \bar{g}_t \\ &\quad - \nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\beta_1 g_{t-1} + m_{t+1}) \\ &\leq -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t + (1 - a\beta_1) M^2 \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right\| - \left\| \eta_t \hat{v}_t^{-1/2} \right\| \right] \\ &\quad - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1}) \end{aligned} \quad (38)$$

455 using Lemma 1 on $\|g_t\|$ and where that $\tilde{g}_t = \bar{g}_t + \beta_1 g_{t-1} + m_{t+1} = g_t - \beta_1 m_t + \beta_1 g_{t-1} + m_{t+1}$.
456 Plugging (38) into (37) yields:

$$\begin{aligned} &\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) \\ &\leq -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t + \frac{1}{1 - \beta_1} (a\beta_1^2 - 2a\beta_1 + \beta_1) M^2 \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right\| - \left\| \eta_t \hat{v}_t^{-1/2} \right\| \right] \\ &\quad - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1}) \end{aligned} \quad (39)$$

457 **Term B.** By Cauchy-Schwarz (CS) inequality we have:

$$(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \|\nabla f(\bar{w}_t) - \nabla f(w_t)\| \|\bar{w}_{t+1} - \bar{w}_t\| \quad (40)$$

458 Using smoothness assumption H2:

$$\begin{aligned} \|\nabla f(\bar{w}_t) - \nabla f(w_t)\| &\leq L \|\bar{w}_t - w_t\| \\ &\leq L \frac{\beta_1}{1 - \beta_1} \|w_t - \tilde{w}_{t-1}\| \end{aligned} \quad (41)$$

459 By Lemma 2 we also have:

$$\begin{aligned} \bar{w}_{t+1} - \bar{w}_t &= \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \left[\eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \\ &= \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} \left[I - (\eta_t \hat{v}_t^{-1/2})(\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \\ &= \frac{\beta_1}{1 - \beta_1} \left[I - (\eta_t \hat{v}_t^{-1/2})(\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1} \right] (\tilde{w}_{t-1} - w_t) - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \end{aligned} \quad (42)$$

where the last equality is due to $\tilde{\theta}_{t-1}\eta_{t-1}\hat{v}_{t-1}^{-1/2} = \tilde{w}_{t-1} - w_t$ by construction of $\tilde{\theta}_t$. Taking the norms on both sides, observing $\left\|I - (\eta_t\hat{v}_t^{-1/2})(\eta_{t-1}\hat{v}_{t-1}^{-1/2})^{-1}\right\| \leq 1$ due to the decreasing stepsize and the construction of \hat{v}_t and using CS inequality yield:

$$\|\bar{w}_{t+1} - \bar{w}_t\| \leq \frac{\beta_1}{1-\beta_1} \|\tilde{w}_{t-1} - w_t\| + \left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\| \quad (43)$$

We recall Young's inequality with a constant $\delta \in (0, 1)$ as follows:

$$\langle X | Y \rangle \leq \frac{1}{\delta} \|X\|^2 + \delta \|Y\|^2$$

Plugging (41) and (43) into (40) returns:

$$\begin{aligned} (\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) &\leq L \frac{\beta_1}{1-\beta_1} \left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\| \|w_t - \tilde{w}_{t-1}\| \\ &\quad + L \left(\frac{\beta_1}{1-\beta_1}\right)^2 \|\tilde{w}_{t-1} - w_t\|^2 \end{aligned} \quad (44)$$

Applying Young's inequality with $\delta \rightarrow \frac{\beta_1}{1-\beta_1}$ on the product $\left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\| \|w_t - \tilde{w}_{t-1}\|$ yields:

$$(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) \leq L \left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\|^2 + 2L \left(\frac{\beta_1}{1-\beta_1}\right)^2 \|\tilde{w}_{t-1} - w_t\|^2 \quad (45)$$

The last term $\frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2$ can be upper bounded using (43):

$$\begin{aligned} \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2 &\leq \frac{L}{2} \left[\frac{\beta_1}{1-\beta_1} \|\tilde{w}_{t-1} - w_t\| + \left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\| \right]^2 \\ &\leq L \left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\|^2 + 2L \left(\frac{\beta_1}{1-\beta_1}\right)^2 \|\tilde{w}_{t-1} - w_t\|^2 \end{aligned} \quad (46)$$

Plugging (39), (45) and (46) into (35) and taking the expectations on both sides give:

$$\begin{aligned} &\mathbb{E} \left[f(\bar{w}_{t+1}) + \frac{1}{1-\beta_1} \tilde{M}^2 \left\|\eta_t\hat{v}_t^{-1/2}\right\| - \left(f(\bar{w}_t) + \frac{1}{1-\beta_1} \tilde{M}^2 \left\|\eta_{t-1}\hat{v}_{t-1}^{-1/2}\right\| \right) \right] \\ &\leq \mathbb{E} \left[-\nabla f(w_t)^\top \eta_{t-1}\hat{v}_{t-1}^{-1/2}\tilde{g}_t - \nabla f(w_t)^\top \eta_t\hat{v}_t^{-1/2}(\beta_1 g_{t-1} + m_{t+1}) \right] \\ &\quad + \mathbb{E} \left[2L \left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\|^2 + 4L \left(\frac{\beta_1}{1-\beta_1}\right)^2 \|\tilde{w}_{t-1} - w_t\|^2 \right] \end{aligned} \quad (47)$$

where $\tilde{M}^2 = (a\beta_1^2 - 2a\beta_1 + \beta_1)M^2$. Note that the expectation of \tilde{g}_t conditioned on the filtration \mathcal{F}_t reads as follows

$$\begin{aligned} \mathbb{E} [\nabla f(w_t)^\top \tilde{g}_t] &= \mathbb{E} [\nabla f(w_t)^\top (g_t - \beta_1 m_t)] \\ &= (1 - a\beta_1) \|\nabla f(w_t)\|^2 \end{aligned} \quad (48)$$

Summing from $t = 1$ to $t = T$ leads to

$$\begin{aligned} &\frac{1}{M} \sum_{t=1}^{T_{\max}} ((1-a\beta_1)\eta_{t-1} + (\beta_1+a)\eta_t) \|\nabla f(w_t)\|^2 \leq \\ &\mathbb{E} \left[f(\bar{w}_1) + \frac{1}{1-\beta_1} \tilde{M}^2 \left\|\eta_0\hat{v}_0^{-1/2}\right\| - \left(f(\bar{w}_{T_{\max}+1}) + \frac{1}{1-\beta_1} \tilde{M}^2 \left\|\eta_{T_{\max}}\hat{v}_{T_{\max}}^{-1/2}\right\| \right) \right] \\ &\quad + 2L \sum_{t=1}^{T_{\max}} \mathbb{E} \left[\left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\|^2 \right] + 4L \left(\frac{\beta_1}{1-\beta_1}\right)^2 \sum_{t=1}^{T_{\max}} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2] \\ &\leq \mathbb{E} \left[\Delta f + \frac{1}{1-\beta_1} \tilde{M}^2 \left\|\eta_0\hat{v}_0^{-1/2}\right\| \right] + 2L \sum_{t=1}^{T_{\max}} \mathbb{E} \left[\left\|\eta_t\hat{v}_t^{-1/2}\tilde{g}_t\right\|^2 \right] + 4L \left(\frac{\beta_1}{1-\beta_1}\right)^2 \sum_{t=1}^{T_{\max}} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2] \end{aligned} \quad (49)$$

where $\Delta f = f(\bar{w}_1) - f(\bar{w}_{T_{\max}+1})$. We note that by definition of \hat{v}_t , and a constant learning rate η_t , we have

$$\begin{aligned}\|\tilde{w}_{t-1} - w_t\|^2 &= \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + h_t) \right\|^2 \\ &= \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + \beta_1 \theta_{t-2} + (1 - \beta_1) m_t) \right\|^2 \\ &\leq \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \theta_{t-1} \right\|^2 + \left\| \eta_{t-2} \hat{v}_{t-2}^{-1/2} \beta_1 \theta_{t-2} \right\|^2 + (1 - \beta_1)^2 \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} m_t \right\|^2\end{aligned}\quad (50)$$

Using Lemma 3 we have

$$\begin{aligned}\sum_{t=1}^{T_{\max}} \mathbb{E} \left[\|\tilde{w}_{t-1} - w_t\|^2 \right] \\ \leq (1 + \beta_1^2) \frac{\eta^2 d T_{\max} (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} + (1 - \beta_1)^2 \sum_{t=1}^{T_{\max}} \mathbb{E} \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} m_t \right\|^2 \right]\end{aligned}\quad (51)$$

And thus, setting the learning rate to a constant value η and injecting in (49) yields:

$$\begin{aligned}\mathbb{E} [\|\nabla f(w_T)\|^2] &= \frac{1}{\sum_{j=1}^{T_{\max}} \eta_j} \sum_{t=1}^{T_{\max}} \eta_t \|\nabla f(w_t)\|^2 \\ &\leq \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_{\max}} \eta_j} \mathbb{E} \left[\Delta f + \frac{1}{1 - \beta_1} \tilde{M}^2 \left\| \eta_0 \hat{v}_0^{-1/2} \right\|^2 \right] \\ &\quad + \frac{4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_{\max}} \eta_j} (1 + \beta_1^2) \frac{\eta^2 d T_{\max} (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \\ &\quad + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_{\max}} \eta_j} (1 - \beta_1)^2 \sum_{t=1}^{T_{\max}} \mathbb{E} \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} m_t \right\|^2 \right] \\ &\quad + \frac{2LM}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_{\max}} \eta_j} \sum_{t=1}^{T_{\max}} \mathbb{E} \left[\left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\|^2 \right]\end{aligned}\quad (52)$$

where T is a random termination number distributed according (6). Setting the stepsize to $\eta = \frac{1}{\sqrt{dT_{\max}}}$ yields :

$$\begin{aligned}\mathbb{E} [\|\nabla f(w_T)\|^2] \\ \leq C_1 \sqrt{\frac{d}{T_{\max}}} + C_2 \frac{1}{T_{\max}} \\ + D_1 \frac{\eta}{T_{\max}} \sum_{t=1}^{T_{\max}} \mathbb{E} \left[\left\| \hat{v}_{t-1}^{-1/2} m_t \right\|^2 \right] + D_2 \frac{\eta}{T_{\max}} \sum_{t=1}^{T_{\max}} \mathbb{E} \left[\left\| \hat{v}_{t-1}^{-1/2} \tilde{g}_t \right\|^2 \right]\end{aligned}\quad (53)$$

where

$$\begin{aligned}C_1 &= \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \Delta f + \frac{4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{(1 + \beta_1^2)(1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \\ C_2 &= \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E} \left[\left\| \hat{v}_0^{-1/2} \right\|^2 \right]\end{aligned}\quad (54)$$

Simple case as in [43]: if $\beta_1 = 0$ then $\tilde{g}_t = g_t + m_{t+1}$ and $g_t = \theta_t$. Also using Lemma 3 we have that:

$$\sum_{t=1}^{T_{\max}} \eta_t^2 \mathbb{E} \left[\left\| \hat{v}_t^{-1/2} g_t \right\|^2 \right] \leq \frac{\eta^2 d T_{\max}}{(1 - \beta_2)} \quad (55)$$

479 which leads to the final bound:

$$\begin{aligned} & \mathbb{E} [\|\nabla f(w_T)\|^2] \\ & \leq \tilde{C}_1 \sqrt{\frac{d}{T_{\max}}} + \tilde{C}_2 \frac{1}{T_{\max}} \end{aligned} \quad (56)$$

480 where

$$\begin{aligned} \tilde{C}_1 &= C_1 + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \left[\frac{a(1 - \beta_1)^2}{1 - \beta_2} + 2L \frac{1}{1 - \beta_2} \right] \\ \tilde{C}_2 &= C_2 = \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E} [\|\hat{v}_0^{-1/2}\|] \end{aligned} \quad (57)$$

481

□

482 E Proof of Lemma 4 (Boundedness of the iterates)

483 **Lemma.** *Given the multilayer model (9), assume the boundedness of the input data and of the loss*
484 *function, i.e., for any $\xi \in \mathbb{R}^p$ and $y \in \mathbb{R}$ there is a constant $T > 0$ such that:*

$$\|\xi\| \leq 1 \quad \text{a.s.} \quad \text{and} \quad |\mathcal{L}'(\cdot, y)| \leq T \quad (58)$$

where $\mathcal{L}'(\cdot, y)$ denotes its derivative w.r.t. the parameter. Then for each layer $\ell \in [1, L]$, there exist a constant $A_{(\ell)}$ such that:

$$\|w^{(\ell)}\| \leq A_{(\ell)}$$

Proof Recall that for any layer index $\ell \in [1, L]$ we denote the output of layer ℓ by $h^{(\ell)}(w, \xi)$:

$$h^{(\ell)}(w, \xi) = \sigma \left(w^{(\ell)} \sigma \left(w^{(\ell-1)} \dots \sigma \left(w^{(1)} \xi \right) \right) \right)$$

485 Given the sigmoid assumption we have $\|h^{(\ell)}(w, \xi)\| \leq 1$ for any $\ell \in [1, L]$ and any $(w, \xi) \in$
486 $\mathbb{R}^d \times \mathbb{R}^p$. Observe that at the last layer L :

$$\begin{aligned} \|\nabla_{w^{(L)}} \mathcal{L}(\text{MLN}(w, \xi), y)\| &= \|\mathcal{L}'(\text{MLN}(w, \xi), y) \nabla_{w^{(L)}} \text{MLN}(w, \xi)\| \\ &= \left\| \mathcal{L}'(\text{MLN}(w, \xi), y) \sigma'(w^{(L)} h^{(L-1)}(w, \xi)) h^{(L-1)}(w, \xi) \right\| \\ &\leq \frac{T}{4} \end{aligned} \quad (59)$$

487 where the last equality is due to mild assumptions (58) and to the fact that the norm of the derivative
488 of the sigmoid function is upperbounded by 1/4.

489 From Algorithm 2, and with $\beta_1 = 0$ for the sake of notation, we have for iteration index $t > 0$:

$$\begin{aligned} \|w_t - \tilde{w}_{t-1}\| &= \left\| -\eta_t \hat{v}_t^{-1/2} (\theta_t + h_{t+1}) \right\| \\ &= \left\| \eta_t \hat{v}_t^{-1/2} (g_t + m_{t+1}) \right\| \\ &\leq \hat{\eta} \left\| \hat{v}_t^{-1/2} g_t \right\| + \hat{\eta} a \left\| \hat{v}_t^{-1/2} g_{t+1} \right\| \end{aligned} \quad (60)$$

where $\hat{\eta} = \max_{t>0} \eta_t$. For any dimension $p \in [1, d]$, using assumption H3, we note that

$$\sqrt{\hat{v}_{t,p}} \geq \sqrt{1 - \beta_2} g_{t,p} \quad \text{and} \quad m_{t+1} \leq a \|g_{t+1}\|$$

490 . Thus:

$$\begin{aligned} \|w_t - \tilde{w}_{t-1}\| &\leq \hat{\eta} \left(\left\| \hat{v}_t^{-1/2} g_t \right\| + a \left\| \hat{v}_t^{-1/2} g_{t+1} \right\| \right) \\ &\leq \hat{\eta} \frac{a + 1}{\sqrt{1 - \beta_2}} \end{aligned} \quad (61)$$

491 In short there exist a constant B such that $\|w_t - \tilde{w}_{t-1}\| \leq B$.

Proof by induction: As in [9], we will prove the containment of the weights by induction. Suppose an iteration index T and a coordinate i of the last layer L such that $w_{T,i}^{(L)} \geq \frac{T}{4\lambda} + B$. Using (59), we have

$$\nabla_i f(w_t^{(L)}) \geq -\frac{T}{4} + \lambda \frac{T}{\lambda 4} \geq 0$$

492 where $f(\cdot)$ is defined by (10) and is the loss of our MLN. This last equation yields $\theta_{T,i}^{(L)} \geq 0$ (given
493 the algorithm and $\beta_1 = 0$) and using the fact that $\|w_t - \tilde{w}_{t-1}\| \leq B$ we have

$$0 \leq w_{T-1,i}^{(L)} - B \leq w_{T,i}^{(L)} \leq w_{T-1,i}^{(L)} \quad (62)$$

which means that $|w_{T,i}^{(L)}| \leq w_{T-1,i}^{(L)}$. So if the first assumption of that induction reasoning holds, i.e., $w_{T-1,i}^{(L)} \geq \frac{T}{4\lambda} + B$, then the next iterates $w_{T,i}^{(L)}$ decreases, see (62) and go below $\frac{T}{4\lambda} + B$. This yields that for any iteration index $t > 0$ we have

$$w_{T,i}^{(L)} \leq \frac{T}{4\lambda} + 2B$$

since B is the biggest jump an iterate can do since $\|w_t - \tilde{w}_{t-1}\| \leq B$. Likewise we can end up showing that

$$|w_{T,i}^{(L)}| \leq \frac{T}{4\lambda} + 2B$$

494 meaning that the weights of the last layer at any iteration is bounded in some matrix norm.

495 Now that we have shown this boundedness property for the last layer L , we will do the same for the
496 previous layers and conclude the verification of assumption H1 by induction.

497 For any layer $\ell \in [1, L - 1]$, we have:

$$\nabla_{w^{(\ell)}} \mathcal{L}(\text{MLN}(w, \xi), y) = \mathcal{L}'(\text{MLN}(w, \xi), y) \left(\prod_{j=1}^{\ell+1} \sigma' \left(w^{(j)} h^{(j-1)}(w, \xi) \right) \right) h^{(\ell-1)}(w, \xi) \quad (63)$$

This last quantity is bounded as long as we can prove that for any layer ℓ the weights $w^{(\ell)}$ are bounded in some matrix norm as $\|w^{(\ell)}\|_F \leq F_\ell$ with the Frobenius norm. Suppose we have shown $\|w^{(r)}\|_F \leq F_r$ for any layer $r > \ell$. Then having this gradient (63) bounded we can use the same lines of proof for the last layer L and show that the norm of the weights at the selected layer ℓ satisfy

$$\|w^{(\ell)}\| \leq \frac{T \prod_{t \geq \ell} F_t}{4^{L-\ell+1}} + 2B$$

498 Showing that the weights of the previous layers $\ell \in [1, L - 1]$ as well as for the last layer L of our
499 fully connected feed forward neural network are bounded at each iteration, leads by induction, to
500 the boundedness (at each iteration) assumption we want to check. \square

F Comparison to some related methods

Comparison to nonconvex optimization works. Recently, [40, 5, 38, 42, 44, 22] provide some theoretical analysis of ADAM-type algorithms when applying them to smooth nonconvex optimization problems. For example, [5] provides a bound, which is $\min_{t \in [T]} \mathbb{E}[\|\nabla f(w_t)\|^2] = O(\log T / \sqrt{T})$. Yet, this data independent bound does not show any advantage over standard stochastic gradient descent. Similar concerns appear in other papers.

To get some adaptive data dependent bound that are in terms of the gradient norms observed along the trajectory) when applying OPT-AMSGRAD to nonconvex optimization, one can follow the approach of [2] or [6]. They provide ways to convert algorithms with adaptive data dependent regret bound for convex loss functions (e.g. ADAGRAD) to the ones that can find an approximate stationary point of nonconvex loss functions. Their approaches are modular so that simply using OPT-AMSGRAD as the base algorithm in their methods will immediately lead to a variant of OPT-AMSGRAD that enjoys some guarantee on nonconvex optimization. The variant can outperform the ones instantiated by other ADAM-type algorithms when the gradient prediction m_t is close to g_t . The details are omitted since this is a straightforward application.

Comparison to AO-FTRL [26]. In [26], the authors propose AO-FTRL, which has the update of the form $w_{t+1} = \arg \min_{w \in \Theta} (\sum_{s=1}^t g_s)^\top w + m_{t+1}^\top w + r_{0:t}(w)$, where $r_{0:t}(\cdot)$ is a 1-strongly convex loss function with respect to some norm $\|\cdot\|_{(t)}$ that may be different for different iteration t . Data dependent regret bound was provided in the paper, which is $r_{0:T}(w^*) + \sum_{t=1}^T \|g_t - m_t\|_{(t)}^*$ for any benchmark $w^* \in \Theta$. We see that if one selects $r_{0:t}(w) := \langle w, \text{diag}\{\hat{v}_t\}^{1/2} w \rangle$ and $\|\cdot\|_{(t)} := \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{1/2} \cdot \rangle}$, then the update might be viewed as an optimistic variant of ADAGRAD. However, no experiments was provided in [26].

Comparison to OPTIMISTIC-ADAM [8]. We are aware that [8] proposed one version of optimistic algorithm for ADAM, which is called OPTIMISTIC-ADAM in their paper. A slightly modified version is summarized in Algorithm 4. Here, OPTIMISTIC-ADAM+ \hat{v}_t is OPTIMISTIC-ADAM in [8] with the additional max operation $\hat{v}_t = \max(\hat{v}_{t-1}, v_t)$ to guarantee that the weighted second moment is monotone increasing.

Algorithm 4 OPTIMISTIC-ADAM [8]+ \hat{v}_t .

- 1: Required: parameter β_1, β_2 , and η_t .
 - 2: Init: $w_1 \in \Theta$ and $\hat{v}_0 = v_0 = \epsilon 1 \in \mathbb{R}^d$.
 - 3: **for** $t = 1$ to T **do**
 - 4: Get mini-batch stochastic gradient vector $g_t \in \mathbb{R}^d$ at w_t .
 - 5: $\theta_t = \beta_1 \theta_{t-1} + (1 - \beta_1) g_t$.
 - 6: $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$.
 - 7: $\hat{v}_t = \max(\hat{v}_{t-1}, v_t)$.
 - 8: $w_{t+1} = \Pi_k[w_t - 2\eta_t \frac{\theta_t}{\sqrt{\hat{v}_t}} + \eta_t \frac{\theta_{t-1}}{\sqrt{\hat{v}_{t-1}}}]$.
 - 9: **end for**
-

We want to emphasize that the motivations are different. OPTIMISTIC-ADAM in their paper is designed to optimize two-player games (e.g. GANs [15]), while the proposed algorithm in this paper is designed to accelerate optimization (e.g. solving empirical risk minimization quickly). [8] focuses on training GANs [15]. GANs is a two-player zero-sum game. There have been some related works in OPTIMISTIC ONLINE LEARNING like [7, 30, 34]) showing that if both players use some kinds of OPTIMISTIC-update, then accelerating the convergence to the equilibrium of the game is possible. [8] was inspired by these related works and showed that OPTIMISTIC-MIRROR-DESCENT can avoid the cycle behavior in a bilinear zero-sum game, which accelerates the convergence. Furthermore, [8] did not provide theoretical analysis of OPTIMISTIC-ADAM.

G Additional Remarks and Runs on the Gradient Prediction Process

Two illustrative examples. We provide two toy examples to demonstrate how OPT-AMSGRAD works with the chosen extrapolation method. First, consider minimizing a quadratic function

540 $H(w) := \frac{b}{2}w^2$ with vanilla gradient descent method $w_{t+1} = w_t - \eta_t \nabla H(w_t)$. The gradient
541 $g_t := \nabla H(w_t)$ has a recursive description as $g_{t+1} = bw_{t+1} = b(w_t - \eta_t g_t) = g_t - b\eta_t g_t$. So,
542 the update can be written in the form of $g_t = Ag_{t-1} + O(\|g_{t-1}\|_2^2)u_{t-1}$, with $A = (1 - b\eta)$ and
543 $u_{t-1} = 0$ by setting $\eta_t = \eta$ (constant step size). Therefore, the extrapolation method should predict
544 well.

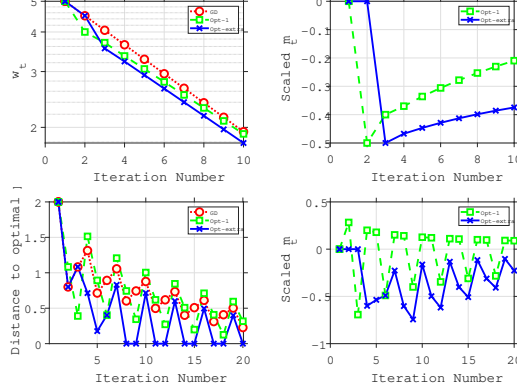


Figure 5: (a): The iterate w_t ; the closer to the optimal point 0 the better. (b): A scaled and clipped version of m_t : $w_t - w_{t-1/2}$, which measures how the prediction of m_t drives the update towards the optimal point. In this scenario, the more negative the better. (c): Distance to the optimal point -1 . The smaller the better. (d): A scaled and clipped version of m_t : $w_t - w_{t-1/2}$, which measures how the prediction of m_t drives the update towards the optimal point. In this scenario, the more negative the better.

545 Specifically, consider optimizing $H(w) := w^2/2$ by the following three algorithms with the same
546 step size. One is Gradient Descent (GD): $w_{t+1} = w_t - \eta_t g_t$, while the other two are OPT-
547 AMSGRAD with $\beta_1 = 0$ and the second moment term \hat{v}_t being dropped: $w_{t+\frac{1}{2}} = \Pi_{\Theta}[w_{t-\frac{1}{2}} - \eta_t g_t]$,
548 $w_{t+1} = \Pi_{\Theta}[w_{t+\frac{1}{2}} - \eta_{t+1} m_{t+1}]$. We denote the algorithm that sets $m_{t+1} = g_t$ as Opt-1, and denote
549 the algorithm that uses the extrapolation method to get m_{t+1} as Opt-extra. We let $\eta_t = 0.1$ and the
550 initial point $w_0 = 5$ for all the three methods. The simulation results are on Figure 5 (a) and (b).
551 Sub-figure (a) plots update w_t over iteration, where the updates should go towards the optimal point
552 0. Sub-figure (b) is about a scaled and clipped version of m_t , defined as $w_t - w_{t-1/2}$, which can be
553 viewed as $-\eta_t m_t$ if the projection (if exists) is lifted. Sub-figure (a) shows that Opt-extra converges
554 faster than the other methods. Furthermore, sub-figure (b) shows that the prediction by the extrap-
555 olation method is better than the prediction by simply using the previous gradient. The sub-figure
556 shows that $-m_t$ from both methods all point to 0 in all iterations and the magnitude is larger for the
557 one produced by the extrapolation method after iteration 2. ²

558 Now let us consider another problem: an online learning problem proposed in [31] ³. Assume the
559 learner's decision space is $\Theta = [-1, 1]$, and the loss function is $\ell_t(w) = 3w$ if $t \bmod 3 = 1$, and
560 $\ell_t(w) = -w$ otherwise. The optimal point to minimize the cumulative loss is $w^* = -1$. We
561 let $\eta_t = 0.1/\sqrt{t}$ and the initial point $w_0 = 1$ for all the three methods. The parameter λ of the
562 extrapolation method is set to $\lambda = 10^{-3} > 0$. The results are on Figure 5 (c) and (d). Sub-figure
563 (c) shows that Opt-extra converges faster than the other methods while Opt-1 is not better than GD.
564 The reason is that the gradient changes from -1 to 3 at $t \bmod 3 = 1$ and it changes from 3 to -1
565 at $t \bmod 3 = 2$. Consequently, using the current gradient as the guess for the next clearly is not a
566 good choice, since the next gradient is in the opposite direction of the current one. Sub-figure (d)
567 shows that $-m_t$ by the extrapolation method always points to $w^* = -1$, while the one by using
568 the previous negative direction points to the opposite direction in two thirds of rounds. It shows
569 that the extrapolation method is much less affected by the gradient oscillation and always makes the
570 prediction in the right direction, which suggests that the method can capture the aggregate effect.

² The extrapolation method needs at least two gradients for prediction. This is why in the first two iterations, m_t is 0.

³ [31] uses this example to show that ADAM [19] fails to converge.