
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 [33], 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 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 $\mathcal{O}(\sqrt{d/T} + d/T)$ non-asymptotic bound indepen-
11 dently of the initialization of the method. We illustrate the practical speedup on
12 several deep learning models through numerical experiments.

1 Introduction

14 Deep learning models have been successful in several applications, from robotics (e.g. [22]), com-
15 puter vision (e.g. [18, 15]), reinforcement learning (e.g. [27]), 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 [33], ADAM [19], RMSPROP [37], ADADELTA [43], 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, 25] and the idea of momentum from NESTEROV’S METHOD
21 [29] or HEAVY BALL method [30]. 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 [30] is an accelerated optimization algorithm whose 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 [33] 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, 31, 36, 1, 26],
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 gradient predictions. We combine the OPTIMISTIC ONLINE LEARNING idea with
35 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 [32]. 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, 32, 36] showing that if both players use an OPTIMISTIC type of update, then accelerating the convergence to the equilibrium of the game is possible. Authors in [8] build on these related works and show 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 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 in related adaptive optimization papers [19, 33]. 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 $w_t \in \Theta \subseteq \mathbb{R}^d$, 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, 31, 36, 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

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

where η is a parameter, $\mathbf{R}(\cdot)$ is a 1-strongly convex function with respect to a given norm 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

¹Imagine 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 [36] 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, 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 [31]. Yet, when the predictions are well designed, 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 introduce in Section 5 a simple, yet effective, predictable process $\{m_t\}_{t \geq 0}$ leading to empirical acceleration.

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 [30] 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, [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 [33] to fix ADAM failures. The difference between ADAM and AMSGRAD lies in line 7 of Algorithm 1. AMSGRAD [33] adds the max operation to guarantee a non-increasing learning rate $\eta_t / \sqrt{\hat{v}_t}$, which helps for the convergence (i.e. average regret $\mathcal{R}_T/T \rightarrow 0$).

Algorithm 1 AMSGRAD [33]

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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
```

3 OPT-AMSGRAD Algorithm

We formulate in this section the proposed optimistic acceleration of AMSGrad, noted as 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 [31]. 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 gradient prediction process plays an important role as discussed in Section 5. The proposed

129 OPT-AMSGRAD inherits three properties: (i) Adaptive learning rate of each dimension as ADA-
 130 GRAD [11]. (line 6, line 8 and line 9). (ii) Exponential moving average of the past gradients as
 131 NESTEROV'S METHOD [29] and the HEAVY-BALL method [30]. (line 5). (iii) Optimistic update
 132 that exploits *prior knowledge* of the next gradient vector as in optimistic online learning algorithms
 133 [7, 31, 36]. (line 9). The first property helps for acceleration when the gradient has a sparse structure.
 134 The second one is from the long-established idea of momentum which can also help for accelera-
 135 tion. The last one can lead to an acceleration when the prediction of the next gradient is good as
 136 mentioned above when introducing the regret bound for the OPTIMISTIC-FTRL algorithm. This
 137 property will be elaborated whilst establishing the theoretical analysis of OPT-AMSGRAD.

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 $h_{t+1} := \beta_1 \theta_{t-1} + (1 - \beta_1) m_{t+1}$ with
 m_{t+1} the guess of g_{t+1} .
 10: **end for**

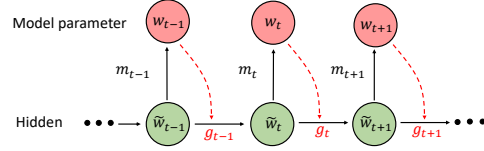


Figure 1: OPT-AMSGRAD Underlying Structure.

4 Global Convergence Analysis of OPT-AMSGRAD

140 For conciseness, we place all the proofs of the following results in the supplementary material.
 141 **Notations.** We denote the Mahalanobis norm $\|\cdot\|_H := \sqrt{\langle \cdot, H \cdot \rangle}$ for some positive semidefinite
 142 (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
 143 $\text{diag}\{\hat{v}_t\}$ represents the diagonal matrix which i_{th} diagonal element is $\hat{v}_t[i]$ defined in Algorithm 2.
 144 We define its corresponding Mahalanobis norm $\|\cdot\|_{\psi_t} := \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{1/2} \cdot \rangle}$, where we abuse
 145 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
 146 convex with respect to the norm $\|\cdot\|_{\psi_t}$. Namely, $\psi_t(\cdot)$ satisfies $\psi_t(u) \geq \psi_t(v) + \langle \psi_t(v), u - v \rangle$
 147 $+ \frac{1}{2} \|u - v\|_{\psi_t}^2$ for any point $(u, v) \in \Theta^2$. A consequence of 1-strongly convexity of $\psi_t(\cdot)$ is
 148 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 $B_{\psi_t}(u, v) :=$
 149 $\psi_t(u) - \psi_t(v) - \langle \psi_t(v), u - v \rangle$ with $\psi_t(\cdot)$ as the distance generating function. We also define the
 150 corresponding dual norm $\|\cdot\|_{\psi_t^*} := \sqrt{\langle \cdot, \text{diag}\{\hat{v}_t\}^{-1/2} \cdot \rangle}$.

4.1 Convex Regret Analysis

152 In this section, we assume that the loss functions $\{\ell_t\}_{t>0}$ are convex. We also assume that Θ has
 153 bounded diameter D_∞ , which is a standard assumption in previous works [33, 19] on adaptive
 154 methods. It is necessary in regret analysis since if the boundedness assumption is lifted, one might
 155 construct a scenario such that the benchmark is $w^* = \infty$ and the learner's regret is infinite.

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

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

158 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
 159 the bounded set Θ . The result holds for any benchmark $w^* \in \Theta$ and any step size sequence $\{\eta_t\}_{t>0}$.

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

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

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

163 We can compare the bound of Corollary 1 with that of AMSGRAD [33] with $\eta_t = \eta/\sqrt{t}$:

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

164 For convex regret minimization, the results above yields that the learner suffers regret of
 165 $\mathcal{O}(\sqrt{\sum_{t=1}^T \|g_t - m_t\|_{\psi_{t-1}^*}^2})$ with an access to an arbitrary predictable process $\{m_t\}_{t>0}$ of the mini-
 166 batch gradients. The better the predictors, the lower the regret, which can be seen from the second
 167 term in Corollary 1 compared to the first term in (2). The construction of the predictable process
 168 $\{m_t\}_{t>0}$ is thus of utmost importance for achieving optimal acceleration and can be learned through
 169 the iterations. We will not deal with the latter in this paper for the sake of space and clarity. Though,
 170 for implementation purposes, we derive a simple, yet effective, gradient prediction algorithm, see
 171 Algorithm 3 in Section 5, embedded in our OPT-AMSGRAD algorithm.

172 4.2 Nonconvex Analysis (Finite-Time Upper Bound)

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

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

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

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

178 where T_M is the maximum number of iteration. The random termination number (4) is inspired by
 179 [14] and is widely used for nonconvex optimization. Assume the following:

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

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

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

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

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

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

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

190 **Lemma 1.** Assume H4, then the quantities defined in Algorithm 2 satisfy for any $w \in \Theta$ and $t > 0$,
 191 $\|\nabla f(w_t)\| < M$, $\|\theta_t\| < M$ and $\|\hat{v}_t\| < M^2$.

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

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

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

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

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

We remark that the bound for our OPT-AMSGrad method matches the complexity bound of $\mathcal{O}\left(\sqrt{d/T_M} + 1/T_M\right)$ of [14] for SGD and [45] 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 ℓ_2 regularization. We consider a fully connected feed forward neural network with L layers modeled by the function $\text{MLN}(w, \xi) : \Theta^d \times \mathbb{R}^p \rightarrow \mathbb{R}$:

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

where $w = [w^{(1)}, w^{(2)}, \dots, w^{(L)}]$ is the vector of parameters, $\xi \in \mathbb{R}^p$ is the input data and σ is the sigmoid activation function. We assume a p dimension input data and a scalar output for simplicity. 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 (can be Huber loss or cross entropy), y are the true labels and $\lambda > 0$ is the regularization parameter. For any index $\ell \in [1, L]$ we denote the output of layer ℓ by

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

The following Lemma proves that assumption H1 is satisfied with a feed forward neural net (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

From 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 [39], MINIMAL POLYNOMIAL EXTRAPOLATION [4], REDUCED RANK EXTRAPOLATION [12]. These methods aim at finding a fixed point g^* and assume that $\{g_t \in \mathbb{R}^d\}_{t>0}$ 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 [34] for details and results. For our numerical experiments, we run OPT-AMSGRAD using Algorithm 3 to construct the sequence $\{m_t\}_{t>0}$ and based on estimating the limit of a sequence using the last iterates [3].

Algorithm 3 REGULARIZED APPROXIMATE MINIMAL POLYNOMIAL EXTRAPOLATION [34]

- 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 a sequence of past r gradients, $\{g_{t-1}, g_{t-2}, \dots, g_{t-r}\}$ as input 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 (6) as $g_t = Ag_{t-1} + \mathcal{O}(\|g_{t-1}\|_2^2)u_{t-1}$, 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.

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 [33]. The other benchmark method is the OPTIMISTIC-ADAM+ \hat{v}_t [8], which details are reported to 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 η 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. We compare different algorithms on *MNIST*, *CIFAR10*, *CIFAR100*, and *IMDB* datasets. For *MNIST*, we use two noisy variants called *MNIST-back-rand* and *MNIST-back-image* from [21] ($n = 12\,000$), *CIFAR10* and *CIFAR100* [20] ($n = 50\,000$) and *IMDB* [24] ($n = 25\,000$).

Network architecture. 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 [35], 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.

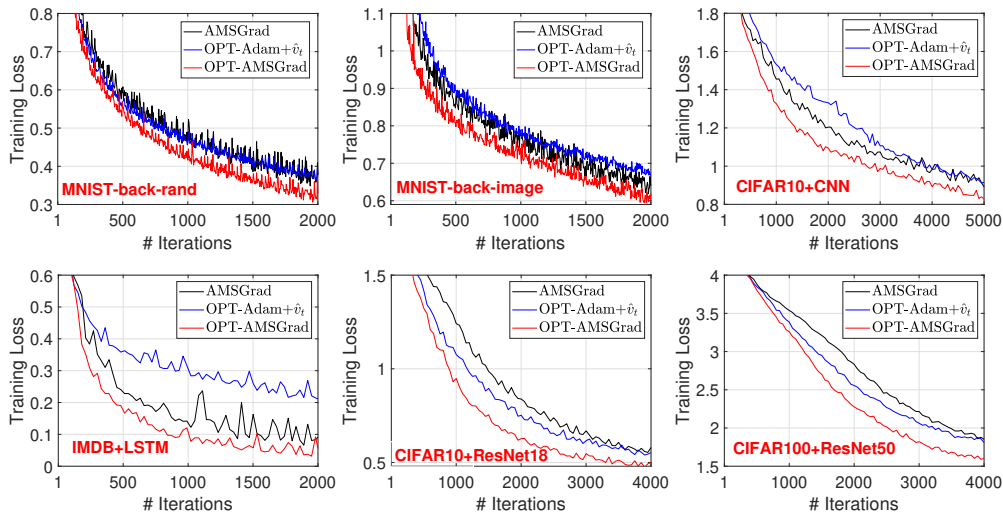


Figure 2: Training loss vs. Number of iterations for fully connected NN, LSTM, CNN and ResNet.

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

262 datasets, the proposed OPT-AMSGRAD converges faster than the other competing methods since
 263 fewer iterations are required to achieve the same precision validating one of the main edges of
 264 OPT-AMSGRAD. We are also curious about the long-term performance and generalization of the
 265 proposed method in test phase. In Figure 3, we plot the results when the model is trained until the
 266 test accuracy stabilizes. We observe: (1) in the long term, OPT-AMSGRAD algorithm may con-
 267 verge to a better point with smaller objective function value, and (2) in these three applications, the
 268 proposed OPT-AMSGRAD also outperforms the competing methods in terms of test accuracy.

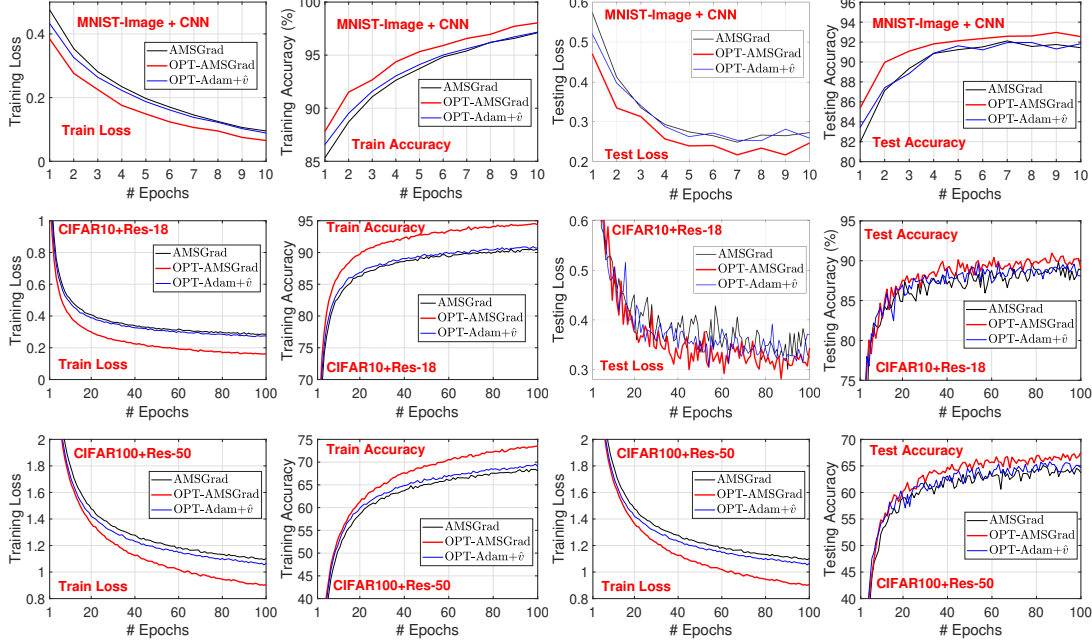


Figure 3: *MNIST-back-image + CNN*, *CIFAR10 + Res-18* and *CIFAR100 + Res-50*. We compare three methods in terms of training (cross-entropy) loss and accuracy, testing loss and accuracy.

269 5.3 Choice of parameter r

270 Since the number of past gradients r is im-
 271 portant in our algorithm, we compare Figure 4
 272 the performance under different values $r = 3, 5, 10$
 273 on two datasets. From the result we see that the
 274 choice of r does not have significant impact on
 275 the training loss. Taking into consideration both
 276 quality of gradient prediction and computational
 277 cost, $r = 5$ is a good choice for most applica-
 278 tions here. We remark that empirically, the per-
 279 formance comparison among $r = 3, 5, 10$ is not
 280 absolutely consistent (i.e. more means better) in
 281 all cases. One possible reason is that for deep neu-
 282 ral networks, the high diversity of gradients com-
 283 puted through the iterations, due to the nonconvex-
 ity of the loss, makes most of them inefficient for
 the predictable process $\{m_t\}_{t>0}$. Only recent ones
 ($r \leq 5$) are useful.

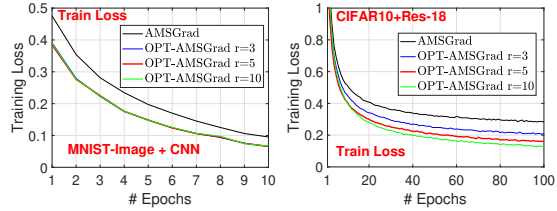


Figure 4: Training loss w.r.t. r .

284 6 Conclusion

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

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

381 **Proof** Beforehand, note:

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

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

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

384 Recall the notation $\psi_t(x)$ and the Bregman divergence $B_{\psi_t}(u, v)$ we defined in the beginning of this
385 section. Now we are going to exploit a useful inequality (which appears in e.g., [38]); for any update
386 of the form $\hat{w} = \arg \min_{w \in \Theta} \langle w, \theta \rangle + B_\psi(w, v)$, it holds that

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

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

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

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

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

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 [41] 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 $\tilde{g}_t = g_t - \beta_1m_t + \beta_1g_{t-1} + m_{t+1}$.

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 $\tilde{g}_t = g_t - \beta_1m_t + \beta_1g_{t-1} + m_{t+1}$. Notice that $\tilde{\theta}_t = \beta_1\tilde{\theta}_{t-1} + (1 -$
421 $\beta_1)(g_t + \beta_1g_{t-1})$.

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

422 \square

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 γ . \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

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

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 (4) and the constants are defined as
438 follows:

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

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

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

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

$$\begin{aligned}\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) &\leq \nabla f(w_t)^\top \left[\frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \left[\eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right] \\ &\leq \frac{\beta_1}{1 - \beta_1} \|\nabla f(w_t)\| \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right\| \left\| \tilde{\theta}_{t-1} \right\| - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t\end{aligned}\quad (30)$$

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

$$\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \frac{\beta_1(1 + \beta_1)}{1 - \beta_1} M^2 \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right\| - \left\| \eta_t \hat{v}_t^{-1/2} \right\| \right] - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \quad (31)$$

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:

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

445 using Lemma 1 on $\|g_t\|$ and where that $\tilde{g}_t = \bar{g}_t + \beta_1 g_{t-1} + m_{t+1} = g_t - \beta_1 m_t + \beta_1 g_{t-1} + m_{t+1}$.
446 Plugging (32) into (31) yields:

$$\begin{aligned}\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) &\leq -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t + \frac{1}{1 - \beta_1} (a\beta_1^2 - 2a\beta_1 + \beta_1) M^2 \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right\| - \left\| \eta_t \hat{v}_t^{-1/2} \right\| \right] \\ &\quad - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1})\end{aligned}\quad (33)$$

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

$$(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \|\nabla f(\bar{w}_t) - \nabla f(w_t)\| \|\bar{w}_{t+1} - \bar{w}_t\| \quad (34)$$

448 Using smoothness assumption H2:

$$\begin{aligned}\|\nabla f(\bar{w}_t) - \nabla f(w_t)\| &\leq L \|\bar{w}_t - w_t\| \\ &\leq L \frac{\beta_1}{1 - \beta_1} \|w_t - \tilde{w}_{t-1}\|\end{aligned}\quad (35)$$

449 By Lemma 3 we also have:

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

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 $\left\| I - (\eta_t \hat{v}_t^{-1/2}) (\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1} \right\| \leq 1$ due to the decreasing stepsize
452 and the construction of \hat{v}_t and using CS inequality yield:

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

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 (35) and (37) into (34) returns:

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

454 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:

$$(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) \leq L \left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\|^2 + 2L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 \|\tilde{w}_{t-1} - w_t\|^2 \quad (39)$$

455 The last term $\frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2$ can be upper bounded using (37):

$$\begin{aligned} \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2 &\leq \frac{L}{2} \left[\frac{\beta_1}{1 - \beta_1} \|\tilde{w}_{t-1} - w_t\| + \left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\| \right] \\ &\leq L \left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\|^2 + 2L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 \|\tilde{w}_{t-1} - w_t\|^2 \end{aligned} \quad (40)$$

456 Plugging (33), (39) and (40) into (29) and taking the expectations on both sides give:

$$\begin{aligned} &\mathbb{E} \left[f(\bar{w}_{t+1}) + \frac{1}{1 - \beta_1} \tilde{M}^2 \left\| \eta_t \hat{v}_t^{-1/2} \right\| - \left(f(\bar{w}_t) + \frac{1}{1 - \beta_1} \tilde{M}^2 \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right\| \right) \right] \\ &\leq \mathbb{E} \left[-\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \tilde{g}_t - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1}) \right] \\ &\quad + \mathbb{E} \left[2L \left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\|^2 + 4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 \|\tilde{w}_{t-1} - w_t\|^2 \right] \end{aligned} \quad (41)$$

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

$$\begin{aligned} \mathbb{E} [\nabla f(w_t)^\top \tilde{g}_t] &= \mathbb{E} [\nabla f(w_t)^\top (g_t - \beta_1 m_t)] \\ &= (1 - a\beta_1) \|\nabla f(w_t)\|^2 \end{aligned} \quad (42)$$

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

$$\begin{aligned} &\frac{1}{M} \sum_{t=1}^{T_M} ((1 - a\beta_1)\eta_{t-1} + (\beta_1 + a)\eta_t) \|\nabla f(w_t)\|^2 \leq \\ &\mathbb{E} \left[f(\bar{w}_1) + \frac{1}{1 - \beta_1} \tilde{M}^2 \left\| \eta_0 \hat{v}_0^{-1/2} \right\| - \left(f(\bar{w}_{T_M+1}) + \frac{1}{1 - \beta_1} \tilde{M}^2 \left\| \eta_{T_M} \hat{v}_{T_M}^{-1/2} \right\| \right) \right] \\ &\quad + 2L \sum_{t=1}^{T_M} \mathbb{E} \left[\left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\|^2 \right] + 4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 \sum_{t=1}^{T_M} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2] \\ &\leq \mathbb{E} \left[\Delta f + \frac{1}{1 - \beta_1} \tilde{M}^2 \left\| \eta_0 \hat{v}_0^{-1/2} \right\| \right] + 2L \sum_{t=1}^{T_M} \mathbb{E} \left[\left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\|^2 \right] + 4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 \sum_{t=1}^{T_M} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2] \end{aligned} \quad (43)$$

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

$$\begin{aligned}\|\tilde{w}_{t-1} - w_t\|^2 &= \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + h_t) \right\|^2 \\ &= \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\theta_{t-1} + \beta_1 \theta_{t-2} + (1 - \beta_1) m_t) \right\|^2 \\ &\leq \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} \theta_{t-1} \right\|^2 + \left\| \eta_{t-2} \hat{v}_{t-2}^{-1/2} \beta_1 \theta_{t-2} \right\|^2 + (1 - \beta_1)^2 \left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} m_t \right\|^2\end{aligned}\quad (44)$$

Using Lemma 4 we have

$$\begin{aligned}\sum_{t=1}^{T_M} \mathbb{E} \left[\|\tilde{w}_{t-1} - w_t\|^2 \right] \\ \leq (1 + \beta_1^2) \frac{\eta^2 d T_M (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} + (1 - \beta_1)^2 \sum_{t=1}^{T_M} \mathbb{E} \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} m_t \right\|^2 \right]\end{aligned}\quad (45)$$

And thus, setting the learning rate to a constant value η and injecting in (43) yields:

$$\begin{aligned}\mathbb{E} [\|\nabla f(w_T)\|^2] &= \frac{1}{\sum_{j=1}^{T_M} \eta_j} \sum_{t=1}^{T_M} \eta_t \|\nabla f(w_t)\|^2 \\ &\leq \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_M} \eta_j} \mathbb{E} \left[\Delta f + \frac{1}{1 - \beta_1} \tilde{M}^2 \left\| \eta_0 \hat{v}_0^{-1/2} \right\|^2 \right] \\ &\quad + \frac{4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_M} \eta_j} (1 + \beta_1^2) \frac{\eta^2 d T_M (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \\ &\quad + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_M} \eta_j} (1 - \beta_1)^2 \sum_{t=1}^{T_M} \mathbb{E} \left[\left\| \eta_{t-1} \hat{v}_{t-1}^{-1/2} m_t \right\|^2 \right] \\ &\quad + \frac{2LM}{(1 - a\beta_1) + (\beta_1 + a)} \frac{1}{\sum_{j=1}^{T_M} \eta_j} \sum_{t=1}^{T_M} \mathbb{E} \left[\left\| \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \right\|^2 \right]\end{aligned}\quad (46)$$

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

$$\begin{aligned}\mathbb{E} [\|\nabla f(w_T)\|^2] \\ \leq C_1 \sqrt{\frac{d}{T_M}} + C_2 \frac{1}{T_M} \\ + D_1 \frac{\eta}{T_M} \sum_{t=1}^{T_M} \mathbb{E} \left[\left\| \hat{v}_{t-1}^{-1/2} m_t \right\|^2 \right] + D_2 \frac{\eta}{T_M} \sum_{t=1}^{T_M} \mathbb{E} \left[\left\| \hat{v}_{t-1}^{-1/2} \tilde{g}_t \right\|^2 \right]\end{aligned}\quad (47)$$

where

$$\begin{aligned}C_1 &= \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \Delta f + \frac{4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a\beta_1) + (\beta_1 + a)} \frac{(1 + \beta_1^2)(1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)} \\ C_2 &= \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E} \left[\left\| \hat{v}_0^{-1/2} \right\|^2 \right]\end{aligned}\quad (48)$$

Simple case as in [45]: if $\beta_1 = 0$ then $\tilde{g}_t = g_t + m_{t+1}$ and $g_t = \theta_t$. Also using Lemma 4 we have that:

$$\sum_{t=1}^{T_M} \eta_t^2 \mathbb{E} \left[\left\| \hat{v}_t^{-1/2} g_t \right\|^2 \right] \leq \frac{\eta^2 d T_M}{(1 - \beta_2)} \quad (49)$$

469 which leads to the final bound:

$$\begin{aligned} & \mathbb{E} [\|\nabla f(w_T)\|^2] \\ & \leq \tilde{C}_1 \sqrt{\frac{d}{T_M}} + \tilde{C}_2 \frac{1}{T_M} \end{aligned} \quad (50)$$

470 where

$$\begin{aligned} \tilde{C}_1 &= C_1 + \frac{M}{(1 - a\beta_1) + (\beta_1 + a)} \left[\frac{a(1 - \beta_1)^2}{1 - \beta_2} + 2L \frac{1}{1 - \beta_2} \right] \\ \tilde{C}_2 &= C_2 = \frac{M}{(1 - \beta_1)((1 - a\beta_1) + (\beta_1 + a))} \tilde{M}^2 \mathbb{E} [\|\hat{v}_0^{-1/2}\|] \end{aligned} \quad (51)$$

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:*

$$\|\xi\| \leq 1 \quad \text{a.s.} \quad \text{and} \quad |\mathcal{L}'(\cdot, y)| \leq T \quad (52)$$

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 $h^{(\ell)}(w, \xi)$:

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

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 $\mathbb{R}^d \times \mathbb{R}^p$. Observe that at the last layer L :

$$\begin{aligned} \|\nabla_{w^{(L)}} \mathcal{L}(\text{MLN}(w, \xi), y)\| &= \|\mathcal{L}'(\text{MLN}(w, \xi), y) \nabla_{w^{(L)}} \text{MLN}(w, \xi)\| \\ &= \left\| \mathcal{L}'(\text{MLN}(w, \xi), y) \sigma'(w^{(L)} h^{(L-1)}(w, \xi)) h^{(L-1)}(w, \xi) \right\| \\ &\leq \frac{T}{4} \end{aligned} \quad (53)$$

477 where the last equality is due to mild assumptions (52) and to the fact that the norm of the derivative
478 of the sigmoid function is upperbounded by 1/4.

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

$$\begin{aligned} \|w_t - \tilde{w}_{t-1}\| &= \left\| -\eta_t \hat{v}_t^{-1/2} (\theta_t + h_{t+1}) \right\| \\ &= \left\| \eta_t \hat{v}_t^{-1/2} (g_t + m_{t+1}) \right\| \\ &\leq \hat{\eta} \left\| \hat{v}_t^{-1/2} g_t \right\| + \hat{\eta} a \left\| \hat{v}_t^{-1/2} g_{t+1} \right\| \end{aligned} \quad (54)$$

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

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

480 . Thus:

$$\begin{aligned} \|w_t - \tilde{w}_{t-1}\| &\leq \hat{\eta} \left(\left\| \hat{v}_t^{-1/2} g_t \right\| + a \left\| \hat{v}_t^{-1/2} g_{t+1} \right\| \right) \\ &\leq \hat{\eta} \frac{a + 1}{\sqrt{1 - \beta_2}} \end{aligned} \quad (55)$$

481 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 (53), we have

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

482 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
483 $\theta_{T,i}^{(L)} \geq 0$ (given the algorithm and $\beta_1 = 0$) and using the fact that $\|w_t - \tilde{w}_{t-1}\| \leq B$ we have

$$0 \leq w_{T-1,i}^{(L)} - B \leq w_{T,i}^{(L)} \leq w_{T-1,i}^{(L)} \quad (56)$$

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 (56) 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

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

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

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

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

$$\nabla_{w^{(\ell)}} \mathcal{L}(\text{MLN}(w, \xi), y) = \mathcal{L}'(\text{MLN}(w, \xi), y) \left(\prod_{j=1}^{\ell+1} \sigma' \left(w^{(j)} h^{(j-1)}(w, \xi) \right) \right) h^{(\ell-1)}(w, \xi) \quad (57)$$

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 (57) 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

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

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

491 F Comparison to some related methods

492 **Comparison to nonconvex optimization works.** Recently, [42, 5, 40, 44, 46, 23] provide some
 493 theoretical analysis of ADAM-type algorithms when applying them to smooth nonconvex opti-
 494 mization problems. For example, [5] provides a bound, which is $\min_{t \in [T]} \mathbb{E}[\|\nabla f(w_t)\|^2] =$
 495 $\mathcal{O}(\log T / \sqrt{T})$. Yet, this data independent bound does not show any advantage over standard
 496 stochastic gradient descent. Similar concerns appear in other papers.

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

506 **Comparison to AO-FTRL [28].** In [28], the authors propose AO-FTRL, which has the update
 507 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
 508 convex loss function with respect to some norm $\|\cdot\|_{(t)}$ that may be different for different iteration t .
 509 Data dependent regret bound was provided in the paper, which is $r_{0:T}(w^*) + \sum_{t=1}^T \|g_t - m_t\|_{(t)}^*$
 510 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.
 511 However, no experiments was provided in [28].

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

518 We want to emphasize that the motivations are different. OPTIMISTIC-ADAM in their paper is
 519 designed to optimize two-player games (e.g. GANs [15]), while the proposed algorithm in this paper
 520 is designed to accelerate optimization (e.g. solving empirical risk minimization quickly). [8] focuses
 521 on training GANs [15]. GANs is a two-player zero-sum game. There have been some related works
 522 in OPTIMISTIC ONLINE LEARNING like [7, 32, 36]) showing that if both players use some kinds of
 523 OPTIMISTIC-update, then accelerating the convergence to the equilibrium of the game is possible.
 524 [8] was inspired by these related works and showed that OPTIMISTIC-MIRROR-DESCENT can avoid
 525 the cycle behavior in a bilinear zero-sum game, which accelerates the convergence. Furthermore,
 526 [8] did not provide theoretical analysis of OPTIMISTIC-ADAM.

527 G Additional Remarks and Runs on the Gradient Prediction Process

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

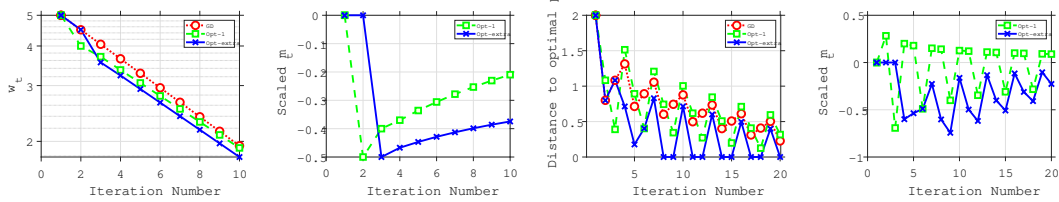


Figure 5: (a): The iterate w_t ; the closer to the optimal point 0 the better. (b): A scaled and clipped version of m_t : $w_t - w_{t-1/2}$, which measures how the prediction of m_t drives the update towards the optimal point. In this scenario, the more negative the better. (c): Distance to the optimal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

535 Specifically, consider optimizing $H(w) := w^2/2$ by the following three algorithms with the same
536 step size. One is Gradient Descent (GD): $w_{t+1} = w_t - \eta_t g_t$, while the other two are OPT-
537 AMSGRAD with $\beta_1 = 0$ and the second moment term \hat{v}_t being dropped: $w_{t+\frac{1}{2}} = \Pi_{\Theta}[w_{t-\frac{1}{2}} - \eta_t g_t]$,
538 $w_{t+1} = \Pi_{\Theta}[w_{t+\frac{1}{2}} - \eta_{t+1} m_{t+1}]$. We denote the algorithm that sets $m_{t+1} = g_t$ as Opt-1, and denote
539 the algorithm that uses the extrapolation method to get m_{t+1} as Opt-extra. We let $\eta_t = 0.1$ and the
540 initial point $w_0 = 5$ for all the three methods. The simulation results are on Figure 5 (a) and (b).
541 Sub-figure (a) plots update w_t over iteration, where the updates should go towards the optimal point
542 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
543 viewed as $-\eta_t m_t$ if the projection (if exists) is lifted. Sub-figure (a) shows that Opt-extra converges
544 faster than the other methods. Furthermore, sub-figure (b) shows that the prediction by the extrap-
545 olation method is better than the prediction by simply using the previous gradient. The sub-figure
546 shows that $-m_t$ from both methods all point to 0 in all iterations and the magnitude is larger for the
547 one produced by the extrapolation method after iteration 2.²

548 Now let us consider another problem: an online learning problem proposed in [33]³. Assume the
549 learner's decision space is $\Theta = [-1, 1]$, and the loss function is $\ell_t(w) = 3w$ if $t \bmod 3 = 1$, and
550 $\ell_t(w) = -w$ otherwise. The optimal point to minimize the cumulative loss is $w^* = -1$. We
551 let $\eta_t = 0.1/\sqrt{t}$ and the initial point $w_0 = 1$ for all the three methods. The parameter λ of the
552 extrapolation method is set to $\lambda = 10^{-3} > 0$. The results are on Figure 5 (c) and (d). Sub-figure
553 (c) shows that Opt-extra converges faster than the other methods while Opt-1 is not better than GD.
554 The reason is that the gradient changes from -1 to 3 at $t \bmod 3 = 1$ and it changes from 3 to -1
555 at $t \bmod 3 = 2$. Consequently, using the current gradient as the guess for the next clearly is not a
556 good choice, since the next gradient is in the opposite direction of the current one. Sub-figure (d)
557 shows that $-m_t$ by the extrapolation method always points to $w^* = -1$, while the one by using
558 the previous negative direction points to the opposite direction in two thirds of rounds. It shows
559 that the extrapolation method is much less affected by the gradient oscillation and always makes the
560 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 [33] uses this example to show that ADAM [19] fails to converge.