Grad-GradaGrad? A Non-Monotone Adaptive Stochastic Gradient Method

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Abstract

The classical AdaGrad method adapts the learning rate by dividing by the square root of a sum of squared gradients. Because this sum on the denominator is increasing, the method can only decrease step sizes over time, and requires a learning rate scaling hyper-parameter to be carefully tuned. To overcome this restriction, we introduce GradaGrad, a method in the same family that naturally grows or shrinks the learning rate based on a different accumulation in the denominator, one that can both increase and decrease. We show that it obeys a similar convergence rate as AdaGrad and demonstrate its non-monotone adaptation capability with experiments.

1 Introduction

We consider stochastic optimization problems of the form

\[
\min_{x \in \mathbb{R}^d} f(x) := \mathbb{E}_\xi [f(x, \xi)],
\]

where \(\xi\) is a random variable. We assume that each \(f(x, \cdot)\) is convex in \(x\) but potentially non-smooth. Problems of this class are most often addressed with stochastic gradient methods (SGD). Aiming to accelerate the convergence of stochastic gradient methods in practice, adaptive rules for adjusting the learning rate have a long history (e.g., Kesten, 1958) and have been extensively studied more recently. The stochastic gradient descent method, a member of the Mirror Descent (MD) family takes the general form:

\[
x_{k+1} = x_k - A_{k+1}^{-1}g_k,
\]

where \(A_{k+1}\) is a dynamically adjusted positive definite matrix. Due to the high dimensionality of modern machine learning applications, \(A_{k+1}\) is usually taken to be a diagonal matrix. AdaGrad (Duchi et al., 2011) uses the choice:

\[
A_{i,k+1}^{-1} = \frac{\gamma}{\sqrt{\sum_{t=0}^{k} g_{i,t}^2}},
\]

where \(A_{i,k+1}\) is the \(i\)th diagonal entry of \(A_{k+1}\), \(g_{i,t}\) is the \(i\)th coordinate of the stochastic gradient \(g_t\), and \(\gamma\) is a hyper-parameter. Another popular and effective algorithm is Adam (Kingma & Ba, 2014), which uses an exponential weighted average instead of a summation, in combination with momentum. Both methods have seen widespread adoption and have been the focus of extensive followup work (e.g., Tieleman & Hinton, 2012; Reddi et al., 2019; Li & Orabona, 2019).

A fundamental limitation of AdaGrad is monotone adaptation. In other words, since the sum in (2) is increasing, it can only decrease the learning rate over time. Therefore, the global learning rate parameter \(\gamma\) must be carefully tuned. In addition, once the learning rate becomes very small, it...
Adaptive stochastic gradient methods have seen heavy investigation on a number of fronts, including where \( \rho > 0 \). \( T \sim B_{\alpha} \). Another line of work that can both increase and decrease the learning rate. Methods that maintain multiple learning rates, such as Metagrad (\cite{vanErvenKoolen2016}) are also potentially non-monotonic. Another line of work that can both increase and decrease the learning rate. Tommasi (2017) proposed a method to adjust the learning rate based on a “coin-betting” strategy.

Throughout this paper, we let \( x, \gamma \) be the initial point. We use the convention that \( g \) be the initial point. We use the convention that \( \alpha \) be the initial point. We use the convention that \( \rho \) be the initial point.

\begin{equation}
A_{i,k+1} \propto \sqrt{\sum_{t=0}^{k} (g_{i,t}^{2} - \rho g_{i,t}g_{i,t-1}),}
\end{equation}

where \( \rho > 0 \) is a constant that can be tuned. The expectation of \( -g_{i,t}g_{i,t-1} \) is the hyper-gradient of \( f \) with respect to the learning rate for the \( i \)th coordinate (see Section 2). Intuitively, if consecutive stochastic gradients are highly positively correlated, then \( g_{i,t}^{2} - \rho g_{i,t}g_{i,t-1} \) can be negative and thus the learning rate will be increased. Similarly, if consecutive gradients are negatively correlated, then the learning rate will be decreased. In the “goldilocks” zone, the hyper-gradient term wobbles around 0 and the learning rate changes in a similar manner to AdaGrad. Compared to AdaGrad, our method is able to rapidly increase the learning rate when it is too small (Figure 2).

However, applying the idea above directly runs into several problems. The most apparent problem is that the sum under the square root may become a negative number. A more subtle problem is how to ensure that the sequences of \( A_{i,k+1} \) increase, in a non-monotone manner, at an appropriate rate to guarantee convergence. After laying out the basic ideas in Section 3, we show in Section 4 how the GradaGrad method addresses these problems with reparameterization and other techniques. As a preview, Algorithm 1 shows a simplified version of GradaGrad using a scalar learning rate.

In the rest of Section 4, we show that GradaGrad obeys a similar convergence bound as the AdaGrad method. In Section 5, preliminary experiments demonstrate that our method matches the practical performance of several benchmark methods and has the advantage of non-monotone adaptation.

\textbf{Notation and Assumptions} Throughout this paper, we let \( g \) denote any minimizer of \( f \) and \( x_{0} \) be the initial point. We use the convention that \( g_{-1} \) is the zero vector. The notation \( B > 0 \) means that \( B \) is a symmetric and positive definite matrix. For \( B > 0 \), we define \( \|x\|_{B} = \sqrt{x^{T}Bx} \) and \( (x,y)_{B} = x^{T}By \). Some of our results will use the Lipschitz smoothness of \( f \), in which case we denote the smoothness constant as \( L \). We define the filtration \( \Phi = (\mathcal{F}_{1}, \mathcal{F}_{2}, \ldots) \), where \( \mathcal{F}_{k} \) is the \( \sigma \)-algebra generated by a sequence of random variables \( \{\xi_{i}, \ldots, \xi_{k-1}\} \). The notation \( \mathbb{E}[\cdot] \) and \( \mathbb{E}[\cdot | \mathcal{F}_{k}] \) denote the expectation conditioned on \( \mathcal{F}_{k} \).

\section{Related Work}

Adaptive stochastic gradient methods have seen heavy investigation on a number of fronts, including non-monotone methods that can both increase and decrease the learning rate. \cite{Schaul2013} proposed a method that combines the estimation of gradient variance and local curvature. \cite{OrabonaTommasi2017} proposed a method to adjust the learning rate based on a “coin-betting” strategy.

\begin{algorithm}
\textbf{Input:} \( \gamma_{0}, \rho, r, x_{0} \)
\textbf{Initialize} \( g_{-1} = 0, \alpha_{0} = 0 \)
\textbf{for} \( k = 0 \) \textbf{to} \( n \) \textbf{do}
\begin{align*}
g_{k} &= \nabla f(x_{k}, \xi_{k}) \\
v_{k} &= \|g_{k}\|^{2} - \rho \langle g_{k}, g_{k-1} \rangle \\
\text{if} \ v_{k} \geq 0 \text{ then} \\
\gamma_{k+1} &= \gamma_{k} \\
\alpha_{k+1} &= \alpha_{k} + v_{k} \\
\text{else} \\
\gamma_{k+1} &= \gamma_{k} \sqrt{1 - \frac{v_{k}}{\alpha_{k}}} \\
\alpha_{k+1} &= \alpha_{k} \\
\text{end if}
\end{align*}
\( A_{k+1} = \sqrt{\alpha_{k+1} / \gamma_{k+1}} \)
\( x_{k+1} = x_{k} - \frac{1}{A_{k+1}} g_{k} \)
\textbf{end for}
\textbf{Algorithm 1: GradaGrad (Simplified Scalar variant)}
\end{algorithm}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure1.png}
\caption{The GradaGrad update (Equation 9) results in a smooth scaling of the learning rate when negative values of \( v_{k} \) are encountered, compared to the naive solution from Equation (3) which quickly explodes.}
\end{figure}
rate are stochastic line search methods [Vaswani et al., 2019; Paquette & Scheinberg, 2020; Zhang et al., 2020]. None of the existing strategies can be considered “drop-in” replacements for AdaGrad in the same way our approach is, as they require either additional gradient evaluations, additional memory overhead or knowledge of problem-dependent constants that make them harder to use in practice than the AdaGrad family of methods.

Methods in the Polyak class [Loizou et al., 2021] compute learning rates using the function value sub-optimality \( f(x_k) - f(x^*) \), or in the stochastic case \( f(x_k, \xi_k) - f^*_{\xi_k} \) where \( f^*_{\xi_k} \) is the minimal value of \( f(\cdot, \xi_k) \). These methods can exhibit impressive performance but rely on knowledge or estimates of the minimal function value \( f^* \) or \( f^*_{\xi_k} \), which is not available for most problems.

The idea of adjusting the learning rate based on inner products of consecutive stochastic gradients goes back to Kesten (1958), and it was extended to the multi-dimensional case by Delyon & Juditsky (1993). Mirzakhormedov & Uryasev (1983) showed that such adaptation schemes can be interpreted as stochastic hyper-gradient methods. Specifically, suppose \( d_k \) is a search direction depending on the random variable \( \xi_k \) (e.g., \( g_k \) itself or combined with momentum). Let’s define a merit function of the learning rate at each iteration

\[
\phi_k(\eta) = \mathbb{E} \left[ f(x_{k+1}) \mid F_k \right] = \mathbb{E} \left[ f(x_k - \eta d_k) \mid F_k \right].
\]

The hypergradient of \( \phi_k \) with respect to \( \eta \) can be derived as

\[
\frac{\partial \phi_k}{\partial \eta} = \mathbb{E} \left[ \frac{\partial}{\partial \eta} f(x_k - \eta d_k) \mid F_k \right] = \mathbb{E} \left[ \langle \nabla f(x_k - \eta d_k), -d_k \rangle \mid F_k \right]
= \mathbb{E} \left[ -\langle g_{k+1}, d_k \rangle \mid F_k \right],
\]

where we assume necessary technical conditions for changing the order of differentiation and expectation. Therefore, \( -\langle g_{k+1}, d_k \rangle \) can be viewed as a stochastic hypergradient. If \( d_k = g_k \), then it becomes \( -\langle g_{k+1}, g_k \rangle \). If in addition the learning rate is different for each coordinate, say \( \eta_i \) for the
we add additional terms which combine with the gradient error term. Inspired by hyper-gradient
methods, we use the following Lemma.

Adaptive stochastic gradient methods based on hyper-gradient descent have been studied in the
machine learning literature before, including Jacobs (1988), Sutton (1992), Schraudolph (1999),
Mahmood et al. (2012), and more recently by Baydin et al. (2018). The major difference between
our work and these previous works is that, although our adaptation scheme carries the intuition of
hyper-gradient, our method is not really a hyper-gradient method and our analysis does not rely on the
hyper-gradient interpretation.

The “without descent” adaptive method of Malitsky & Mishchenko (2019) is the most direct inspi-
ration for our work. In a footnote, they suggest the following rule for learning rate \( \eta_k \), when the
denominator is positive:

\[
\eta_k^2 \leq \frac{\|x_k - x_{k-1}\|^2}{3\|g_k\|^2 - 4(\langle g_k, g_{k-1} \rangle)}.
\]

Our method arose from attempts to adapt this learning rate to the stochastic case.

3 Augmenting AdaGrad

For simplicity we consider the Euclidean step setting, with an unconstrained domain. In this situation,
as shown by Duchi et al. (2011), the AdaGrad update

\[
g_k = \nabla f(x_k, \xi_k),
\]

\[
x_{k+1} = x_k - A_{k+1}^{-1}g_k,
\]

obey the inequality:

\[
2E \sum_{k=0}^{n} (f(x_k) - f_\star) \leq \|x_0 - x_\star\|^2_{A_1} + E \sum_{k=1}^{n} \|x_k - x_\star\|^2_{(A_{k+1} - A_k)} + E \sum_{k=0}^{n} \|g_k\|^2_{A_{k+1}^{-1}}.
\]

The right-hand side of this inequality consists of some initial conditions (first term), an iterate distance
error term (second term) and a gradient norm term (third term). The key insight of the AdaGrad
method is that the gradient error term’s growth can be restricted to a \( O(\sqrt{n}) \) rate over time if the
matrices \( A_k \) are carefully chosen. For simplicity of notation, consider the one-dimensional case for
the remainder of this section. The gradient error term grows each step by \( g_k^2/A_{k+1} \), and the overall
growth is controlled by using an inductive bound of the form: \( qA_k + g_k^2/A_{k+1} \leq qA_{k+1} \). AdaGrad
uses the choice \( A_{k+1}^2 = \sum_{i=0}^{k} g_i^2 \) and \( q = 2 \) to keep the overall growth rate \( O(\sqrt{n}) \). In our approach,
we add additional terms which combine with the gradient error term. Inspired by hyper-gradient
methods, we use the following Lemma.

Lemma 1. For any \( A_k \geq 0 \) and \( \rho > 0 \), the sequences generated by (5) obey:

\[
0 \leq -E \left[ \rho \langle g_k, g_{k-1} \rangle_{A_k^{-1}} | F_k \right] + \rho \left[ f(x_{k-1}) - f(x_k) \right].
\]

The first term is a scaling of the hyper-gradient; see Equation (4). Usually this quantity is used to
adapt the learning rate by applying stochastic gradient descent on the learning rate, treating the
hyper-parameter as a parameter (hence the name). Our approach here is different, we introduce
the term into our convergence rate bound directly. The second term is a function value difference
between the current and previous points. This term is particularly nice as it may be telescoped, and
so it introduces an error term that doesn’t grow over time. The degree of adaptivity is controlled by
\( \rho \), which is a tunable parameter of our method. The theory we develop in Section 4.4 suggests that
\( \rho = 2 \) is the best default choice, although larger values can lead to greater adaptivity.

Using Lemma 1 and the AdaGrad result (5), we may derive the following bound.
Theorem 2. For $k \geq 1$, Algorithm 1 satisfies:

$$2\mathbb{E} \sum_{k=0}^{n} |f(x_k) - f_*| \leq \|x_0 - x_*\|^2 + \rho \|f(x_0) - f_*\| + \mathbb{E} \sum_{k=1}^{n} \|x_k - x_*\|^2 (A_{k+1} - A_k)$$

$$+ \mathbb{E} \sum_{k=0}^{n} \left[ \frac{\|g_k\|_{A_{k+1}}^2}{A_{k+1} - 1} - \rho \langle g_k, g_{k-1} \rangle A_{k+1} - 1 \right].$$

Compared to the bound for AdaGrad in Equation (6), the gradient norm error term now grows each step by a term:

$$\|g_k\|_{A_{k+1}}^2 - \rho \langle g_k, g_{k-1} \rangle A_{k+1} - 1 \text{ v.s. } \|g_k\|_{A_{k+1}}^2 - \rho \langle g_k, g_{k-1} \rangle A_{k+1} - 1.$$

This error term is potentially much smaller, or even negative, when consecutive gradients are highly positively correlated. This corresponds to the situation in hyper-gradient methods where the learning rate should be increased. This error term is larger in the opposite situation, where consecutive gradients are negatively correlated, and the learning rate should be decreased. In the “goldilocks” zone, the hyper-gradient term will wobble around 0, and should not contribute significantly to the accumulated error over time.

Ideally, we would like to apply a similar inductive bound to this error term as was applied for AdaGrad:

$$qA_k + \frac{\|g_k\|^2}{A_{k+1} - 1} - \rho \frac{\langle g_k, g_{k-1} \rangle}{A_{k}} \leq qA_{k+1},$$

with $A$ given by (3). This schema is the motivation for development of our GradaGrad method. Applied directly we run into a number of problems that must be solved to arrive at a practical method:

i) The above update can potentially yield the square root of a negative number. The approach we develop in the following sections, shown in Figure 1, steadily grows the learning rate, avoiding the divergence towards infinity encountered in the naive implementation in Equation (3).

ii) When $A_k$ is allowed to both expand and shrink, generally, the iterate-distance error term, i.e., second line in (6), may grow at a $O(n)$ rate, rather than the $O(\sqrt{n})$ rate required for a non-trivial convergence rate bound. It’s this term that prevents the use of arbitrary step-size sequences. Our approach maintains the $O(\sqrt{n})$ rate by construction.

iii) The hyper-gradient term is divided by $A_{k-1}$ not $A_k$, which significantly breaks the bounding approach used by AdaGrad. The bound may be violated both when the error term is positive and negative.

4 The GradaGrad Method

In this section, we show how to address the issues listed above through a reparametrization technique, present the full version of GradaGrad with momentum, and establish its convergence properties.

4.1 Controlling error through reparameterization

The key to controlling the error terms that arise in the GradaGrad method is the use of reparameterization of the learning rate. Like AdaGrad, our learning rate will take the form:

$$A_{k+1}^{-1} = \frac{\gamma_{k+1}}{\sqrt{\alpha_{k+1}}},$$

where $\alpha_{k+1}$ is updated from $\alpha_k$ each step by adding some additional term $v_k$. In GradaGrad, we allow the numerator $\gamma_{k+1}$ to change over time, compared to the fixed numerator used in AdaGrad. The purpose of this additional flexibility is to allow us to reparameterize the learning rate before applying the AdaGrad like additive update to $\alpha_k$. We still consider coordinate-wise updates of the form:

$$\alpha_{k+1} = \alpha_k + v_k, \quad (7)$$
AdaGrad variants (such as AdaGrad-DA) for the theory and can usually be omitted from practical implementations of the method.

`v_k` approximation, as the gradients match at

The scalar version of GradaGrad is detailed in Algorithm 1. It’s straightforward to extend the method to per-coordinate adaptivity (diagonal scaling), and to include the use of momentum and projection onto a convex set $\mathcal{X}$. This full version is given in Algorithm 2. The full version includes 2 other changes needed to facilitate the analysis: firstly, the $v_0$ update uses a maximum element-wise gradient bound $G$ rather than the observed gradient $g_0$. This kind of change is also needed by other AdaGrad variants (such as AdaGrad-DA) for the theory and can usually be omitted from practical implementations of the method.

4.2 GradaGrad with momentum

The scalar version of GradaGrad is detailed in Algorithm 1. It’s straightforward to extend the method to per-coordinate adaptivity (diagonal scaling), and to include the use of momentum and projection onto a convex set $\mathcal{X}$. This full version is given in Algorithm 2. The full version includes 2 other changes needed to facilitate the analysis: firstly, the $v_0$ update uses a maximum element-wise gradient bound $G$ rather than the observed gradient $g_0$. This kind of change is also needed by other AdaGrad variants (such as AdaGrad-DA) for the theory and can usually be omitted from practical implementations of the method.

Input: $\gamma_0, \rho, x_0, \beta, G_\infty, D_\infty$

Initialize $z_0 = x_0$

for $k = 0$ to $n$ do

g_k = \nabla f(x_k, \xi_k)

for $i = 1$ to $D$ do

if $k = 0$ then

$v_{i,k} = G^2_\infty$

else if $\gamma_{i,k} = D_\infty$ then

$v_{i,k} = g^2_{i,k}$$^\gamma$

else

$v_{i,k} = g^2_{i,k} - \rho g_{i,k} m_{i,k-1}$

end if

if $v_{i,k} \geq 0$ then

$\gamma_{i,k+1} = \gamma_{i,k}$

$\alpha_{i,k+1} = \alpha_{i,k} + v_{i,k}$

else

$r_{i,k} = \left(\frac{\rho m_{i,k-1}}{g_{i,k}}\right)^2 - 1$

$v_{i,k} = \max(v_{i,k}, -r_{i,k} \alpha_{i,k})$

$\gamma_{i,k+1} = \min(\gamma_{i,k} \sqrt{1 - \frac{v_{i,k}}{\alpha_{i,k}}}, D_\infty)$

$\alpha_{i,k+1} = \alpha_{i,k}$

end if

$A_{i,k+1} = \sqrt{\alpha_{i,k+1}/\gamma_{i,k+1}}$

end for

$z_{k+1} = \text{proj}_\mathcal{X}(z_k - A_{k+1}^{-1}_i g_k)$

$x_{k+1} = \beta x_k + (1 - \beta) z_{k+1}$

$m_k = A_{k+1} (x_k - x_{k+1})$

end for

Algorithm 2: GradaGrad

where $v_k = \|g_k\|^2$ in AdaGrad and $v_k = \|g_k\|^2 - \rho \langle g_k, g_{k-1} \rangle$ in GradaGrad. However, we apply these updates after a reparameterization:

\[
\frac{\gamma_{k+1}}{\sqrt{\alpha'_{k+1}}} = \frac{\gamma_k}{\sqrt{\alpha_k}}, \tag{8}
\]

that leaves the learning rate the same but changes the effect of adding $v_k$. The update then consists of $\alpha_{k+1} = \alpha'_{k+1} + v_k$. We choose our reparameterization so that when $v_k$ is negative, $\alpha_{k+1} = \alpha_k$ regardless of the value of $v_k$. Solving Equation (8) under this condition gives the update

\[
\gamma_{k+1} = \gamma_k \sqrt{\frac{\alpha'_{k+1}}{\alpha_k}} = \gamma_k \sqrt{\frac{\alpha_{k+1} - v_k}{\alpha_k}} = \gamma_k \sqrt{\frac{\alpha_k - v_k}{\alpha_k}} = \gamma_k \sqrt{1 - \frac{v_k}{\alpha_k}}. \tag{9}
\]

This results in the behavior observed in Figure 1 where the learning rates smoothly increase as $v_k$ becomes more negative. Note that this correction is only used when $v_k$ is negative, for positive $v_k$ the standard AdaGrad update in Equation (7) is used without any reparameterization. This update is well behaved, the learning rate matches the value from using $\alpha_{k+1} = \alpha_k - v_k$ up to a first order approximation, as the gradients match at $v_k = 0$ (this can be seen in Figure 1). The ratio $v_k/\alpha_k$ is typically very small at the later stages of optimization, so its behavior differs from the naive variant only at the beginning of optimization.
Secondly, we derive an explicit expression for the hyper-parameter $\rho$ rather than using a fixed value. This is a trade-off, as it adds some additional complexity to the method but reduces the number of hyper-parameters. The necessity of this parameter is detailed in Section 4.3. We establish the following $O(1/\sqrt{n})$ convergence rate bound for the diagonal scaling variant, the scalar variant can be analysed using the same techniques.

**Theorem 3.** Define $G_\infty = \max_k \|g_k\|_\infty^2$, $D_\infty = \sup_{x \in X} \|x - x_*\|_\infty$ then the function value at the average iterate $\bar{x}$ of GradaGrad converges at a $O(1/\sqrt{n})$ rate:

$$E[f(\bar{x}_{n+1}) - f_*] \leq \frac{1}{2(n+1)} \left( \frac{2\beta}{1 - \beta} + \rho \right) [f(x_0) - f_*] + 3\sqrt{2 + \rho} \frac{dG_\infty D_\infty^2}{\gamma_0 \sqrt{n} + 1},$$

where $\rho > 0$ is a hyper-parameter and $\beta \in [0, 1)$ is the classical momentum parameter.

**4.3 The restricted increase constraint**

As mentioned in point (iii), care must be taken to control the growth of the gradient noise term:

$$\|g_k\|^2_{A_k^{-1}} - \rho \langle g_{k-1}, g_k \rangle A_k^{-1}.$$  

The AdaGrad approach to bounding the accumulated error:

$$q A_k + \|g_k\|^2_{A_k^{-1}} - \rho \langle g_{k-1}, g_k \rangle A_k^{-1} \leq q A_{k+1},$$

breaks down when $v_k = \|g_k\|^2 - \rho \langle g_{k-1}, g_k \rangle$ is negative, as this inequality can become impossible to satisfy for any choice of $A_k < A_{k-1}$, preventing us from using increasing learning rate sequences. Instead, we will impose the following restriction:

$$\|g_k\|^2_{A_k^{-1}} - \rho \langle g_{k-1}, g_k \rangle A_k^{-1} \leq 0. \quad \text{(10)}$$

This is not always satisfied, even when $\|g_k\|^2 - \rho \langle g_{k-1}, g_k \rangle \leq 0$, as the gradient norm square term may grow very large if the learning rate $A_k^{-1}$ is allowed to increase significantly between steps. By rearranging terms, we see that this bound is satisfied when the ratio $A_{k+1}/A_k$ is controlled:

$$A_{k+1}A_k^{-1} \geq \frac{\|g_k\|^2}{\rho \langle g_{k-1}, g_k \rangle}.$$  

We satisfy this constraint by using the following update in the GradaGrad method:

**Lemma 4.** Inequality (10) is satisfied if we clip $v_k$ using:

$$v_k = \max(v_k, -r\alpha_k) \text{ where } r = \left( \frac{\rho \langle g_{k-1}, g_k \rangle}{\|g_k\|^2} \right)^2 - 1.$$  

**4.4 The $\rho$ hyper-parameter**

There are two values of $\rho$ for which the update has special properties worth further discussion. Consider the use of $\rho = 1$. The $\alpha_k$ sequence (without reparameterization) can be written as

$$\alpha_{n+1} = g_0^2 + \sum_{k=1}^{n} [g_k^2 - g_k g_{k-1}] = \frac{1}{2} g_0^2 + \frac{1}{2} g_n^2 + \frac{1}{2} \sum_{k=0}^{n-1} (g_{k+1} - g_k)^2.$$  

Although individual steps may increase or decrease the rate, the overall growth will be dominated by the summation term, and so GradaGrad with $\rho = 1$ will not result in significant learning rate growth. The accumulation of differences of gradients instead of gradients has been explored before, under the name of optimistic online gradient descent (Rakhlin & Sridharan [2013], Bach & Levy [2019], Antonakopoulos & Mertikopoulos [2021]).

This method is still of interest as it can be used as a drop-in replacement for AdaGrad, without the need for the complexities of reparameterization that larger $\rho$ require. It can behave quite differently than AdaGrad, for instance on the absolute value function example in Figure 2, it will make much more rapid progress, the learning rate initially stays constant rather than decreasing as $g_{k+1} - g_k$ is zero until it overshoots the minimum, and starts decreasing from there. The case of $\rho = 2$ is the most natural as it results in simplifications of the constants in the bounds. We would recommend $\rho = 2$ as the default choice in the GradaGrad method, as it results in adaptivity without introducing excessive instability during training.
5 Experiments

We evaluated GradaGrad on 6 baseline problems widely used in the optimization literature ([Chang & Lin, 2011]; [Dua & Graff, 2017]): Glass, Letter, Protein, USPS, Vehicle and Vowel. We tested a binary logistic regression model, with no further data preprocessing, using the scaled versions of each dataset (when applicable) retrieved from the LIBSVM dataset repository. We compare our method against Adam, SGD and AdaGrad, where for each method the learning rate is chosen via grid search on a power-of-2 grid to give the highest final accuracy averaged over the last 10 epochs. This tuning is extremely advantageous to these baselines methods, and provides a difficult benchmark to beat. We plot the average of 10 runs with different random seeds, with a 2 standard-error range overlaid. As shown in Figure 3, GradaGrad is able to match these baseline methods using the same default hyper-parameters $\gamma_0 = 1$.0, and $\rho = 2$ across all problems.

To illustrate the effect of the $\rho$ hyperparameter, we performed experiments on the DLRM ([Naumov et al., 2019] model on the Criteo Kaggle Display Advertising Challenge Dataset, using the scalar
variant of GradaGrad. This model has more than 300 million parameters and is representative of models used in industry. Batch size 128 and embedding dimension 16 were used, with no regularization. Whereas the diagonal scaling variant of GradaGrad performs well with $\rho = 2$, the scalar variant requires larger $\rho$ for large or high noise problems. Figure 4 shows the results of using $\gamma_0$ equal to 1, 1e-2, 1e-4, 1e-6 with different $\rho$ values. Values of $\rho = 2$ and $\rho = 10$ show a significant lack of adaptivity, whereas for large $\rho$ each of these rates performs similarly.

6 Discussion

Although GradaGrad’s learning rate is more adaptive than that of AdaGrad, it still inherits many of the same limitations. The “any-time” sequences that have a square-root growth denominator give optimal rates up to a constant factor, but they sometimes give noticeably worse rates in practice than more heavily hand-tuned learning rate schedules such as MADGRAD. (Defazio & Jelassi, 2021).

The GradaGrad method is also limited in its ability to adjust $\gamma$. The updates only increase $\gamma$, so the initial $\gamma_0$ must be no larger than the optimal $\gamma$. The GradaGrad update allows $\gamma$ to grow at an exponential rate, which means that small initial values can potentially be used. Care must be taken when initializing with $\gamma_0$ that are very small as numerical issues may come into play. Values below roughly $10^{-6}$ will likely result in loss of precision and no adaptivity when using single precision floating point.

Conclusion

The GradaGrad method has promising theoretical and practical properties that make it a viable drop-in replacement for the AdaGrad method. It exhibits greater adaptivity to the gradient sequence as it is able to exploit correlations between consecutive gradients, going beyond the simple gradient magnitudes used in the AdaGrad method. There are many open problems relating to the $v_k$ sequence we described. Can the same sequence be used in other AdaGrad family methods? We believe that $v_k$ sequences of the form we describe here could have widespread applications. Can the upper bound on $\gamma$ be removed? It does not appear to be necessary in practice.
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A Convergence Theory

We define the ancillary quantity \( z' \), so that the update in Algorithm 2 may be written as

\[
\begin{align*}
z'_{k+1} &= z_k - A_{k+1}^{-1} g_k, \\
z_{k+1} &= \text{proj}_X(z'_{k+1}), \\
x_{k+1} &= \beta x_k + (1 - \beta) z_{k+1}.
\end{align*}
\]

(11)

Then define \( m_k \) via

\[ x_{k+1} = x_k - A_{k+1}^{-1} m_k. \]

Note that \( m_k = A_k(x_k - x_{k+1}) \).

Lemma 5. For \( k \geq 1 \):

\[ E \xi_k \langle g_k, m_{k-1} \rangle_{A_k^{-1}} \leq [f(x_{k-1}) - f(x_k)]. \]

Proof. Using \( x_k = x_{k-1} - A_{k-1}^{-1} m_{k-1} \),

\[
E \xi_k \langle g_k, m_{k-1} \rangle_{A_k^{-1}} = E \xi_k \langle g_k, x_{k-1} - x_k \rangle = (\nabla f(x_k), x_{k-1} - x_k) \leq f(x_{k-1}) - f(x_k).
\]

Lemma 6. Consider \( k \geq 1 \) and \( \rho \geq 1 \). Then the iterate sequence generated by Equation (11) obeys the following bound:

\[
2 \left[ f(x_k) - f_* \right] \leq E \xi_k \| z_k - x_* \|^2_{A_{k+1}} - E \xi_k \| z_{k+1} - x_* \|^2_{A_{k+1}} - \frac{2 \beta}{1 - \beta} \left[ f(x_k) - f_* \right] + \left( \frac{2 \beta}{1 - \beta} + \rho \right) \left[ f(x_{k-1}) - f_* \right]
\]

\[
+ E \xi_k \left[ \| g_k \|^2_{A_{k+1}} - \rho \langle g_k, m_{k-1} \rangle_{A_k^{-1}} \right].
\]

Proof. We start by expanding \( x_{k+1} \) around \( x_* \).

\[
E \xi_k \| z_{k+1} - x_* \|^2_{A_{k+1}} \\
\leq E \xi_k \| z'_{k+1} - x_* \|^2_{A_{k+1}} \\
= E \xi_k \| z_k - x_* + z'_{k+1} - z_k \|^2_{A_{k+1}} \\
= E \xi_k \| z_k - x_* \|^2_{A_{k+1}} + 2E \xi_k \langle A_{k+1} (z'_{k+1} - z_k), z_k - x_* \rangle + E \xi_k \| z'_{k+1} - z_k \|^2_{A_{k+1}} \\
= E \xi_k \| z_k - x_* \|^2_{A_{k+1}} - 2E \xi_k \langle g_k, z_k - x_* \rangle + E \| g_k \|^2_{A_{k+1}} \\
= E \xi_k \| z_k - x_* \|^2_{A_{k+1}} - 2 \langle \nabla f(x_k), 1 - \frac{\beta}{1 - \beta} x_k - \frac{\beta}{1 - \beta} x_{k-1} - x_* \rangle + E \xi_k \| g_k \|^2_{A_{k+1}} \\
= E \xi_k \| z_k - x_* \|^2_{A_{k+1}} - 2 \langle \nabla f(x_k), \beta x_k - \frac{\beta}{1 - \beta} x_{k-1} + x_k - x_* \rangle + E \xi_k \| g_k \|^2_{A_{k+1}} \\
= E \xi_k \| z_k - x_* \|^2_{A_{k+1}} - 2 \langle \nabla f(x_k, x_k - x_* \rangle - \frac{2 \beta}{1 - \beta} \langle \nabla f(x_k), x_k - x_{k-1} \rangle + E \xi_k \| g_k \|^2_{A_{k+1}} \\
\leq E \xi_k \| z_k - x_* \|^2_{A_{k+1}} - 2 \left[ f(x_k) - f_* \right] - \frac{2 \beta}{1 - \beta} \left[ f(x_k) - f(x_{k-1}) \right] + E \xi_k \| g_k \|^2_{A_{k+1}}.
\]
We prove a more general form of Theorem 2, covering the use of momentum and projection. The
We combine with Lemma 5 multiplied by \( \rho \):
\[
E_{\xi_k} \| z_{k+1} - x_\star \|_{A_{k+1}}^2 \leq E_{\xi_k} \| z_k - x_\star \|_{A_{k+1}}^2 - 2 [f(x_k) - f_\star] + \left( \frac{2\beta}{1 - \beta} + \rho \right) [f(x_{k-1}) - f(x_k)]
+ E_{\xi_k} \left[ \| g_k \|^2_{A_{k+1}} - \rho \langle g_k, m_{k-1} \rangle_{A_{k+1}} \right].
\]

A.1 Proof of Theorem 2

We prove a more general form of Theorem 2 covering the use of momentum and projection. The
variant listed in the body of the paper is the special case where \( \mathcal{X} = \mathbb{R}^d \) and \( \beta = 0 \). Consider the case where \( k = 0 \). Then:
\[
E_{\xi_0} \| z_1 - x_\star \|_{A_1}^2 \leq E_{\xi_0} \| z_0 - x_\star \|_{A_1}^2
= E_{\xi_0} \| z_0 - x_\star \|_{A_1}^2 + 2 \langle A_1 (z'_0 - z_0), z_0 - x_\star \rangle + E_{\xi_0} \| z'_0 - z_0 \|_{A_1}^2
= E_{\xi_0} \| z_0 - x_\star \|_{A_1}^2 - 2E \langle g_0, z_0 - x_\star \rangle + E_{\xi_0} \| g_0 \|_{A_1}^2
\leq E_{\xi_0} \| z_0 - x_\star \|_{A_1}^2 - 2 [f(x_0) - f_\star]
+ E_{\xi_0} \| g_0 \|_{A_1}^2.
\]

Using the law of total expectation, we telescope Lemma 6 together with the base case from \( k = 0 \) to \( n \):
\[
2E \sum_{k=0}^n [f(x_k) - f_\star] \leq E \| z_0 - x_\star \|_{A_1}^2 + \left( \frac{2\beta}{1 - \beta} + \rho \right) [f(x_0) - f_\star]
+ E \sum_{k=1}^n \| z_k - x_\star \|_{(A_{k+1} - A_k)}^2
+ E \sum_{k=0}^n \left[ \| g_k \|^2_{A_{k+1}^{-1}} - \rho \langle g_k, m_{k-1} \rangle_{A_{k+1}^{-1}} \right].
\]

Lemma 7. Define \( D_\infty = \sup_{x \in \mathcal{X}} \| x - x_\star \| \). The GradaGrad update satisfies:
\[
\| z_0 - x_\star \|^2_{A_1} + E \sum_{k=1}^n \| z_k - x_\star \|^2_{(A_{k+1} - A_k)} \leq \frac{D_\infty^2}{\gamma_0} E \sum_{i=1}^d \sqrt{\alpha_{i,n+1}}.
\]

Proof. We consider the 1D case for simplicity as the bound is separable in the dimension of the
problem. This allows us to simplify the left hand side to
\[
\| z_0 - x_\star \|^2_{A_1} + E \sum_{k=1}^n \left[ \left( \frac{\sqrt{\alpha_{k+1}}}{\gamma_{k+1}} - \frac{\sqrt{\alpha_k}}{\gamma_k} \right) \| z_k - x_\star \|^2 \right].
\]

We will prove this by induction. Consider the base case, \( v_0 \) is always positive so:
\[
\| z_0 - x_\star \|^2_{A_1} \leq \frac{D_\infty^2}{\gamma_0} \sqrt{\alpha_1} \leq \frac{D_\infty^2}{\gamma_0} \sqrt{\alpha_1}.
\]

Now consider \( k > 0 \). We have two cases corresponding to the sign of \( v_k \). If \( v_k \) is negative, then \( \gamma_{k+1} \) and \( \alpha_{k+1} \) are rescaled, and \( A_{k+1} \) decreases from \( A_k \) so \( \gamma_{k+1} > \gamma_k \). If \( v_k \) is negative, then \( \gamma_{k+1} \) and \( \alpha_{k+1} \) are rescaled, and \( A_{k+1} \) decreases from \( A_k \) so \( \gamma_{k+1} > \gamma_k \). If \( v_k \) is positive, then \( \gamma_{k+1} \) and \( \alpha_{k+1} \) are rescaled, and \( A_{k+1} \) decreases from \( A_k \) so \( \gamma_{k+1} > \gamma_k \).

Now consider the remaining case, where \( v_k \) is positive, in which case \( \gamma \) increases and \( \alpha \) stays unchanged:
\[
\frac{D_\infty^2}{\gamma_0} \sqrt{\alpha_k} + E \left( \frac{\sqrt{\alpha_{k+1}}}{\gamma_{k+1}} - \frac{\sqrt{\alpha_k}}{\gamma_k} \right) \| z_k - x_\star \|^2 \leq \frac{D_\infty^2}{\gamma_0} \sqrt{\alpha_k}
= \frac{D_\infty^2}{\gamma_0} \sqrt{\alpha_{k+1}}.
\]

\( \square \)
A.2 Gradient error bounding

Lemma 8. When $v_k \leq 0$:
\[
\|g_k\|^2_{A_k^{-1}} - \rho \langle m_{k-1}, g_k \rangle_{A_k^{-1}} \leq 0,
\]
when
\[
v_k \geq -r\alpha_k,
\]
\[
r = \frac{1}{h_k^2} - 1,
\]
\[
h_k = \frac{g_k^2}{\rho m_{k-1}g_k}.
\]

We again consider the 1D case as the inequality is separable in the dimension. So the required inequality is:
\[
\frac{g_k^2}{A_{k+1}} - \rho \frac{g_k}{A_{k}} \leq 0.
\]  \hspace{1cm} (12)

Rearranging:
\[
\frac{g_k^2}{A_k} \leq \rho \frac{g_k}{A_{k+1}} m_{k-1}g_k,
\]
\[
\frac{A_{k+1}}{A_k} \geq \frac{g_k^2}{\rho m_{k-1}g_k},
\]
Define:
\[
h_k = \frac{g_k^2}{\rho m_{k-1}g_k} \geq 0.
\]

We want to find a value of $r$ such that:
\[
\frac{A_{k+1}}{A_k} \geq h_k.
\]

Using $v_k = -r\alpha_k$ we have:
\[
\frac{\sqrt{\alpha_{k+1}}}{\sqrt{\alpha_k}} \geq h_k,
\]
\[
\frac{g_k}{\sqrt{\gamma_k}} \geq h_k,
\]
\[
\frac{\gamma_k}{\frac{\gamma_k}{\frac{\gamma_k}{\alpha_k}}} \geq h_k,
\]
\[
\frac{1}{\sqrt{\alpha_k}} \geq \frac{1}{h_k},
\]
\[
\frac{1}{h_k} \geq \frac{1}{\sqrt{1 + r}},
\]
\[
r \leq \frac{1}{h_k^2} - 1.
\]

Therefore any $r$ value smaller than $1/h_k^2 - 1$ is sufficient.

Lemma 9. Consider the 1D case, with $k \geq 1$. Let $q \geq 2\sqrt{2 + \rho \gamma_{k+1}^2}$ if $v_k \geq 0$:
\[
qA_k + \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_k} \leq qA_{k+1}.
\]

Proof. We start by applying a case argument. Consider when $-g_k m_{k-1} \geq 0$. From the fact that $\alpha_0 = G_\infty^2$ we have $\frac{1}{A_k} \leq \frac{\sqrt{\alpha_0}}{A_{k+1}}$, and therefore:
\[
qA_k + \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_k} \leq qA_k + \frac{g_k^2}{A_{k+1}} - \sqrt{2 + \rho g_k m_{k-1}}
\]
\[
\leq qA_k + \frac{g_k^2}{A_{k+1}} - \sqrt{2 + \rho m_{k-1}}.
\]
In the other case, where \(-g_k m_{k-1} < 0\), then we can instead use \(A_{k+1} \geq A_k\) and thus \(-\frac{1}{A_k} \leq -\frac{1}{A_{k+1}}\) (given that \(v_k\) is assumed positive), so:

\[
qA_k + \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_k} \leq qA_k + \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_{k+1}} \\
\leq qA_k + \sqrt{2 + \rho} \left[ \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_{k+1}} \right].
\]

Using the notation \(A_k = \gamma_{k+1}^{-1} \sqrt{b_k - \alpha_k}\), where \(b_k = \sum_{t=0}^{k} (g_t^2 - \rho g_t m_{t-1})\) and \(\alpha_k = g_k^2 - \rho g_k m_{k-1}\). We have from the concavity of the square-root function that:

\[
\sqrt{b_k - \alpha_k} \leq \sqrt{b_k} + \frac{b_k - \alpha_k - b_k}{2\sqrt{b_k}} \\
= \sqrt{b_k} - \frac{\alpha_k}{2\sqrt{b_k}}.
\]

Therefore:

\[
qA_k + \sqrt{2 + \rho} \left[ \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_{k+1}} \right] \\
\leq qA_{k+1} - \frac{q}{2\gamma_{k+1}} \left[ \frac{g_k^2}{\sqrt{b_k}} - \frac{\rho g_k m_{k-1}}{\sqrt{b_k}} \right] + \sqrt{2 + \rho} \left[ \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_{k+1}} \right] \\
= qA_{k+1} - \frac{q}{2\gamma_{k+1}} \left[ \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_{k+1}} \right] + \sqrt{2 + \rho} \left[ \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_{k+1}} \right] \\
= qA_{k+1} + \left( -\frac{2\sqrt{2 + \rho}}{2\gamma_{k+1}} \right) + \sqrt{2 + \rho} \left[ \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_{k+1}} \right] \\
= qA_{k+1}. 
\]

\[\square\]

**Lemma 10.** Let \(q = 2\sqrt{2 + \rho}\gamma_n^2\). Then:

\[
\sum_{k=0}^{n} \left[ \|g_k\|_{A_k^{-1}}^2 - \rho \langle g_{k-1}, g_k \rangle_{A_k^{-1}} \right] \leq q \sum_{i=1}^{d} A_{i+1} + \frac{q}{\gamma_0} \sum_{i=1}^{d} \sqrt{\alpha_{i,n+1}}.
\]

**Proof.** Without loss of generality, we again consider the 1D case. Recall that if \(v_k < 0\) (which can only occur when \(k \geq 1\)):

\[
qA_k + \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_k} \leq qA_k \\
= qA_{k+1} + q (A_k - A_{k+1}),
\]

and if \(v_k > 0\) and \(k \geq 1\):

\[
qA_k + \frac{g_k^2}{A_{k+1}} - \frac{\rho g_k m_{k-1}}{A_k} \leq qA_{k+1}.
\]

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We will telescope this bound from the base-case $\frac{q^2}{A_1} \leq qA_1$ (which is trivially true) to $A_{n+1}$. Combining we have:

\[
\sum_{k=0}^{n} \left[ \frac{g_k^2}{A_{k+1}} - \rho g_k m_{k-1} \right] \leq qA_{n+1} + q \sum_{k=1}^{n} I [v_k \leq 0] (A_k - A_{k+1}) \\
= qA_1 - q \sum_{k=1}^{n} (A_k - A_{k+1}) + q \sum_{k=1}^{n} I [v_k \leq 0] (A_k - A_{k+1}) \\
= qA_1 - q \sum_{k=1}^{n} I [v_k \geq 0] (A_k - A_{k+1}) \\
= qA_1 + q \sum_{k=1}^{n} I [v_k > 0] (A_{k+1} - A_k) \\
= qA_1 + q \sum_{k=1}^{n} I [v_k > 0] \frac{1}{\gamma_k} \left( \sqrt{\alpha_{k+1} - \sqrt{\alpha_k}} \right) \\
\leq qA_1 + \frac{q}{\gamma_0} \sum_{k=1}^{n} I [v_k > 0] \left( \sqrt{\alpha_{k+1} - \sqrt{\alpha_k}} \right) \\
= qA_1 + \frac{q \sqrt{\alpha_{n+1}}}{\gamma_0}.
\]

\[\square\]

A.3 Proof of Theorem 3

Recall the general form of Theorem 2 from Section A.1:

\[
2E \sum_{k=0}^{n} \left[ f(x_k) - f_* \right] \leq E \|z_0 - x_*\|^2_{A_1} + \left( \frac{2\beta}{1-\beta} + \rho \right) [f(x_0) - f_*] \\
+ E \sum_{k=1}^{n} \|z_k - x_*\|^2 (A_{k+1} - A_k) \\
+ E \sum_{k=0}^{n} \left[ \|g_k\|^2_{A_{k+1}} - \rho (g_k, m_{k-1}) A_k^2 \right].
\]

We apply the iterate error bound (Lemma 7) and the gradient bound (Lemma 10) to give:

\[
2E \sum_{k=0}^{n} \left[ f(x_k) - f_* \right] \leq \left( \frac{2\beta}{1-\beta} + \rho \right) [f(x_0) - f_*] \\
+ \frac{D^2}{\gamma_0} E \sum_{i=1}^{d} \sqrt{\alpha_{i,n+1}} + qE \sum_{i=1}^{d} A_{i,1} + E \frac{q}{\gamma_0} \sum_{i=1}^{d} \sqrt{\alpha_{i,n+1}}.
\]

Now using $f(x_{n+1}) - f_* \leq \frac{1}{n+1} \sum_{k=0}^{n} [f(x_k) - f_*]$, we have:

\[
E [f(x_{n+1}) - f_*] \leq \frac{1}{2(n+1)} \left( \frac{2\beta}{1-\beta} + \rho \right) [f(x_0) - f_*] \\
+ \left( \frac{D^2}{2\gamma_0(n+1)} + \frac{q}{2\gamma_0(n+1)} \right) E \sum_{i=1}^{d} \sqrt{\alpha_{i,n+1}} + \frac{q}{2(n+1)} E \sum_{i=1}^{d} A_{i,1}.
\]

Now using that $\alpha_{i,n+1} \leq (n+1)G_*^2$, and $A_{i,1} \leq G_* / \gamma_0$ and the definition of $q$:

\[
E [f(x_{n+1}) - f_*] \leq \frac{1}{2(n+1)} \left( \frac{2\beta}{1-\beta} + \rho \right) [f(x_0) - f_*] \\
+ \left( \frac{D^2}{2\gamma_0(n+1)} + \frac{q}{2\gamma_0(n+1)} \right) d\sqrt{n+1}G_* + \frac{qd}{2(n+1)^2} G_*.
\]

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Simplifying:

\[ \mathbb{E}[f(\bar{x}_{n+1}) - f_*] \leq \frac{1}{2(n+1)} \left( \frac{2\beta}{1 - \beta} + \rho \right) [f(x_0) - f_*] \]
\[ + \left( \frac{D_\infty^2}{2} + q \right) \frac{dG_\infty}{\gamma_0 \sqrt{n+1}}. \]

Now further using that \( q = 2\sqrt{2 + \rho \gamma_n^2} \leq 2\sqrt{2 + \rho D_\infty^2} \):

\[ \mathbb{E}[f(\bar{x}_{n+1}) - f_*] \leq \frac{1}{2(n+1)} \left( \frac{2\beta}{1 - \beta} + \rho \right) [f(x_0) - f_*] \]
\[ + 3\sqrt{2 + \rho} \frac{dG_\infty D_\infty^2}{\gamma_0 \sqrt{n+1}}. \]

B Further experimental details

For the convex experiments, we trained in PyTorch using CPU training. Each training run took several minutes at most, depending on the dataset. Our DLRM training was run on a V100 GPU, and took approximately 6 hours per training run.