
An Optimistic Acceleration of AMSGrad for Nonconvex Optimization

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Abstract

We propose a new variant of AMSGrad [30], a popular adaptive gradient based optimization algorithm widely used for training deep neural networks. Our algorithm adds prior knowledge about the sequence of consecutive mini-batch gradients and leverages its underlying structure making the gradients sequentially predictable. By exploiting the predictability and ideas from optimistic online learning, the proposed algorithm can accelerate the convergence and increase sample efficiency. After establishing a tighter upper bound under some convexity conditions on the regret, we offer a complimentary view of our algorithm which generalizes the offline and stochastic version of nonconvex optimization. In the nonconvex case, we establish a non-asymptotic convergence bound independent of the initialization. We illustrate, via numerical experiments, the practical speedup on several deep learning models and benchmark datasets.

1 Introduction

Deep learning models have been successful in several applications, from robotics (e.g., [21]), computer vision (e.g. [18, 15]), reinforcement learning (e.g., [25]) and natural language processing (e.g., [16]). With the sheer size of modern datasets and the dimension of neural networks, speeding up training is of utmost importance. To do so, several algorithms have been proposed in recent years, such as AMSGRAD [30], ADAM [19], RMSPROP [34], ADADELTA [40], and NADAM [10]. All the prevalent algorithms for training deep networks mentioned above combine two ideas: the idea of adaptivity from ADAGRAD [11, 23] and the idea of momentum from NESTEROV’S METHOD [27] or HEAVY BALL method [28]. ADAGRAD is an online learning algorithm that works well compared to the standard online gradient descent when the gradient is sparse. Its update has a notable feature: it leverages an anisotropic learning rate depending on the magnitude of the gradient for each dimension which helps in exploiting the geometry of the data. On the other hand, NESTEROV’S METHOD or HEAVY BALL Method [28] is an accelerated optimization algorithm which update not only depends on the current iterate and gradient but also depends on the past gradients (i.e. momentum). State-of-the-art algorithms such as AMSGRAD [30] and ADAM [19] leverage these ideas to accelerate the training of nonconvex objective functions, for instance deep neural networks losses.

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

A single work along that direction stands out. [8] develop OPTIMISTIC-ADAM 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. [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 our 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 model parameter estimates leveraging a predictable process able to provide guesses of gradients through the iterations; (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 adapts to the informative dimensions, exhibits momentum, and also exploits a good guess of the next gradient to facilitate acceleration. Besides the complete convergence analysis of OPT-AMSGRAD, we conduct numerical experiments and show that the proposed algorithm not only accelerates the training procedure, but also leads to better empirical generalization performance.

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 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 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 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, called OPTIMISTIC-FTRL and developed in [33] reads

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

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.

where $\{m_t\}_{t>0}$ is a predictable process incorporating (possibly arbitrary) knowledge about the sequence of gradients $\{g_t := \nabla \ell_t(w_t)\}_{t>0}$. Under the assumption that the 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 $\{m_t\}_{t>0}$ 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], under certain boundedness assumptions on Θ detailed below. Yet, when the predictors $\{m_t\}_{t>0}$ are well designed, the resulting 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 $\{m_t\}_{t>0}$ 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 $\sqrt{\sum_{t=1}^T g_t[j]^2}$, where $g_t[j]$ is the j -th element of the gradient vector g_t at time t .

This adaptive learning rate helps accelerating the convergence when the gradient vector is sparse [11], yet, when applying ADAGRAD to train deep neural networks, it is observed that the learning rate might decay too fast, see [19] for more details. Therefore, [19] put forward ADAM that uses a moving average of the gradients divided by the square root of the second moment of this 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 $\mathcal{R}_T/T \rightarrow 0$).

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

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 this 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 OPT-AMSGRAD algorithm inherits three properties: (i) Adaptive learn-

ing rate of each dimension as ADAGRAD [11] (line 6, line 8 and line 9). (ii) Exponential moving average of the past gradients as NESTEROV'S METHOD [27] and the HEAVY-BALL method [28] (line 5). (iii) Optimistic update that exploits *prior knowledge* of the next gradient vector as in optimistic online learning algorithms [7, 29, 33] (line 9). The first property helps for acceleration when the gradient has a sparse structure. The second one is from the long-established idea of momentum which can also help for acceleration. The last property can lead to an acceleration when the prediction of the next gradient is good as mentioned above when introducing the regret bound for the OPTIMISTIC-FTRL algorithm. This 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**

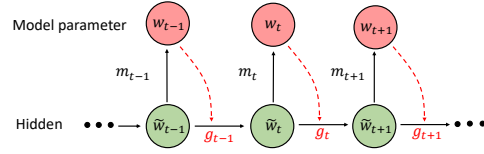


Figure 1: OPT-AMSGRAD underlying structure.

4 Non-Asymptotic Convergence Analysis

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

4.1 Convex Regret Analysis

In the following, we assume convexity of $\{\ell_t\}_{t \geq 0}$ and that Θ has a bounded diameter D_∞ , which is a standard assumption for adaptive methods [30, 19] and is necessary in regret analysis.

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

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

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

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

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

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

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

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

160 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
 161 access to an arbitrary predictable process $\{m_t\}_{t>0}$ of the mini-batch gradients. We notice from
 162 the second term in Corollary 1 compared to the first term in (2) that better predictors lead to lower
 163 regret. The construction of the predictions $\{m_t\}_{t>0}$ is thus of utmost importance for achieving
 164 optimal acceleration and can be learned through the iterations [29]. In Section 5, we derive a basic,
 165 yet effective, gradient prediction algorithm, see Algorithm 3, embedded in OPT-AMSGRAD.

166 4.2 Finite-Time Analysis in the Nonconvex Case

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

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

170 for a fixed batch of n samples $\{\xi_i\}_{i=1}^n$. Set the terminating number, $T \in \{0, \dots, T_M - 1\}$, as a
 171 discrete r.v. with:

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

172 where T_M is the maximum number of iteration. The random termination number (4) is inspired by
 173 [14] and is widely used for nonconvex optimization. Assume the following:

174 **H1.** For any $t > 0$, the estimated parameter w_t stays within a ℓ_∞ -ball. There exist a constant
 175 $W > 0$ such that $\|w_t\|_\infty \leq W$ almost surely.

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

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

179 **H3.** For any $t > 0$, $0 < \langle m_t | g_t \rangle = a_t \|g_t\|^2$ with some $0 < a_t \leq 1$, and $\|m_t\| \leq \|g_t\|$, where $\langle \cdot | \cdot \rangle$
 180 denotes the inner product.

181 Lastly, We make a classical assumption in nonconvex optimization on the magnitude of the gradient:

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

183 We now derive important results for our global analysis. The first one ensures bounded norms of
 184 quantities of interests (resulting from the bounded stochastic gradient assumption):

185 **Lemma 1.** Assume H4, then the quantities defined in Algorithm 2 satisfy for any $w \in \Theta$ and $t > 0$,
 186 $\|\nabla f(w_t)\| < M$, $\|\theta_t\| < M$ and $\|\hat{v}_t\| < M^2$.

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

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

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

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

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

192 where $\Delta f = f(\bar{w}_1) - f(\bar{w}_{T_M+1})$ and $a_m = \min_{t=1, \dots, T} a_t$.

193 Firstly, the bound for our OPT-AMSGrad method matches the complexity bound of $\mathcal{O}(\sqrt{d/T_M} +$
 194 $1/T_M)$ of [14] for SGD considering the dependence of T only, and of [41] for AMSGrad method. To
 195 see the influence of prediction quality, we can show that when $(1 - \beta_1)(\beta_2 - \beta_1^2 - 2L(1 - \beta_1)) -$
 196 $\frac{4L\beta_1^2(1+\beta_1^2)}{1-\gamma} < 0$, \tilde{C}_1 and \tilde{C}_2 both decrease as a_m approaches 1, i.e. as the prediction gets more accu-
 197 rate. Therefore, similar to the convex case, our bound also improves with better gradient prediction.

198 4.3 Checking H1 for a Deep Neural Network

199 As boundedness assumption H1 is generally hard to verify, we now show, for illustrative purposes,
 200 that the weights of a fully connected feed forward neural network stay in a bounded set when being
 201 trained using our method. The activation function for this section will be sigmoid function and we
 202 use a ℓ_2 regularization. We consider a fully connected feed forward neural network with L layers
 203 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 σ 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

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

204 where $\mathcal{L}(\cdot, y)$ is the loss function (e.g., cross-entropy), y are the true labels and $\lambda > 0$ is the regular-
 205 ization parameter. We establish that the boundedness assumption H1 is satisfied with model (5):

206 **Lemma 2.** *Given the multilayer model (5), assume the boundedness of the input data and of the*
 207 *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.*
 208 *and $|\mathcal{L}'(\cdot, y)| \leq T$ where $\mathcal{L}'(\cdot, y)$ denotes its derivative w.r.t. the parameter. Then for each layer*
 209 *$\ell \in [1, L]$, there exist a constant $A_{(\ell)}$ such that $\|w^{(\ell)}\| \leq A_{(\ell)}$*

210 5 Numerical Experiments

211 5.1 Gradient Estimation

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

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

217 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
 218 matrix, see [31] for details and results. For our numerical experiments, we run OPT-AMSGRAD
 219 using Algorithm 3 to construct the sequence $\{m_t\}_{t>0}$ which is based on estimating the limit of a
 220 sequence using the last iterates [3].

221 Specifically, at iteration t , m_t is ob-
 222 tained by (a) calling Algorithm 3
 223 with a sequence of r past gradi-
 224 ents, $\{g_{t-1}, g_{t-2}, \dots, g_{t-r}\}$ as input
 225 yielding the vector $c = [c_0, \dots, c_{r-1}]$
 226 and (b) setting $m_t := \sum_{i=0}^{r-1} c_i g_{t-r+i}$.
 227 To understand why the output from
 228 the extrapolation method may be a
 229 reasonable estimation, assume that

Algorithm 3 Regularized Approximated Minimal Poly-
 nomial Extrapolation [31]

- 1: **Input:** sequence $\{g_s \in \mathbb{R}^d\}_{s=0}^{r-1}$, 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^* .
-

230 the update converges to a stationary point (i.e. $g^* := \nabla f(w^*) = 0$ for the underlying function
 231 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
 232 equation suggests that the next gradient vector g_t is a linear transform of g_{t-1} plus an error vector
 233 that may not be in the span of A . If the algorithm converges to a stationary point, the magnitude of
 234 the error will converge to zero. We note that prior known gradient prediction methods are mainly

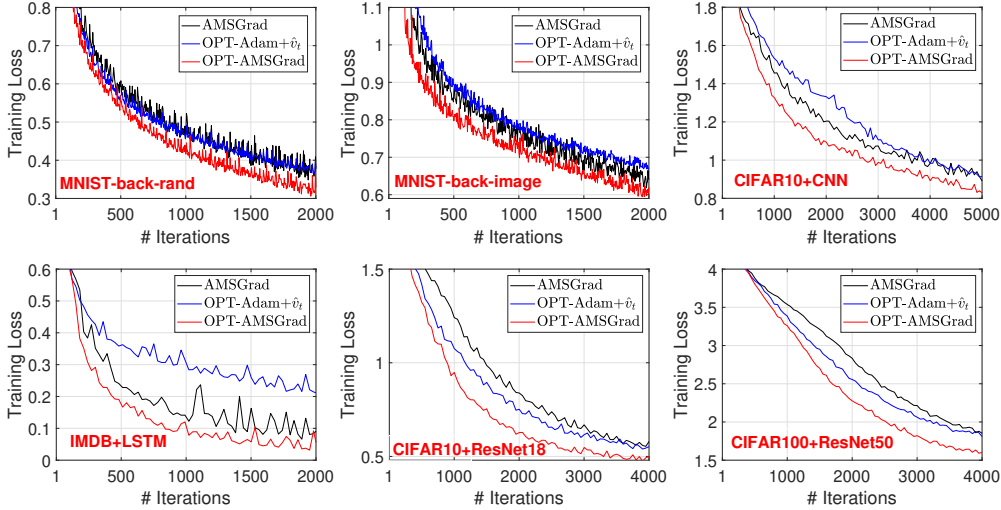


Figure 2: Training loss vs. Number of iterations for fully connected NN, CNN, LSTM and ResNet.

designed for convex functions. Algorithm 3 is employed in our following numerical applications given its empirical success in Deep Learning, see [32], nevertheless, any gradient prediction method can be embedded in our OPT-AMSGRAD framework. The search for the optimal prediction process in order to accelerate even more OPT-AMSGRAD is an interesting research direction, which is left as future work.

Computational cost: This extrapolation step consists in: (a) Constructing the linear system ($U^T U$) 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) can be parallelized in the final implementation.

5.2 Classification Experiments

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 described Algorithm 4. 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. In our implementation, 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 (28×28) 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 32×32 . The *IMDB* movie review dataset, popular for text classification, is a binary dataset with 25 000 training and testing samples respectively.

Network architectures. We adopt a multi-layer fully connected neural network with hidden layers of 200 connected to another layer with 100 neurons (using ReLU activations and Softmax output). This network is tested on *MNIST* variants. For convolutional networks, we adopt a simple four layer CNN which has 2 convolutional layers following by a fully connected layer. In addition, we also

270 apply residual networks, Resnet-18 and Resnet-50 [18], which have achieved state-of-the-art results.
 271 For the texture *IMDB* dataset, we consider a Long-Short Term Memory (LSTM) network [13]. The
 272 latter network includes a word embedding layer with 5 000 input entries representing most frequent
 273 words embedded into a 32 dimensional space. The output of the embedding layer is passed to 100
 274 LSTM units then connected to 100 fully connected ReLU layers.

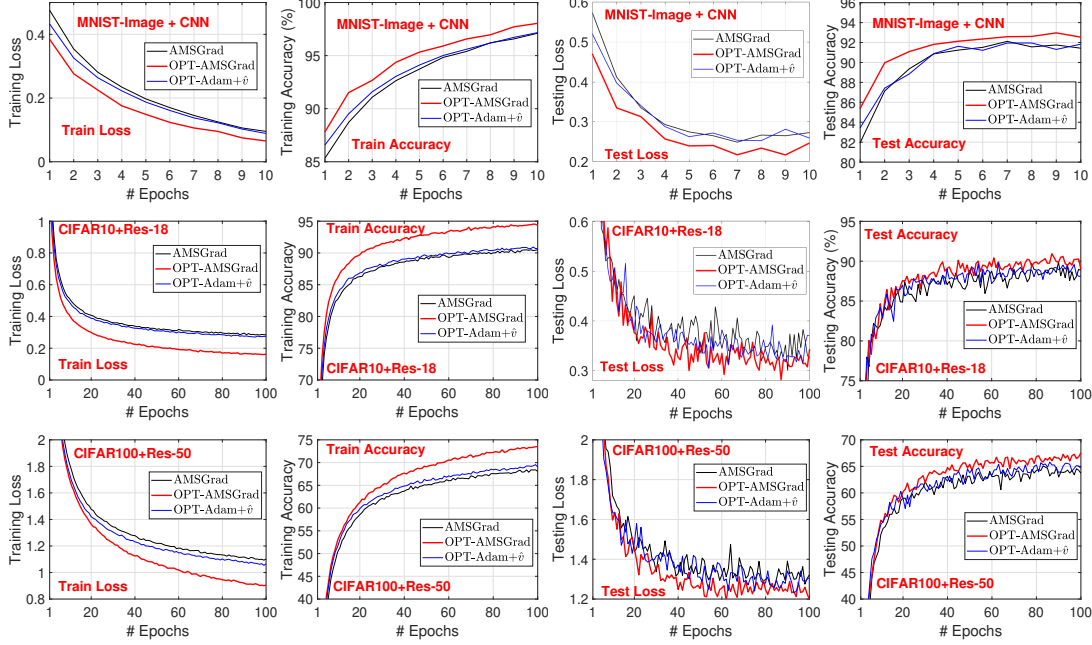


Figure 3: *MNIST-back-image* + CNN, *CIFAR10* + Res-18 and *CIFAR100* + Res-50 . We compare three methods in terms of training (cross-entropy) loss and accuracy, testing loss and accuracy.

275 **Results.** Firstly, to illustrate the acceleration effect of OPT-AMSGRAD at early stage, we pro-
 276 vide the training loss against number of iterations in Figure 2. We clearly observe that on all
 277 datasets, the proposed OPT-AMSGRAD converges faster than the other competing methods since
 278 fewer iterations are required to achieve the same precision, validating one of the main edges of
 279 OPT-AMSGRAD. We are also curious about the long-term performance and generalization of the
 280 proposed method in test phase. In Figure 3, we plot the results when the model is trained until the test
 281 accuracy stabilizes. We observe: (1) in the long term, OPT-AMSGRAD algorithm may converge to
 282 a better point with smaller loss value, and (2) in these applications, our proposed OPT-AMSGRAD
 283 also outperforms the competing methods in terms of test accuracy.

284 5.3 Choice of parameter r

285 Since the number of past gradients r is im-
 286 portant in gradient prediction (Algorithm
 287 3), we compare Figure 4 the performance
 288 under different values $r = 3, 5, 10$ on two
 289 datasets. From the results we see that, tak-
 290 ing into consideration both quality of gra-
 291 dient prediction and computational cost,
 292 $r = 5$ is a good choice for most applica-
 293 tions. We remark that, empirically, the per-
 294 formance comparison among $r = 3, 5, 10$
 295 is not absolutely consistent (i.e. more means better) in all cases. We suspect one possible reason
 296 is that for deep neural networks, the diversity of computed gradients through the iterations, due to
 297 the highly nonconvex loss, makes them inefficient for sequentially building the predictable process
 298 $\{m_t\}_{t>0}$. Thus, sometimes, the recent gradient vectors (e.g. $r \leq 5$) can be more informative.
 299 Yet, in some sense, this characteristic, very specific to deep neural networks, is itself a fundamental
 300 problem of gradient prediction methods.

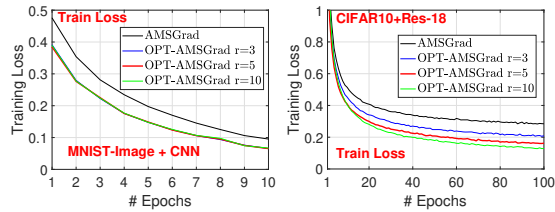


Figure 4: Training loss w.r.t. r .

301 6 Conclusion

302 In this paper, we propose OPT-AMSGRAD, which combines optimistic online learning and AMS-
303 GRAD to improve sample efficiency and accelerate the training process, in particular for fitting deep
304 neural networks on a finite batch of observations. Given a well-designed gradient prediction pro-
305 cess, we theoretically show that the regret, through the iterations, can be smaller than that of standard
306 AMSGRAD. We also establish a finite-time convergence bound on the second order moment of the
307 gradient of the objective loss function matching that of state-of-the-art adaptive gradient methods.
308 Experiments on several benchmark datasets using various deep learning models demonstrate the ef-
309 fectiveness of the proposed algorithm in accelerating the empirical risk minimization procedure and
310 empirically show better generalization properties of our method OPT-AMSGRAD.

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Appendix: An Optimistic Acceleration of AMSGrad for Nonconvex Optimization

A Proof of Theorem 1

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

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

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

Proof Beforehand, we denote:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

415 which is further bounded by

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

416 where the inequality is due to $\|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}} \|g_t - m_t\|_{\psi_{t-1}^*} = \inf_{\beta > 0} \frac{1}{2\beta} \|w_t - \tilde{w}_{t+1}\|_{\psi_{t-1}}^2 +$
417 $\frac{\beta}{2} \|g_t - m_t\|_{\psi_{t-1}^*}^2$ by Young's inequality and the 1-strongly convex of $\psi_{t-1}(\cdot)$ with respect to $\|\cdot\|_{\psi_{t-1}}$
418 which yields that $B_{\psi_{t-1}}(\tilde{w}_{t+1}, w_t) \geq \frac{1}{2} \|\tilde{w}_{t+1} - w_t\|_{\psi_t}^2 \geq 0$.

419 To proceed, notice that

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

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

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

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

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

422 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
423 proof.

424 □

425 B Proof of Corollary 1

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

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

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

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

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

430 The second term reads:

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

431 To interpret the bound, let us make a rough approximation such that $\sum_{s=1}^{t-1} \beta_2^{t-1-s} (g_s[i] - m_s[i])^2 \simeq$
 432 $(g_t[i] - m_t[i])^2$. Then, we can further get an upper-bound as

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

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

434 □

435 C Proofs of Auxiliary Lemmas

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

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

437 **Lemma 3.** Assume a strictly positive and non increasing sequence of stepsizes $\{\eta_t\}_{t>0}$, $\beta_1 < \beta_2 \in$
 438 $[0, 1)$, then the following holds:

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

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

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

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

441 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 $\tilde{\theta}_t = \beta_1 \tilde{\theta}_{t-1} + (1 -$
 442 $\beta_1)(g_t + \beta_1 g_{t-1})$.

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

443 □

444 **Lemma 4.** Assume H4, a strictly positive and a sequence of constant stepsizes $\{\eta_t\}_{t>0}$, $(\beta_1, \beta_2) \in$
 445 $[0, 1]$, then the following holds:

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

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

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

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

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

449 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:

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

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

451 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:

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

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

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

Using the same induction reasoning we prove that

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

454

□

455 D Proof of Theorem 2

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

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

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

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

459 where $\Delta f = f(\bar{w}_1) - f(\bar{w}_{T_M+1})$ and $a_m = \min_{t=1, \dots, T} a_t$.

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

$$\begin{aligned} f(\bar{w}_{t+1}) &\leq f(\bar{w}_t) + \nabla f(\bar{w}_t)^\top (\bar{w}_{t+1} - \bar{w}_t) + \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2 \\ &\leq f(\bar{w}_t) + \underbrace{\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t)}_A \\ &\quad + \underbrace{(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t)}_B + \frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|. \end{aligned} \quad (27)$$

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

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

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

$$\nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \frac{\beta_1 (1 + \beta_1)}{1 - \beta_1} M^2 [\|\eta_{t-1} \hat{v}_{t-1}^{-1/2}\| - \|\eta_t \hat{v}_t^{-1/2}\|] - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t, \quad (28)$$

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

$$\begin{aligned} -\nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} \tilde{g}_t &= -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \tilde{g}_t - \nabla f(w_t)^\top \left[\eta_t \hat{v}_t^{-1/2} - \eta_{t-1} \hat{v}_{t-1}^{-1/2} \right] \tilde{g}_t \\ &\quad - \nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} (\beta_1 g_{t-1} + m_{t+1}) \\ &\leq -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \tilde{g}_t + (1 - a_t \beta_1) M^2 [\|\eta_{t-1} \hat{v}_{t-1}^{-1/2}\| - \|\eta_t \hat{v}_t^{-1/2}\|] \\ &\quad - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1}), \end{aligned} \quad (29)$$

where we have used Lemma 1 on $\|g_t\|$ and where that $\tilde{g}_t = \bar{g}_t + \beta_1 g_{t-1} + m_{t+1} = g_t - \beta_1 m_t + \beta_1 g_{t-1} + m_{t+1}$. Plugging (29) into (28) yields:

$$\begin{aligned} & \nabla f(w_t)^\top (\bar{w}_{t+1} - \bar{w}_t) \\ & \leq -\nabla f(w_t)^\top \eta_{t-1} \hat{v}_{t-1}^{-1/2} \bar{g}_t + \frac{1}{1 - \beta_1} (a_t \beta_1^2 - 2a_t \beta_1 + \beta_1) \mathbf{M}^2 [\|\eta_{t-1} \hat{v}_{t-1}^{-1/2}\| - \|\eta_t \hat{v}_t^{-1/2}\|] \\ & \quad - \nabla f(w_t)^\top \eta_t \hat{v}_t^{-1/2} (\beta_1 g_{t-1} + m_{t+1}) . \end{aligned} \quad (30)$$

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

$$(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) \leq \|\nabla f(\bar{w}_t) - \nabla f(w_t)\| \|\bar{w}_{t+1} - \bar{w}_t\| . \quad (31)$$

Using smoothness assumption H2:

$$\begin{aligned} \|\nabla f(\bar{w}_t) - \nabla f(w_t)\| & \leq L \|\bar{w}_t - w_t\| \\ & \leq L \frac{\beta_1}{1 - \beta_1} \|w_t - \tilde{w}_{t-1}\| . \end{aligned} \quad (32)$$

By Lemma 3 we also have:

$$\begin{aligned} \bar{w}_{t+1} - \bar{w}_t & = \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \left[\eta_{t-1} \hat{v}_{t-1}^{-1/2} - \eta_t \hat{v}_t^{-1/2} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \\ & = \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{t-1} \eta_{t-1} \hat{v}_{t-1}^{-1/2} \left[I - (\eta_t \hat{v}_t^{-1/2})(\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1} \right] - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t \\ & = \frac{\beta_1}{1 - \beta_1} \left[I - (\eta_t \hat{v}_t^{-1/2})(\eta_{t-1} \hat{v}_{t-1}^{-1/2})^{-1} \right] (\tilde{w}_{t-1} - w_t) - \eta_t \hat{v}_t^{-1/2} \tilde{g}_t , \end{aligned} \quad (33)$$

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

$$\|\bar{w}_{t+1} - \bar{w}_t\| \leq \frac{\beta_1}{1 - \beta_1} \|\tilde{w}_{t-1} - w_t\| + \|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\| . \quad (34)$$

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

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

Plugging (32) and (34) into (31) returns:

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

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:

$$(\nabla f(\bar{w}_t) - \nabla f(w_t))^\top (\bar{w}_{t+1} - \bar{w}_t) \leq L \|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\|^2 + 2L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 \|\tilde{w}_{t-1} - w_t\|^2 . \quad (35)$$

The last term $\frac{L}{2} \|\bar{w}_{t+1} - \bar{w}_t\|^2$ can be upper bounded using (34):

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

477 Plugging (30), (35) and (36) into (27) and taking the expectations on both sides give:

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

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

$$\mathbb{E} [\nabla f(w_t)^\top \tilde{g}_t] = \mathbb{E} [\nabla f(w_t)^\top (g_t - \beta_1 m_t)] = (1 - a_t \beta_1) \|\nabla f(w_t)\|^2. \quad (37)$$

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

$$\begin{aligned}
& \frac{1}{M} \sum_{t=1}^{T_M} ((1 - a_t \beta_1) \eta_{t-1} + (\beta_1 + a_t) \eta_t) \|\nabla f(w_t)\|^2 \leq \\
& \mathbb{E} \left[f(\bar{w}_1) + \frac{1}{1-\beta_1} \tilde{M}_t^2 \|\eta_0 \hat{v}_0^{-1/2}\| - \left(f(\bar{w}_{T_M+1}) + \frac{1}{1-\beta_1} \tilde{M}_t^2 \|\eta_{T_M} \hat{v}_{T_M}^{-1/2}\| \right) \right] \\
& + 2L \sum_{t=1}^{T_M} \mathbb{E} [\|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\|^2] + 4L \left(\frac{\beta_1}{1-\beta_1} \right)^2 \sum_{t=1}^{T_M} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2] \quad (38) \\
& \leq \mathbb{E} \left[\Delta f + \frac{1}{1-\beta_1} \tilde{M}_t^2 \|\eta_0 \hat{v}_0^{-1/2}\| \right] + 2L \sum_{t=1}^{T_M} \mathbb{E} [\|\eta_t \hat{v}_t^{-1/2} \tilde{g}_t\|^2] \\
& + 4L \left(\frac{\beta_1}{1-\beta_1} \right)^2 \sum_{t=1}^{T_M} \mathbb{E} [\|\tilde{w}_{t-1} - w_t\|^2],
\end{aligned}$$

481 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
482 learning rate η_t , we have

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

483 Using Lemma 4 we have

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

484 Assume $a_m = \min_{1, \dots, T_M} a_t$ and denote $\tilde{M}_m^2 = (a_m \beta_1^2 + \beta_1) M^2$. Setting a constant learning rate
 485 $\eta_t = \eta$ and plugging in (38) yields:

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

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

$$\mathbb{E}[\|\nabla f(w_T)\|^2] \leq C_{1,m} \sqrt{\frac{d}{T_M}} + C_{2,m} \frac{1}{T_M} + \frac{\eta}{T_M} D_{1,m} \mathbb{E}[\|\hat{v}_{t-1}^{-1/2} m_t\|] + \frac{\eta}{T_M} D_{2,m} \mathbb{E}[\|\hat{v}_{t-1}^{-1/2} \tilde{g}_t\|],$$

488 where

$$\begin{aligned} C_{1,m} &= \frac{M}{(1 - a_m \beta_1) + (\beta_1 + a_m)} \Delta f + \frac{4L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 M}{(1 - a_m \beta_1) + (\beta_1 + a_m)} \frac{(1 + \beta_1^2)(1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)}, \\ C_{2,m} &= \frac{M}{(1 - \beta_1)((1 - a_m \beta_1) + (\beta_1 + a_m))} (a_m \beta_1^2 + \beta_1) M^2 \mathbb{E}[\|\hat{v}_0^{-1/2}\|]. \end{aligned}$$

489 **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
 490 that:

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

491 which leads to the final bound:

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

492 where

$$\begin{aligned} \tilde{C}_{1,m} &= C_{1,m} + \frac{M}{(1 - a_m \beta_1) + (\beta_1 + a_m)} \left[\frac{a_m (1 - \beta_1)^2}{1 - \beta_2} + 2L \frac{1}{1 - \beta_2} \right], \\ \tilde{C}_{2,m} &= C_{2,m} = \frac{M}{(1 - \beta_1)((1 - a_m \beta_1) + (\beta_1 + a_m))} \tilde{M}_m^2 \mathbb{E}[\|\hat{v}_0^{-1/2}\|]. \end{aligned}$$

493

□

494 E Proof of Lemma 2 (Boundedness of the iterates H1)

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

$$\|\xi\| \leq 1 \quad \text{a.s.} \quad \text{and} \quad |\mathcal{L}'(\cdot, y)| \leq T, \quad (39)$$

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 ℓ by

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

497 Given the sigmoid assumption we have $\|h^{(\ell)}(w, \xi)\| \leq 1$ for any $\ell \in [1, L]$ and any $(w, \xi) \in$
 498 $\mathbb{R}^d \times \mathbb{R}^p$. We also recall that $\mathcal{L}(\cdot, y)$ is the loss function, which can be Huber loss or cross entropy.
 499 Observe that at the last layer L :

$$\begin{aligned} \|\nabla_{w^{(L)}} \mathcal{L}(\text{MLN}(w, \xi), y)\| &= \|\mathcal{L}'(\text{MLN}(w, \xi), y) \nabla_{w^{(L)}} \text{MLN}(w, \xi)\| \\ &= \|\mathcal{L}'(\text{MLN}(w, \xi), y) \sigma'(w^{(L)} h^{(L-1)}(w, \xi)) h^{(L-1)}(w, \xi)\| \\ &\leq \frac{T}{4} , \end{aligned} \quad (40)$$

500 where the last equality is due to mild assumptions (39) and to the fact that the norm of the derivative
 501 of the sigmoid function is upperbounded by $1/4$.

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

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

503 Thus:

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

504 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 (40), we have

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

505 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
 506 $\theta_{T,i}^{(L)} \geq 0$ (given the algorithm and $\beta_1 = 0$) and using the fact that $\|w_t - \tilde{w}_{t-1}\| \leq B$ we have

$$0 \leq w_{T-1,i}^{(L)} - B \leq w_{T,i}^{(L)} \leq w_{T-1,i}^{(L)} , \quad (41)$$

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 (41) 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

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

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

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

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

$$\nabla_{w^{(\ell)}} \mathcal{L}(\text{MLN}(w, \xi), y) = \mathcal{L}'(\text{MLN}(w, \xi), y) \left(\prod_{j=1}^{\ell+1} \sigma' \left(w^{(j)} h^{(j-1)}(w, \xi) \right) \right) h^{(\ell-1)}(w, \xi) . \quad (42)$$

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 (42) 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

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

511 Showing that the weights of the previous layers $\ell \in [1, L-1]$ as well as for the last layer L of our
 512 fully connected feed forward neural network are bounded at each iteration, leads by induction, to
 513 the boundedness (at each iteration) assumption we want to check, thus proving Lemma 2. \square

514 F Comparison to related methods

515 **Comparison to nonconvex optimization methods.** Recently, [39, 5, 37, 41, 42, 22] provide
 516 some theoretical analysis of ADAM-type algorithms when applying them to smooth nonconvex op-
 517 timization problems. For example, [5] provide the following bound $\min_{t \in [T]} \mathbb{E}[\|\nabla f(w_t)\|^2] =$
 518 $\mathcal{O}(\log T / \sqrt{T})$. Yet, this data independent bound does not show any advantage over standard
 519 stochastic gradient descent. Similar concerns appear in other related works. To get some adap-
 520 tive data dependent bound written in terms of the gradient norms observed along the trajectory when
 521 applying OPT-AMSGRAD to nonconvex optimization, one can follow the approach of [2] or [6].
 522 They provide a modular approach to convert algorithms with adaptive data dependent regret bound
 523 for convex loss functions (e.g., ADAGRAD) to algorithms that can find an approximate stationary
 524 point of nonconvex objectives. These variants can outperform the ones instantiated by other ADAM-
 525 type algorithms when the gradient prediction m_t is close to the true gradient g_t .

526 **Comparison to AO-FTRL [26].** In [26], the authors propose AO-FTRL, which update reads
 527 $w_{t+1} = \arg \min_{w \in \Theta} (\sum_{s=1}^t g_s)^\top w + m_{t+1}^\top w + r_{0:t}(w)$, where $r_{0:t}(\cdot)$ is a 1-strongly convex loss
 528 function with respect to some norm $\|\cdot\|_{(t)}$ that may be different for different iteration t . Data depen-
 529 dent regret bound provided in [26] reads $r_{0:T}(w^*) + \sum_{t=1}^T \|g_t - m_t\|_{(t)}^*$ for any benchmark $w^* \in \Theta$.
 530 We remark 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
 531 the update might be viewed as an optimistic variant of ADAGRAD. However, no experiments were
 532 provided in [26] to back those findings.

533 **Comparison to OPTIMISTIC-ADAM [8].** This is an optimistic variant of ADAM,
 534 namely OPTIMISTIC-ADAM. A slightly modified version is summarized in Algorithm 4.
 535 Here, OPTIMISTIC-ADAM+ \hat{v}_t corresponds to OPTIMISTIC-ADAM with the additional max
 536 operation $\hat{v}_t = \max(\hat{v}_{t-1}, v_t)$ to guarantee that the weighted second moment is monotone
 537 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**
-

538 We want to emphasize that the motivations of our optimistic algorithm are different. OPTIMISTIC-
 539 ADAM is designed to optimize two-player games (e.g., GANs [15]), while our proposed algorithm
 540 OPT-AMSGRAD is designed to accelerate optimization (e.g., solving empirical risk minimization).
 541 [8] focuses on training GANs [15] as a two-player zero-sum game. [8] is inspired by these related
 542 works and shows that OPTIMISTIC-MIRROR-DESCENT can avoid the cycle behavior in a bilinear
 543 zero-sum game thus accelerating convergence.

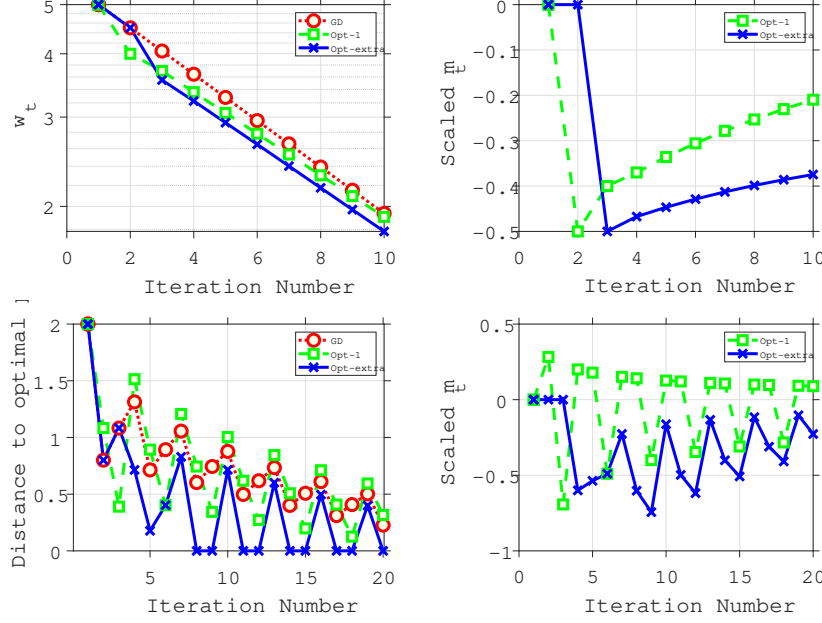


Figure 5: (a): The iterate w_t ; the closer to the optimal point 0 the better. (b): A scaled and clipped version of m_t : $w_t - w_{t-1/2}$, which measures how the prediction of m_t drives the update towards the optimal point. In this scenario, the more negative the better. (c): Distance to the optimal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

544 G Additional Remarks and Runs on the Gradient Prediction Process

Two illustrative examples. We provide two toy examples to demonstrate how OPT-AMSGRAD works with the chosen extrapolation method. First, consider minimizing a quadratic function $H(w) := \frac{b}{2}w^2$ with vanilla gradient descent method $w_{t+1} = w_t - \eta_t \nabla H(w_t)$. The gradient $g_t := \nabla H(w_t)$ can be recursively expressed as $g_{t+1} = bw_{t+1} = b(w_t - \eta_t g_t) = g_t - b\eta_t g_t$. Thus, the update can be written in the form of

$$g_t = Ag_{t-1} + \mathcal{O}(\|g_{t-1}\|_2^2)u_{t-1},$$

545 where $A = (1 - b\eta)$ and $u_{t-1} = 0$ by setting $\eta_t = \eta$ (constant step size). Therefore, the extrapolation
 546 method should predict well. Specifically, consider optimizing $H(w) := w^2/2$ by the following
 547 three algorithms with the same step size. One is Gradient Descent (GD): $w_{t+1} = w_t - \eta_t g_t$, while
 548 the other two are OPT-AMSGRAD with $\beta_1 = 0$ and the second moment term \hat{v}_t being dropped:
 549 $w_{t+\frac{1}{2}} = \Pi_{\Theta}[w_{t-\frac{1}{2}} - \eta_t g_t]$, $w_{t+1} = \Pi_{\Theta}[w_{t+\frac{1}{2}} - \eta_{t+1} m_{t+1}]$. We denote the algorithm that sets
 550 $m_{t+1} = g_t$ as OPT-1, and denote the algorithm that uses the extrapolation method to get m_{t+1} as
 551 OPT-EXTRA. We let $\eta_t = 0.1$ and the initial point $w_0 = 5$ for all three methods. The simulation
 552 results are on Figure 5 (a) and (b). Sub-figure (a) plots update w_t over iteration, where the updates
 553 should go towards the optimal point 0. Sub-figure (b) displays a scaled and clipped version of m_t ,
 554 defined as $w_t - w_{t-1/2}$, which can be viewed as $-\eta_t m_t$ if the projection (if exists) is lifted. Sub-
 555 figure (a) shows that OPT-EXTRA converges faster than the other methods. Furthermore, sub-figure
 556 (b) shows that the prediction by the extrapolation method is better than the prediction by simply
 557 using the previous gradient. The sub-figure shows that $-m_t$ from both methods points to 0 for each
 558 iteration and the magnitude is larger for the one produced by the extrapolation method after iteration
 559 2.²

560 Now let us consider another problem: an online learning problem proposed in [30]³. Assume the
 561 learner's decision space is $\Theta = [-1, 1]$, and the loss function is $\ell_t(w) = 3w$ if $t \bmod 3 = 1$, and
 562 $\ell_t(w) = -w$ otherwise. The optimal point to minimize the cumulative loss is $w^* = -1$. We let

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

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

563 $\eta_t = 0.1/\sqrt{t}$ and the initial point $w_0 = 1$ for all three methods. The parameter λ of the extrapolation
 564 method is set to $\lambda = 10^{-3} > 0$. The results are reported Figure 5 (c) and (d). Sub-figure (c) shows
 565 that OPT-EXTRA converges faster than the other methods while OPT-1 is not performing better than
 566 GD. The reason is that the gradient changes from -1 to 3 at $t \bmod 3 = 1$ and it changes from 3 to -1
 567 at $t \bmod 3 = 2$. Consequently, using the current gradient as the guess for the next is empirically not
 568 a good choice, since the next gradient is in the opposite direction of the current one, according to our
 569 experiments. Sub-figure (d) shows that $-m_t$, obtained with the extrapolation method, always points
 570 to $w^* = -1$, while the one obtained by using the previous negative direction points to the opposite
 571 direction in two thirds of rounds. It shows that the extrapolation method is much less affected by the
 572 gradient oscillation and always makes the prediction in the right direction, which suggests that the
 573 method can capture the aggregate effect.