BGD: Generalization Using Large Step Sizes to Attract Flat Minima

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Keywords: Generalization, Optimization Method, Deep Neural Network, Bouncing Gradient Descent, Heuristic Algorithm, Large Step Sizes, Local Minima, Basin Flatness and Sharpness.

Abstract: In the digital age of ever-increasing data sources, accessibility, and collection, the demand for *generalizable* machine learning models that are effective at capitalizing on given limited training datasets is unprecedented due to the labor-intensiveness and expensiveness of data collection. The deployed model must efficiently exploit patterns and regularities in the data to achieve desirable predictive performance on new, unseen datasets. Naturally, due to the various sources of data pools within different domains from which data can be collected, such as in Machine Learning, Natural Language Processing, and Computer Vision, *selection bias* will evidently creep into the gathered data, resulting in distribution (domain) shifts. In practice, it is typical for learned deep neural networks to yield sub-optimal generalization performance as a result of pursuing sharp local minima when simply solving empirical risk minimization (ERM) on highly complex and non-convex loss functions. Hence, this paper aims to tackle the generalization error by first introducing the notion of a local minimum's *sharpness*, which is an attribute that induces a model's non-generalizability and can serve as a simple guiding heuristic to theoretically distinguish satisfactory (flat) local minima from poor (sharp) local minima. Secondly, motivated by the introduced concept of variance-stability $\sim$ exploration-exploitation tradeoff, we propose a novel gradient-based adaptive optimization algorithm that is a variant of SGD, named *Bouncing Gradient Descent* (BGD). BGD's primary goal is to ameliorate SGD's deficiency of getting trapped in suboptimal minima by utilizing relatively *large* step sizes and "unorthodox" approaches in the weight updates in order to achieve better model generalization by attracting flatter local minima. We empirically validate the proposed approach on several benchmark classification datasets, showing that it contributes to significant and consistent improvements in model generalization performance and produces state-of-the-art results when compared to the baseline approaches.

1 INTRODUCTION

Generalization refers to how well a trained generic parameterized candidate learner (usually a deep neural network (DNN)) can categorize or predict data that has not yet been seen. Deep learning (DL), which utilizes the generalization power of deep neural networks, has recently caused paradigm shifts in various academic and industrial fields. Therefore, one of the primary goals of many studies pertaining to deep learning has been to increase the generalization power of deep neural networks through the implementation of appropriate training techniques, and optimization algorithms (Cha et al., 2021). One way to achieve this goal is by finding a *flat* local minimum of a given loss surface of training data (Lengyel et al., 2021), (Lengyel et al., 2021), which indirectly induces minimization of the generalization error, as shown explicitly in the following generalization risk upper bound (Ben-David et al., 2010):

$$R^T(h) \leq R_s^{emp}(h) + 2d(P_X^s, P_X^t) + min_{P_X \in \{P_X^s, P_X^t\}} \{\mathrm{E}_{\mathbf{x}\sim P_X}[|h^{*s}(\mathbf{x}) - h^{*t}(\mathbf{x})|]\}, \quad (1)$$

where $R_s^{emp}(h)$ is the tractable source risk, $R^T(h)$ is the target risk, and $d(P_X^s, P_X^t) := \min_{\mathcal{A}\in\mathcal{X}} |P_X^s[\mathcal{A}] - P_X^t[\mathcal{A}]|$ signifies how the source and target distributions are varied.

Flatness of a local minimum also induces minimization of the generalization error implicitly in following bias-variance decomposition (James et al.,

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Ali, M., Alsuwaidi, O. and Khan, S.
BGD: Generalization Using Large Step Sizes to Attract Flat Minima.
DOI: 10.5220/0011771700003417
In *Proceedings of the 18th International Joint Conference on Computer Vision, Imaging and Computer Graphics Theory and Applications (VISIGRAPP 2023) - Volume 5: VISAPP*, pages 239-249
ISBN: 978-989-758-634-7; ISSN: 2184-4321

2013):

$$\mathrm{E}_{\hat{y}\sim P_{XY}(\hat{y}|\mathbf{x})}[(\hat{y}-y)^2\,|\,\mathbf{x}] = \underbrace{(\mathrm{E}[\hat{y}\,|\,\mathbf{x}]-y^*)^2}_{\text{bias}} + \underbrace{\mathrm{Var}[\hat{y}\,|\,\mathbf{x}]}_{\text{variance}} + \underbrace{\mathrm{Var}[y\,|\,\mathbf{x}]}_{\text{Bayes error}}. \quad (2)$$

The bias term can be correlated with the depth of the loss landscape's local minima, where attaining a "deeper" basin of a local minimum corresponds to a lower bias value, lowering the generalization error. Similarly, attracting a *flat* basin of the loss landscape's minimum corresponds to an insensitive candidate learner, which results in diminishing the variance term, consequently reducing the overall generalization error. Another popular way of achieving model generalization is by utilizing vast overparameterization in network models (Neyshabur et al.,). It was shown by (Simsek et al., 2021) that in vastly overparameterized networks, the number of global minima subspaces dominates that of the critical subspaces, so that symmetry-induced saddles play only a marginal role in the loss landscape. Hence, the gradient trajectory will have an easier time converging towards a more desirable (generalizable) local minimum. Therefore, adequate optimization of non-convex neural network loss landscapes can be achieved via a combination of model attraction towards flat local minima and model overparameterization. Although they are gaining in popularity, stochastic gradient descent (SGD) optimization algorithms are frequently implemented as *black-box* optimizers because it is challenging to propose concrete explanations of the benefits and drawbacks of using these algorithms in the different domains (Ruder, 2016) without making several assumptions. However, SGD is widely celebrated for its ability to converge to more generalizable local minima as compared to other optimization algorithms such as ADAM (Kingma and Ba, 2014) and RMSProp (Dauphin et al., 2015). SGD's ability to generalize has been attributed to its capability of escaping undesirable sharp local minima in favor of more generalizable flat ones due to the inherent stochasticity (noise) in its training process. Therefore, the flatness of the loss surface has become an appealing measure of generalizability for neural networks as a result of the intuitive connection to robustness and predictor insensitivity, as well as the convincing empirical evidence surrounding it. (Lengyel et al., 2021) has provided quantifiable empirical evidence that, under the cross-entropy loss, once a neural network reaches a non-trivial training error, the flatness correlates (via Pearson Correlation Coefficient) well to the classification margins. Accordingly, many researchers have proposed improved variants of Vanilla GD that aim to generalize better and converge faster, which are primarily driven by postulating numerous assumptions, empirical experiments, and intuitive, yet not necessarily rigorous, theoretical justifications. Our proposed method improved convergence while maintaining accuracy. we present a new gradient-based adaptive optimization process that we call Bouncing Gradient Descent. This approach is a version of SGD (BGD). The primary objective of BGD is to improve upon SGD's weakness of becoming stuck in suboptimal minima. This will be accomplished by employing relatively large step sizes and "unorthodox" approaches in the weight update process. The end result we obtain is improved model generalisation achieved through the attraction of flatter local minima. This helps in achieving stable convergence and improved accuracies. We provide empirical validation of the proposed method on many benchmark classification data-sets, demonstrating that it is effective.

2 RELATED WORK

One key aspect that most of the variants of SGD attempted to ameliorate was their ability to indirectly or directly reduce the amount *variance* (noise) in the approximated gradients of the weight updates while simultaneously improving their *stability* (Netrapalli, 2019). The motivation behind reducing the gradient's variance was based on the perception that it would lead to a better approximation of the true (full) gradient and, as a result, it would allow the algorithm to achieve faster and more stable convergence. This ultimately leads to better loss landscape and hence improved accuracies. Furthermore, most proposed SGD variants rely heavily on local information about the loss surface through the exploitation of gradients and Hessians to draw global conclusions. Some examples of such algorithms that attempt to reduce the inherent variance present in SGD include: SVRG (Johnson and Zhang, 2013), SAG (Konečnỳ and Richtárik, 2013), SAGA (Defazio et al., 2014), and SARAH (Nguyen et al., 2017).

While reducing the variance in the utilized gradients can lead to more stabilized weight updates during training, potentially improving convergence time, it does not guarantee that the converged set of weights will be better (more generalizable) weight candidates than otherwise. When diminishing the variance in the deployed gradients to a large extent, we consequently narrow down the region of uncertainty (confusion) around where a local minimum can be located; therefore, it probabilistically leads to a reduction in the number of explored regions in the loss (fitness) land-

scape that can contain a local minimum, thereby hindering overall weight exploration for local minima. The latter can be a primary cause of overfitting because a reduction in the probability of discovering local minima could potentially force the optimizer to search and converge within a limited region of the weight (search) space, which could contain unfavorable narrow (sharp) local minima. The optimization algorithm is therefore prevented from further exploring other regions in the weight space that could have corresponded to flatter more favorable local minima, where the coinciding weights would have been more generalizable and insensitive to more extensive input data distributions, as proven by (Cha et al., 2021) and (He et al., 2019) under mild assumptions. Furthermore, (Keskar et al., 2016) showed that small-batch SGD consistently converges to flatter, more generalizable minimizers as compared to large-batch SGD, which tends to converge to sharp minimizers of the training and testing functions. Additionally, they attributed this reduction in the generalization gap when performing small-batch SGD to the inherent noise in the gradient estimation when performing the weight updates.

Having said that, one can observe an apparent tradeoff between the variance (noise) and stability of the gradients. The gradient's variance-stability tradeoff can be closely linked to the popular exploration-exploitation tradeoff that occurs in reinforcement learning systems, where exploration involves movements such as discovery, variation, risk-taking, and search, while exploitation involves actions such as refinement, efficiency, and selection. When searching for local minima of the loss landscape in the weight space, the amount of variance in the gradient is analogous to exploration, while the gradient's stability is analogous to exploitation. That is because the high variance in the gradients causes the weight updates to be noisy, which coincides with oscillations in the loss function, either due to bouncing off some local minimum's basin or skipping over sharp ones. In contrast, higher gradient stability implies an exploitative approach to the local geometry of the loss landscape, which can be achieved by considering more gradient statistics (a larger batch size) or by relying on a history of past gradients, such as incorporating a momentum factor or using a previous fixed mini-batch gradient direction as an anchor in order to stabilize future SGD updates. The latter is implemented in algorithms such as SVRG and SARAH in a double-loop fashion, with the fixed mini-batch gradient being updated in the outer loop $\frac{1}{k}$ times the number of updates in the inner loop, where k corresponds to the number of individual SGD updates in the inner loop.

One common and straightforward way that is used to pseudo-reduce the amount of variance in the weight updates is by altering the step size. Where to reduce the noise in the gradients, an extremely small step size is used, or a decaying factor on the gradient's step size is employed accordingly, such that the step size shrinks continuously as the training proceeds in order to reduce the amount of fluctuation in the weight updates, thereby inducing stabilization (exploitation). In a similar fashion, employing a large step size would correspond to a pseudo-increase in the amount of variance in our weight updates, leading to further exploration in the weight space. However, picking the right step size is a labor-intensive, non-trivial problem, as its appropriate value widely varies from model to model and task to task and requires tedious manual hyperparameter tuning depending on multiple factors such as the data type, the dataset used, the selected choice of optimization algorithm, and other factors.

Furthermore, there exists a surplus of research to relate flatness with generalizability, such as the works conducted by (Keskar et al., 2016), (He et al., 2019), (Wen et al., 2018), and (Izmailov et al., 2018), where they demonstrate the effectiveness of finding a flatter local minima of the loss surface in improving the model's generalizability, and hence, one must seek to formulate techniques that can either smoothen and flatten the loss landscape on the training dataset, or lead to convergence towards a flatter local minimum.

Accordingly, we can condense our primary goal of achieving model generalization to having the optimizer converge to the best possible generalizable local minimum by finding and attracting the *flattest* one, because seeking flat minima can achieve better generalizability by maximizing classification margins in both in-domain and out-of-domain (Cha et al., 2021).

3 METHODOLOGY

Motivated by the *variance-stability* $\sim$ *exploration-exploitation tradeoff* as well as the particular findings of (Lengyel et al., 2021), (Cha et al., 2021), and (Nar and Sastry, 2018), we propose a novel adaptive variant of SGD, presented in Algorithm 1, named *Bouncing Gradient Descent* (BGD), which aims to ameliorate SGD's deficiency of getting trapped in suboptimal minima by using "unorthodox" approaches in the weight updates to achieve better model generalization by attracting flat local minima. The authors of (Lengyel et al., 2021) established a strong correlation between the flatness of a loss surface's basin and the wideness of the classification margins associated with it, and (Cha et al., 2021)

theoretically and empirically showed that attracting flatter minima will result in smaller generalization gaps and lower model overfitting. Furthermore, the authors of (Nar and Sastry, 2018) demonstrated that the step size of the GD algorithm (and its variants) influences the dynamics of the algorithm substantially. More specifically, they showed a crucial relationship: that the step size value *restricts* and *limits* the set of possible local minima to which the algorithm can converge. In addition, they demonstrated that if the gradient descent algorithm is able to converge to a solution while utilizing a large step size, then the function that is estimated by the deep linear network must have small singular values, and consequently, the estimated function must have a small Lipschitz constant. With the aforementioned statements in mind, the BGD optimization algorithm is constructed to leverage relatively large step sizes to its advantage, allowing the optimizer to better explore the loss landscape in search of a flatter set of local minima. BGD also makes use of overshooting oracles, which enable the optimizer to bounce across the loss landscape's basins and avoid as many undesirable sharp local minima as possible in order to eventually settle on a sufficiently flat local minimum, which induces model generalizability. Firstly, we introduce the notion of a local minimum's sharpness, which is an attribute that induces a model's non-generalizability and can serve as a simple guiding heuristic to theoretically distinguish good (flat) local minima from bad (sharp) local minima. The concept of sharpness $\psi : W^* \to \mathbb{R}^+$ of a given local minima $\mathbf{w}^*$ in non-convex functions $\mathcal{L} : W \to \mathbb{R}^+$ is defined by the following formulation:

Let

$$\mathbf{w}_c := \underbrace{\underset{\|\delta\|_p \leq \rho}{\arg\max} \{\mathcal{L}(\mathbf{w}^* + \delta) - \mathcal{L}(\mathbf{w}^*)\}}_{\delta^*} + \mathbf{w}^*. \quad (3)$$

Let

$$\mathbf{w}_I := \inf_{\lambda \in (0,1)} \{\mathbf{w}^* + \lambda \delta^*\} \quad (4)$$

such that: $\nabla^2 \mathcal{L}(\mathbf{w}_I)$ is singular and $\|\nabla \mathcal{L}(\mathbf{w}_I)\|_p \neq 0$.

Then:

$$\psi(\mathbf{w}^*) := \frac{\mathcal{L}(\mathbf{w}_c) - \mathcal{L}(\mathbf{w}^*)}{\|\mathbf{w}_c - \mathbf{w}^*\|_p} + \frac{\|\mathbf{w}_c - \mathbf{w}_I\|_p}{\|\mathbf{w}_c - \mathbf{w}^*\|_p} \quad (5)$$

$$\psi(\mathbf{w}^*) := \frac{1}{\|\mathbf{w}_c - \mathbf{w}^*\|_p} \Big(\underbrace{\mathcal{L}(\mathbf{w}_c) - \mathcal{L}(\mathbf{w}^*)}_{>0} + \|\mathbf{w}_c - \mathbf{w}_I\|_p \Big) \quad (6)$$

$$\psi(\mathbf{w}^*) := \frac{1}{\|\delta^*\|_p} \Big(\mathcal{L}(\mathbf{w}_c) - \mathcal{L}(\mathbf{w}^*) + , \|\mathbf{w}_c - \mathbf{w}_I\|_p \Big) \quad (7)$$

where $\mathbf{w}_c$ corresponds to the set of weights in the weight space representing the *pseudo-critical* point that is in proximity to a given local minimum $\mathbf{w}^*$ defined by a ball of radius ρ, and $\mathbf{w}_I$ refers to the set of weights that represents the *pseudo-inflection* point that is the closest to that given local minimum. Note that there exists at least one inflection point between any two critical points, as given by applying Rolle's Theorem to any differentiable function f': where if $f'(a) = f'(b)$, then there exists $x \in (a, b)$ such that $f''(x) = 0$, implying x is an inflection point. The first term in Equation 5 resembles the *slope* of an embedded one-dimensional manifold line, and it will always be positive, trivially because by construction: $\mathcal{L}(\mathbf{w}_c) > \mathcal{L}(\mathbf{w}^*)$, $\forall \mathbf{w}^* \in W^*$. Moreover, the second term serves as a metric that measures a local minimum's upwards concavity, where a smaller value for the term indicates that the minimum's basin holds its upwards concavity for longer before starting to concave downwards. Given the formulation above, the goal of our optimization algorithm would be to capture the loss function's local minimum with the smallest degree of sharpness, which corresponds to finding the smallest attainable value for Equation 7:

$$\psi^* = \inf_{\mathbf{w}^*} \{\psi(\mathbf{w}^*)\}.$$

However, optimizing a non-convex function to attain the best local minimum in terms of generalizability, represented by ψ^* can be infeasible. Thus, we should consider a "good enough" local minimum that satisfies the following condition:

$$\psi(\mathbf{w}^*) \leq k\psi^*, \; k > 1. \quad (8)$$

Looking at Equations 7 and 8, one can remark that the common denominator term $\|\delta^*\|_p := \underset{\|\delta\|_p \leq \rho}{\arg\max} \{\mathcal{L}(\mathbf{w}^* + \delta) - \mathcal{L}(\mathbf{w}^*)\}$ can serve as a significant, yet simple guiding heuristic in discriminating flat minima from sharp ones, since the other terms are more complicated to analyze and compute. Observing that $\|\delta^*\|_p$ is inversely proportional to a local minimum's sharpness:

$$\psi(\mathbf{w}^*) \propto \frac{1}{\|\delta^*\|_p},$$

we can hence use $\|\delta^*\|_p$ as a rough measure to distinguish out and avoid undesirable local minima. Therefore, we can postulate that any local minima with $\|\delta^*\|_p$ satisfying the following criteria:

$$\|\delta^*\|_p \leq \gamma, \; \gamma > 0, \quad (9)$$

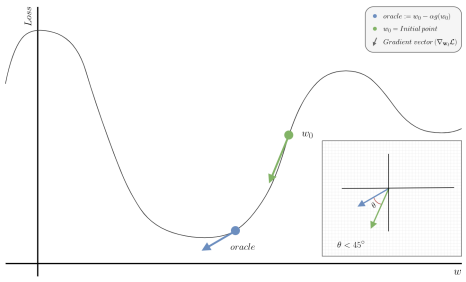
will be classified as a bad one. Thus, our objective now becomes to avoid any local minima that satisfy Equation 9. Since the magnitude of a weight update in the direction of a local minimum is given by: $\alpha\|\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w})\|$ in GD algorithms, the probability of a weight update at step t skipping over a bad local minimum, given by: $\|\delta^*\|_p \leq \gamma$ can be modeled on the order of the following:

$$\mathbf{Pr}[\alpha\|\nabla_{\mathbf{w}_t}\mathcal{L}(\mathbf{w}_t)\|_p > \gamma + \|\mathbf{w}_t - \mathbf{w}^*\|_p]. \quad (10)$$

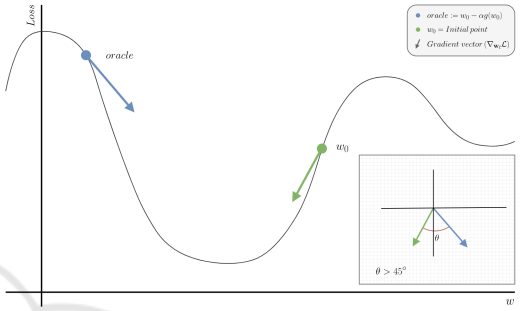
From Equation 10, it is evident that increasing the step size α will probabilistically increase the chances of the optimizer skipping over the bad local minimum while, at the same time, exploring the search space further. Consequently, the integral aspect behind the BGD algorithm is to use a substantial set of step sizes $\alpha \gg \mathbf{0}$ in order to increase the odds of skipping over as many sharp, ungeneralizable local minima as possible, as given in Equation 10.

Algorithm 1: Bouncing Gradient Descent (BGD).

Parameters: the step size vector $\alpha \gg \mathbf{0}$, the mini-batch size m, the exponential decay rate for the second moment estimate $\beta \geq 0.999$, and the threshold value $\tau \in (0.5, 1)$
Require: Stochastic objective function $f : \mathbb{R}^d \to \mathbb{R}$ with parameters $\mathbf{w}$
Require: Distance-measuring function $dist : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{+2}_{<1}$ mapping gradients g_i, g_j to positive scalars respectively, where large gradient magnitudes result in small scalar values and vice versa.
Initialize: $\mathbf{w}_0$ (Initial parameter vector)
Initialize: $\upsilon_0 \leftarrow \mathbf{1}$ (2^{nd} moment vector)
Initialize: $t \leftarrow 0$ (timestep)
  while $\mathbf{w}_t$ not converged **do**
    $g_t = \nabla_{\mathbf{w}_t} f\left(\mathbf{w}_t; x^{i:i+m}\right)$
    $\upsilon_{t+1} = \upsilon_t + \beta \cdot \sqrt{g_t \odot g_t}$
    oracle = $\mathbf{w}_t - \alpha \odot g_t$
    $g_{orc} = \nabla_{\text{orc}} f\left(\text{oracle}; x^{i:i+m}\right)$
    if $\langle g_t, g_{orc} \rangle \leq 0$ **then** ▷ Indicates the optimizer has bounced off
      $d_1, d_2 = dist(g_t, g_{orc})$ ▷ $d_1 + d_2 = 1$
      if $d_1 > \tau$ **then** ▷ Implies the step size taken is too big
        $\alpha = \alpha / \upsilon_{t+1}$
      end if
      $\mathbf{w}_{t+1} = d_1 \cdot \mathbf{w}_t + d_2 \cdot \text{oracle}$
    else
      $\mathbf{w}_{t+1} = \text{oracle} - \alpha \odot g_{orc}$
    end if
    $t = t + 1$
  end while
Return: $\mathbf{w}_{t+1}$



(a) The weight update results in both the previous weight w_0 and the *oracle* to be on the same side of the loss surface. In such case, the first **if** statement would be evaluated as *False*.



(b) The weight update results in the *oracle* bouncing off from the side where the previous weight w_0 was on the loss surface. In such case, the first **if** statement would be evaluated as *True*.

Figure 1: An elementary example to showcase the two possible cases of the first **if** statement in Algorithm 1.

As presented in Algorithm 1, BGD leverages relatively significant step sizes in order to maximize its regional search in the weight space for a generalizable set of weights that coincide with a flatter local minimum in the fitness landscape. The first **if** statement is used to determine whether the optimizer's initial weight update: oracle $= \mathbf{w}_t - \alpha \odot g_t$ has caused the oracle to bounce off from one side of the loss surface to another, indicated by the vector dot product $\langle g_t, g_{orc} \rangle$ being non-positive. Additionally, we provide several figures to help visualize the geometry of the dot product **if** condition, as well as the possible trajectory dynamics that BGD can follow. Figure 1 presents a simplified illustrative example, showcasing the two possible conditions of the first **if** statement.

Additionally, since BGD is an adaptive algorithm (based on the second moment of gradients) that deploys per-parameter step sizes, we explicitly capture this notion in the step size α hyperparameter. Where α is now a *vector* with relatively large step sizes corresponding to each weight, and the adaptivity of these step sizes will become apparent when the second **if** statement in Algorithm 1 is first triggered, specifically when $\alpha = \alpha / \upsilon_{t+1}$, indicating an element-wise division.

Furthermore, the *dist* function is a vector-valued distance-measuring (score) function that serves the purpose of evaluating the *relative quality* of the two given gradient vectors in order to yield two respective distances summing up to one; resembling a weighted sum of distances corresponding to each gradient vector.

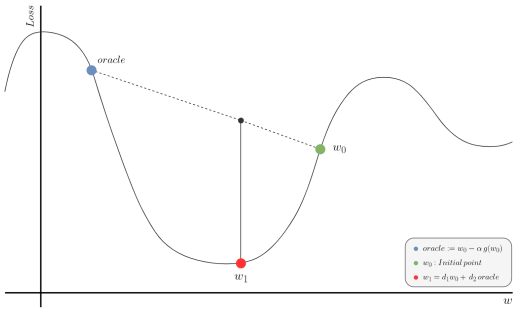
The quality of a gradient degrades as its vector norm increases and vice versa; here, the L2 norm was used for the evaluation. A weight vector that yields a smaller gradient norm will result in a comparatively large distance value, and hence; the weight update will lean closer towards that weight vector, allowing the optimizer to quickly jump to attracting basins given the large step sizes. The *dist* function can take many forms, though the formulation used for the *dist* function in the experiments was a simple and straightforward one, taking the following form:

$$dist\,(g_i, g_j) = [\frac{\|g_j\|}{\|g_i\| + \|g_j\| + \varepsilon}, \frac{\|g_i\|}{\|g_i\| + \|g_j\| + \varepsilon}], \tag{11}$$

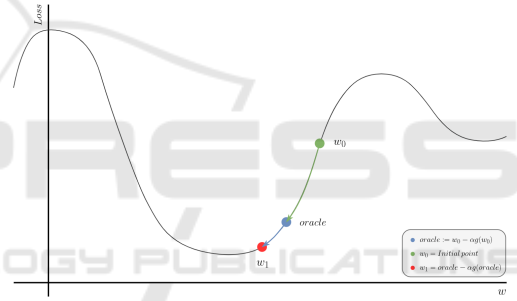
where for numerical stability purposes, $\varepsilon > 0$ is a small value added to the denominator. The threshold value τ is an additional tunable hyperparameter in BGD that determines when to adaptively shrink the value of the step size vector α based on the second moment of gradients υ in order to stabilize the future weight updates. Execution of the second **if** statement indicates that the overshooting oracle has landed on a loss surface with a sharp (steep) curvature as compared to its previous point $\mathbf{w}_t$, characterized by a large gradient norm, and thus; the d_1 value corresponding to $\mathbf{w}_t$ will be relatively large. Hence, using a low threshold value will be more suitable for highly non-convex surfaces, as it will cause the second **if** statement to trigger more often, consequently reducing the overall step size vector α. In practice, a threshold value of $\tau \in [0.7, 0.9]$ was determined to work best empirically.

As apparent in Algorithm 1, BGD contains two versions of the weight update. Where if the first **if** statement was triggered, the first version of the form $\mathbf{w}_{t+1} = d_1 \cdot \mathbf{w}_t + d_2 \cdot \text{oracle}$ will occur; implying that the oracle has bounced off from the side of the loss surface where the previous weight $\mathbf{w}_t$ was at. The updated weight $\mathbf{w}_{t+1}$ in the first version will be a weighted average of previous weight $\mathbf{w}_t$ and the oracle, causing $\mathbf{w}_{t+1}$ to land somewhere in between the two valleys around the loss basin. However, if the first **if** statement was not triggered, the second version of the weight update will take place, which basically is a gradient descent step from the oracle's position towards the local minimum. Both versions of the weight update are illustrated in Figure 2.

Finally, since the step size for BGD does not need to decay continuously to achieve stable convergence as it does for SGD, allowing for a relatively large step size to be utilized, which in turn leads to faster convergence and the potential to converge to flatter local minima due to the random exploration of the loss landscape.



(a) Description of the first version of the weight update which is applied when the first **if** statement is evaluated as *True*.



(b) Description of the second version of the weight update which is applied when the first **if** statement is evaluated as *False*.

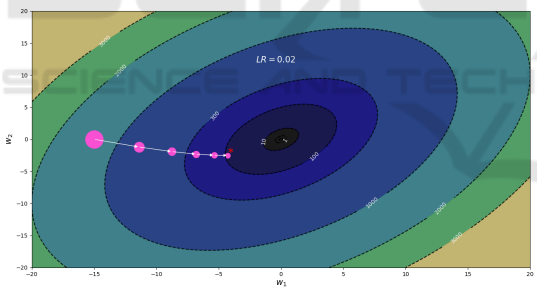
Figure 2: A simplified example that demonstrates the two versions of the weight update presented in Algorithm 1.

4 EXPERIMENTATION AND RESULTS

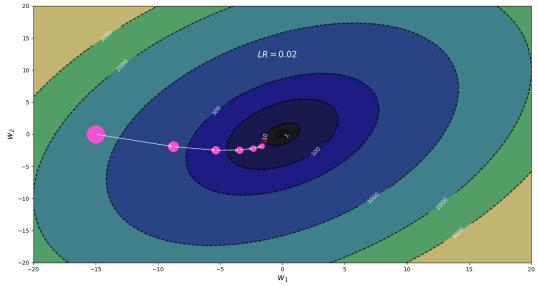
To begin, a comparison between GD and BGD is made in terms of minimizing a simple β-smooth α-strongly convex quadratic function $f : \mathbb{R}^2 \to \mathbb{R}$ for five iterations, in order to demonstrate the behavior of the paths taken by each algorithm across different step size values. As shown in the contour plots of Figure 3, when a relatively proper step size is chosen, GD weight updates follow a smooth trajectory toward the minimum point of the function. Even though this choice of step size does not fully capitalize on the bouncing properties of BGD, it still manages to outperform GD significantly thanks to its advantageous

use of oracles. Figure 4 depicts the same comparison made between the two algorithms, but this time, we opted for a comparatively larger step size than the one in Figure 3. As a result, we can see GD starting to demonstrate oscillating behavior caused by bounces around the basin of the function's local minimum, indicating that GD's weight updates are overshooting the minimum. On the other hand, BGD managed not to overshoot the function's minimum and bounce off to the other side due to its utilization of the first version of the weight update in BGD, resulting in faster and more stable convergence.

Finally, Figure 5 shows the most unfavorable case for GD, yet the most favorable case for BGD, where a relatively large step size is deployed. Consequently, GD started diverging away from the function's minimum and would require additional manual intervention in order to stabilize its weight updates by incorporating a step size decay per iteration. Again, however, BGD faces no issues and is successfully able to leverage the large step size to its advantage, converging stably in much fewer steps than usual. Furthermore, surprisingly, BGD is able to handle much larger step sizes than those used in the figures. However, when using such step sizes, GD starts to diverge heavily and goes beyond the visible bounds of the contour plots.

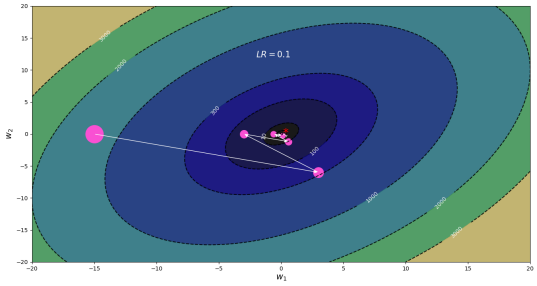


(a) Trajectory of the weight updates taken by GD.

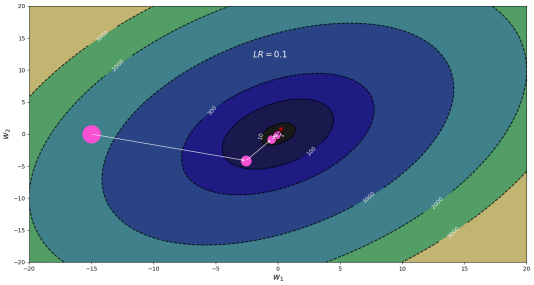


(b) Trajectory of the weight updates taken by BGD.

Figure 3: A comparison between the trajectories taken by GD versus BGD when minimizing the function: $f(w_1, w_2) = 6w_1^2 + 4w_2^2 - 4w_1w_2$ using a relatively small step size of 0.02. The the final point is represented by the asterisk symbol.

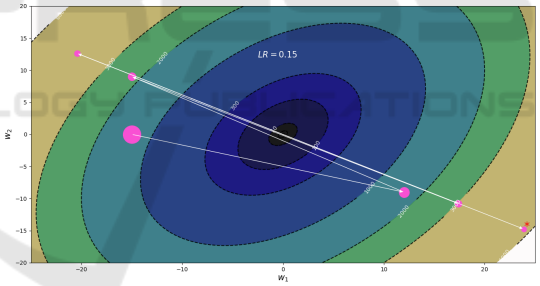


(a) Trajectory of the weight updates taken by GD.

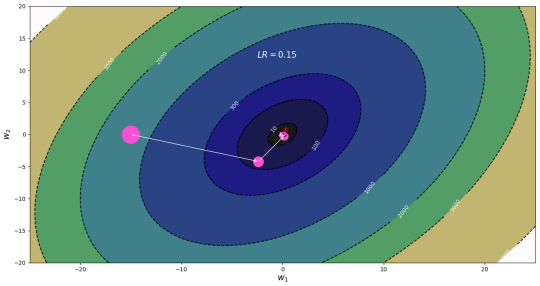


(b) Trajectory of the weight updates taken by BGD.

Figure 4: A comparison between the trajectories taken by GD and BGD when minimizing the function: $f(w_1, w_2) = 6w_1^2 + 4w_2^2 - 4w_1w_2$ using a relatively modest step size (learning rate) of 0.1. The the final point is represented by the asterisk symbol.



(a) Trajectory of the weight updates taken by GD.



(b) Trajectory of the weight updates taken by BGD.

Figure 5: A comparison between the trajectories taken by GD and BGD when minimizing the function: $f(w_1, w_2) = 6w_1^2 + 4w_2^2 - 4w_1w_2$ using a relatively large step size (learning rate) of 0.15. The the final point is represented by the asterisk symbol.

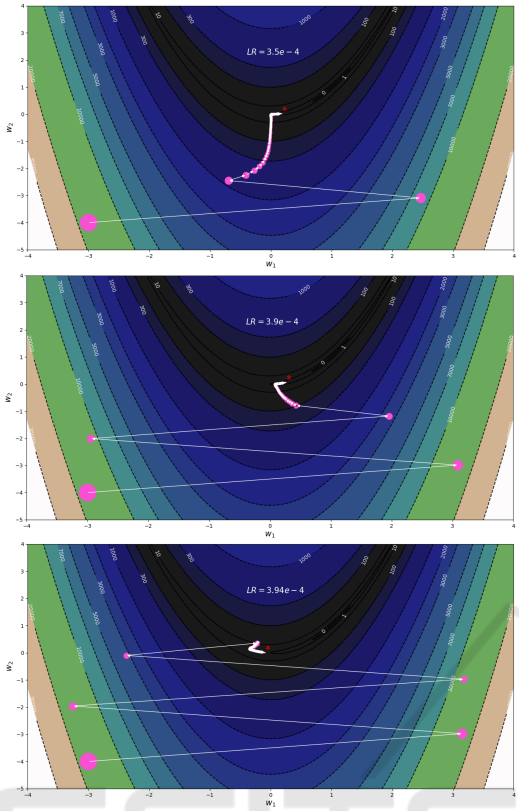


Figure 6: The trajectories taken by GD when minimizing the Rosenbrock function: $f(x,y) = (1-x)^2 + 100\left(y-x^2\right)^2$ across different values of the step size hyperparameter α, where the final point is represented by the asterisk symbol.

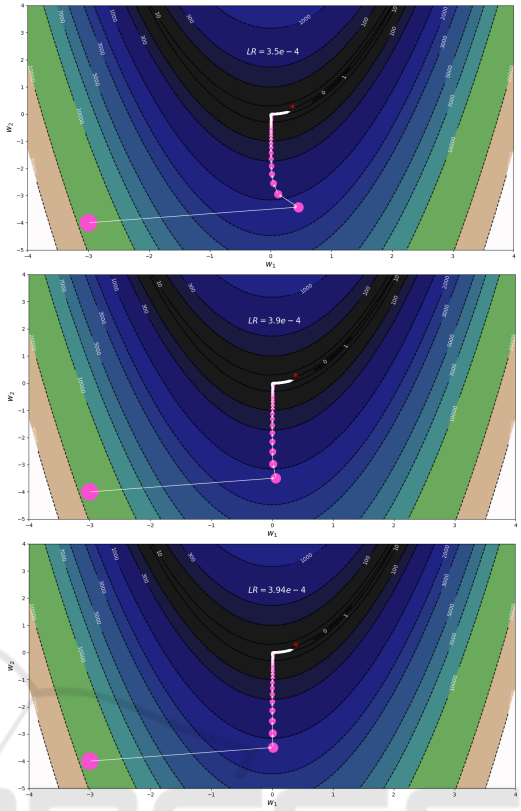


Figure 7: The trajectories taken by BGD when minimizing the Rosenbrock function: $f(x,y) = (1-x)^2 + 100\left(y-x^2\right)^2$ across different values of the step size hyperparameter α, where the final point is represented by the asterisk symbol.

In addition, a comparison of the trajectory dynamics of both algorithms GD and BGD on minimizing the Rosenbrock function $f : \mathbb{R}^2 \to \mathbb{R}$ for 325 iterations is conducted. The Rosenbrock function is unimodal, and its global minimum lies in a narrow, parabolic valley, which is notoriously difficult to converge to for gradient-based optimization algorithms. As shown in Figure 6, GD's convergence performance deteriorates as the step size increases due to the oscillations around the valley of the function, failing to utilize the increase in step size when approaching the minimum of the Rosenbrock function. Moreover, GD's convergence performance is extremely sensitive to the step size used, as relatively small adjustments made to the step size result in extreme changes in the trajectories and convergence of GD due to the non-convexity of the Rosenbrock function. On the other hand, as illustrated in Figure 7, BGD's convergence actually improves as the step size increases, since BGD is able to quickly land in the valley of the Rosenbrock function thanks to its first version of the weight update (illustrated in Figure 2 (a)). Another important thing to note is that GD started to diverge to infinity when the step size was slightly altered to 3.95e−4, while conversely, BGD demonstrated faster convergence towards the minimum.

Furthermore, BGD can handle exceptionally large step sizes, achieving remarkable performance even when using a step size of α =1e5, resulting in a solution with a function value of 0.319 in 325 iterations as demonstrated in Figure 8 This shows that even while algorithm tested for the extreme cases gives stable

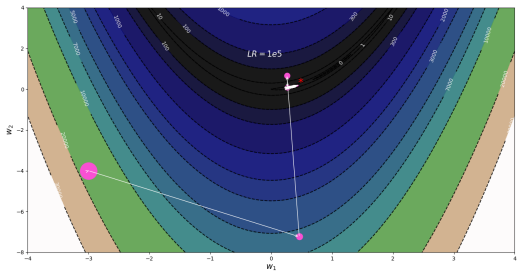
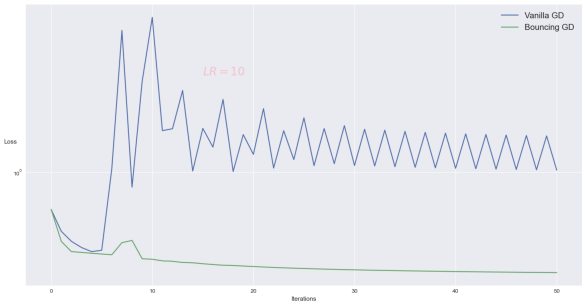
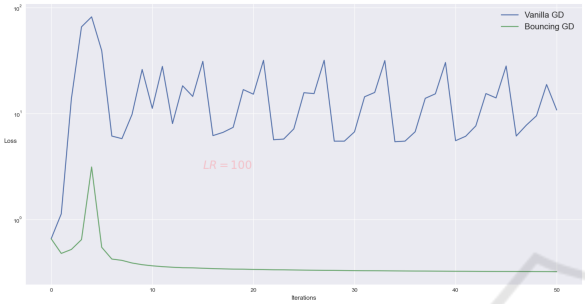


Figure 8: The trajectories taken by BGD when minimizing the Rosenbrock function: $f(x,y) = (1-x)^2 + 100\left(y-x^2\right)^2$ using an exaggerated value of 100000 for the step size hyperparameter α, where the final point is represented by the asterisk symbol.



(a) Minimizing the logistic loss using a step size of 10.



(b) Minimizing the logistic loss using a step size of 100.

Figure 9: The log-scaled loss curves of each algorithm when minimizing the logistic loss on the **a1a** dataset using two different step sizes (learning rates).

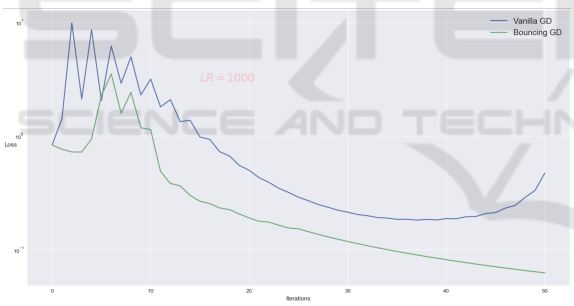


Figure 10: The log-scaled loss curves of each algorithm when minimizing the logistic loss on the **news.20.binary** dataset using an exaggerated step size (learning rate) of 1000.

performance and it doesnot crash.

Next, we demonstrate yet another optimization comparison between GD and BGD, though this time, by observing how each algorithm minimizes the logistic loss on two different binary classification datasets taken from the LIBSVM library (Chang and Lin, 2011). The first dataset is the simple **a1a** dataset, which consists of 1,605 training examples, where each example contains 123 input features. Figure 9 illustrates the loss curves generated by training on each algorithm. The second dataset is the more extensive **news.20.binary** dataset, which contains 19,996 training examples and 1,355,191 input features per example. Its loss curves are depicted in Figure 10; even though both algorithms suffered from loss oscillations initially, they eventually managed to find a relatively smoother loss surface. However, GD started diverging towards the end of the training phase, indicating that the attracting basin of the loss function's local minimum was relatively sharp; hence, GD bounced off the minimum's basin which resulted in a cascading diverging effect, because unlike BGD, GD is unable to handle large values of the step size α. Therefore we cannot use very large learning rates with GD as it will crash. While for the case of BGD we prove the handling of even large learning rates with improved convergence. That shows consistent performance of our algorithm.

Figure 11: The classification accuracy of the different optimization algorithms evaluated on multiple benchmark classification datasets when using a batch-size of 1000.

Finally, we conducted classification performance comparisons between SGD (with and without momentum), BGD, and ADAM on popular benchmark image classification datasets by minimizing the categorical cross-entropy loss of a three-layer non-linear feedforward neural network, also known as a multi-

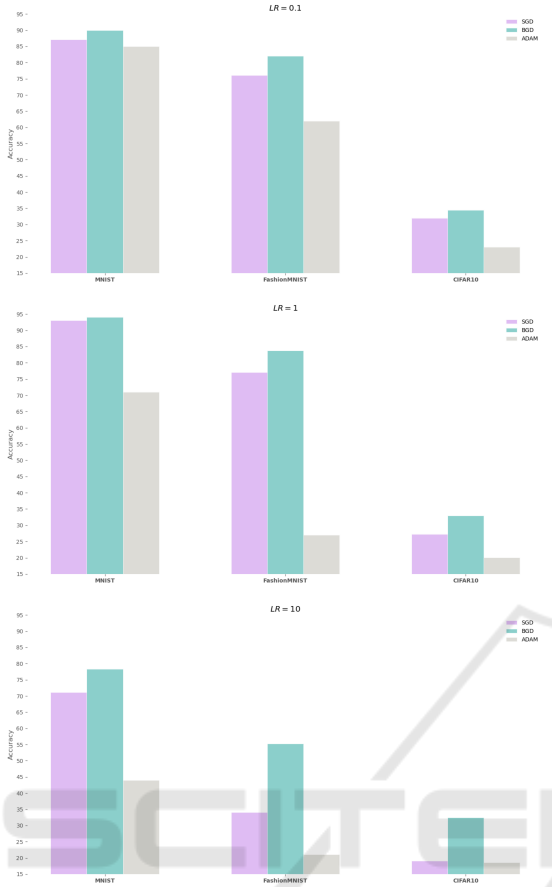


Figure 12: The classification accuracy of the different optimization algorithms evaluated on multiple benchmark classification datasets when using a batch-size of 100.

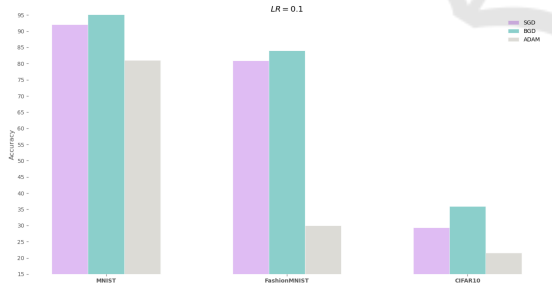


Figure 13: The classification accuracy of the different optimization algorithms evaluated on multiple benchmark classification datasets when using a batch-size of 10.

layer perceptron (MLP). For SGD, the best result between SGD versus SGD with momentum was chosen for SGD's performance evaluation. Each optimizer was run using the same weight initialization, same number of epochs, identical learning rates in each run, and with the proper image normalization for each dataset. Moreover, all the experiments were run for five epochs while using the tanh non-linear activation for the hidden layers of the NN (other activation functions where also used such as ReLU and sigmoid in the Appendix). Firstly, in Figure 11, a batch-size of 1000 was used across different step sizes to demonstrate each algorithms performance when utilizing relatively stable gradients. Secondly, in Figure 12, a batch-size of 100 was used across different step sizes, and finally, in Figure 13, a small batch-size of 10 was used with a relatively small learning rate to demonstrate each algorithms performance when dealing with comparatively high-variance (noisy) gradients. As illustrated in all the Figures, BGD consistently outperforms both GD and ADAM under all settings, and specifically, when a relatively large step size is used, confirming BGD's superiority in utilizing large step sizes. This algorithm shows stable performance in all the different settings shown and proved the usefulness of this algorithm. With better and optimized learning rates this algorithm can be utilized for downstream tasks with improved convegence.

5 CONCLUSION

The primary goal of this paper was to tackle the significantly practical problem of being able to train a generic model that can generalize efficiently by learning predictive knowledge from a limited training dataset, given that the gathered data is not a statistically significant representation of the population data due to selection bias. We introduced the BGD algorithm, a novel and robust gradient-based optimization algorithm aimed at capturing flatter local minima as compared to SGD and its variants for non-convex objective functions. The BGD algorithm is constructed in such a way as to leverage relatively large step sizes to its advantage since the step size restricts the set of local minima that the algorithm can converge to, allowing the optimizer to better explore the loss landscape in search of a flatter set of local minima. BGD also makes use of overshooting oracles, which enable the optimizer to bounce across the loss landscape's basins and avoid as many undesirable sharp local minima as possible in order to eventually settle on a sufficiently flat local minimum, which induces model generalizability. This paper also aims to push for intuitive, unorthodox approaches that utilize large step sizes in weight updates to balance the variance-stability $\sim$ exploration-exploitation tradeoff. Currently, most proposed SGD variants rely heavily on *exploiting* the local information about the loss surface to stabilize training and convergence rather than utilizing the inherent variance advantageously to further *explore* the loss landscape, exposing the opti-

mizer to a broader set of minima in the hopes of attracting a flatter local minimum. The experimentations conducted empirically validate the superiority and consistency of the proposed algorithm over the baseline methods in improving classification accuracy and achieving model generalization. They also reveal the robustness of BGD and demonstrate that it is well-suited to a wide range of non-convex optimization problems in machine learning.

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