Improving the convergence of SGD through adaptive batch sizes

Scott Sievert\(^1\) and Shrey Shah\(^2\)

\(^1\)Air Force Research Laboratory\(^†\)
\(^2\)University of Wisconsin–Madison

Abstract

Mini-batch stochastic gradient descent (SGD) and variants thereof approximate the objective function’s gradient with a small number of training examples, aka the batch size. Small batch sizes require little computation for each model update but can yield high-variance gradient estimates, which poses some challenges for optimization. Conversely, large batches require more computation but can yield higher precision gradient estimates. This work presents a method to adapt the batch size to the model’s training loss. For various function classes, we show that our method requires the same order of model updates as gradient descent while requiring the same order of gradient computations as SGD. This method requires evaluating the model’s loss on the entire dataset every model update. However, the required computation is greatly reduced by approximating the training loss. We provide experiments that illustrate our methods require fewer model updates without increasing the total amount of computation.

1 Introduction

Mini-batch SGD and variants thereof (Bottou et al., 2018) are extremely popular in machine learning (e.g., Zou et al. (2017); Szegedy et al. (2017); Simon et al. (2016)). These methods attempt to minimize a function $F(w) := \frac{1}{n} \sum_{i=1}^{n} f(w; z_i)$ where the function $f$ measures the loss of a model $w$ on example $z_i$. For example, if performing linear regression on $d$ features, $z_i = (x_i, y_i)$ which includes a feature vector $x_i \in \mathbb{R}^d$ and scalar output variable $y_i \in \mathbb{R}$. To minimize $F$, mini-batch SGD uses $B$ examples to compute a model update via

$$w_{k+1} = w_k - \frac{\gamma_k}{B} \sum_{i=1}^{B} \nabla f(w_k; z_i)$$

(1)

where $\gamma_k$ is the step-size or learning rate at model update $k$ and $i_s$ is chosen uniformly at random. This update approximates $F$’s gradient with $B$ examples in order to make the complexity of each model update scale with $B$, typically much smaller than $n$ (Bottou, 2012).

In practice, the batch size $B$ is a hyper-parameter and is often constant throughout the optimization (e.g., Alistarh et al. (2017); Zagoruyko and Komodakis (2016); Goyal et al. (2017)). There is a clear tradeoff between small and large batch sizes for each model update: using small batch sizes reduces the computation required for each model update while yielding imprecise estimates of the objective function’s gradient. Conversely, large batch sizes yield more precise gradient estimates, but fewer model updates can be performed with the same computation budget.

\(^*\)Corresponding author. Email: scott.sievert.3@us.af.mil
\(^†\)Relevant work performed while at the University of Wisconsin–Madison
1.1 Contributions

Why should the batch size remain static as an optimization proceeds? With poor initialization, the optimal model for each example is in the same direction. In this case, approximating the objective function’s gradient with more examples will have little benefit because each gradient is similar. By that measure, perhaps large batch sizes will provide utility near the optimum because the optimum depends on all training examples.

This work expands upon the idea by adaptively growing the batch size with model performance\(^1\) as the optimization proceeds. Specifically, this work does the following:

- Provides methods to adapt the batch size to the model performance. These methods require significant computation because they require computing model performance before every model update.
- Shows that adapting the batch size to the model performance can require significantly fewer model updates and approximately the same number of gradient computations when compared with standard SGD.\(^2\)
- Provides a practical implementation that circumvents the requirement to evaluate the objective function before every model update.
- Provides experimental results on both methods. These experiments show that the methods above require fewer model updates and the same number of gradient computations as standard mini-batch SGD to reach a particular accuracy.

The benefit of reducing the number of model updates isn’t apparent at first glance. One benefit is that the wall-clock time required for any one model update is agnostic to the batch size with a certain distributed system configuration\(^3\) (Goyal et al., 2017, Sec. 5.5). When the batch size grows geometrically, the number of model updates is a “meaningful measure of the training time” in a similar system (Smith et al., 2018, Sec. 5.4). Additionally, larger batch sizes improve distributed system performance (Qi et al., 2016; Yin et al., 2018).\(^4\)

Our adaptive method receives the function value in addition to the gradients, which is more information than SGD and variants thereof receive (Nemirovsky and Yudin, 1983). However, in practice, our proposed practical implementation largely ignores the gradient norm and essentially only receives the function value.

In Section 3, some preliminary notions are introduced before the presentation of the adaptive batch size method and the corresponding convergence results in Section 4. We address some practical implementation issues and provide validating experiments in Section 5.

2 Related work

Mini-batch SGD with small batch sizes tends to bounce around the optimum because the gradient estimate has high variance – the optimum depends on all examples, not a few examples. Common methods to circumvent this issue include some step size decay schedule (Bottou, 1998, Sec. 4) and averaging model iterates with averaged SGD (ASGD) (Polyak and Juditsky, 1992). Less common methods include stochastic average gradient (SAG) and stochastic variance reduction (SVRG) because they present memory and computational restrictions respectively (Schmidt et al., 2013; Johnson and Zhang, 2013). Our work is more similar in spirit to variance reduction techniques that use variable learning rates and batch sizes, discussed below.

Adaptive learning rates  Adaptive learning rates or step sizes can help adapt the optimization to the most informative features with Adagrad (Ward et al., 2019; Duchi et al., 2011) or to estimate the first and second moments of the gradients with Adam (Kingma and Ba, 2014). Adagrad has inspired Adadelta (Zeiler, 2012) which makes some modifications to average over a certain window and approximate the Hessian. Such methods are useful for convergence and a reduction in hyperparameter tuning.\(^5\) AdaGrad and variants

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1"Model performance" defined as the objective function loss over the entire training set for convex and strongly-convex functions.

2At least for convex and strongly-convex functions.

3Specifically when the number of workers is proportional to the batch size.

4See [https://talwalkarlab.github.io/paleo/](https://talwalkarlab.github.io/paleo/) with “strong scaling.”

5The original work on SGD stated that the learning rate should decay to meet some conditions, but did not specify the decay schedule (Robbins and Monro, 1951).
Increasing batch sizes Increasing the batch size as an optimization proceeds is another method of variance reduction. Strongly convex functions provably benefit from geometrically increasing batch sizes in terms of the number of model updates while requiring no more gradient computations than SGD (Bottou et al., 2018, Ch. 5). The number of model updates required for strongly convex, convex and non-convex functions is improved with batch sizes that increase like $O(r^k)$, $O(k^2)$ and $O(k)$ respectively (Zhou et al., 2018).6

Smith et al. perform variance reduction by geometrically increasing the batch size or decreasing the learning rate by the same factor, both in discrete steps (e.g., every 60 epochs) (Smith et al., 2018). Specifically, Smith et al. motivate their method by connecting variance reduction to simulated annealing, in which reducing the SGD model update variance or “noise scale” in a series of discrete steps enhances the likelihood of reaching a “robust” minima (Smith et al., 2018, Sec. 3). Smith et al. show that increasing the batch size yields similar results to decaying the learning rate by the same amount, which suggests that “it is the noise scale which is relevant, not the learning rate” (Smith et al., 2018, Sec. 5.1). By that measure, adaptive batch sizes are to geometrically increasing batch sizes as adaptive learning rate methods are to SGD learning rate decay schedules.

Adaptive batch sizes Several schemes to adapt the batch size to the model have been developed, ranging from model specific schemes (Orr, 1997) to more general schemes (De et al., 2016; Balles et al., 2017; Byrd et al., 2012). These methods tend to look at the sample variance of every individual gradient, which involves the computation of a single gradient norm $\|\nabla f_i(x)\|$ for every example $i$ in the current batch (Byrd et al., 2012; Balles et al., 2017; De et al., 2016). Naively, this requires feeding every example through the model individually. This can be circumvented; Balles et al. present an approximation method to avoid the variance estimation that requires about 1.25× more computation than the standard mini-batch SGD update, with some techniques to avoid memory constraints (Balles et al., 2017, Sec. 4.2).

Friedlander et al. use adaptive batch sizes to prove linear convergence for strongly convex functions and a $O(1/k)$ convergence rate for convex functions (Friedlander and Schmidt, 2012). Their adaptive approach relies on providing a batch size that satisfies certain error bounds on the gradient residual (in Eq. 2.6), which provides motivation for geometrically increasing batch sizes (Friedlander and Schmidt, 2012, Sec. 3).

Work developed concurrently with this work includes an SVRG modification (Ji et al., 2019), which involves modifying the outer-loop of SVRG. Instead of calculating the gradient for all examples during every loop, they propose a scheme to calculate the gradient for $N_s$ examples where $N_s$ is inversely proportional to the average gradient variance.7

3 Preliminaries

First, some basic definitions:

Definition 1. A function $F$ is $L$-Lipschitz if $\|F(w_1) - F(w_2)\| \leq L \|w_1 - w_2\|$ $\forall w_1, w_2$.

Definition 2. A function $F$ is $\beta$-smooth if the gradients are $\beta$-Lipschitz, or if $\|\nabla F(w_1) - \nabla F(w_2)\| \leq \beta \|w_1 - w_2\|$ $\forall w_1, w_2$.

The class of $\beta$-smooth functions is a result of the gradient norm being bounded, or that all the eigenvalues of the Hessian are smaller than $\beta$. If a function $F$ is $\beta$-smooth, the function also obeys $\forall x_1, x_2$, $F(w_1) \leq F(w_2) + \langle \nabla F(w_2), w_1 - w_2 \rangle + \frac{\beta}{2} \|w_1 - w_2\|^2$ (Bubeck et al., 2015, Lemma 3.4).

6In HSGD, convex functions require $O(\epsilon^{-3})$ gradient computations (Zhou et al., 2018, Cor. 2). As illustrated in Table 1, this work and SGD require $O(\epsilon^{-2})$ gradient computations.

7In later revisions of their work, they provide a comparison with this work, which includes a similar proof to Theorem 4 (Ji et al., 2019, Appendix D).
**Theorem 1.** Let work shows that mini-batch SGD with appropriately chosen adaptive batch sizes requires the same number of 2016, Thm. 1), as does SGD with geometrically increasing batch sizes for strongly convex functions (Bottou 2016, Thm. 4). Gradient descent with a constant learning rate requires

\[
\alpha - \text{PL functions.}
\]

For simplicity, we refer to these functions \( F \) satisfying this condition as being “\( \alpha \)-PL.” The class of \( \alpha \)-PL functions includes \( \alpha \)-strongly convex functions and a certain class non-convex functions (Karimi et al., 2016). One important constraint of \( \alpha \)-PL functions is that every stationary point must be a global minimizer, though stationary points are not necessarily unique. Recent work has shown similar convergence rates for \( \alpha \)-PL and \( \alpha \)-strongly convex functions for a variety of different algorithms (Karimi et al., 2016).

A bound on the expected gradient norm will also be useful because it will appear in theorem statements. For ease of notation, let’s define \( f_i(w) := f(w; z_i) \).

**Definition 5.** For model \( w \), let \( M^2(w) := 1/n \sum_{i=1}^{n} \| \nabla f_i(w) \|^2 \) and let \( M := \{ M^2(w_k) : k \in \mathbb{N} \cup \{0\} \text{ and } k < T \} \) when \( T \) model updates are performed. Let \( M^2_L := \min M \) and \( M^2_U := \max M \).

## 4 Convergence

In this section we will prove convergence rates for mini-batch SGD with adaptive batch sizes and give bounds on the number of gradient computations needed. Our main results are summarized in Table 1. In general, this work shows that mini-batch SGD with appropriately chosen adaptive batch sizes requires the same number of model updates as gradient descent (up to constants) while not requiring more gradient computations than serial SGD (up to constants).

In general, the adaptive batch sizes are inversely proportional to the current model’s loss. This method is motivated by an approximate measure of gradient dissimilarity as detailed in Appendix A. Section 4.1 analyzes the required number of model updates, and Section 4.2 analyzes the required number of gradient computations. The theory in this section might require significant computation; methods in Section 5 circumvent some of these issues.

### 4.1 Model updates

Let’s start in the context of \( \alpha \)-PL functions. In this setting, SGD requires \( O(1/\varepsilon) \) model updates (Karimi et al., 2016, Thm. 4). Gradient descent with a constant learning rate requires \( \log(1/\varepsilon) \) model updates (Karimi et al., 2016, Thm. 1), as does SGD with geometrically increasing batch sizes for strongly convex functions (Bottou et al., 2018, Cor. 5.2). We show that \( \log(1/\varepsilon) \) model updates are also required when the adaptive batch size is chosen appropriately:

**Theorem 1.** Let \( x_k \) denote the \( k \)-th iterate of mini-batch SGD with step-size \( \gamma \) on a \( \beta \)-smooth and \( \alpha \)-PL function \( F \). If the batch size \( B_k \) at each iteration \( k \) is given by

\[
B_k = \left[ \frac{c}{F(w_k) - F^*} \right]
\]

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8In this theoretical discussion, the batch size will not require any computation.

9This computation is impractical but possible. The model updates in Eq. 1 produce model \( w_{k+1} \) from model \( w_k \), and the batch size \( B_k \) depends on model \( w_k \).
Table 1: The number of model updates or gradient computations required to reach a model of error at most $\varepsilon$. Error is defined with loss $F(w_T) - F^* \leq \varepsilon$ for smooth & convex functions and $\alpha$-strongly convex ($\alpha$-SC) functions, and with gradient norm for smooth functions, $\min_{k=0,...,T-1} \| \nabla F(w_k) \| \leq \varepsilon$. All function classes are $\beta$-smooth, and for $\alpha$-strongly convex functions the condition number $\kappa$ is given by $\kappa = \beta/\alpha$. The function class column in Table 1a is shared with Table 1b. See Section 4 for details and references. Cells with minimum model updates/gradient computations (up to constants) with $n = 60 \cdot 10^3$, $\varepsilon = 0.01$, $\alpha = 0.1$ and $\beta = 1$ are highlighted.

| Function class | SGD | Adaptive batch sizes | Gradient descent | SGD | Adaptive batch sizes | Gradient descent |
|----------------|-----|----------------------|------------------|-----|----------------------|------------------|
| $\alpha$-SC    | $O(\alpha/\varepsilon)$ | $O(\alpha \log(1/\varepsilon))$ | $O(\alpha/2)$ | $O(\alpha/\varepsilon)$ | $O(\alpha \log(1/\varepsilon))$ | $O(\alpha/2)$ |
| Convex         | $O(1/\varepsilon)$      | $O(1/\varepsilon)$           | $O(1/\varepsilon)$ | $O(1/\varepsilon)$      | $O(1/\varepsilon)$           | $O(1/\varepsilon)$ |
| Smooth         | $O(1/\varepsilon)$      | $O(1/\varepsilon)$           | $O(1/\varepsilon)$ | $O(1/\varepsilon)$      | $O(1/\varepsilon)$           | $O(1/\varepsilon)$ |

(a) Total number of **model updates** required during optimization. (b) Total number of **gradient computations** required during optimization.

and the learning rate $\gamma = \alpha/\beta (\alpha + M_\alpha^2/2c)$ for some constant $c > 0$, then

$$\mathbb{E}[F(w_T)] - F^* \leq (1 - r)^T (F(w_0) - F^*)$$

where $r := \alpha^2/(\beta (\alpha + M_\alpha^2/2c))$. This implies $T \geq O(\log(1/\varepsilon))$ model updates are required to obtain $w_T$ such that $\mathbb{E}[F(w_T)] - F^* \leq \varepsilon$.

The proof is detailed in Appendix B.1 and follows from the definition of $B_k$, $\beta$-smooth and $\alpha$-PL. This theorem can also be applied to Euclidean distance from the optimal model for $\alpha$-strongly convex functions because $\alpha/2 \| w_k - w^* \|^2 \leq F(w_k) - F(w^*)$. The learning rate $\gamma$ is typically a user-specified hyperparameter determined through trial-and-error (e.g., (Schaul et al., 2013; Smith, 2015)). This theorem makes a fairly standard assumption that the optimal training loss $F^*$ is known, which influences $\gamma$ in Ward et al. (2019, Sec. 1.1) and Orr (1997, Eq. 15).10

When $F$ is convex, the same adaptive batch size method obtains comparable convergence rates to gradient descent. SGD requires $O(1/\varepsilon)$ model updates (Bubeck et al., 2015, Thm. 6.3). Gradient descent with constant learning rate requires $O(1/\varepsilon)$ model updates (Bubeck et al., 2015, Thm. 3.3), and has linear convergence if an exact line search is used (Boyd and Vandenberghe, 2004, Eq. 9.18). Using adaptive batch sizes with SGD also requires $O(1/\varepsilon)$ model updates:

**Theorem 2.** Let $x_k$ denote the $k$-th iterate of mini-batch SGD with step size $\gamma$ on some $\beta$-smooth and convex function $F$. If the batch size $B_k$ at each iteration is given by Equation 2 and $\gamma = (\beta + 1/c)^{-1}$, then for any $T \geq 1$,$$
\mathbb{E}[F(\overline{w}_T)] - F^* \leq \frac{r}{T}
$$

where $r := \|w_0 - w^*\|^2 \left( \beta + \frac{M_\alpha^2}{\varepsilon} \right) + F(w_0) - F^* \enspace and \enspace \overline{w}_T := \frac{1}{T} \sum_{i=0}^{T-1} w_{i+1}$. This implies $T \geq r/\varepsilon$ model updates are required to obtain $w_T$ such that $\mathbb{E}[F(w_T)] - F^* \leq \varepsilon$.

This proof adapts classic convergence analysis of SGD (Bubeck et al., 2015) and is in Appendix B.2.

**Key Lemma** Theorems 1 and 2 rely on a key lemma, one that controls the gradient approximation error $\mathbb{E}[\| \nabla F(w_k) - g_k \|^2]$ as a function of the number of model updates $k$ and batch size $B_k$. When the batch size is grown according to Eq. 2, the gradient approximation error for model update $k$ is bounded by the loss of model $w_k$:

10For most overparameterized neural nets, the optimal training loss is 0 or close to 0 (Belkin et al., 2018; Zhang et al., 2017; Salakhutdinov, 2017).
Lemma 3. Let the batch size $B_k$ be chosen as in Eq. 2. Then when the gradient estimate $g_k = 1 / B_k \sum_{i=1}^{B_k} \nabla f_i(w_k)$ is created with $i_k$ chosen uniformly at random, then

$$\mathbb{E} \left[ \| \nabla F(w_k) - g_k \|_2^2 \mid w_k \right] \leq (F(w_k) - F^*) M_f^2 \gamma^{-1}$$

The proof is Appendix B and relies on substituting the definition of the batch size $B_k$ into the gradient approximation error, $\mathbb{E} \left[ \| \nabla F(w_k) - g_k \|_2^2 \right]$.

When $F$ is smooth and non-convex, we’ll provide an upper bound on the number of model updates required to find an $\varepsilon$-approximate critical point so that $\| \nabla F(x) \| \leq \varepsilon$, which requires computing the adaptive batch size differently. In this setting, SGD requires $O\left( \frac{1}{\varepsilon^4} \right)$ model updates (Yin et al., 2018, Thm. 2), and gradient descent requires $O\left( \frac{1}{\varepsilon^2} \right)$ model updates (Jin et al., 2017, Thm. 2). Adaptive batch sizes require $O\left( \frac{1}{\varepsilon^2} \right)$ model updates:

Theorem 4. Let $x_k$ denote the $k$-th iterate of mini-batch SGD on a $\beta$-smooth function $F$. If the batch size $B_k$ at each iteration satisfies

$$B_k = \left[ \frac{c}{\| \nabla F(w_k) \|_2^2} \right]$$

for some $c > 0$ and the step size $\gamma = \beta^{-1} \cdot c / (c + M_f^2)$, then for any $T \geq 1$,

$$\min_{k=0, \ldots, T-1} \| \nabla F(w_k) \| \leq \sqrt{\frac{r}{T}}$$

where $r := 2(F(w_0) - F^*) \cdot \beta (M_f^2 \gamma^{-1} + 1)$. This implies $T \geq r^2 / \varepsilon^2$ model updates are required to obtain $w_T$ such that $\min_{k=0, \ldots, T-1} \| \nabla F(w_k) \| \leq \varepsilon$.

The proof adapts a proof by Yin et al. (2018, Thm. 2) to the batch size in Equation 3 and is detailed in Appendix B.3.

4.2 Number of gradient computations

While the convergence rates above show that adaptively chosen batch sizes can lead to fast convergence in terms of the number of model updates, this is not a good metric for the total amount of work performed. When the model is close to the optimum, the batch size will be large but only one model update will be computed. A better metric for the amount of work performed is on the number of gradient computations required to reach a model of a particular error.

The number of gradient computations required by the adaptive batch size method is similar to the number of gradient computations for SGD. The number of gradient computations for SGD and gradient descent are reflected in the model update count; SGD and gradient descent require computing 1 and $n$ gradients per model update respectively. These values are concisely summarized in Table 1.11

Let’s start with $\alpha$-PL and convex functions. When increasing the batch size geometrically for $\alpha$-strong convex functions, only $O\left( \frac{1}{\varepsilon} \right)$ gradient computations are required (Bottou et al., 2018, Thm. 5.3).

Corollary 5. When $F$ is $\alpha$-PL, no more than $4cr \log (1/\varepsilon) / \varepsilon$ gradient computations are required in Theorem 1 for $c$ and $r$ defined therein.

Corollary 6. For convex and $\beta$-smooth functions $F$, no more than $4cr / \varepsilon^2$ gradient computations are required in Theorem 2 for $c$ and $r$ defined therein.

Now, let’s look at the gradient computations required for smooth functions. For illustration, let’s assume the batch size in Eq. 3 is given by an oracle and does not require any gradient computation.

11In this table, line searches are not performed for gradient descent on convex functions.
Corollary 7. For $\beta$-smooth functions $F$, no more than $4cr/\varepsilon^3$ gradient computations are required to estimate the loss function’s gradient in Theorem 4 for $c$ and $r$ therein.

Proof is delegated to Appendix C. Corollaries 5, 6 and 7 rely on Lemma 14, which is not tight. Tightening this bound requires finding lower bounds on model loss, a statement of the form $F(w_k) - F^* \geq g(\varepsilon, k)$ for some function $g$. There are classical bounds of this sort for gradient descent (Nesterov, 2013, Thms. 2.1.7 and 2.1.13), and more recent lower bounds for SGD (Nguyen et al., 2019). However, deriving a comprehensive understanding of lower bounds for mini-batch SGD remains an open problem.

5 Experimental results & Practical considerations

In this section, we first show that the theory above works as expected: far fewer model are required to obtain a model of a particular loss, and the total number of gradient computations is the same as standard mini-batch SGD. However, the implementation above is impractical: the batch size requires significant computation. We suggest some workarounds to address these practical issues, and provide experiments that compare the proposed method with relevant work.

In this section, two performance metrics are relevant: the number of gradient computations and model updates to reach a particular accuracy. These two metrics can be treated as proxies for energy and time respectively. A single gradient computation requires a fixed number of floating point operations, which requires a fixed amount of energy. As discussed in Section 1.1, the wall-clock time required to complete one model update can be (almost) agnostic to the batch size with certain distributed systems.

5.1 Synthetic simulations

First, let’s train a neural network with linear activations to illustrate our theoretical contributions. Practically speaking, this is an extremely inefficient and roundabout way to compute a linear function. However, the associated loss function is non-convex and more difficult to optimize. Despite the non-convexity it satisfies the PL inequality almost everywhere in a measure–theoretic sense (Charles and Papailiopoulos, 2018, Thm. 13).
This section will focus on this optimization:

$$\hat{w}_1, \hat{W}_2, \hat{W}_3 = \arg\min_{w_1, w_2, w_3} \sum_{i=1}^{n} (y_i - w_i^T W_2 W_3 x_i)^2$$

(4)

where there are $n = 10^4$ observations and each feature vector has $d = 100$ dimensions, and $w_1 \in \mathbb{R}^d$, $W_2, W_3 \in \mathbb{R}^{d,d}$. The synthetic data $x_i$ is generated with coordinates drawn independently from $\mathcal{N}(0, 1)$. Each label $y_i$ is given by $y_i = x_i^T w^* + n_i$ where $n_i \sim \mathcal{N}(0, \sigma^2/100)$ and $w^* \sim \mathcal{N}(0, 1)$. Of the $n = 10^4$ observations, 2,000 observations are used as test data.

In order to understand our adaptive batch size method, we compare the model updates in Theorem 1 (aka “Adaptive Batch SGD”) with mini-batch SGD to standard mini-batch SGD with decaying step size (SGD), AdaGrad (Duchi et al., 2011). Adagrad requiring more data than SGD but far less than gradient descent. Figure 1c shows that the batch size grows nearly exponentially, which is unsurprising given Bottou et al. (2018, Eq. 5.7).

### 5.2 Functional implementation

A practical issue immediately presents itself: the computation of the batch size $B_k$. This is clearly infeasible because it requires evaluating the entire training dataset every model update. To work around this issue, let’s approximate the training loss with a rolling-average of batch losses. Additionally, generalization and GPU memory concerns may be present. To address these concerns, prior work sets a maximum batch size and decays the learning rate or batch size. Specifically, let’s compare the optimization algorithms that either passively or adaptively change the learning rate or batch size.

#### Algorithm 1: RADA-DAMP

```plaintext
1: for $k \in [0, 1, 2, \ldots]$ do
2: $\gamma' \leftarrow \gamma$
3: if $B_k \geq B_{\text{max}}$ then
4: $\gamma' \leftarrow \gamma B_{\text{max}}/B_k$
5: $B_k \leftarrow B_{\text{max}}$
6: end if
7: $\tilde{L}_B \leftarrow 1/B_k \sum_{i=1}^{B_k} f_i(x_k)$
8: $w_{k+1} \leftarrow w_k - \gamma'\nabla \tilde{L}_B$
9: $t_k \leftarrow \tilde{L}_B + \lambda \|\nabla \tilde{L}_B\|_2$
10: if $k > 0$ then
11: $\hat{d}_k \leftarrow \rho \cdot \hat{d}_{k-1} + (1 - \rho)t_k$
12: else
13: $\hat{d}_0 \leftarrow t_k$
14: end if
15: $B_{k+1} \leftarrow \lceil B_0 \hat{d}_0/\hat{d}_k \rceil$
16: end for
17: return $w_{k+1}$
```

There are concerns with large static batch sizes (Smith and Le, 2018; Jastrzębski et al., 2017); it’s unclear what happens for variable batch sizes.

All optimizers use the same learning rate, momentum and initial/max batch size, and basic tuning on the batch size increase/learning rate decay schedule is performed.
size increase schedule for RADADAMP/GeoDamp, and use the same schedule for the corresponding algorithms that only decay the learning rate (“RADADAMP-LR” and SGD respectively). Details are in Appendix D.

Our experimental results are shown in Figure 2, details of which are in Appendix D. As expected, they show that RADADAMP and GeoDamp require far fewer model updates than RADADAMP-LR and SGD, and similar performance is obtained for all methods in terms of epochs. If the “noise scale” of the model updates is relevant as Smith et al. hypothesize (Smith et al., 2018), then perhaps the relevant comparison is between passive and adaptive methods of changing the “noise scale” (i.e., RADADAMP is to Adagrad as GeoDamp is to SGD).

RADADAMP requires far fewer model updates than GeoDamp to reach any test accuracy RADADAMP obtains (though GeoDamp obtains a final test accuracy that is approximately 0.4% higher). Of course, Both Adagrad and RADADAMP require far less tuning than GeoDamp and SGD because of the adaptivity to the (estimated) training loss.

Figure 2c shows that both RADADAMP and GeoDamp (approximately) increase the batch size exponentially as functions of model updates, at least initially. However GeoDamp’s learning rate decays much more and far quicker than RADADAMP’s (perhaps a reason for GeoDamp’s increased performance).

### 6 Conclusion & Future work

This work presents a method to have the batch size depend on the model training loss, and provides convergence results. However, this method requires significant computation. This complexity is mitigated by the presentation of a approximation to the adaptive method. Experimental results validate the theoretical results.

Future work involves studying why GeoDamp outperforms RADADAMP. This will likely motivate the design of a method similar to RADADAMP that might incorporate second-order information (Zeiler, 2012) and/or line searches (Vaswani et al., 2019; De et al., 2016; 2017).

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15With the exception of Adagrad.
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A Gradient diversity bounds

Yin et al. introduced a measure of gradient dissimilarity called “gradient diversity” (Yin et al., 2018):

**Definition 6.** The gradient diversity of a model $w$ with respect to $F$ is given by

$$
\Delta(w) := \frac{\sum_{i=1}^{n} \| \nabla f_i(w) \|_2^2}{\| \sum_{i=1}^{n} \nabla f_i(w) \|_2^2} = \frac{\sum_{i=1}^{n} \| \nabla f_i(w) \|_2^2}{\sum_{i=1}^{n} \| \nabla f_i(w) \|_2^2 + \sum_{i \neq j} (f_i(w), f_j(w))},
$$

(5)

when $f_i(w) = f(w; x_i)$. Let $\Delta_k := \Delta(w_k)$ given iterates $\{w_i\}_{i=1}^T$.

When the gradients are orthogonal, then $\Delta_k = 1$ and when all the gradients are exactly the same, then $\Delta_k = 1/n$.

Yin et al. show that serial SGD and mini-batch SGD produce similar results with the same number of gradient evaluations (Yin et al., 2018, Theorem 3). In this result, the batch size must obey a bound proportional to the maximum gradient diversity over all iterates. Let’s see how gradient diversity changes as an optimization proceeds:

**Theorem 8.** If $F$ is $\beta$-smooth, the gradient diversity $\Delta_k$ obeys $\Delta_k \geq \|w_k - w^*\|_2^2 / (1 + \delta)\gamma^2 M^2(w_k)$ for $c = M^2 / \beta^2 n$.

**Theorem 9.** If $F$ is $\alpha$-strongly convex, the gradient diversity $\Delta_k$ obeys $\Delta_k \leq \|w_k - w^*\|_2^2 / (1 + \delta)\gamma^2 M^2(w_k)$ for $c = M^2 / \alpha^2 n$.

**Corollary 10.** If $F$ is $\alpha$-PL, then the gradient diversity $\Delta_k$ obeys $\Delta_k \leq \|w_k - F(w_k) - F^*\|_2^2 / (1 + \delta)\gamma^2 M^2(w_k)$ for $c = M^2 / 2\alpha^2 n$.

Straightforward proofs of the above are given in Appendix A.1 and A.2. These proofs will rely on

**Lemma 11.** If a function $f$ is $\lambda$-strongly convex, then $f$ is also $\lambda$-PL.

and

**Corollary 12** (from Lemma 1 on (Yin et al., 2018)). Let $w_k$ be a model after $k$ updates. Let $w_{k+1}$ be the model after a mini-batch iteration given by Equation 1 with batch size $B_k \leq n\delta \Delta_k + 1$ for an arbitrary $\delta$. Then,

$$
E \left[ \|w_{k+1} - w^*\|_2^2 \mid w_k \right] \leq \|w_k - w^*\|_2^2 - 2\gamma_k \langle \nabla F(w_k), w_k - w^* \rangle + \frac{(1 + \delta)\gamma^2 M^2(w_k)}{B_k}
$$

with equality when there are no projections.

Proof is in Appendix A.3.

### A.1 Proof of Theorem 8

**Proof.** First, let’s expand the gradient diversity term and exploit that $\nabla F(w^*) = 0$ when $w^*$ is a local minimizer or saddle point:

$$
\Delta_k = \frac{\sum_i \| \nabla f_i(w_k) \|_2^2}{\| \sum_i \nabla f_i(w_k) \|_2^2} = \frac{\sum_i \| \nabla f_i(w_k) \|_2^2}{\| n \nabla F(w_k) \|_2^2} = \frac{1}{n} \frac{\sum_i \| \nabla f_i(w_k) \|_2^2}{\| \nabla F(w_k) - \nabla F(w^*) \|_2^2}
$$

Because $F$ is $\beta$-smooth, $\| \nabla F(w_1) - \nabla F(w_2) \| \leq \beta \| w_1 - w_2 \|$. Then,

$$
\Delta_k \geq \frac{M^2(w_k)}{n \| \nabla F(w_k) - \nabla F(w^*) \|_2^2} \geq \frac{M^2(w_k)}{n \beta^2 \| w_k - w^* \|_2^2} \geq \frac{M_L^2}{n \beta^2 \| w_k - w^* \|_2^2}
$$

$\square$
A.2 Proof of Theorem 9

Proof. Now, define expand gradient diversity and take advantage that $\nabla F(x^\star) = 0$ when $x^\star$ is a local minima or saddle point:

$$
\Delta_k = \frac{\sum_i \|\nabla f_i(w_k)\|^2}{\|\sum_i \nabla f_i(w_k)\|^2} \\
= \frac{\frac{1}{n} \sum_i \|\nabla f_i(w_k)\|^2}{n \|\nabla F(w_k)\|^2} \\
= \frac{M^2(w_k)}{n \|\nabla F(w_k)\|^2} \\
\leq \frac{M^2(w_k)}{2\alpha n (F(w_k) - F(x^\star))}
$$

In the context of Theorem 9, the function $F$ is assumed to be $\alpha$-strongly convex. This implies that the function $F$ is also $\alpha$-PL as shown in Lemma 11. With this, the fact that strongly convex functions grow at least quadratically can be used, so

$$
\frac{M^2(w_k)}{2\alpha n (F(w_k) - F(x^\star))} \leq \frac{M^2(w_k)}{\alpha^2 n \|w_k - w^\star\|^2}
$$

Then, by definition of $M^2$ and $M^2_U$, there’s also

$$
\Delta_k \leq \frac{M^2}{2\alpha n (F(w_k) - F(x^\star))} \leq \frac{M^2}{\alpha^2 n \|w_k - w^\star\|^2}
$$

A.3 Proof of Lemma 11

There is a brief proof of this in Appendix B of (Karimi et al., 2016). It is expanded here for completeness.

Proof. Recall that $\lambda$-strongly convex means $\forall x, y$

$$
f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{\lambda}{2} \|y - x\|^2
$$

and $\lambda$-PL means that $\frac{1}{2} \|\nabla f(x)\|^2 \geq \lambda(f(x) - f(x^\star))$.

Let’s start off with the definition of strong convexity, and define $g(y) = \nabla f(x)^T (y - x) + \frac{\lambda}{2} \|y - x\|^2$. Then, it’s simple to see that

$$
f(x^\star) - f(x) \geq \nabla f(x)^T (x^\star - x) + \frac{\lambda}{2} \|x^\star - x\|^2 \\
\geq \min_y g(y)
$$

g is a convex function, so the minimum can be obtained by setting $\nabla g(y) = 0$. When the minimum of $g(y)$ is found, $y = x - \frac{1}{\lambda} \nabla f(x)$. That means that

$$
\min_y g(y) = g(x - \lambda^{-1} \nabla f(x)) \\
= \frac{-1}{\lambda} \|f(x)\|^2 + \frac{1}{2\lambda} \|\nabla f(x)\|^2 \\
\geq \frac{-1}{2\lambda} \|\nabla f(x)\|^2
$$
because \( y - x = \frac{1}{
abla f(x)} \).

\[ \Box \]

B Convergence

This section will analyze the convergence rate of mini-batch SGD on \( F(w) \). In this, at every iteration \( k \), \( B_k \) examples are drawn uniformly at random with repetition via \( i_1^{(k)}, \ldots, i_{B_k}^{(k)} \) from the possible example indices \{1, \ldots, n\}. Let \( S_k = \{i_1^{(k)}, \ldots, i_{B_k}^{(k)}\} \). The model is updated with \( w_{k+1} = w_k - \gamma_k g_k \) where

\[
g_k = \frac{1}{B_k} \sum_{i \in S_k} \nabla f_i(w_k).
\]

Note that \( E[g_k] = \nabla F(w_k) \).

Now, let’s prove Lemma 3. Here’s the statement again:

**Lemma.** Let \( c' = c/M_U^2 \). When the gradient estimate \( g_k = 1/B_k \sum_{i=1}^{B_k} \nabla f_i(w_k) \) is created with batch size \( B_k \) in Eq. 2 with \( i_s \) chosen uniformly at random, then the expected variance

\[
E \left[ \| \nabla F(w_k) - g_k \|_2^2 \right] \leq \frac{F(w_k) - F^*}{c'}.
\]

**Proof.**

\[
E \left[ \| \nabla F(w_k) - g_k \|_2^2 \right] = E \left[ \frac{1}{B_k} \sum_{i=1}^{B_k} \left( \nabla f_i(w_k) - g_k \right) \right]^2 = \frac{1}{B_k} \sum_{i=1}^{B_k} \| \nabla f_i(w_k) - g_k \|_2^2
\]

\[
\leq \frac{B_k}{B_k} \| \nabla f(w_k) \|_2^2 + \frac{B_k - 1}{B_k} \frac{M^2(w_k)}{B_k} \leq \frac{\| \nabla f(w_k) \|_2^2}{c'M_U^2}
\]

when the batch size \( B_k = \lceil c(F(w_k) - F^*)^{-1} \rceil \) and with \( c = c'M_U^2 \).

\[ \Box \]

B.1 Proof of Theorem 1

**Proof.** From definition of \( \beta \)-smooth (Definition 2) and with the mini-batch SGD iterations,

\[
F(w_{k+1}) \leq F(w_k) - \gamma \left( \nabla F(w_k), \frac{1}{B} \sum_{i=1}^{B} \nabla f_i(w) \right) + \frac{\beta \gamma^2}{2} \left( \nabla F(w_k), \frac{1}{B} \sum_{i=1}^{B} \nabla f_i(w) \right)_2^2
\]

Wrapping with conditional expectation and noticing that \( \sum_{i=1}^{B} a_i, \sum_{i=1}^{B} a_i \) = \( \sum_{i=1}^{B} \| a_i \|^2 + \sum_{i=1}^{B} \sum_{j=1,j \neq i} a_i a_j \),
when \( c = c' M_0^2 \) by Lemma 3. Then choose \( \gamma < \frac{2}{\beta} \) so \( \frac{\gamma^2}{2} - \gamma < 0 \). Then because \( F \) is \( \alpha \)-PL,

\[
\begin{align*}
\leq F(w_k) - F^* - \left( \gamma - \frac{\beta \gamma^2}{2} \right) &\cdot 2\alpha (F(w_k) - F(w^*)) + \frac{\beta \gamma^2}{2} \frac{F(w_k) - F(w^*)}{c'} \\
= &\left( 1 - 2a\gamma + 2b\gamma^2 + \frac{\beta \gamma^2}{2c'} \right) (F(w_k) - F(w^*)) \\
= &\left( 1 - a\gamma + b\gamma^2 \right) (F(w_k) - F(w^*))
\end{align*}
\]

when \( a = 2\alpha \) and \( b = \beta \left( \alpha + \frac{1}{2\gamma^2} \right) \). Choose the step size \( \gamma = a/2b = \alpha/\left[ \beta \left( \alpha + \frac{1}{2\gamma^2} \right) \right] < 1/\beta \). Then

\[
\begin{align*}
= &\left( 1 - \frac{\alpha^2}{4b} \right) (F(w_k) - F(w^*)) \\
= &\left( 1 - \frac{\alpha^2}{\beta \left( \alpha + \frac{1}{2\gamma^2} \right)} \right) (F(w_k) - F(w^*))
\end{align*}
\]

This holds for any \( k \). Then, by law of iterated expectation:

\[
\begin{align*}
\mathbb{E} \left[ F(w_2) - F^* \mid w_0 \right] = \mathbb{E} \left[ \mathbb{E} \left[ F(w_2) - F^* \mid w_1 \right] \mid w_0 \right] \\
\leq \mathbb{E} \left[ (1 - r) \mathbb{E} \left[ F(w_1) - F^* \mid w_1 \right] \mid w_0 \right] \\
= (1 - r) \mathbb{E} \left[ F(w_1) - F^* \mid w_0 \right] \\
\leq (1 - r) \mathbb{E} \left[ (1 - r)(F(w_0) - F^*) \mid w_0 \right] \\
= (1 - r)^2 (F(w_0) - F^*)
\end{align*}
\]

when \( r := \left( 1 - \frac{\alpha^2}{\beta \left( \alpha + \frac{1}{2\gamma^2} \right)} \right) \). Continuing this process to iteration \( T \),

\[
\begin{align*}
\mathbb{E} \left[ F(w_T) - F^* \mid w_0 \right] \leq \left( 1 - \frac{\alpha^2}{\beta \left( \alpha + \frac{1}{2\gamma^2} \right)} \right)^T (F(w_0) - F(w^*))
\end{align*}
\]
Noticing that $1-x \leq e^{-x}$ for all $x \geq 0$, $\mathbb{E}[F(w_T) - F(w^*)] \leq \varepsilon$ when

$$T \geq \log \left( \frac{F(w_0) - F(w^*)}{\varepsilon} \right) \left( \frac{\beta (\alpha + \frac{1}{2\varepsilon})}{\alpha^2} \right)$$

(6)

B.2 Proof of Theorem 2

Proof. Suppose we use a step-size of $\gamma = 1/(\beta + 1/\eta)$ for $\eta > 0$. Then, we have the following relation, extracted from the proof of Theorem 6.3 of (Bubeck et al., 2015).

$$\mathbb{E}[F(w_{k+1}) - F^*] \leq \frac{(\beta + 1/\eta)}{2} (\mathbb{E}\|w_k - w^*\| - \mathbb{E}\|w_{k+1} - w^*\|) + \frac{\eta}{2} \mathbb{E}\|\nabla F(w_k) - g_k\|^2.$$

By Lemma 3, and taking $\eta = c'$, we have

$$\mathbb{E}[F(w_{k+1}) - F^*] \leq \frac{(\beta + 1/c')}{2} (\mathbb{E}\|w_k - w^*\| - \mathbb{E}\|w_{k+1} - w^*\|) + \frac{\eta}{2} \mathbb{E}[F(w_k) - F^*]$$

Summing $k = 0$ to $k = T - 1$ we have

$$\sum_{k=0}^{T-1} \mathbb{E}[F(w_{k+1}) - F^*] \leq \frac{(\beta + 1/c')}{2} (\mathbb{E}\|w_0 - w^*\| - \mathbb{E}\|w_{k+1} - w^*\|) + \frac{1}{2} \sum_{k=0}^{T-1} \mathbb{E}[F(w_k) - F^*]$$

$$\leq \frac{(\beta + 1/c')}{2} R^2 + \frac{1}{2} \sum_{k=0}^{T-1} \mathbb{E}[F(w_k) - F^*].$$

Rearranging, we have

$$\sum_{k=0}^{T-1} \mathbb{E}[F(w_{k+1}) - F^*] = (\beta + 1/c') R^2 + F(w_0) - F^* - 2(F(w_T) - F^*)$$

$$\leq (\beta + 1/c') R^2 + F(w_0) - F^*$$

This implies the desired result after applying the law of iterated expectation and convexity.

B.3 Proof of Theorem 4

Proof. By definition of $\beta$-smooth,

$$F(w_{k+1}) \leq F(w_k) + \langle \nabla F(w_k), w_{k+1} - w_k \rangle + \frac{\beta}{2} \|w_{k+1} - w_k\|^2$$

Then substitution of $w_{k+1} = w_k - \frac{\gamma}{B_k} \sum_{i=1}^{B_k} \nabla f_i(w_k)$, the following is obtained:

$$\gamma \left( \nabla F(w_k), \frac{1}{B_k} \sum_{i=1}^{B_k} \nabla f_i(w_k) \right) \leq F_k - F_{k+1} + \frac{\beta \gamma^2}{2} \left( \frac{1}{B_k} \sum_{i=1}^{B_k} \nabla f_i(w_k) \right)^2$$

Wrapping in conditional expectation given $w_k$,
\[ \gamma \| \nabla F(w_k) \|^2 \leq \mathbb{E} \left[ F_k - F_{k+1} \mid w_k \right] + \frac{\beta \gamma^2}{2} \mathbb{E} \left[ \left\| \frac{1}{B_k} \sum_{i=1}^{B_k} \nabla f_i(w_k) \right\|_2^2 \mid w_k \right] \]

\[ \leq \mathbb{E} \left[ F_k - F_{k+1} \mid w_k \right] + \frac{\beta \gamma^2}{2B_k} \mathbb{E} \left[ \sum_{i=1}^{B_k} \sum_{j=1}^{B_k} \langle \nabla f_i, \nabla f_j \rangle \mid w_k \right] \]

\[ \leq \mathbb{E} \left[ F_k - F_{k+1} \mid w_k \right] + \frac{\beta \gamma^2}{2B_k^2} \mathbb{E} \left[ \sum_{i=1}^{B_k} \| f_i \|^2 + \sum_{i=1}^{B_k} \sum_{j=1}^{B_k} \langle \nabla f_i, \nabla f_j \rangle \mid w_k \right] \]

because the indices \( i_s \) and \( j_s \) are chosen independently and \( \mathbb{E} [ \nabla f_i(w) ] = F(w) \). Then, substituting the definition of \( B_k \) in Eq. 3,

\[ \leq \mathbb{E} [ F_k - F_{k+1} ] + \frac{\beta \gamma^2}{2} \left( \frac{\| \nabla F(w_k) \|^2}{c} + \mathbb{E} \| \nabla F(w_k) \|^2 \right) \]

when \( c = c'M_2^2 \). Then this inequality is obtained after rearranging:

\[ \| \nabla F(w_k) \|^2 \left( \gamma - \frac{\gamma^2 \beta}{2} \left( c' - 1 \right) + 1 \right) \leq \mathbb{E} [ F_k - F_{k+1} ] \]

Then with this result and iterated expectation

\[ \min_{k=0, \ldots, T-1} \| \nabla F(w_k) \|^2 \leq \frac{1}{T} \sum_{k=0}^{T-1} \| \nabla F(w_k) \|^2 \]

\[ \leq \frac{F_0 - F^*}{T} \left( \gamma - \frac{\gamma^2 \beta}{2} \left( c' - 1 \right) + 1 \right)^{-1} \]

\[ \leq \frac{F_0 - F^*}{T} 2 \beta \left( \frac{1}{c' + 1} \right) \]

when \( \gamma = \beta^{-1}c/(c + M_2^2) \).

\[ \square \]

**Corollary 13.**

\[ \sum_{k=0}^{T-1} \| \nabla F(w_k) \|^2 \leq 2 \beta (F_0 - F^*) \left( \frac{1}{c' + 1} \right) \]

**C Number of examples**

The number of examples required to be processed is the sum of batch sizes:

\[ \sum_{i=1}^{T} B_i \]

over \( T \) iterations. This section will assume an oracle provides the batch size \( B_i \).
C.1 Proof of Corollaries 5 and 6

These proofs require another lemma that will be used in both proofs:

**Lemma 14.** If a model is trained so the loss difference from optimal $F(w) - F^* \in [\varepsilon/2, \varepsilon]$, then $4B_0(F(w_0) - F^*)T/\varepsilon$ examples need to be processed when there are $T$ model updates the initial batch size is $B_0$.

C.1.1 Proof of Corollary 5

Proof. This case requires $T \ge c_{\alpha, \beta} \log(\delta_0/\varepsilon)$ iterations for some constant $c$ when $F$ is $\alpha$-PL and $\beta$-smooth by Equation 6 when $\delta_0 = F(w_0) - F^*$. Applying Lemma 14 gives that AdaDamp requires no more then the number of examples

$$\sum_{k=0}^{T-1} B_k \le \frac{\log(\delta_0/\varepsilon)}{\varepsilon} \cdot 4c_{\alpha, \beta} B_0 \delta_0$$

C.1.2 Proof of Corollary 6

Proof. This case requires $T \ge r_{\beta}/\varepsilon$ iterations when $F$ is convex and $\beta$-smooth by Theorem 1. Applying Lemma 14 gives that AdaDamp requires no more then the number of examples

$$\sum_{k=0}^{T-1} B_k \le \frac{1}{\varepsilon^2} \cdot 4r_{\beta} B_0 \delta_0$$

when $\delta_0 := F(w_0) - F^*$.

C.2 Proof of Lemma 14

Proof.

$$\sum_{k=1}^{T} B_k = \sum_{k=1}^{T} \left[ \frac{B_0(F(w_0) - F^*)}{F(w_k) - F^*} \right]$$

$$\le 2B_0(F(w_0) - F^*) \sum_{k=1}^{T} \frac{1}{F(w_k) - F^*}$$

$$\le 4B_0(F(w_0) - F^*)T/\varepsilon$$

C.3 Proof of Corollary 7

Proof. Following the proof of Lemma 14,

$$\sum_{k=1}^{T} B_k = \sum_{k=1}^{T} \left[ \frac{c}{\|\nabla F(w_k)\|_2} \right]$$

$$\le 2c \sum_{k=1}^{T} \frac{1}{\|\nabla F(w_k)\|_2^2}$$

$$\le 4cT/\varepsilon$$

$$\le 4cr/\varepsilon^3$$

using Theorem 4 when $\|\nabla F(w_k)\| \le \varepsilon$ (and not when $\|\nabla F(w_k)\|_2^2 \le \varepsilon$).
D  Experiments

PyTorch (Paszke et al., 2017) is used to implement all optimization.

D.1 Synthetic dataset

All optimizers use learning rate $\gamma = 2.5 \cdot 10^{-3}$ unless explicitly noted otherwise.

- **SGD with adaptive batch sizes.** Batch size: $B_k = \left[ B_0 (F(x_0) - F^*) (F(x_k) - F^*)^{-1} \right], B_0 = 2$.

- **SGD with decaying step sizes:** Static batch size $B = 64$, decaying step size $\gamma_k = 10 \gamma/k$ at iteration $k$ (Murata, 1998).

- **AdaGrad** is used with a batch size of $B = 64$ and PyTorch 1.1’s default hyperparameters, $\gamma = 0.01$ and 0 for all other hyperparameters.

- **Gradient descent.** No other hyperparameters are required past learning rate.

These hyperparameters were not tuned past ensuring the convergence of each optimizer.

D.2 Fashion MNIST

Fashion MNIST is a dataset with 60,000 training examples and 10,000 testing examples. Each example includes a $28 \times 28$ image that falls in one of 10 classes (e.g., “coat” or “bag”) (Xiao et al., 2017). The standard pre-processing in PyTorch’s MNIST example is used.\(^{16}\)

The CNN used has about 111,000 parameters that specify 3 convolutional layers with max-pooling and 2 fully-connected layers, with ReLU activations after every layer.

The hyperparameter optimization process followed the data flow below for each optimizer:

- Randomly sample hyperparameters, and train the model for 200 epochs on 80% of the training set (using the remaining 20% for validation).

- Refine hyperparameters based on the hyperparameters that had validation loss within 0.005 of the minimum, and had fewer model updates than the mean number of model updates.

- Repeat steps 1 and 2 until satisfied with validation performance.

- Manually choose one set of hyperparameters for each optimizer, and train for 200 epochs with the entire training set, and report performance on the test set.

Step (4) has only been run once for RADAAMP. For GeoDamp, we sampled at least 268 hyperparameters, and for Adagrad we sampled at least 179 hyperparameters. We spent a while on step (3) for RADAAMP\(^{17}\)

Both GeoDamp and Adagrad required fewer iterations of step (3).

Hyperparameter sampling space, and tuned values are below. After some initial sampling, the learning rate is fixed at to be 0.005 and initial/maximum batch sizes to be 256/1024 respectively for all optimizers. We tuned the value of weight decay more for RADAAMP, and set it to be 0.003 for all optimizers.

With those fixed hyperparameters, in our last run of hyperparameter optimization we sampled from these hyperparameters:

- **Adagrad:**
  - Batch size: [16, 32, 64, 128, 256] (tuned value: 256)

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\(^{16}\)The transform at [http://github.com/pytorch/examples/.../mnist/main.py#L105](http://github.com/pytorch/examples/.../mnist/main.py#L105) is used; the resulting pixels value have a mean of 0.504 and a standard deviation of 1.14, not zero mean and unit variance as is typical for preprocessing. The model used has about 110 thousand parameters and includes bias in all layers, likely resolving any issues.

\(^{17}\)Primarily to tune the regularization balance between loss and gradient norm, $\lambda$. We didn’t have much success with large $\lambda$. 

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GeoDamp:
- Damping delay (epochs): (2, 5, 10, 20, 30, 60) (tuned value: 10)
- Damping factor: log-uniform between 1 to 10 (tuned value: 1.219231)

RadaDamp:
- “Dwell”: [1, 10, 20, 30, 50, 100] (tuned value: 1)
- Memory $\rho$: [0.95, 0.99, 0.995, 0.999] (tuned value: 0.999)

“Dwell” is the frequency at which to update the batch size; if dwell= 7, then the batch size will be updated every 7 model updates. Because we found the best value of dwell to be 1, it is not included in the description of Algorithm 1.

GeoDamp and RadaDamp change the batch size/learning rate for SGD with Nesterov momentum (and a momentum value 0.9). GeoDamp-LR aka SGD and RadaDamp-LR change the learning rate by the same amount the batch size would have changed; if RadaDamp increases the batch size by a factor of $f$, RadaDamp-LR will decay the learning rate by a factor of $f$ instead. When the maximum batch size is reached for RadaDamp and GeoDamp, the learning rate is decayed instead of the batch size increasing by the same scheme.

If the damping factor is $d$ and the damping delay is $e$ epochs, the batch size increases by a factor of $d$ or the step size decays by a factor of $d$ every $e$ epochs.