Optimistic Acceleration of AMSGrad for Nonconvex Optimization.

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1 Nonconvex Analysis

We tackle the following classical optimization problem:

$$\min_{w \in \Theta} f(w) := \mathbb{E}[f(w, \xi)] \tag{1}$$

- where ξ is some random noise and only noisy versions of the objective function are accessible in
- 4 this work. The objective function f(w) is (potentially) nonconvex and has Lipschitz gradients.
- 5 Optimistic Algorithm We present here the algorithm studied in this paper to tackle problem (1).
- Set the terminating iteration number, $K \in \{0, \dots, K_{\text{max}} 1\}$, as a discrete r.v. with:

$$P(K = k) = \frac{\eta_k}{\sum_{f=0}^{K_{\text{max}}-1} \eta_f}.$$
 (2)

- 7 where $K_{\text{max}} \leftarrow$ is the maximum number of iteration. The random termination number (2) is inspired
- 8 by [Ghadimi and Lan, 2013] which enables one to show non-asymptotic convergence to stationary
- 9 point for non-convex optimization. Consider constants $(\beta_1, \beta_2) \in [0, 1]$, a sequence of decreasing
- stepsizes $\{\eta_k\}_{k>0}$, Algorithm 1 introduces the new optimistic AMSGrad method.

Algorithm 1 OPTIMISTIC-AMSGRAD

- 1: **Input:** Parameters $\beta_1, \beta_2, \epsilon, \eta_k$ 2: **Init.:** $w_1 = w_{-1/2} \in \mathcal{K} \subseteq \mathbb{R}^d$ and $v_0 = \epsilon \mathbf{1} \in \mathbb{R}^d$ 3: **for** $k = 0, 1, 2, \dots, K$ **do** 4: Get mini-batch stochastic gradient g_k at w_k 5: $\theta_k = \beta_1 \theta_{k-1} + (1 - \beta_1) g_k$ 6: $v_k = \beta_2 v_{k-1} + (1 - \beta_2) g_k^2$ 7: $\hat{v}_k = \max(\hat{v}_{k-1}, v_k)$ 8: $w_{k+\frac{1}{2}} = \Pi_K \left[w_k - \eta_k \frac{\theta_k}{\sqrt{\hat{v}_k}} \right]$ 9: $w_{k+1} = \Pi_K \left[w_{k+\frac{1}{2}} - \eta_k \frac{h_{k+1}}{\sqrt{\hat{v}_k}} \right]$ 10: where $h_{k+1} := \beta_1 \theta_{k-1} + (1 - \beta_1) m_{k+1}$ 11: and m_{k+1} is a guess of g_{k+1} 12: **end for** 13: **Return**: w_{K+1} .
- The final update at iteration k can be summarized as:

$$w_{k+1} = w_k - \eta_k \frac{\theta_k}{\sqrt{\hat{v}_k}} - \eta_k \frac{h_{k+1}}{\sqrt{v}_k}$$
(3)

We make the following assumptions:

Submitted to 34th Conference on Neural Information Processing Systems (NeurIPS 2020). Do not distribute.

- 13 **H1.** The loss function f(w) is nonconvex w.r.t. the parameter w.
- 14 **H2.** For any k>0, the estimated weight w_k stays within a ℓ_∞ -ball. There exists a constant W>0
- 15 such that.

$$||w_k|| \le W$$
 almost surely (4)

H3. The function f(w) is L-smooth w.r.t. the parameter w. There exist some constant L > 0 such that for $(w, \vartheta) \in \Theta^2$:

$$f(w) - f(\vartheta) - \nabla f(\vartheta)^{\top} (w - \vartheta) \le \frac{L}{2} \|w - \vartheta\|^2 . \tag{5}$$

H4. There exists a constant a > 0 such that for any k > 0:

$$||m_{k+1}|| \le a ||g_{k+1}||$$

- 18 Classically (see [Ghadimi and Lan, 2013]) in nonconvex optimization, we make an assumption on
- 19 the magnitude of the gradient:
 - **H5.** There exists a constant M > 0 such that

$$\|\nabla f(w,\xi)\| < \mathsf{M}$$
 for any w and ξ

- 20 We begin with some auxiliary Lemmas important for the analysis. The first one ensures bounded
- 21 norms of various quantities of interests (boiling down from the classical stochastic gradient bound-
- 22 edness assumption):

Lemma 1. Assume assumption H 5, then the quantities defined in Algorithm 1 satisfy for any $w \in \Theta$ and k > 0:

$$\|\nabla f(w_k)\| < \mathsf{M}, \quad \|\theta_k\| < \mathsf{M}^2, \quad \|\hat{v}_k\| < \mathsf{M}.$$

Proof Assume assumption H 5 we have:

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

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

$$\|\theta_{k+1}\| = \|\beta_1 \theta_k + (1 - \beta_1) g_{k+1}\| \le \beta_1 \|\theta_k\| + (1 - \beta_1) \|g_{k+1}\| \le \mathsf{M}$$
 (6)

Using the same induction reasoning we prove that

$$\|\hat{v}_{k+1}\| = \|\beta_2 \hat{v}_k + (1 - \beta_2) g_{k+1}^2\| \le \beta_2 \|\hat{v}_k\| + (1 - \beta_1) \|g_{k+1}^2\| \le \mathsf{M}^2 \tag{7}$$

25

- Then, following [Yan et al., 2018] and their study of the SGD with Momentum (not AMSGrad but
- simple momentum) we denote for any k > 0:

$$\overline{w}_k = w_k + \frac{\beta_1}{1 - \beta_1} (w_k - w_{k-1}) = \frac{1}{1 - \beta_1} w_k - \frac{\beta_1}{1 - \beta_1} w_{k-1} , \qquad (8)$$

- 28 and derive an important Lemma:
- Lemma 2. Assume a strictly positive and non increasing sequence of stepsizes $\{\eta_k\}_{k>0}$, $\beta_{\in}[0,1]$,
- 30 then the following holds:

$$\overline{w}_{k+1} - \overline{w}_k = \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{k-1} \left[\eta_{k-1} \hat{v}_{k-1}^{-1/2} - \eta_k \hat{v}_k^{-1/2} \right] - \eta_k \hat{v}_k^{-1/2} \tilde{g}_k , \qquad (9)$$

- 31 where $\tilde{\theta}_k = \theta_k + \beta_1 \theta_{k-1} + (1 \beta_1) m_{k+1}$ and $\tilde{g}_k = g_k \beta_1 g_{k-1}$.
- Proof By definition (8) and using the Algorithm updates, we have:

$$\overline{w}_{k+1} - \overline{w}_k = \frac{1}{1 - \beta_1} (w_{k+1} - w_k) - \frac{\beta_1}{1 - \beta_1} (w_k - w_{k-1})
= -\frac{1}{1 - \beta_1} \eta_k \hat{v}_k^{-1/2} (\theta_k + h_{k+1}) + \frac{\beta_1}{1 - \beta_1} \eta_{k-1} \hat{v}_{k-1}^{-1/2} (\theta_{k-1} + h_k)
= -\frac{1}{1 - \beta_1} \eta_k \hat{v}_k^{-1/2} (\theta_k + \beta_1 \theta_{k-1}) - \frac{1}{1 - \beta_1} \eta_k \hat{v}_k^{-1/2} (1 - \beta_1) m_{k+1}
+ \frac{\beta_1}{1 - \beta_1} \eta_{k-1} \hat{v}_{k-1}^{-1/2} (\theta_{k-1} + \beta_1 \theta_{k-2}) + \frac{\beta_1}{1 - \beta_1} \eta_{k-1} \hat{v}_{k-1}^{-1/2} (1 - \beta_1) m_k$$
(10)

Denote $\tilde{\theta}_k=\theta_k+\beta_1\theta_{k-1}+(1-\beta_1)m_{k+1}$ and $\tilde{g}_k=g_k-\beta_1g_{k-1}.$ Notice that $\tilde{\theta}_k=\beta_1\tilde{\theta}_{k-1}+(1-\beta_1)(g_k+\beta_1g_{k-1}).$

$$\overline{w}_{k+1} - \overline{w}_k = \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{k-1} \left[\eta_{k-1} \hat{v}_{k-1}^{-1/2} - \eta_k \hat{v}_k^{-1/2} \right] - \eta_k \hat{v}_k^{-1/2} \tilde{g}_k$$
 (11)

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Lemma 3. Assume H 5, a strictly positive and non increasing sequence of stepsizes $\{\eta_k\}_{k>0}$, $\beta \in [0,1]$, then the following holds:

$$\sum_{k=1}^{K} \eta_k^2 \mathbb{E}\left[\left\| \hat{v}_k^{-1/2} \theta_k \right\|_2^2 \right] \le \frac{\eta^2 dK (1 - \beta_1)}{(1 - \beta_2)(1 - \gamma)}$$
(12)

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

$$\eta_{k}^{2} \mathbb{E} \left[\left\| \hat{v}_{k}^{-1/2} \theta_{k} \right\|_{2}^{2} \right] = \eta_{k}^{2} \mathbb{E} \left[\sum_{p=1}^{d} \frac{\theta_{k,p}^{2}}{\hat{v}_{k,p}} \right] \\
\leq \eta_{k}^{2} \mathbb{E} \left[\sum_{i=1}^{d} \frac{\theta_{k,p}^{2}}{v_{k,p}} \right] \\
\leq \eta_{k}^{2} \mathbb{E} \left[\sum_{i=1}^{d} \frac{\left(\sum_{t=1}^{k} (1 - \beta_{1}) \beta_{1}^{k-t} g_{t,p} \right)^{2}}{\sum_{t=1}^{k} (1 - \beta_{2}) \beta_{2}^{k-t} g_{t,p}^{2}} \right]$$
(13)

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

$$\eta_{k}^{2} \mathbb{E} \left[\left\| \hat{v}_{k}^{-1/2} \theta_{k} \right\|_{2}^{2} \right] \leq \frac{\eta_{k}^{2} (1 - \beta_{1})^{2}}{1 - \beta_{2}} \mathbb{E} \left[\sum_{i=1}^{d} \frac{\left(\sum_{t=1}^{k} \beta_{1}^{k-t} g_{t,p} \right)^{2}}{\sum_{t=1}^{k} \beta_{2}^{k-t} g_{t,p}^{2}} \right] \\
\stackrel{(a)}{\leq} \frac{\eta_{k}^{2} (1 - \beta_{1})}{1 - \beta_{2}} \mathbb{E} \left[\sum_{i=1}^{d} \frac{\sum_{t=1}^{k} \beta_{1}^{k-t} g_{t,p}^{2}}{\sum_{t=1}^{k} \beta_{2}^{k-t} g_{t,p}^{2}} \right] \\
\leq \frac{\eta_{k}^{2} (1 - \beta_{1})}{1 - \beta_{2}} \mathbb{E} \left[\sum_{i=1}^{d} \sum_{t=1}^{k} \gamma^{k-t} \right] = \frac{\eta_{k}^{2} d (1 - \beta_{1})}{1 - \beta_{2}} \mathbb{E} \left[\sum_{t=1}^{k} \gamma^{k-t} \right]$$

$$(14)$$

where (a) is due to $\sum_{t=1}^k \beta_1^{k-t} \le \frac{1}{1-\beta_1}$. Summing from k=1 to k=K on both sides yields:

$$\sum_{k=1}^{K} \eta_{k}^{2} \mathbb{E} \left[\left\| \hat{v}_{k}^{-1/2} \theta_{k} \right\|_{2}^{2} \right] \leq \frac{\eta_{k}^{2} d (1 - \beta_{1})}{1 - \beta_{2}} \mathbb{E} \left[\sum_{k=1}^{K} \sum_{t=1}^{k} \gamma^{k-t} \right] \\
\leq \frac{\eta^{2} d K (1 - \beta_{1})}{1 - \beta_{2}} \mathbb{E} \left[\sum_{t=t}^{k} \gamma^{k-t} \right] \\
\leq \frac{\eta^{2} d K (1 - \beta_{1})}{(1 - \beta_{2})(1 - \gamma)} \tag{15}$$

where the last inequality is due to $\sum_{t=1}^{k} \gamma^{k-t} \leq \frac{1}{1-\gamma}$ as a consequence of the definition of γ .

- We now formulate the main result of our paper giving a finite-time upper bound of the quantity
- 44 $\mathbb{E}\left[\|\nabla f(w_K)\|^2\right]$ where K is a random termination number distributed according to 2, see [Ghadimi
- 45 and Lan, 2013].
- **Theorem 1.** Assume H 3-H 5, $(\beta_1, \beta_2) \in [0, 1]$ and a sequence of decreasing stepsizes $\{\eta_k\}_{k>0}$,
- 47 then the following result holds:

$$\mathbb{E}\left[\|\nabla f(w_K)\|^2\right] \le tocomplete \tag{16}$$

Proof Using H 3 and the iterate \overline{w}_k we have:

$$f(\overline{w}_{k+1}) \leq f(\overline{w}_k) + \nabla f(\overline{w}_k)^{\top} (\overline{w}_{k+1} - \overline{w}_k) + \frac{L}{2} \|\overline{w}_{k+1} - \overline{w}_k\|^2$$

$$\leq f(\overline{w}_k) + \underbrace{\nabla f(w_k)^{\top} (\overline{w}_{k+1} - \overline{w}_k)}_{A} + \underbrace{(\nabla f(\overline{w}_k) - \nabla f(w_k))^{\top} (\overline{w}_{k+1} - \overline{w}_k)}_{B} + \underbrace{\frac{L}{2} \|\overline{w}_{k+1} - \overline{w}_k\|}_{(17)}$$

Term A. Using Lemma 2, we have that:

$$\nabla f(w_{k})^{\top}(\overline{w}_{k+1} - \overline{w}_{k}) = \nabla f(w_{k})^{\top} \left[\frac{\beta_{1}}{1 - \beta_{1}} \tilde{\theta}_{k-1} \left[\eta_{k-1} v_{k-1}^{-1/2} - \eta_{k} v_{k}^{-1/2} \right] - \eta_{k} v_{k}^{-1/2} \tilde{g}_{k} \right]$$

$$\leq \frac{\beta_{1}}{1 - \beta_{1}} \left\| \nabla f(w_{k}) \right\| \left\| \eta_{k-1} v_{k-1}^{-1/2} - \eta_{k} v_{k}^{-1/2} \right\| \left\| \tilde{\theta}_{k-1} \right\| - \nabla f(w_{k})^{\top} \eta_{k} v_{k}^{-1/2} \tilde{g}_{k}$$

$$(18)$$

where the inequality is due to trivial inequality for positive diagonal matrix. Using Lemma 1 and

assumption H4 we obtain:

$$\nabla f(w_k)^{\top} (\overline{w}_{k+1} - \overline{w}_k) \le \frac{\beta_1 (1 + \beta_1 + a)}{1 - \beta_1} \mathsf{M}^2 \left[\left\| \eta_{k-1} v_{k-1}^{-1/2} \right\| - \left\| \eta_k v_k^{-1/2} \right\| \right] - \nabla f(w_k)^{\top} \eta_k v_k^{-1/2} \tilde{g}_k$$
(19)

where we have used the fact that $\eta_k v_k^{-1/2}$ is a diagonal matrix such that $\eta_{k-1} v_{k-1}^{-1/2} \succcurlyeq \eta_k v_k^{-1/2} \succcurlyeq 0$ (decreasing stepsize and max operator). Also note that:

$$-\nabla f(w_{k})^{\top} \eta_{k} v_{k}^{-1/2} \tilde{g}_{k} = -\nabla f(w_{k})^{\top} \eta_{k-1} v_{k-1}^{-1/2} \tilde{g}_{k} - \nabla f(w_{k})^{\top} \left[\eta_{k} v_{k}^{-1/2} - \eta_{k-1} v_{k-1}^{-1/2} \right] \tilde{g}_{k}$$

$$\leq -\nabla f(w_{k})^{\top} \eta_{k-1} v_{k-1}^{-1/2} \tilde{g}_{k} + (1 - \beta_{1}) \mathsf{M}^{2} \left[\left\| \eta_{k-1} v_{k-1}^{-1/2} \right\| - \left\| \eta_{k} v_{k}^{-1/2} \right\| \right]$$
(20)

using Lemma 1 on $||g_k||$ and recalling that $\tilde{g}_k = g_k - \beta_1 g_{k-1}$. Plugging (20) into (19) yields:

$$\nabla f(w_k)^{\top} (\overline{w}_{k+1} - \overline{w}_k)$$

$$\leq -\nabla f(w_k)^{\top} \eta_{k-1} v_{k-1}^{-1/2} \tilde{g}_k + \frac{1}{1-\beta_1} (\beta_1^2 + a\beta_1 + 1) \mathsf{M}^2 \left[\left\| \eta_{k-1} v_{k-1}^{-1/2} \right\| - \left\| \eta_k v_k^{-1/2} \right\| \right]$$
(21)

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

$$\left(\nabla f(\overline{w}_{k}) - \nabla f(w_{k})\right)^{\top} \left(\overline{w}_{k+1} - \overline{w}_{k}\right) \leq \left\|\nabla f(\overline{w}_{k}) - \nabla f(w_{k})\right\| \left\|\overline{w}_{k+1} - \overline{w}_{k}\right\| \tag{22}$$

Using smoothness assumption H 3:

$$\|\nabla f(\overline{w}_k) - \nabla f(w_k)\| \le L \|\overline{w}_k - w_k\|$$

$$\le L \frac{\beta_1}{1 - \beta_1} \|w_k - w_{k-1}\|$$
(23)

By Lemma 2 we also have:

$$\overline{w}_{k+1} - \overline{w}_k = \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{k-1} \left[\eta_{k-1} v_{k-1}^{-1/2} - \eta_k v_k^{-1/2} \right] - \eta_k v_k^{-1/2} \tilde{g}_k
= \frac{\beta_1}{1 - \beta_1} \tilde{\theta}_{k-1} \eta_{k-1} v_{k-1}^{-1/2} \left[I - (\eta_k v_k^{-1/2}) (\eta_{k-1} v_{k-1}^{-1/2})^{-1} \right] - \eta_k v_k^{-1/2} \tilde{g}_k
= \frac{\beta_1}{1 - \beta_1} \left[I - (\eta_k v_k^{-1/2}) (\eta_{k-1} v_{k-1}^{-1/2})^{-1} \right] (w_{k-1} - w_k) - \eta_k v_k^{-1/2} \tilde{g}_k$$
(24)

where the last equality is due to $\tilde{\theta}_{k-1}\eta_{k-1}v_{k-1}^{-1/2}=w_{k-1}-w_k$ by construction of $\tilde{\theta}_k$. Taking the

norms on both sides, observing $\left\|I-(\eta_k v_k^{-1/2})(\eta_{k-1}v_{k-1}^{-1/2})^{-1}\right\| \leq 1$ due to the decreasing stepsize and the construction of \hat{v}_k and using CS inequality yield:

$$\|\overline{w}_{k+1} - \overline{w}_k\| \le \frac{\beta_1}{1 - \beta_1} \|w_{k-1} - w_k\| + \|\eta_k v_k^{-1/2} \tilde{g}_k\|$$
 (25)

61 Plugging (23) and (25) into (22) returns:

$$(\nabla f(\overline{w}_{k}) - \nabla f(w_{k}))^{\top} (\overline{w}_{k+1} - \overline{w}_{k}) \leq L \frac{\beta_{1}}{1 - \beta_{1}} \| \eta_{k} v_{k}^{-1/2} \tilde{g}_{k} \| \| w_{k} - w_{k-1} \| + L \left(\frac{\beta_{1}}{1 - \beta_{1}} \right)^{2} \| w_{k-1} - w_{k} \|^{2}$$
(26)

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

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

Applying Young's inequality with $\delta o rac{eta_1}{1-eta_1}$ on the product $\left\|\eta_k v_k^{-1/2} \tilde{g}_k\right\| \|w_k - w_{k-1}\|$ yields:

$$\left(\nabla f(\overline{w}_{k}) - \nabla f(w_{k})\right)^{\top} \left(\overline{w}_{k+1} - \overline{w}_{k}\right) \leq L \left\| \eta_{k} v_{k}^{-1/2} \tilde{g}_{k} \right\|^{2} + 2L \left(\frac{\beta_{1}}{1 - \beta_{1}} \right)^{2} \left\| w_{k-1} - w_{k} \right\|^{2}$$
(27)

The last term $\frac{L}{2} \|\overline{w}_{k+1} - \overline{w}_k\|$ can be upper bounded using (25):

$$\frac{L}{2} \|\overline{w}_{k+1} - \overline{w}_k\|^2 \le \frac{L}{2} \left[\frac{\beta_1}{1 - \beta_1} \|w_{k-1} - w_k\| + \left\| \eta_k v_k^{-1/2} \tilde{g}_k \right\| \right]
\le L \left\| \eta_k v_k^{-1/2} \tilde{g}_k \right\|^2 + 2L \left(\frac{\beta_1}{1 - \beta_1} \right)^2 \|w_{k-1} - w_k\|^2$$
(28)

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Plugging (21), (27) and (28) into (17) and taking the expectations on both sides give:

$$\mathbb{E}\left[f(\overline{w}_{k+1}) + \frac{1}{1-\beta_{1}}\widetilde{\mathsf{M}}^{2} \left\| \eta_{k}v_{k}^{-1/2} \right\| - \left(f(\overline{w}_{k}) - \frac{1}{1-\beta_{1}}\widetilde{\mathsf{M}}^{2} \left\| \eta_{k-1}v_{k-1}^{-1/2} \right\| \right) \right] \\
\leq \mathbb{E}\left[-\nabla f(w_{k})^{\mathsf{T}} \eta_{k-1}v_{k-1}^{-1/2} \tilde{g}_{k} + 2L \left\| \eta_{k}v_{k}^{-1/2} \tilde{g}_{k} \right\|^{2} + 4L \left(\frac{\beta_{1}}{1-\beta_{1}} \right)^{2} \left\| w_{k-1} - w_{k} \right\|^{2} \right] \tag{29}$$

where $\tilde{\mathsf{M}}^2=(\beta_1^2+a\beta_1+1)\mathsf{M}^2$. Note that $w_{k-1}-w_k=-\eta_{k-1}\hat{v}_{k-1}^{-1/2}(\theta_{k-1}+h_k)$ with $h_k=\beta_1\theta_{k-2}+(1-\beta_1)m_k$ and that the expectation of \tilde{g}_k conditioned on the filtration \mathcal{F}_k reads as follows

$$\mathbb{E}\left[\tilde{g}_{k}\right] = \mathbb{E}\left[g_{k} - \beta_{1}g_{k-1}\right]$$

$$= \nabla f(w_{k}) - \beta_{1}\nabla f(w_{k-1})$$
(30)

2 Containment of the iterates for a Deep Neural Network

- 70 We show in this section that the weights satisfy assumption H 2 and stay in a bounded set when
- 71 the model we are fitting, using our method, is a fully connected feed forward neural network. The
- 72 activation function for this section will be sigmoid function and we add a ℓ_2 regularization.
- For the sake of notation, we assume $\beta_1=0$. We consider a fully connected feed forward neural
- network with L layers modeled by the function $\mathsf{MLN}(w,\xi):\mathbb{R}^l\to\mathbb{R}$:

$$\mathsf{MLN}(w,\xi) = \sigma\left(w^{(L)}\sigma\left(w^{(L-1)}\dots\sigma\left(w^{(1)}\xi\right)\right)\right) \tag{31}$$

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

$$f(w,\xi) = \mathcal{L}(\mathsf{MLN}(w,\xi), y) + \frac{\lambda}{2} \|w\|^2$$
(32)

where $\mathcal{L}(\cdot,y)$ is the loss function (can be Huber loss or cross entropy), y are the true labels and $\lambda>0$

79 is the regularization parameter. Beforehand, two following mild conditions on the boundedness of

the input data and of the loss function should be verified. For any $\xi \mathbb{R}^l$ and $y \in \mathbb{R}$ there is a constant

T > 0 such that:

$$\|\xi\| \le 1$$
 a.s. and $|\mathcal{L}'(\cdot, y)| \le T$ (33)

where $\mathcal{L}'(\cdot,y)$ denotes its derivative *w.r.t.* the paramer. For any layer index $\ell \in [1,L]$ we denote the output of layer ℓ by $h^{(\ell)}(w,\xi)$:

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

Given the sigmoid assumption we have $\|h^{(\ell)}(w,\xi)\| \leq 1$ for any $\ell \in [1,L]$ and any $(w,\xi) \in$

83 $\mathbb{R}^d \times \mathbb{R}^l$.

Observe that at the last layer L:

$$\begin{split} \|\nabla_{w^{(L)}}\mathcal{L}(\mathsf{MLN}(w,\xi),y)\| &= \|\mathcal{L}'(\mathsf{MLN}(w,\xi),y)\nabla_{w^{(L)}}\mathsf{MLN}(w,\xi)\| \\ &= \left\|\mathcal{L}'(\mathsf{MLN}(w,\xi),y)\sigma'(w^{(L)}h^{(L-1)}(w,\xi))h^{(L-1)}(w,\xi)\right\| \\ &\leq \frac{T}{4} \end{split} \tag{34}$$

where the last equality is due to mild assumptions (33) and to the fact that the norm of the derivative of the sigmoid function is upperbounded by 1/4.

From Algorithm 1, with $\beta_1 = 0$ we have for iteration index k > 0:

$$\|w_{k} - w_{k-1}\| = \left\| -\eta_{k} \hat{v}_{k}^{-1/2} (\theta_{k} + h_{k+1}) \right\|$$

$$= \left\| \eta_{k} \hat{v}_{k}^{-1/2} (g_{k} + m_{k+1}) \right\|$$

$$\leq \hat{\eta} \left\| \hat{v}_{k}^{-1/2} g_{k} \right\| + \hat{\eta} a \left\| \hat{v}_{k}^{-1/2} g_{k+1} \right\|$$
(35)

where $\hat{\eta} = \max_{k>0} \eta_k$. For any dimension $p \in [1, d]$, using assumption H 4, we note that

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

88 . Thus:

$$||w_{k} - w_{k-1}|| \leq \hat{\eta} \left(\left\| \hat{v}_{k}^{-1/2} g_{k} \right\| + a \left\| \hat{v}_{k}^{-1/2} g_{k+1} \right\| \right)$$

$$\leq \hat{\eta} \frac{a+1}{\sqrt{1-\beta_{2}}}$$
(36)

In short there exist a constant B such that $||w_k - w_{k-1}|| \le B$.

Proof by induction: As in [Défossez et al., 2020], we will prove the containment of the weights by induction. Suppose an iteration index K and a coordinate i of the last layer L such that $w_{K,i}^{(L)} \geq \frac{T}{4\lambda} + B$. Using (34), we have

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

where $f(\cdot)$ is defined by (32) and is the loss of our MLN. This last equation yields $\theta_{K,i}^{(L)} \geq 0$ (given

91 the algorithm and $\beta_1=0$) and using the fact that $\|w_k-w_{k-1}\|\leq B$ we have

$$0 \le w_{K-1,i}^{(L)} - B \le w_{K,i}^{(L)} \le w_{K-1,i}^{(L)}$$
(37)

which means that $|w_{K,i}^{(L)}| \leq w_{K-1,i}^{(L)}$. So if the first assumption of that induction reasoning holds, i.e., $w_{K-1,i}^{(L)} \geq \frac{T}{4\lambda} + B$, then the next iterates $w_{K,i}^{(L)}$ decreases, see (37) and go below $\frac{T}{4\lambda} + B$. This yields that for any iteration index k > 0 we have

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

since B is the biggest jump an iterate can do since $||w_k - w_{k-1}|| \le B$. Likewise we can end up showing that

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

- meaning that the weights of the last layer at any iteration is bounded in some matrix norm.
- Now that we have shown this boundedness property for the last layer L, we will do the same for the
- previous layers and conclude the verification of assumption H 2 by induction.
- 95 For any layer $\ell \in [1, L-1]$, we have:

$$\nabla_{w^{(\ell)}} \mathcal{L}(\mathsf{MLN}(w,\xi),y) = \mathcal{L}'(\mathsf{MLN}(w,\xi),y) \left(\prod_{j=1}^{\ell+1} \sigma'\left(w^{(j)}h^{(j-1)}(w,\xi)\right) \right) h^{(\ell-1)}(w,\xi) \quad (38)$$

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 (38) 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

$$\left\| w^{(\ell)} \right\| \le \frac{T \prod_{k>\ell} F_k}{4L - \ell + 1} + 2B$$

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

99 References

- A. Défossez, L. Bottou, F. Bach, and N. Usunier. On the convergence of adam and adagrad. *arXiv* preprint arXiv:2003.02395, 2020.
- S. Ghadimi and G. Lan. Stochastic first-and zeroth-order methods for nonconvex stochastic programming. *SIAM Journal on Optimization*, 23(4):2341–2368, 2013.
- Y. Yan, T. Yang, Z. Li, Q. Lin, and Y. Yang. A unified analysis of stochastic momentum methods for deep learning. *arXiv preprint arXiv:1808.10396*, 2018.