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# 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 [30], a popular adaptive gra-  
2 dient based optimization algorithm widely used for training deep neural networks.  
3 Our algorithm adds prior knowledge about the sequence of consecutive mini-batch  
4 gradients and leverages its underlying structure making the gradients sequentially  
5 predictable. By exploiting the predictability and ideas from Optimistic Online  
6 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 version of nonconvex optimization. In the  
10 nonconvex case, we establish a non-asymptotic convergence bound independently  
11 of the initialization of the method. We illustrate the practical speedup on several  
12 deep learning models through numerical experiments.

## 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]) and natural language processing (e.g.  
16 [16]). With the sheer size of modern datasets 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 [30], ADAM [19], RMSPROP [34], ADADELTA [40], 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 the 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 [30] 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, 33, 1, 24],  
31 which assumes that, in each round of online learning, a *predictable process* of the gradient of the  
32 loss function is available. Then an action is played exploiting these predictors. By capitalizing on  
33 this (possibly) arbitrary process, algorithms in OPTIMISTIC ONLINE LEARNING enjoy smaller re-  
34 gret than the ones without gradient predictions. We combine the OPTIMISTIC ONLINE LEARNING  
35 idea with the adaptivity and the momentum ideas to design a new algorithm — OPT-AMSGRAD.

36 A single work along that direction stands out. Daskalakis et al. [8] develop OPTIMISTIC-ADAM  
37 leveraging optimistic online mirror descent [29]. Yet, OPTIMISTIC-ADAM is specifically designed

to optimize two-player games, e.g. GANs [15] which is in particular a two-player zero-sum game. There have been some related works in OPTIMISTIC ONLINE LEARNING [7, 29, 33] showing that if both players use an OPTIMISTIC type of update, then accelerating the convergence to the equilibrium of the game is possible. Daskalakis et al. [8] build on these related works and show that OPTIMISTIC-MIRROR-DESCENT can avoid the cycle behavior in a bilinear zero-sum game accelerating 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 guesses of gradients through the iterations and (II) the construction of a *double update* algorithm done sequentially. We interpret this two-projection step as the learning of the global parameter and of an underlying scheme which makes the gradients sequentially predictable.
- We focus on the *theoretical* justifications of our method by establishing novel *non-asymptotic* and *global* convergence rates in both convex and nonconvex cases. Based on *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 convergence rate  $\mathcal{O}(\sqrt{d/T} + d/T)$ , where  $g_t$  is the gradient and  $m_t$  is its prediction.

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 the training procedure, 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, namely 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 problems in Section 5. The supplementary material of this paper is devoted to the proofs of our theoretical results.

**Notations:** We follow the notations of adaptive optimization [19, 30]. For any  $u, v \in \mathbb{R}^d$ ,  $u/v$  represents the element-wise division,  $u^2$  the element-wise square,  $\sqrt{u}$  the element-wise square-root. We denote  $g_{1:T}[i]$  as the sum of the  $i_{th}$  element of  $g_1, \dots, g_T \in \mathbb{R}^d$  and  $\|\cdot\|$  as the Euclidean norm.

## 2 Preliminaries

**Optimistic Online learning.** The standard setup of ONLINE LEARNING is that, in each round  $t$ , an online learner selects an action  $w_t \in \Theta \subseteq \mathbb{R}^d$ , observes  $\ell_t(\cdot)$  and suffers the associated 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, 33, 1]) is as follows. In each round  $t$ , the learner exploits a guess  $m_t(\cdot)$  of the gradient  $\nabla \ell_t(\cdot)$  to choose an action  $w_t$ <sup>1</sup>. Consider the FOLLOW-THE-REGULARIZED-LEADER (FTRL, [17]) online learning algorithm which update reads

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

where  $\eta$  is a parameter,  $\mathbf{R}(\cdot)$  is a 1-strongly convex function with respect to a given norm on the constraint set  $\Theta$ , and  $L_{t-1} := \sum_{s=1}^{t-1} g_s$  is the cumulative sum of gradient vectors of the loss functions

<sup>1</sup>Imagine that if the learner would have 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 minimize the regret.

up to round  $t - 1$ . It has been shown that FTRL has regret at most  $\mathcal{O}(\sqrt{\sum_{t=1}^T \|g_t\|_*^2})$ . The update of its optimistic variant, noted OPTIMISTIC-FTRL and developed in [33] reads

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

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, it has been shown in [33] that the regret of OPTIMISTIC-FTRL is at most  $\mathcal{O}(\sqrt{\sum_{t=1}^T \|g_t - m_t\|_*^2})$ .

*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 bound up to a factor 2 [29]. Yet, when the predictors  $\{m_t\}_{t \geq 0}$  are well designed, the regret will be lower. We will have a similar argument when comparing OPT-AMSGRAD and AMSGRAD regret bounds in Section 4.1. 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 introduce in Section 5 a simple predictable process  $\{m_t\}_{t \geq 0}$  leading to empirical acceleration on various applications.

**Adaptive optimization methods.** Adaptive optimization has been popular in various deep learning applications due to their superior empirical performance. ADAM [19], a popular adaptive algorithm, combines momentum [28] and anisotropic learning rate of ADAGRAD [11]. More specifically, the learning rate of ADAGRAD at time  $t$  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 neural networks, it is observed that the learning rate might decay too fast [19]. Therefore, Kingma and Ba [19] propose ADAM that uses a moving average of the 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 [30] to fix ADAM failures. The difference between ADAM and AMSGRAD lies in Line 7 of Algorithm 1. The AMSGRAD algorithm [30] applies the max operation on the second moment to guarantee a non-increasing learning rate  $\eta_t / \sqrt{\hat{v}_t}$ , which helps for the convergence (i.e. average regret  $\mathcal{R}_T/T \rightarrow 0$ ).

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#### Algorithm 1 AMSGRAD [30]

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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, namely 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  $w_{t+1}$  (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  $w_{t+1} = \tilde{w}_t - \eta_t(\theta_t + h_{t+1})/\sqrt{\hat{v}_t}$ .

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. 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

127 gradient prediction process plays an important role as discussed in Section 5. The proposed OPT-  
 128 AMSGRAD inherits three properties: (i) Adaptive learning rate of each dimension as ADAGRAD  
 129 [11] (line 6, line 8 and line 9). (ii) Exponential moving average of the past gradients as NESTEROV'S  
 130 METHOD [27] and the HEAVY-BALL method [28] (line 5). (iii) Optimistic update that exploits *prior*  
 131 *knowledge* of the next gradient vector as in optimistic online learning algorithms [7, 29, 33] (line 9).  
 132 The first property helps for acceleration when the gradient has a sparse structure. The second one is  
 133 from the long-established idea of momentum which can also help for acceleration. The last one can  
 134 lead to an acceleration when the prediction of the next gradient is good as mentioned above when  
 135 introducing the regret bound for the OPTIMISTIC-FTRL algorithm. This property will be elaborated  
 136 whilst establishing the theoretical analysis of OPT-AMSGRAD.

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**Algorithm 2** OPT-AMSGRAD

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1: **Required:** parameter  $\beta_1, \beta_2, \epsilon$ , and  $\eta_t$ .  
 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  $h_{t+1} := \beta_1 \theta_{t-1} + (1 - \beta_1) m_{t+1}$  with  
      $m_{t+1}$  the guess of  $g_{t+1}$ .  
 10: **end for**

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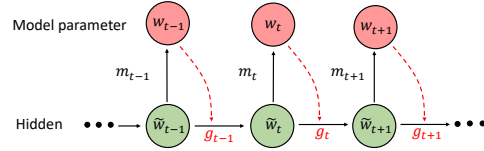


Figure 1: OPT-AMSGRAD Underlying Structure.

## 138 4 Global Convergence Analysis of OPT-AMSGRAD

139 **More 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  $H_t^{1/2} := \text{diag}\{\hat{v}_t\}^{1/2}$ ,  
 140 where  $\text{diag}\{\hat{v}_t\}$  represents the diagonal matrix which  $i_{th}$  diagonal element is  $\hat{v}_t[i]$  defined in Al-  
 141 gorithm 2. We define its corresponding Mahalanobis norm  $\|\cdot\|_{\psi_t} := \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{1/2} \cdot \rangle}$ , where  
 142 we abuse the notation  $\psi_t$  to represent the PSD matrix  $H_t^{1/2} := \text{diag}\{\hat{v}_t\}^{1/2}$ . Note that  $\psi_t(\cdot)$  is  
 143 1-strongly convex with respect to the norm  $\|\cdot\|_{\psi_t}$ . A consequence of 1-strongly convexity of  
 144  $\psi_t(\cdot)$  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  
 145  $B_{\psi_t}(u, v) := \psi_t(u) - \psi_t(v) - \langle \psi_t(v), u - v \rangle$  with  $\psi_t(\cdot)$  as the distance generating function. We  
 146 also define the corresponding dual norm  $\|\cdot\|_{\psi_t^*} := \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{-1/2} \cdot \rangle}$ .  
 147

### 148 4.1 Convex Regret Analysis

149 In this section, we assume convexity of  $\{\ell_t\}_{t \geq 0}$  and that  $\Theta$  has a bounded diameter  $D_\infty$ , which is a  
 150 standard assumption for adaptive methods [30, 19] and is necessary in regret analysis.

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

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

153 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  $D_\infty^2$  is the diameter of  
 154 the bounded set  $\Theta$ . The result holds for any benchmark  $w^* \in \Theta$  and any step size sequence  $\{\eta_t\}_{t \geq 0}$ .

155 **Corollary 1.** Suppose  $\beta_1 = 0$  and  $\{v_t\}_{t \geq 0}$  is a monotonically increasing sequence, then we obtain  
 156 the following regret bound for any  $w^* \in \Theta$  and sequence of stepsizes  $\{\eta_t = \eta/\sqrt{t}\}_{t \geq 0}$ :

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

157 where  $B_{\psi_1} := B_{\psi_1}(w^*, \tilde{w}_1)$ ,  $g_t := \nabla \ell_t(w_t)$  and  $\eta_{\min} := \min_t \eta_t$ .

158 We can compare the bound of Corollary 1 with that of AMSGRAD [30] with  $\eta_t = \eta/\sqrt{t}$ :

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

159 For convex regret minimization, Corollary 1 yields a regret of  $\mathcal{O}(\sqrt{\sum_{t=1}^T \|g_t - m_t\|_{\psi_{t-1}^*}^2})$  with an  
 160 access to an arbitrary predictable process  $\{m_t\}_{t \geq 0}$  of the mini-batch gradients. We notice from  
 161 the second term in Corollary 1 compared to the first term in (2) that better predictors lead to lower  
 162 regret. The construction of the predictions  $\{m_t\}_{t \geq 0}$  is thus of utmost importance for achieving  
 163 optimal acceleration and can be learned through the iterations [29]. In Section 5, we derive a basic,  
 164 yet effective, gradients prediction algorithm, see Algorithm 3, embedded in OPT-AMSGRAD.

## 165 4.2 Finite-Time Analysis in the Nonconvex Case

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

$$\min_{w \in \Theta} f(w) := \mathbb{E}[f(w, \xi)] = n^{-1} \sum_{i=1}^n \mathbb{E}[f(w, \xi_i)], \quad (3)$$

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

$$P(T = \ell) = \frac{\eta_\ell}{\sum_{j=0}^{T_M-1} \eta_j}, \quad (4)$$

171 where  $T_M$  is the maximum number of iteration. The random termination number (4) is inspired by  
 172 [14] and is widely used for nonconvex optimization. Assume the following:

173 **H1.** For any  $t > 0$ , the estimated parameter  $w_t$  stays within a  $\ell_\infty$ -ball. There exists a constant  
 174  $W > 0$  such that  $\|w_t\|_\infty \leq W$  almost surely.

175 **H2.** The function  $f$  is  $L$ -smooth (has  $L$ -Lipschitz gradients) w.r.t. the parameter  $w$ . There exists  
 176 some constant  $L > 0$  such that for  $(w, \vartheta) \in \Theta^2$ ,  $f(w) - f(\vartheta) - \nabla f(\vartheta)^\top (w - \vartheta) \leq \frac{L}{2} \|w - \vartheta\|^2$ .

177 We assume that the optimistic guess  $m_t$  at iteration  $t$  and the true gradient  $g_t$  are correlated:

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

179 We make a classical assumption in nonconvex optimization [14] on the magnitude of the gradient:

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

181 We now derive important auxiliary Lemmas for our global analysis. The first one ensures bounded  
 182 norms of quantities of interests (resulting from the bounded stochastic gradient assumption):

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

185 We now formulate the main result of our paper yielding a finite-time upper bound of the subopti-  
 186 mality condition  $\mathbb{E}[\|\nabla f(w_T)\|^2]$  (set as the convergence criterion of interest, see [14]):

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

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

189 where  $T$  is a random termination number distributed according (4). The constants are defined as:

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

190 The bound for our OPT-AMSGrad method matches the complexity bound of  $\mathcal{O}(\sqrt{d/T_M} + 1/T_M)$   
 191 of [14] for SGD considering the dependence of  $T$  only, and of [41] for AMSGrad method.



### 4.3 Checking H1 for a Deep Neural Network

As boundedness assumption H1 is generally hard to verify, we now show, for illustrative purposes, that the weights of a fully connected feed forward neural network stay in a bounded set when being trained using our method. The activation function for this section will be sigmoid function and we use a  $\ell_2$  regularization. We consider a fully connected feed forward neural network with  $L$  layers modeled by the function  $\text{MLN}(w, \xi) : \Theta^d \times \mathbb{R}^p \rightarrow \mathbb{R}$  defined as:

$$\text{MLN}(w, \xi) = \sigma \left( w^{(L)} \sigma \left( w^{(L-1)} \dots \sigma \left( w^{(1)} \xi \right) \right) \right), \quad (5)$$

where  $w = [w^{(1)}, w^{(2)}, \dots, w^{(L)}]$  is the vector of parameters,  $\xi \in \mathbb{R}^p$  is the input data and  $\sigma$  is the sigmoid activation function. We assume a  $p$  dimension input data and a scalar output for simplicity. In this setting, the stochastic objective function (3) reads

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

where  $\mathcal{L}(\cdot, y)$  is the loss function (e.g., cross-entropy),  $y$  are the true labels and  $\lambda > 0$  is the regularization parameter. We establish that assumption H1 is satisfied with a neural network as in (5):

**Lemma 2.** *Given the multilayer model (5), 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

Based on the analysis in the previous section, we understand that the choice of the prediction  $m_t$  plays an important role in the convergence of OPTIMISTIC-AMSGRAD. Some classical works in gradient prediction methods include ANDERSON acceleration [36], MINIMAL POLYNOMIAL EXTRAPOLATION [4] and REDUCED RANK EXTRAPOLATION [12]. These methods aim at finding a fixed point  $g^*$  and assume that  $\{g_t \in \mathbb{R}^d\}_{t \geq 0}$  has the following linear relation:

$$g_t - g^* = A(g_{t-1} - g^*) + e_t, \quad (6)$$

where  $e_t$  is a second order term satisfying  $\|e_t\|_2 = \mathcal{O}(\|g_{t-1} - g^*\|_2^2)$  and  $A \in \mathbb{R}^{d \times d}$  is an unknown matrix, see [31] for details and results. For our numerical experiments, we run OPT-AMSGRAD using Algorithm 3 to construct the sequence  $\{m_t\}_{t \geq 0}$  which is based on estimating the limit of a sequence using the last iterates [3].

Specifically, at iteration  $t$ ,  $m_t$  is obtained by (a) calling Algorithm 3 with a sequence of  $r$  past gradients,  $\{g_{t-1}, g_{t-2}, \dots, g_{t-r}\}$  as input yielding the vector  $c = [c_0, \dots, c_{r-1}]$  and (b) setting  $m_t := \sum_{i=0}^{r-1} c_i g_{t-r+i}$ .

To understand 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 (6) as  $g_t = A g_{t-1} + \mathcal{O}(\|g_{t-1}\|_2^2) u_{t-1}$ , for some unit vector  $u_{t-1}$ . This 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 converges to a stationary point, the magnitude of the error will converge to zero.

**Computational cost:** This extrapolation step consists in: (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.

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#### Algorithm 3 Regularized Approximated Minimal Polynomial Extrapolation [31]

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- 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  $g^*$ .
-

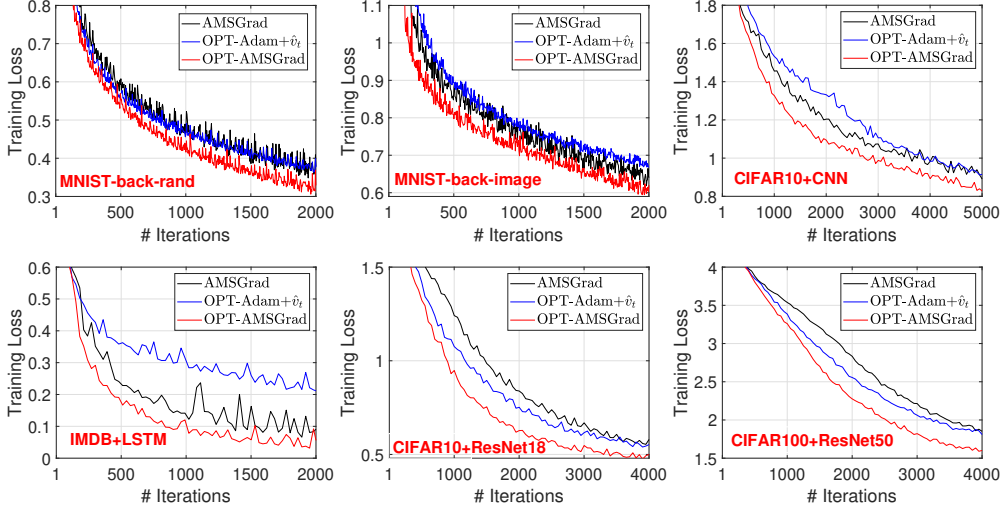


Figure 2: Training loss vs. Number of iterations for fully connected NN, CNN, LSTM and ResNet.

## 5.2 Classification Experiments

In this section, we provide experiments on classification tasks with various neural network architectures and datasets to demonstrate the effectiveness of OPT-AMSGRAD.

**Methods.** We consider two baselines. The first one is the original AMSGRAD. The hyperparameters are set to be  $\beta_1 = 0.9$  and  $\beta_2 = 0.999$ , see [30]. The other benchmark method is the OPTIMISTIC-ADAM+ $\hat{v}_t$  [8], which details are given in the supplementary material. We use cross-entropy loss, a mini-batch size of 128 and tune the learning rates over a fine grid and report the best result for all methods. For OPT-AMSGRAD, we use  $\beta_1 = 0.9$  and  $\beta_2 = 0.999$  and the best step size  $\eta$  of AMSGRAD for a fair evaluation of the optimistic step. OPT-AMSGRAD has an additional parameter  $r$  that controls the number of previous gradients used for gradient prediction. We use  $r = 5$  past gradient for empirical reasons, see Section 5.3. The algorithms are initialized at the same point and the results are averaged over 5 repetitions.

**Datasets.** Following [30] and [19], we compare different algorithms on *MNIST*, *CIFAR10*, *CIFAR100*, and *IMDB* datasets. For *MNIST*, we use two noisy variants namely *MNIST-back-rand* and *MNIST-back-image* from [20]. They both have 12 000 training samples and 50 000 test samples, where random background is inserted to the original *MNIST* hand-written digit images. For *MNIST-back-rand*, each image is inserted with a random background, which pixel values are generated uniformly from 0 to 255, while *MNIST-back-image* takes random patches from a black and white noisy background. The input dimension is 784 ( $28 \times 28$ ) and the number of classes is 10. *CIFAR10* and *CIFAR100* are popular computer-vision datasets of 50 000 training images and 10 000 test images, of size  $32 \times 32$ . The *IMDB* movie review dataset is a binary classification dataset with 25 000 training and testing samples respectively. It is a popular datasets for text classification.

**Network architectures.** We adopt a multi-layer fully connected neural network with hidden layers of 200 then 100 neurons (using ReLU activations and Softmax output) on *MNIST* variants. For *CIFAR* datasets, we adopt ALL-CNN network proposed by [32], built with convolutional blocks and dropout layers. In addition, we also apply residual networks, Resnet-18 and Resnet-50 [18], which have achieved state-of-the-art results. For the texture *IMDB* dataset, we consider a Long-Short Term Memory (LSTM) network [13] including a word embedding layer with 5 000 input entries representing most frequent words embedded into a 32 dimensional space. The output of the embedding layer is passed to 100 LSTM units then connected to 100 fully connected ReLU layers.

**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 since fewer iterations are required to achieve the same precision, validating one of the main edges of OPT-AMSGRAD. We are also curious about the long-term performance and generalization of the proposed method in test phase. In Figure 3, we plot the results when the model is trained until the

test accuracy stabilizes. We observe: (1) in the long term, OPT-AMSGRAD algorithm may converge to a better point with smaller objective function value, and (2) in these three applications, the proposed OPT-AMSGRAD also outperforms the competing methods in terms of test accuracy.

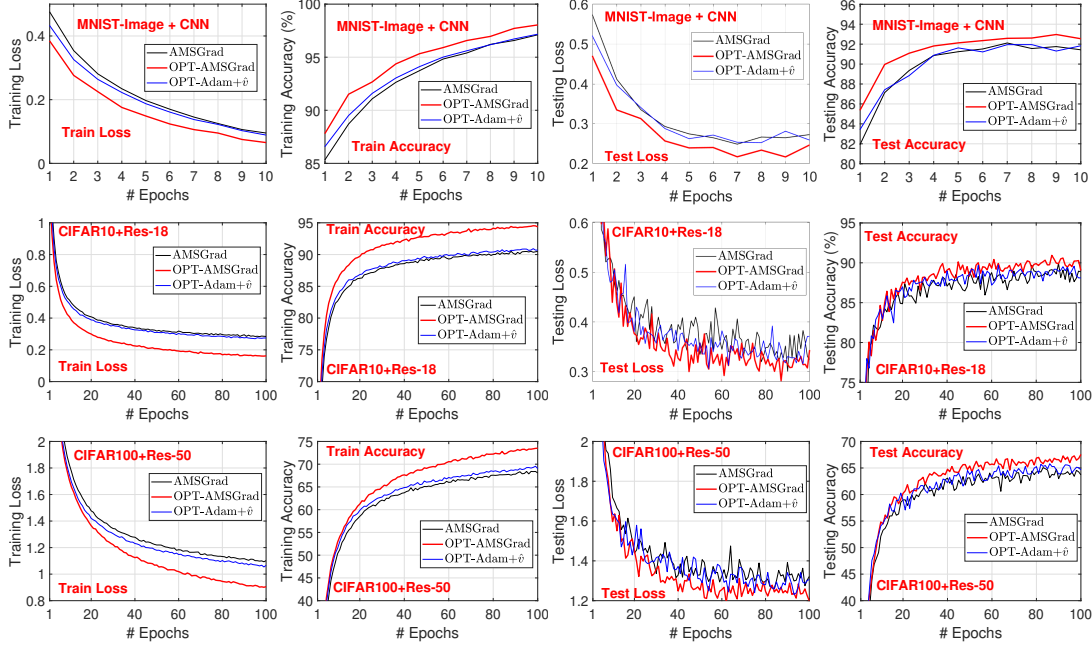


Figure 3: *MNIST-back-image + CNN*, *CIFAR10 + Res-18* and *CIFAR100 + Res-50*. We compare three methods in terms of training (cross-entropy) loss and accuracy, testing loss and accuracy.

### 5.3 Choice of parameter $r$

Since the number of past gradients  $r$  is important in our algorithm, we compare Figure 4 the performance under different values  $r = 3, 5, 10$  on two datasets. From the results we see 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,  $r = 5$  is a good choice for most applications. We remark that, empirically, the performance comparison among  $r = 3, 5, 10$  is not absolutely consistent (i.e. more means better) in all cases. One possible reason is that for deep neural networks, the high diversity of computed gradients through the iterations, due to the highly nonconvex loss, makes them inefficient for sequentially building the predictable process  $\{m_t\}_{t>0}$ . Thus, only recent ones ( $r \leq 5$ ) are used.

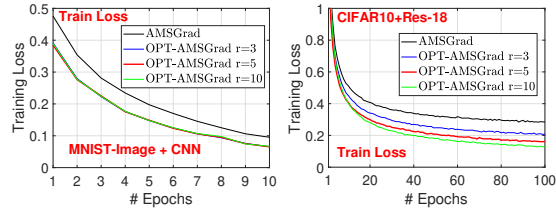


Figure 4: Training loss w.r.t.  $r$ .

## 6 Conclusion

In this paper, we propose OPT-AMSGRAD, which combines optimistic online learning and AMSGRAD to improve sample efficiency and accelerate the process of training, in particular for deep neural networks. Given a good gradient prediction process, we demonstrate that the regret can be smaller than that of standard AMSGRAD. We also establish finite-time convergence bound on the second order moment of the gradient of the objective function matching that of state-of-the-art algorithms. Experiments on various deep learning problems demonstrate the effectiveness of the proposed algorithm in accelerating the empirical risk minimization procedure and empirically show better generalization properties of OPT-AMSGRAD.



## 7 Broader Impact

Broader Impact discussion is not applicable for this paper given the generality of both methods and numerical examples presented.

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## 376 A Proof of Theorem 1

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

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

379 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  $D_\infty^2$  is the diameter of  
380 the bounded set  $\Theta$ . The result holds for any benchmark  $w^* \in \Theta$  and any step size sequence  $\{\eta_t\}_{t>0}$ .

381 **Proof** Beforehand, we denote:

$$\begin{aligned} \tilde{g}_t &= \beta_1 \theta_{t-1} + (1 - \beta_1) g_t, \\ \tilde{m}_{t+1} &= \beta_1 \theta_{t-1} + (1 - \beta_1) m_{t+1}, \end{aligned} \quad (7)$$

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

$$\begin{aligned} \mathcal{R}_T &:= \sum_{t=1}^T \ell_t(w_t) - \min_{w \in \Theta} \sum_{t=1}^T \ell_t(w) \\ &\leq \sum_{t=1}^T \langle w_t - w^*, \nabla \ell_t(w_t) \rangle \\ &= \sum_{t=1}^T \langle w_t - \tilde{w}_{t+1}, g_t - \tilde{m}_t \rangle + \langle w_t - \tilde{w}_{t+1}, \tilde{m}_t \rangle + \langle \tilde{w}_{t+1} - w^*, \tilde{g}_t \rangle + \langle \tilde{w}_{t+1} - w^*, g_t - \tilde{g}_t \rangle. \end{aligned} \quad (8)$$

384 Recall the notation  $\psi_t(x)$  and the Bregman divergence  $B_{\psi_t}(u, v)$  defined Section 4. We exploit a  
385 useful inequality (which appears in e.g., [35]). For any update of the form  $\hat{w} = \arg \min_{w \in \Theta} \langle w, \theta \rangle +$   
386  $B_\psi(w, v)$ , it holds that

$$\langle \hat{w} - u, \theta \rangle \leq B_\psi(u, v) - B_\psi(u, \hat{w}) - B_\psi(\hat{w}, v) \quad \text{for any } u \in \Theta. \quad (9)$$

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

$$\tilde{w}_{t+1} = \arg \min_{w \in \Theta} \eta_t \langle w, \tilde{g}_t \rangle + B_{\psi_t}(w, \tilde{w}_t). \quad (10)$$

388 By using (9) for (10) with  $\hat{w} = \tilde{w}_{t+1}$  (the output of the minimization problem),  $u = w^*$  and  $v = \tilde{w}_t$ ,  
389 we have

$$\langle \tilde{w}_{t+1} - w^*, \tilde{g}_t \rangle \leq \frac{1}{\eta_t} [B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1}) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t)]. \quad (11)$$

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

$$w_{t+1} = \arg \min_{w \in \Theta} \eta_{t+1} \langle w, \tilde{m}_{t+1} \rangle + B_{\psi_t}(w, \tilde{w}_{t+1}). \quad (12)$$

391 and, by using (9) for (12) (written at iteration  $t$ ), with  $\hat{w} = w_t$  (the output of the minimization  
392 problem),  $u = \tilde{w}_{t+1}$  and  $v = \tilde{w}_t$ , we have

$$\langle w_t - \tilde{w}_{t+1}, \tilde{m}_t \rangle \leq \frac{1}{\eta_t} [B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_{t-1}}(\tilde{w}_{t+1}, w_t) - B_{\psi_{t-1}}(w_t, \tilde{w}_t)]. \quad (13)$$

393 By (8), (11), and (13), we obtain

$$\begin{aligned} \mathcal{R}_T &\stackrel{(8)}{\leq} \sum_{t=1}^T \langle w_t - \tilde{w}_{t+1}, g_t - \tilde{m}_t \rangle + \langle w_t - \tilde{w}_{t+1}, \tilde{m}_t \rangle + \langle \tilde{w}_{t+1} - w^*, \tilde{g}_t \rangle + \langle \tilde{w}_{t+1} - w^*, g_t - \tilde{g}_t \rangle \\ &\stackrel{(11), (13)}{\leq} \sum_{t=1}^T \|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}} \|g_t - \tilde{m}_t\|_{\psi_{t-1}^*} + \|\tilde{w}_{t+1} - w^*\|_{\psi_{t-1}} \|g_t - \tilde{g}_t\|_{\psi_{t-1}^*} \\ &\quad + \frac{1}{\eta_t} [B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_{t-1}}(\tilde{w}_{t+1}, w_t) - B_{\psi_{t-1}}(w_t, \tilde{w}_t) \\ &\quad + B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1}) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t)], \end{aligned} \quad (14)$$

394 which is further bounded by

$$\begin{aligned}
\mathcal{R}_T \leq & \sum_{t=1}^T \left\{ \frac{1}{2\eta_t} \|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}}^2 + \frac{\eta_t}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2 + \|\tilde{w}_{t+1} - w^*\|_{\psi_{t-1}} \|g_t - \tilde{g}_t\|_{\psi_{t-1}^*} \right. \\
& + \frac{1}{\eta_t} \underbrace{\left( B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t) \right)}_{A_1} - \frac{1}{2} \|\tilde{w}_{t+1} - w_t\|_{\psi_{t-1}}^2 \\
& \left. + \underbrace{B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1})}_{A_2} \right\}, \tag{15}
\end{aligned}$$

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

398 To proceed, notice that

$$\begin{aligned}
A_1 &:= B_{\psi_{t-1}}(\tilde{w}_{t+1}, \tilde{w}_t) - B_{\psi_t}(\tilde{w}_{t+1}, \tilde{w}_t) \\
&= \langle \tilde{w}_{t+1} - \tilde{w}_t, \text{diag}(\hat{v}_{t-1}^{1/2} - \hat{v}_t^{1/2})(\tilde{w}_{t+1} - \tilde{w}_t) \rangle \leq 0, \tag{16}
\end{aligned}$$

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

$$\begin{aligned}
A_2 &:= B_{\psi_t}(w^*, \tilde{w}_t) - B_{\psi_t}(w^*, \tilde{w}_{t+1}) = \langle w^* - \tilde{w}_{t+1}, \text{diag}(\hat{v}_{t+1}^{1/2} - \hat{v}_t^{1/2})(w^* - \tilde{w}_{t+1}) \rangle \\
&\leq (\max_i (w^*[i] - \tilde{w}_{t+1}[i])^2) \cdot \left( \sum_{i=1}^d \hat{v}_{t+1}^{1/2}[i] - \hat{v}_t^{1/2}[i] \right). \tag{17}
\end{aligned}$$

400 Therefore, by (15),(17),(16), we have

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

401 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  
402 proof.

403 □

## 404 B Proof of Corollary 1

405 **Corollary.** Suppose  $\beta_1 = 0$  and  $\{v_t\}_{t \geq 0}$  is a monotonically increasing sequence, then we obtain  
406 the following regret bound for any  $w^* \in \Theta$  and sequence of stepsizes  $\{\eta_t = \eta/\sqrt{t}\}_{t \geq 0}$ :

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

407 where  $B_{\psi_1} := B_{\psi_1}(w^*, \tilde{w}_1)$ ,  $g_t := \nabla \ell_t(w_t)$  and  $\eta_{\min} := \min_t \eta_t$ .

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

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

409 The second term reads:

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

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

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

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

413

□

## 414 C Proofs of Auxiliary Lemmas

415 Following [38] and their study of the SGD with Momentum we denote for any  $t > 0$ :

$$\bar{w}_t = w_t + \frac{\beta_1}{1-\beta_1} (w_t - \tilde{w}_{t-1}) = \frac{1}{1-\beta_1} w_t - \frac{\beta_1}{1-\beta_1} \tilde{w}_{t-1}. \quad (18)$$

416 **Lemma 3.** Assume a strictly positive and non increasing sequence of stepsizes  $\{\eta_t\}_{t>0}$ ,  $\beta_1 < \beta_2 \in$   
417  $[0, 1)$ , then the following holds:

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

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

419 **Proof** By definition (18) and using the Algorithm updates, we have:

$$\begin{aligned}
\bar{w}_{t+1} - \bar{w}_t &= \frac{1}{1-\beta_1} (w_{t+1} - \tilde{w}_t) - \frac{\beta_1}{1-\beta_1} (w_t - \tilde{w}_{t-1}) \\
&= -\frac{1}{1-\beta_1} \eta_t \hat{v}_t^{-1/2} (\theta_t + h_{t+1}) + \frac{\beta_1}{1-\beta_1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + h_t) \\
&= -\frac{1}{1-\beta_1} \eta_t \hat{v}_t^{-1/2} (\theta_t + \beta_1 \theta_{t-1}) - \frac{1}{1-\beta_1} \eta_t \hat{v}_t^{-1/2} (1-\beta_1) m_{t+1} \\
&\quad + \frac{\beta_1}{1-\beta_1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + \beta_1 \theta_{t-2}) + \frac{\beta_1}{1-\beta_1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} (1-\beta_1) m_t.
\end{aligned} \quad (19)$$

420 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  $\tilde{\theta}_t = \beta_1 \tilde{\theta}_{t-1} + (1 -$   
421  $\beta_1)(g_t + \beta_1 g_{t-1})$ .

$$\bar{w}_{t+1} - \bar{w}_t \leq \frac{\beta_1}{1-\beta_1} \tilde{\theta}_{t-1} \left[ \eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t. \quad (20)$$

422

□



423 **Lemma 4.** Assume H4, a strictly positive and a sequence of constant stepsizes  $\{\eta_t\}_{t>0}$ ,  $\beta \in [0, 1]$ ,  
 424 then the following holds:

$$\sum_{t=1}^{T_M} \eta_t^2 \mathbb{E} \left[ \left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] \leq \frac{\eta^2 d T_M (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)}. \quad (21)$$

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

$$\begin{aligned} \eta_t^2 \mathbb{E} \left[ \left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] &= \eta_t^2 \mathbb{E} \left[ \sum_{p=1}^d \frac{\theta_{t,p}^2}{\hat{v}_{t,p}} \right] \\ &\leq \eta_t^2 \mathbb{E} \left[ \sum_{i=1}^d \frac{\theta_{t,p}^2}{v_{t,p}} \right] \\ &\leq \eta_t^2 \mathbb{E} \left[ \sum_{i=1}^d \frac{(\sum_{r=1}^t (1 - \beta_1) \beta_1^{t-r} g_{r,p})^2}{\sum_{r=1}^t (1 - \beta_2) \beta_2^{t-r} g_{r,p}^2} \right], \end{aligned} \quad (22)$$

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

$$\begin{aligned} \eta_t^2 \mathbb{E} \left[ \left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] &\leq \frac{\eta_t^2 (1 - \beta_1)^2}{1 - \beta_2} \mathbb{E} \left[ \sum_{i=1}^d \frac{(\sum_{r=1}^t \beta_1^{t-r} g_{r,p})^2}{\sum_{r=1}^t \beta_2^{t-r} g_{r,p}^2} \right] \\ &\stackrel{(a)}{\leq} \frac{\eta_t^2 (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[ \sum_{i=1}^d \frac{\sum_{r=1}^t \beta_1^{t-r} g_{r,p}^2}{\sum_{r=1}^t \beta_2^{t-r} g_{r,p}^2} \right] \\ &\leq \frac{\eta_t^2 (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[ \sum_{i=1}^d \sum_{r=1}^t \gamma^{t-r} \right] = \frac{\eta_t^2 d (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[ \sum_{r=1}^t \gamma^{t-r} \right], \end{aligned} \quad (23)$$

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

$$\begin{aligned} \sum_{t=1}^{T_M} \eta_t^2 \mathbb{E} \left[ \left\| \hat{v}_t^{-1/2} \theta_t \right\|_2^2 \right] &\leq \frac{\eta_t^2 d (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[ \sum_{t=1}^{T_M} \sum_{r=1}^t \gamma^{t-r} \right] \\ &\leq \frac{\eta^2 d T (1 - \beta_1)}{1 - \beta_2} \mathbb{E} \left[ \sum_{t=t}^t \gamma^{t-r} \right] \\ &\leq \frac{\eta^2 d T (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)}, \end{aligned} \quad (24)$$

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

### 430 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:

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

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

$$\|\theta_{t+1}\| = \|\beta_1 \theta_t + (1 - \beta_1) g_{t+1}\| \leq \beta_1 \|\theta_t\| + (1 - \beta_1) \|g_{t+1}\| \leq M. \quad (25)$$

432 Using the same induction reasoning we prove that

$$\|\hat{v}_{t+1}\| = \|\beta_2 \hat{v}_t + (1 - \beta_2) g_{t+1}^2\| \leq \beta_2 \|\hat{v}_t\| + (1 - \beta_1) \|g_{t+1}^2\| \leq M^2. \quad (26)$$

433  $\square$

## 434 D Proof of Theorem 2

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

$$\mathbb{E}[\|\nabla f(w_T)\|^2] \leq \tilde{C}_1 \sqrt{\frac{d}{T_M}} + \tilde{C}_2 \frac{1}{T_M}, \quad (27)$$

437 where  $T$  is a random termination number distributed according to (4) and the constants are defined  
 438 as follows:

$$\begin{aligned} \tilde{C}_1 &= C_1 + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \left[ \frac{a(1 - \beta_1)^2}{1 - \beta_2} + 2L \frac{1}{1 - \beta_2} \right] \\ C_1 &= \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \Delta f + \frac{4L \left( \frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{(1 + \beta_1^2)(1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \\ \tilde{C}_2 &= \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E}[\|\hat{v}_0^{-1/2}\|] \end{aligned} \quad (28)$$

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

$$\begin{aligned} f(\bar{w}_{t+1}) &\leq f(\bar{w}_t) + \nabla f(\bar{w}_t)^\top (\bar{w}_{t+1} - \bar{w}_t) + \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2 \\ &\leq f(\bar{w}_t) + \underbrace{\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t)}_A \\ &\quad + \underbrace{(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t)}_B + \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2. \end{aligned} \quad (29)$$

440 **Term A.** Using Lemma 3, we have that:

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

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

$$\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \frac{\beta_1(1 + \beta_1)}{1 - \beta_1} M^2 [\|\eta_{t-1} \hat{v}_{t-1}^{-1/2}\| - \|\eta_t \hat{v}_t^{-1/2}\|] - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t, \quad (30)$$

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

$$\begin{aligned} -\nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t &= -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t - \nabla f(w_t)^\top [\eta_t \hat{v}_t^{-1/2} - \eta_{t-1} \hat{v}_{t-1}^{-1/2}] \bar{g}_t \\ &\quad - \nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\beta_1 g_{t-1} + m_{t+1}) \\ &\leq -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t + (1 - a\beta_1) M^2 [\|\eta_{t-1} \hat{v}_{t-1}^{-1/2}\| - \|\eta_t \hat{v}_t^{-1/2}\|] \\ &\quad - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1}), \end{aligned} \quad (31)$$

445 where we have used Lemma 1 on  $\|g_t\|$  and where that  $\tilde{g}_t = \bar{g}_t + \beta_1 g_{t-1} + m_{t+1} = g_t - \beta_1 m_t +$   
 446  $\beta_1 g_{t-1} + m_{t+1}$ . Plugging (31) into (30) yields:

$$\begin{aligned} &\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) \\ &\leq -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t + \frac{1}{1 - \beta_1} (a\beta_1^2 - 2a\beta_1 + \beta_1) M^2 [\|\eta_{t-1} \hat{v}_{t-1}^{-1/2}\| - \|\eta_t \hat{v}_t^{-1/2}\|] \\ &\quad - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1}). \end{aligned} \quad (32)$$

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

$$(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \|\nabla f(\bar{w}_t) - \nabla f(w_t)\| \|\bar{w}_{t+1} - \bar{w}_t\|. \quad (33)$$

448 Using smoothness assumption H2:

$$\begin{aligned} \|\nabla f(\bar{w}_t) - \nabla f(w_t)\| &\leq L \|\bar{w}_t - w_t\| \\ &\leq L \frac{\beta_1}{1 - \beta_1} \|w_t - \tilde{w}_{t-1}\|. \end{aligned} \quad (34)$$

449 By Lemma 3 we also have:

$$\begin{aligned} \bar{w}_{t+1} - \bar{w}_t &= \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \left[ \eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \\ &= \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} \left[ I - (\eta_t \hat{v}_t^{-1/2})(\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \\ &= \frac{\beta_1}{1 - \beta_1} \left[ I - (\eta_t \hat{v}_t^{-1/2})(\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1} \right] (\tilde{w}_{t-1} - w_t) - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t, \end{aligned} \quad (35)$$

450 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  
451 norms on both sides, observing  $\|I - (\eta_t \hat{v}_t^{-1/2})(\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1}\| \leq 1$  due to the decreasing stepsize  
452 and the construction of  $\hat{v}_t$  and using CS inequality yield:

$$\|\bar{w}_{t+1} - \bar{w}_t\| \leq \frac{\beta_1}{1 - \beta_1} \|\tilde{w}_{t-1} - w_t\| + \|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\|. \quad (36)$$

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

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

453 Plugging (34) and (36) into (33) returns:

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

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

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

455 The last term  $\frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2$  can be upper bounded using (36):

$$\begin{aligned} \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2 &\leq \frac{L}{2} \left[ \frac{\beta_1}{1 - \beta_1} \|\tilde{w}_{t-1} - w_t\| + \|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\| \right]^2 \\ &\leq L \|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\|^2 + 2L \left( \frac{\beta_1}{1 - \beta_1} \right)^2 \|\tilde{w}_{t-1} - w_t\|^2. \end{aligned} \quad (38)$$

456 Plugging (32), (37) and (38) into (29) and taking the expectations on both sides give:

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

457 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  $\mathcal{F}_t$   
 458 reads as follows

$$\mathbb{E} [\nabla f(w_t)^\top \tilde{g}_t] = \mathbb{E} [\nabla f(w_t)^\top (g_t - \beta_1 m_t)] = (1 - a\beta_1) \|\nabla f(w_t)\|^2. \quad (39)$$

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

$$\begin{aligned} & \frac{1}{M} \sum_{t=1}^{T_M} ((1 - a\beta_1)\eta_{t-1} + (\beta_1 + a)\eta_t) \|\nabla f(w_t)\|^2 \leq \\ & \mathbb{E} \left[ f(\bar{w}_1) + \frac{1}{1 - \beta_1} \tilde{M}^2 \|\eta_0 \hat{v}_0^{-1/2}\| - \left( f(\bar{w}_{T_M+1}) + \frac{1}{1 - \beta_1} \tilde{M}^2 \|\eta_{T_M} \hat{v}_{T_M}^{-1/2}\| \right) \right] \\ & + 2L \sum_{t=1}^{T_M} \mathbb{E} [\|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\|^2] + 4L \left( \frac{\beta_1}{1 - \beta_1} \right)^2 \sum_{t=1}^{T_M} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2] \\ & \leq \mathbb{E} \left[ \Delta f + \frac{1}{1 - \beta_1} \tilde{M}^2 \|\eta_0 \hat{v}_0^{-1/2}\| \right] + 2L \sum_{t=1}^{T_M} \mathbb{E} [\|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\|^2] \\ & + 4L \left( \frac{\beta_1}{1 - \beta_1} \right)^2 \sum_{t=1}^{T_M} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2], \end{aligned} \quad (40)$$

460 where we denote  $\Delta f := f(\bar{w}_1) - f(\bar{w}_{T_M+1})$ . We note that by definition of  $\hat{v}_t$ , and a constant  
 461 learning rate  $\eta_t$ , we have

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

462 Using Lemma 4 we have

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

463 And thus, setting the learning rate to a constant value  $\eta$  and injecting in (40) yields:

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

464 where  $T$  is a random termination number distributed according (4). Setting the stepsize to  $\eta = \frac{1}{\sqrt{dT_M}}$   
 465 yields :

$$\mathbb{E} [\|\nabla f(w_T)\|^2] \leq C_1 \sqrt{\frac{d}{T_M}} + C_2 \frac{1}{T_M} + D_1 \frac{\eta}{T_M} \sum_{t=1}^{T_M} \mathbb{E} [\|\hat{v}_{t-1}^{-1/2} m_t\|] + D_2 \frac{\eta}{T_M} \sum_{t=1}^{T_M} \mathbb{E} [\|\hat{v}_{t-1}^{-1/2} \tilde{g}_t\|],$$

466 where

$$C_1 = \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \Delta f + \frac{4L \left( \frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{(1 + \beta_1^2)(1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)},$$

$$C_2 = \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E}[\|\hat{v}_0^{-1/2}\|].$$

467 **Simple case as in [41]:** if  $\beta_1 = 0$  then  $\tilde{g}_t = g_t + m_{t+1}$  and  $g_t = \theta_t$ . Also using Lemma 4 we have  
468 that:

$$\sum_{t=1}^{T_M} \eta_t^2 \mathbb{E} \left[ \left\| \hat{v}_t^{-1/2} g_t \right\|_2^2 \right] \leq \frac{\eta^2 d T_M}{(1 - \beta_2)};$$

469 which leads to the final bound:

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

470 where

$$\tilde{C}_1 = C_1 + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \left[ \frac{a(1 - \beta_1)^2}{1 - \beta_2} + 2L \frac{1}{1 - \beta_2} \right],$$

$$\tilde{C}_2 = C_2 = \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E}[\|\hat{v}_0^{-1/2}\|].$$

471

□

## 472 E Proof of Lemma 2 (Boundedness of the iterates)

473 **Lemma.** *Given the multilayer model (5), assume the boundedness of the input data and of the loss*  
474 *function, i.e., for any  $\xi \in \mathbb{R}^p$  and  $y \in \mathbb{R}$  there is a constant  $T > 0$  such that:*

$$\|\xi\| \leq 1 \quad \text{a.s.} \quad \text{and} \quad |\mathcal{L}'(\cdot, y)| \leq T, \quad (41)$$

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** For any index  $\ell \in [1, L]$  we denote the output of layer  $\ell$  by

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

475 Given the sigmoid assumption we have  $\|h^{(\ell)}(w, \xi)\| \leq 1$  for any  $\ell \in [1, L]$  and any  $(w, \xi) \in$   
476  $\mathbb{R}^d \times \mathbb{R}^p$ . We also recall that  $\mathcal{L}(\cdot, y)$  is the loss function, which can be Huber loss or cross entropy.  
477 Observe that at the last layer  $L$ :

$$\begin{aligned} \|\nabla_{w^{(L)}} \mathcal{L}(\text{MLN}(w, \xi), y)\| &= \|\mathcal{L}'(\text{MLN}(w, \xi), y) \nabla_{w^{(L)}} \text{MLN}(w, \xi)\| \\ &= \|\mathcal{L}'(\text{MLN}(w, \xi), y) \sigma'(w^{(L)} h^{(L-1)}(w, \xi)) h^{(L-1)}(w, \xi)\| \\ &\leq \frac{T}{4}, \end{aligned} \quad (42)$$

478 where the last equality is due to mild assumptions (41) and to the fact that the norm of the derivative  
479 of the sigmoid function is upperbounded by  $1/4$ .

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

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



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

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

481 Thus:

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

482 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 (42), we have

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

483 where  $f(w, \xi) = \mathcal{L}(\text{MLN}(w, \xi), y) + \frac{\lambda}{2} \|w\|^2$  and is the loss of our MLN. This last equation yields

484  $\theta_{T,i}^{(L)} \geq 0$  (given the algorithm and  $\beta_1 = 0$ ) and using the fact that  $\|w_t - \tilde{w}_{t-1}\| \leq B$  we have

$$0 \leq w_{T-1,i}^{(L)} - B \leq w_{T,i}^{(L)} \leq w_{T-1,i}^{(L)} , \quad (43)$$

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 (43) 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

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

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

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

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

$$\nabla_{w^{(\ell)}} \mathcal{L}(\text{MLN}(w, \xi), y) = \mathcal{L}'(\text{MLN}(w, \xi), y) \left( \prod_{j=1}^{\ell+1} \sigma' \left( w^{(j)} h^{(j-1)}(w, \xi) \right) \right) h^{(\ell-1)}(w, \xi) . \quad (44)$$

This last quantity is bounded as long as we can prove that for any layer  $\ell$  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 (44) 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  $\ell$  satisfy

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

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

## 492 F Comparison to some related methods

493 **Comparison to nonconvex optimization works.** Recently, [39, 5, 37, 41, 42, 22] provide some  
 494 theoretical analysis of ADAM-type algorithms when applying them to smooth nonconvex opti-  
 495 mization problems. For example, [5] provides a bound, which is  $\min_{t \in [T]} \mathbb{E}[\|\nabla f(w_t)\|^2] =$   
 496  $\mathcal{O}(\log T / \sqrt{T})$ . Yet, this data independent bound does not show any advantage over standard  
 497 stochastic gradient descent. Similar concerns appear in other papers.

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

507 **Comparison to AO-FTRL [26].** In [26], the authors propose AO-FTRL, which has the update  
 508 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  
 509 convex loss function with respect to some norm  $\|\cdot\|_{(t)}$  that may be different for different iteration  $t$ .  
 510 Data dependent regret bound was provided in the paper, which is  $r_{0:T}(w^*) + \sum_{t=1}^T \|g_t - m_t\|_{(t)}^*$   
 511 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  $\|\cdot\|_{(t)}$   
 512  $:= \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{1/2} \cdot \rangle}$ , then the update might be viewed as an optimistic variant of ADAGRAD.  
 513 However, no experiments was provided in [26].

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

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

---

- 1: Required: parameter  $\beta_1, \beta_2$ , and  $\eta_t$ .
  - 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**
- 

519 We want to emphasize that the motivations are different. OPTIMISTIC-ADAM in their paper is  
 520 designed to optimize two-player games (e.g. GANs [15]), while the proposed algorithm in this paper  
 521 is designed to accelerate optimization (e.g. solving empirical risk minimization quickly). [8] focuses  
 522 on training GANs [15]. GANs is a two-player zero-sum game. There have been some related works  
 523 in OPTIMISTIC ONLINE LEARNING like [7, 29, 33]) showing that if both players use some kinds of  
 524 OPTIMISTIC-update, then accelerating the convergence to the equilibrium of the game is possible.  
 525 [8] was inspired by these related works and showed that OPTIMISTIC-MIRROR-DESCENT can avoid  
 526 the cycle behavior in a bilinear zero-sum game, which accelerates the convergence. Furthermore,  
 527 [8] did not provide theoretical analysis of OPTIMISTIC-ADAM.

## 528 G Additional Remarks and Runs on the Gradient Prediction Process

529 **Two illustrative examples.** We provide two toy examples to demonstrate how OPT-AMSGRAD  
 530 works with the chosen extrapolation method. First, consider minimizing a quadratic function  
 531  $H(w) := \frac{b}{2}w^2$  with vanilla gradient descent method  $w_{t+1} = w_t - \eta_t \nabla H(w_t)$ . The gradient  
 532  $g_t := \nabla H(w_t)$  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,  
 533 the update can be written in the form of  $g_t = Ag_{t-1} + \mathcal{O}(\|g_{t-1}\|_2^2)u_{t-1}$ , with  $A = (1 - b\eta)$  and  
 534  $u_{t-1} = 0$  by setting  $\eta_t = \eta$  (constant step size). Therefore, the extrapolation method should predict  
 535 well.

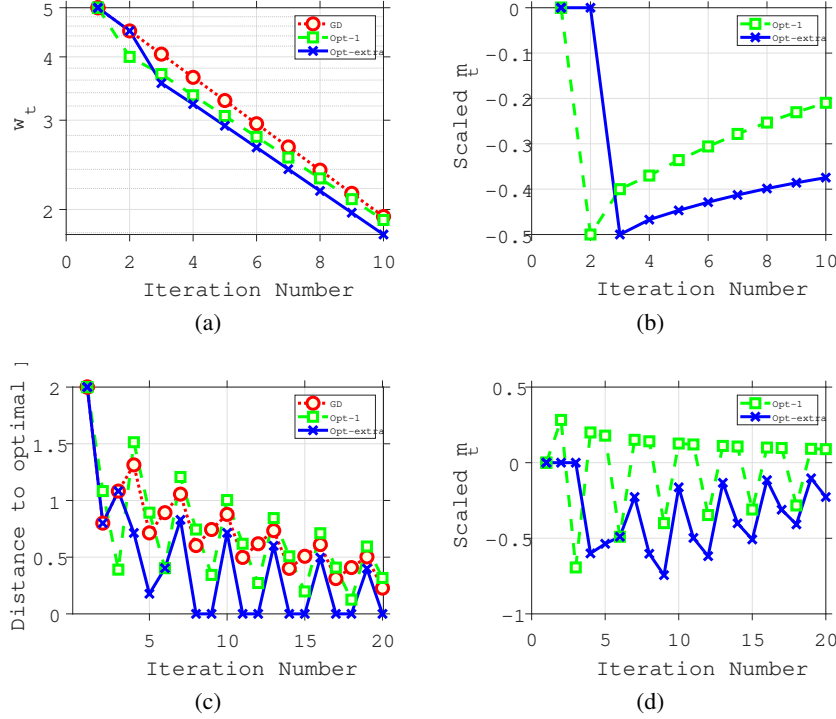


Figure 5: (a): The iterate  $w_t$ ; the closer to the optimal point 0 the better. (b): A scaled and clipped version of  $m_t$ :  $w_t - w_{t-1/2}$ , which measures how the prediction of  $m_t$  drives the update towards the optimal point. In this scenario, the more negative the better. (c): Distance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

536 Specifically, consider optimizing  $H(w) := w^2/2$  by the following three algorithms with the same  
 537 step size. One is Gradient Descent (GD):  $w_{t+1} = w_t - \eta_t g_t$ , while the other two are OPT-  
 538 AMSGRAD with  $\beta_1 = 0$  and the second moment term  $\hat{v}_t$  being dropped:  $w_{t+\frac{1}{2}} = \Pi_{\Theta}[w_{t-\frac{1}{2}} - \eta_t g_t]$ ,  
 539  $w_{t+1} = \Pi_{\Theta}[w_{t+\frac{1}{2}} - \eta_{t+1} m_{t+1}]$ . We denote the algorithm that sets  $m_{t+1} = g_t$  as Opt-1, and denote  
 540 the algorithm that uses the extrapolation method to get  $m_{t+1}$  as Opt-extra. We let  $\eta_t = 0.1$  and the  
 541 initial point  $w_0 = 5$  for all the three methods. The simulation results are on Figure 5 (a) and (b).  
 542 Sub-figure (a) plots update  $w_t$  over iteration, where the updates should go towards the optimal point  
 543 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  
 544 viewed as  $-\eta_t m_t$  if the projection (if exists) is lifted. Sub-figure (a) shows that Opt-extra converges  
 545 faster than the other methods. Furthermore, sub-figure (b) shows that the prediction by the extrap-  
 546 olation method is better than the prediction by simply using the previous gradient. The sub-figure  
 547 shows that  $-m_t$  from both methods all point to 0 in all iterations and the magnitude is larger for the  
 548 one produced by the extrapolation method after iteration 2.<sup>2</sup>

<sup>2</sup>The extrapolation needs at least two gradients for prediction. Thus, in the first two iterations,  $m_t = 0$ .

549 Now let us consider another problem: an online learning problem proposed in [30]<sup>3</sup>. Assume the  
 550 learner’s decision space is  $\Theta = [-1, 1]$ , and the loss function is  $\ell_t(w) = 3w$  if  $t \bmod 3 = 1$ , and  
 551  $\ell_t(w) = -w$  otherwise. The optimal point to minimize the cumulative loss is  $w^* = -1$ . We  
 552 let  $\eta_t = 0.1/\sqrt{t}$  and the initial point  $w_0 = 1$  for all the three methods. The parameter  $\lambda$  of the  
 553 extrapolation method is set to  $\lambda = 10^{-3} > 0$ . The results are on Figure 5 (c) and (d). Sub-figure  
 554 (c) shows that Opt-extra converges faster than the other methods while Opt-1 is not better than GD.  
 555 The reason is that the gradient changes from  $-1$  to  $3$  at  $t \bmod 3 = 1$  and it changes from  $3$  to  $-1$   
 556 at  $t \bmod 3 = 2$ . Consequently, using the current gradient as the guess for the next clearly is not a  
 557 good choice, since the next gradient is in the opposite direction of the current one. Sub-figure (d)  
 558 shows that  $-m_t$  by the extrapolation method always points to  $w^* = -1$ , while the one by using  
 559 the previous negative direction points to the opposite direction in two thirds of rounds. It shows  
 560 that the extrapolation method is much less affected by the gradient oscillation and always makes the  
 561 prediction in the right direction, which suggests that the method can capture the aggregate effect.

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<sup>3</sup>[30] uses this example to show that ADAM [19] fails to converge.