On Avoiding Local Minima Using Gradient Descent With Large Learning Rates

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Abstract

It has been widely observed in training of neural networks that when applying gradient descent (GD), a large step size is essential for obtaining superior models. However, the effect of large step sizes on the success of GD is not well understood theoretically. We argue that a complete understanding of the mechanics leading to GD’s success may indeed require considering effects of using a large step size. To support this claim, we prove on a certain class of functions that GD with large step size follows a different trajectory than GD with a small step size, leading to convergence to the global minimum. We also demonstrate the difference in trajectories for small and large learning rates when GD is applied on a neural network, observing effects of an escape from a local minimum with a large step size, which shows this behavior is indeed relevant in practice. Finally, through a novel set of experiments, we show even though stochastic noise is beneficial, it is not enough to explain success of SGD and a large learning rate is essential for obtaining the best performance even in stochastic settings.

1 Introduction

While using variants of gradient descent (GD) has become standard for optimizing neural networks, the reason behind the success of GD is not yet fully understood. One example is the practical observation that using a large learning rate in the initial phase of training is necessary for obtaining well performing models [20]. Though this has been widely observed, most theoretical frameworks only rely on an upper bound to provide a convergence guarantee, suggesting a mismatch between theoretical assumptions and practice. In this paper, we show that when relaxing some of the assumptions, allowing them to not hold globally, the benefits of using a large learning rate become apparent, allowing GD to converge to the global minimum.

More particularly, similar to how gradient descent will diverge with a very large learning rate, using an intermediate value of learning rate can allow gradient descent to escape some sharp local minima through a “controlled divergence”, leading it to more flat areas. Additionally, we show that gradient descent with random initialization can avoid encountering certain (small) regions of the landscape with some probability and that this probability increases with a higher learning rate. Note that this behavior does not happen when using the continuous version of GD, i.e. gradient flow which corresponds to using infinitesimal step sizes. The difference remains even after adding the implicit regularization term identified in [30] in order to bring trajectories of gradient flow and gradient descent closer. Using these two properties, we prove that under certain assumptions, randomly initialized gradient descent with a high learning rate escapes or avoids certain local minima which can lead to convergence to global minimum.

We would like to note that throughout the paper, we sometimes misuse the terms “global” and “local” minimum to refer to desirable and undesirable minima respectively. For example when discussing generalization, a desirable minimum might not have the lowest objective value but enjoy properties such as flatness.

To our knowledge, this is the first theoretical work that builds on a lower bound on the learning rate to show convergence for generic optimization problems to a global minimum without relying on stochastic noise.

We also provide experimental evidence to show the changes in trajectory that we prove happen as a result of using large learning rates, are indeed relevant in practice. In addition to illustrating our
results on a simple function, we demonstrate similar effects happen in neural network training by showing that a high learning rate allows the optimization to escape local minima. Our observations prove the relevance of our theoretical results in practice and signify the importance of considering the effects of high learning rates for understanding the success of GD. This is further supported by evidence also present in the literature, such as results in [3] showing that the sharpness of the trajectory traversed by GD is controlled by the learning rate.

Recent works have shown that induced noise on trajectory can be beneficial for optimization [15, 34, 37]. This is also used as a possible explanation for the success of SGD [27], the stochastic version of GD which is usually used in practice. Since the effect of stochastic noise on the trajectory is controlled by the learning rate, it is reasonable to ask whether, at least in the stochastic settings, this is the main benefit of using a high learning rate. In this paper, we develop a training method that allows maintaining the impact of the stochastic noise while reducing the learning rate. We observe that while this improves the final model, it is not enough to match the superior performance of a high learning rate. Thus, we provide experimental evidence that the effects of learning rate goes beyond controlling stochastic noise, showing that understanding these effects is also relevant in the stochastic settings.

Overall, our contributions can be summarized as follows:

- Theoretically proving the effect of large learning rates in allowing GD to converge to different minima under certain assumptions.
- Demonstrating gradient descent escapes from local minima in neural network training when using a large learning rate, showing the relevance of our theoretical results in practice.
- Providing experimental evidence that the effect of learning rate in SGD goes beyond stochastic noise, showing the importance of considering the effects of large learning rate even in stochastic settings.

2 Related Work

Extensive literature exists on studying the effect of stochastic noise on the convergence of GD. Several works have focused on the smoothing effect of injected noise [2, 15, 24, 34]. In [33] it has been shown that by perturbing the parameters at every step (called perturbed GD) it is possible to converge to the minimum of a function $f$ while receiving gradients of $f + g$, assuming certain bounds on $g$. Other works use different models for the stochastic noise in SGD and use it to obtain convergence bounds or to show SGD prefers certain type (usually flat) of minima [36, 37]. In order to better understand the effect of various hyperparameters on convergence, Jastrzębski et al. [12, 13] show the learning rate (and its ratio to batch size) plays an important role in determining the minima found by SGD. In [25] it was shown that SGD has an implicit bias in comparison with gradient flow and its magnitude depends on the learning rate. While this shows one benefit of using large learning rates, in this work, we provide evidence that the effect of learning rate on optimization goes beyond controlling the amount of induced stochastic noise.

Prior work also experimentally establish existence of different phases during training of a neural network. Cohen et al. [3] show that initially Hessian eigenvalues tend to grow until reaching the convergence threshold for the used learning rate. This growth is also reported in [18] for the maximum eigenvalue of the Neural Tangent Kernel [11] where it has also been observed that this value decreases later in training, leading to convergence. These observations suggest that gradient descent with a large learning rate follow a different trajectory than one with a small learning rate. Therefore, the conjecture in [6] that gradient descent and gradient flow have close trajectories might not hold for general networks. The difference in trajectory is also supported by the practical observation that a large learning rate leads to a better model [20]. Comparing gradient flow and gradient descent, Barrett and Dherin [1] identify an implicit regularization term on gradient norm induced by using discrete steps. Still, this term is not enough to remove a local minimum from the landscape. Other implicit regularization terms specific to various problems have also been proposed in the literature [22, 26, 35]. In this paper, we provide experimental evidence and showcase the benefits of using
large step sizes that are unlikely to be representable through a regularization term, suggesting that considering discrete steps might be necessary to understand the success of GD.

The type of obstacles encountered during optimization of a neural network is a long-standing question in the literature. Lee et al. [17] show that gradient descent with random initialization almost surely avoids saddle points. However it is still unclear whether local minima are encountered during training. In [7] it was observed that the loss decreases monotonically over the line between the initialization and the final convergence points. This observation was shown not to hold when using larger learning rates [21]. Swirszcz et al. [31] also show that it is possible to create datasets which lead to a landscape containing local minima. Furthermore, better visualization of the landscape shows non-convexities can be observed on some loss functions [19]. For the concrete case of two layer ReLU networks, Safran and Shamir [28] show gradient descent converges to local minima quite often without the help of over-parameterization. Also, it was shown that in the over-parameterized setting, the network is not locally convex around any differentiable global minimum and one-point strong convexity only holds in most but not all directions [29]. We use these observations to make assumptions that are practically justifiable.

There also exists a body of work on which properties of a minimum leads to better generalization [4, 5, 14, 32]. In this work, our goal is to show the ability of gradient descent to avoid certain minima when using a high learning rate. However, we do not argue about whether these minima offer better or worse generalization.

3 Main Results

Let us focus on optimizing the minimization problem

$$f_\star := \min_{x \in \mathbb{R}^d} f(x)$$

using (full-batch) gradient descent with random initialization. For completeness, we provide a pseudo code in the Appendix A, Algorithm 1.

As is done widely in the literature, we assume $f$ is $L_{\text{global}}$-smooth where smoothness is defined in Definition 1.

**Definition 1** ($L$-smoothness). A function $f: \mathbb{R}^d \to \mathbb{R}$ is $L$-smooth if it is differentiable and there exists a constant $L > 0$ such that:

$$\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\|, \quad \forall x, y \in \mathbb{R}^d.$$  \hspace{1cm} (1)

The following definition also commonly appears in the literature:

**Definition 2** ($\mu$-one-point-strongly-convex (OPSC) with respect to $x_\star$ over $M$). A function $f: \mathbb{R}^d \to \mathbb{R}$ is one-point strongly convex with respect to $x_\star$ if it is differentiable and there exists a constant $\mu > 0$ such that:

$$\langle \nabla f(x), x - x_\star \rangle \geq \mu \|x - x_\star\|^2, \quad \forall x \in M.$$  \hspace{1cm} (2)

If $M$ is not explicitly stated, the definition for $M = \mathbb{R}^d$ is used.

Assuming OPSC property is common in the literature and has been shown to guarantee convergence to $x_\star$ [15, 17, 29]. More importantly, recent works have verified both theoretically and empirically that landscapes of neural networks satisfy this property to some extent [15, 29]. For example, Safran et al. [29] show that the condition is satisfied with high probability over the trajectory of perturbed gradient descent on over-parameterized two-layer ReLU networks when initialized in a neighborhood of a global minimum. We also note that there exists other variants of this definition such as quasi-strong convexity [23] or $(1, \mu)$-(strong) quasar convexity [9], which are similar but slightly stronger. In this paper, we only need OPSC property to hold locally around a local minimum to obtain our results.
3.1 Avoiding Regions in Landscape

Various assumptions have been considered in the literature to study the convergence of GD. However, these conditions may not hold globally. In this section, we provide results that show that when using random initialization, for an arbitrary (but small) region of the landscape (e.g. finite number of points), there is a (high) chance that GD will not encounter that region. Therefore, even if a property needed for establishing convergence holds almost globally but not everywhere, it might still be enough to show convergence.

Figure 1 provides an example of this phenomenon. We will discuss this in more details in Section 3.3 and proceed by stating this formally as the following theorem:

**Theorem 1.** Assume gradient descent is initialized randomly on the set $W$ and is run with learning rate $\gamma \leq \frac{1}{2L}$. Let $X \subseteq R^d$ be the set of points that should not be encountered by GD and assume $f$ is $L$-smooth over $R^d \setminus X$. Let $L(S)$ denote the Lebesgue measure of any set $S$. The probability of encountering any points of $X$ in the first $T$ steps of gradient descent, i.e. $x_t \in X$ for some $1 \leq t \leq T$ is at most $2^{(T+1)-d} \cdot \frac{L(X)}{L(W)}$.

We provide the complete proof in Appendix B. Note that while the bound grows exponentially with $T$, it is possible to obtain better bounds in various cases. We provide the following corollaries as examples.

**Corollary 1.** Let $f$ be $L$ smooth. If $X$ is a set with $L(X) = 0$, for example when it is a finite set of points, the probability of encountering $X$ throughout training with gradient descent using $\gamma \leq \frac{1}{2L}$ and random initialization over a set $W$ with $L(W) > 0$ is 0.

The corollary directly follows from Theorem 1. We use this corollary in proving Theorem 2 to avoid cases where we directly land on a minimum with $\nabla f(x) = 0$.

When there is additional guarantee on the speed of convergence, it is also possible to improve on the bound provided by Theorem 1. The reason is that if the algorithm is guaranteed to get closer to somewhere in the landscape (such as a global minimum) than any point on the set $X$ after a number of steps $T_1$, it is only necessary to compute the probability of avoiding $X$ in the first $T_1$ steps. Such guarantee for example can be obtained by assuming $f$ is one-point strongly convex over $R^d \setminus X$ towards some minimum $x_\star$, as defined in Definition 2, leading to the following corollary.

**Corollary 2.** Let $f$ be $L$-smooth and $\mu_\star$-OPSC with respect to a minima $x_\star$ over $R^d \setminus X$. Define $c_X := \inf \{ \|x - x_\star\| \mid x \in X\}$ and $r_W := \sup \{ \|x - x_\star\| \mid x \in W\}$. The probability of encountering any points of $X$ during running gradient descent with $\gamma \leq \frac{c_X}{2L}$ is upper bounded by $2^{1-\frac{c_X}{2L} + \log_2 \left( \frac{r_W}{2L} \right)} \cdot \frac{L(X)}{L(W)}$ when $c_X \leq r_W$ and is zero otherwise.

We provide the proof in Appendix C. Note that in this setting, GD has a higher probability of avoiding parts of the landscape that are closer to the point of initialization. As learning rate controls
the speed of convergence, increasing it lowers the probability of encountering these parts. This establishes one example of how a large learning rate can help avoiding local minima and change the trajectory of optimization.

3.2 Escaping Sharp Regions in Landscape

Theorem 1 shows GD is able to completely avoid parts of the landscape. However, the probability of avoiding a region depends exponentially on $T$ and therefore it may become more likely to fall into local minima as the training progresses. We now show a different effect of high learning rate that does not depend on $T$ and holds deterministically. More particularly, we show GD becomes resilient to falling into some sharp minima by using a large learning rate in Theorem 2. We first state an informal version of the theorem:

**Theorem 2 (Informal).** Let $M$ be a region around a local minimum where the gradients point sharply toward the minimum. Assume there exists a large enough region around $M$ which is much more smooth (less sharp) than $M$ and where gradients point toward a different (global) minimum. If $M$ is far enough from this global minimum, when the learning rate is chosen large enough, GD will either not encounter $M$ or get closer to the global minimum than any point in $M$.

Note that the theorem allows for multiple local minima to exist on the landscape and only applies constraints around each local minimum. Furthermore, we point out that the theorem only ensures that GD will exit the local minima after some steps. In order to obtain convergence guarantees to the global minimum, it is necessary to assume a convergence property on the rest of the landscape as well. We mention an example in a corollary later in this section. To build further intuition, Figure 2 provides an example of how GD with large learning rate may escape a sharp minimum. We now state the formal version of this theorem:

**Theorem 2 (Formal).** Let $f$ be a function that is $L_{\text{global}}$-smooth and consider running GD with learning rate $\gamma$ randomly initialized over a set $W$ with $\mathcal{L}(W) > 0$. Let $M$ be a set with diameter $r$, containing a local minimum $x^\dagger$ and define $P(M) := \{x \notin M \mid \|x - x^\dagger\|_2 \leq r \sqrt{\gamma^2 L_{\text{global}}^2 - 3}\}$ to be the set surrounding $M$. Assume $f$ is $L < L_{\text{global}}$-smooth and $\mu_\star$-OPSC over $P(M)$ with respect to a (global) minimum $x_\star$ that is sufficiently far from $M$, formally, $\|x_\star - x^\dagger\|_2 \geq r \cdot \frac{\gamma \sqrt{\gamma^2 L_{\text{global}}^2 - 3}(1 - \gamma \mu_\star)}{1 - \frac{\gamma \mu_\star}{\mu_\star}}$. Finally, assume $f$ is $\mu^\dagger$-OPSC with respect to $x^\dagger$ over $M$ where $\mu^\dagger > \frac{2L^2}{\mu_\star}$. Then, using a suitable learning rate $\frac{\mu_\star}{\mu^\dagger} < \gamma \leq \frac{\mu_\star}{\mu^\dagger}$, if GD reaches a point $M$, it will escape $M$ and reach a point with distance to $x_\star$ of less than $\|x^\dagger - x_\star\| - r$ almost surely.

Figure 4 provides an illustration of different regions defined in Theorem 2. We provide a complete proof in Appendix D and proceed by discussing some of our assumptions:
OPSC condition inside $M$ We assume $f$ is OPSC with respect to a different minima inside $M$ in order to ensure GD will escape from $M$. However, other conditions might also ensure the same effect. The theorem would also hold with those assumptions. Note that the sharpness of $M$ with respect to the rest of landscape is reflected through the lower bound on $\mu^*$ and is necessary so we can set the learning rate in the given range. As an example, when $f$ is a quadratic function everywhere except $M$ (such as in Figure 4), we have $\mu^* = L$ and the lower bound becomes $\mu^* > 2L$.

OPSC condition around $M$ We already justified the assumption on one-point strong convexity of $f$ towards a global minimum at the beginning of Section 3, both from a theoretical and practical point of view. Here, we combine this assumption with the assumption on $M$ not being very close to the global minimum, in order to ensure that once GD escapes from a local minima, the gradient points strongly towards $x^*$. This ensures that GD will reach a point closer to the global minimum after escaping $M$. While this assumption is not necessary to show GD will never converge to $M$, an assumption on distance might be necessary to show GD will not return to $M$. For example, consider a quadratic function where the region around minimum is replaced by a sharper quadratic function, as plotted in Figure 3. In this case, GD with a high learning rate will keep returning to $M$ though it will never converge to it. Still, it is possible to relax this assumption. For example, one can assume GD converges in at most a fixed number of steps (which Corollary 1 states can not be to any point in $M$ almost surely) or assume directly that the gradient points strongly away from $M$. Finding similar assumptions is grounds for future work.

Similar to our results in Section 3.1, using Theorem 2, it is possible to ignore existence of the set $M$ in the landscape. Therefore, if GD satisfies convergence conditions everywhere else, it will still converge to the global minimum. One example of such settings is the following corollary:

**Corollary 3.** If $f$ is $L$-smooth and $\mu^*$-OPSC with respect to $x^*$ over $\mathbb{R}^d \setminus M$ (instead of only on $P(M)$) where $M$ satisfies the conditions in Theorem 2, GD with random initialization over a set $W$ with $\mathcal{L}(W) > 0$ will converge to $x^*$ almost surely.

We emphasize that, to the best of our knowledge, this is the first result to theoretically prove a large learning rate is necessary to converge to global minima on a class of non-convex functions. Together with Theorem 1, our results allow proving convergence of GD to global minimum on functions where previously known conditions for convergence of GD such as OPSC might not hold in some parts of the landscape. We demonstrate both of these effects in practice for a toy example in our experiments in Section 3.3.
3.3 Toy Example

In order to demonstrate the effects discussed in Section 3, we experiment with running GD over a simple function. The landscape of this function is plotted in Figure 5a and its formula is presented in Appendix E. The function has two minima, one near the initialization and one further away. Since the near-init minimum is almost completely flat, i.e. gradient is constant and equal to zero (except for the edges which are extremely sharp lines in order to ensure the function remains continuous), if GD reaches a point in this region, it will remain there. However, as this region is very close to the initialization, Theorem 1 (more particularly Corollary 2) suggests that GD with large enough learning rate, will probably not reach any points in this region. To demonstrate this more clearly, we plot the trajectory of GD from several initialization points in Figure 1. It is worth noting that even with large learning rate it is possible for GD to get stuck in this region while it is possible to avoid this region even with a small learning rate. However, as suggested by our theoretical upper bound, the probability of this phenomenon increases with the learning rate.

The other minimum is much sharper than the rest of the function and therefore we can expect an escaping behavior similar to the one described by Theorem 2. This behavior is demonstrated in Figure 2. Note that unlike the previous case, GD with large learning rate always (except when landing directly at the minimum) escapes the sharp minimum while GD with small learning rate converges.

We measure rate of convergence of GD for 100 different random initialization to each of these three regions for different learning rates. The results are plotted in Figure 5b. We observe that as the learning increases, the rate of avoiding the near initialization minimum increases. While the learning rate is not still high enough, GD will converge to the sharp minimum while as the learning rate increases further, it is also able to escape the sharp minimum and converge to the global minimum. This behavior is completely compatible with what can be expected based on the results and effects discussed in Section 3.

4 Experiments

We now provide practical evidence to show the effects of high learning rate also apply and are essential in optimization of neural networks. In our experiments we train a ResNet-18 [8] on CIFAR10 [16] dataset. We disable all batch normalization layers [10] in order to avoid any confounding effects. We apply 0.0005 weight decay, 0.9 momentum, and decay the learning rate at epochs 80, 120, and 160 by 0.1.
4.1 Disentangling Effects of Stochastic Noise and Learning Rate

While previous work already established the necessity of using high learning rates for obtaining superior models using SGD, it is not clear if this dependency is only because the learning rate is controlling the impact of stochastic noise on the optimization trajectory. We answer this question through the following experiment.

**SGD with Repeats**  In order to simulate the same magnitude of noise while still using a smaller learning rate, every time a mini-batch is drawn, we use it for \( k \) steps before drawing another mini-batch. Note that when \( k = 1 \), we recover standard SGD. Re-using the same batch \( k \) times, allows the bias of the mini-batch to be amplified \( k \) times, so when reducing learning rate by \( \frac{1}{k} \) the overall magnitude remains unchanged.

We compare standard SGD with learning rate 0.01, standard SGD with learning rate 0.001, and SGD with \( k = 10 \) and learning rate 0.001. When training with standard SGD and learning rate 0.001 we train the model for 10 times more epochs (2000 epochs) in order to obtain a fair comparison and rescale its plot to 200 epochs. Furthermore, when we have \( k > 1 \) we train the model for 10 more epochs at the end and use each batch only once (as in standard SGD) during the additional epochs. We perform these additional steps since training for several steps on one batch at the end of training might lead to overfitting on that batch which is not desirable for test performance. In Appendix F we also experiment with turning off repeats earlier in the training and observe no significant improvement. Finally, we ensure that the experiment with \( k = 10 \) uses the same initialization point and the same ordering of batches used for training with learning rate 0.01.

The results (averaged over 3 runs) are plotted in Figure 6. The first clear observation is that SGD with learning rate 0.01 leads to a much better model than SGD with learning rate 0.001. More importantly, while amplifying the noise through repeats helps lower the gap, it still has a performance below training with the large learning rate.

Explaining the positive effect of using SGD over GD on convergence has been the focus of several prior work. For example, Kleinberg et al. [15] argue that applying SGD allows optimization to be done over a smoothed version of the function which empirically satisfies good convergence properties, particularly, one-point strong convexity toward a minimum. We argue that our observation provides a more complete overview and suggests that even after applying stochastic noise (which for example can lead to a smoothing of the function), there might be certain regions of the landscape that can only be avoided using a high learning rate. As we described above, one can consider the effect of stochastic noise to be the improvement observed when using repeats with a small learning rate in comparison with training in a standard way which still does not close the gap with training using a high learning rate. Therefore, the effects of using a high learning rate, such as those described in Section 3, are still important in determining the optimization trajectory even in the presence of stochastic noise.

4.2 Comparing Trajectories of Large and Small Learning Rates

In Section 3, we showed some of the effects of using large step sizes in avoiding or escaping certain minima in the landscape and demonstrated it on a toy problem in Section 3.3. We now demonstrate that these effects of using large learning can be observed in real world applications such as training neural networks. To be able to observe the effect of large learning rate more clearly, we first warm-start the optimization by running SGD with a small learning rate 0.001 with \( k = 10 \) repeats (as described in Section 4.1) for 20 epochs to obtain parameters \( \mathbf{x}_{\text{warm}} \). We do this to get near a minimum that would be found when using the small learning rate. Then, we start full-batch GD from \( \mathbf{x}_{\text{warm}} \) with two different learning rate 0.001 (small) and 0.01 (large). Similar to [19], we obtain the first two principal components of the vectors \( \mathbf{x}_1 - \mathbf{x}_0, \mathbf{x}_2 - \mathbf{x}_0, \ldots, \mathbf{x}_t - \mathbf{x}_0 \) and plot the trajectory along these two directions in Figure 7. We can clearly observe that GD with a large learning rate changes path and moves toward a different place in the landscape. GD continues on the different path even when the learning rate is reduced back to 0.001 after 400 steps. Furthermore, looking at the loss values, we can observe a peak at the beginning of training that closely resembles what we expect to observe
Figure 6: Comparison between performance of SGD with different learning rates. The gap in performance between large and small learning rates, even after repeatedly using the same batch to maintain the effect of stochastic noise, suggests that learning rate has an effect on trajectory beyond controlling stochastic noise. Repeating batches is turned off at epoch 200 and 10 additional epochs are performed (green). For the experiment with 2000 epochs (orange), the plot is normalized to 200 epochs.

(a) Trajectory of (full-batch) GD with small and large learning rate.

(b) The value of train loss when using different values of learning rate.

Figure 7: Behavior of GD for learning rates 0.001 (small) and 0.01 (large). The initialization is obtained by warm-starting the network using SGD with a small learning rate 0.001. Using a large learning rate changes the trajectory sharply and even if the learning rate is reduced again after several steps (blue line) we move toward a different direction in the landscape. This is accompanied by a sharp increase of loss at the beginning that can be attributed to GD escaping from a local sharp region in the landscape.

when GD is escaping from a local sharp region. This clearly shows that these behaviors of GD are not merely theoretical and are also relevant in real world applications.

Note that while we do not observe similar high spikes in the loss in the next steps, we conjecture that this behavior of escaping sharp regions is constantly happening throughout training. This is also confirmed by observations in [3] which show sharpness increases throughout training until reaching a threshold which depends on the inverse of the learning rate. Hence, with a smaller learning rate, GD traverses through sharper regions. However, the mechanics of avoiding sharp regions is not clear since symptoms of an escape such as a spike in loss is not observed. While we observe smaller increases in the loss, these can be due to oscillations also observed in [3] along the highest eigenvectors. However, results in the same work show that in these cases the parameters do not move in these directions and only oscillate around the same center. Developing better visualization techniques or identifying other effects of using a high learning rate on GD’s trajectory can help explain this behavior further and both of these directions are ground for future work.
5 Future Work

Obtaining further insight on how GD avoids locally sharp regions, for example by developing better methods for visualization of the landscape and trajectory, is grounds for future work. Furthermore, there are various extensions possible on the theoretical results obtained in this paper. For example, it might be possible to show other effects of using a large learning rate on trajectory or other settings where a minima can be avoided. It might also be possible to relax some of the assumptions. For example, while our results also cover functions with several local minima, these minima need to be spaced far from each other. Removing this restriction would also be an interesting direction of research.

6 Conclusion

In this paper, we highlight that a high learning rate can provably lead to avoiding or escaping local minima and reaching a global minimum. Based on this result, we argue that analyzing GD with infinitesimally small learning rate is not sufficient to understand its success unlike what was suggested in prior work [6]. Furthermore, by designing a method to amplify stochastic noise without increasing the learning rate, we disentangle the effects of stochastic noise and high learning rates. We observe that while a higher stochastic noise leads to a better model, it is not enough to close the gap with the model obtained using a high learning rate. Therefore, we argue that the effect of learning rate goes beyond controlling the impact of stochastic noise even in SGD. In contrast, recent works on analyzing success of SGD focus on continuous settings [37] and only take step size into account when modeling the noise [25]. We hope that our results will encourage future work on large step size regime. Finally, we demonstrate that the escape from sharp regions can happen in training of neural networks, hence signifying the relevance of the effects of large learning rate in real world applications.
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A Gradient Descent with Random Initialization

Algorithm 1 Gradient Descent with Random Initialization

1: Pick $x_0$ randomly from the set $W$.
2: for $t = 1 \ldots T$ do
3: \hspace{1em} $x_t \leftarrow x_{t-1} - \gamma \nabla f(x_{t-1})$
4: end for

B Proof of Theorem 1

Theorem. Assume gradient descent is initialized randomly on the set $W$ and is run with learning rate $\gamma \leq \frac{1}{2L}$. Let $X \subseteq \mathbb{R}^d$ be the set of points that should not be encountered by GD and assume $f$ is $L$-smooth over $\mathbb{R}^d \setminus X$. Let $\mathcal{L}(S)$ denote the Lebesgue measure of any set $S$. The probability of encountering any points of $X$ in the first $T$ steps of gradient descent, i.e., $x_i \in X$ for some $1 \leq i \leq T$ is at most $2^{T+1} \cdot \frac{L(X)}{L(W)}$.

Proof. Define $g(x) := x - \gamma \nabla f(x)$. When $\gamma < \frac{1}{2L}$, since $f$ is $L$-smooth over $\mathcal{D}_g := \mathbb{R}^d \setminus X$, results of Lee et al. [17] show $g(x)$ is a diffeomorphism over $\mathcal{D}_g$. As a result, the function $g^T$ obtained by applying $g$ for $T$ times is also a diffeomorphism over the set

$$\mathcal{D}_{g^T} := \mathbb{R}^d \setminus (X \cup g^{-1}(X) \cup \ldots \cup (g^{T-1})^{-1}(X)).$$

According to the change of variable formula for Lebesgue measure (for example, see [38, Eq. (3.7.2)]), for any measurable set $Y \subset \mathcal{D}_{g^T}$

$$\mathcal{L}(g^T(Y)) = \int_Y |\det \nabla g^T(y)| dy.$$

Since $\gamma \leq \frac{1}{2L}$, we have for any $y \in \mathcal{D}_g$,

$$|\det \nabla g(y)| = |\det(I - \gamma \nabla^2 f(y))| \geq 2^{-d}.$$

The last equality holds because smoothness ensures all eigenvalues of $\nabla^2 f(x)$ are at most $L$. So for any eigenvalue $\lambda_i$, $1 - \gamma \lambda_i \geq \frac{1}{2}$. Using this result, we also can obtain $|\det \nabla g^T(y)| \geq 2^{-Td}$ for any $y \in \mathcal{D}_{g^T}$. Thus, we have

$$\mathcal{L}(g^T(Y)) \geq 2^{-Td} \mathcal{L}(Y),$$

which means,

$$\mathcal{L}((g^T)^{-1}(X) \cap \mathcal{D}_{g^T}) \leq 2^{Td} \mathcal{L}(X).$$

Note that while the above argument works for $T \geq 1$, the former inequality also trivially holds for
\[ T = 0. \text{ Hence} \]

\[
\mathcal{L}(\cup_{t=0}^{T}((g^t)^{-1}(X) \cap W)) \leq \mathcal{L}(\cup_{t=0}^{T}(g^t)^{-1}(X))
\]

\[
= \mathcal{L}(\cup_{t=0}^{T}((g^t)^{-1}(X) \cap D_{g^t}))
\]

\[
\leq \sum_{t=0}^{T} \mathcal{L}((g^t)^{-1}(X) \cap D_{g^t})
\]

\[
\leq \sum_{t=0}^{T} 2^{td} \mathcal{L}(X)
\]

\[
\leq \mathcal{L}(X) \left( \sum_{t=0}^{T} 2^{td} \right)
\]

\[
\leq 2^{(T+1)d} \mathcal{L}(X),
\]

where in the last inequality we used \(2^0 + 2^1 + \ldots + 2^T < 2^{T+1}.\) The theorem follows directly from this result. \( \square \)

### C Proof of Corollary 2

**Corollary.** Let \( f \) be \( L \)-smooth and \( \mu_* \)-OPSC with respect to a minima \( x_* \) over \( \mathbb{R}^d \setminus X. \) Define \( c_X := \inf \{ \|x - x_*\| \mid x \in X \} \) and \( r_W := \sup \{ \|x - x_*\| \mid x \in W \}. \) The probability of encountering any points of \( X \) during running gradient descent with \( \gamma \leq \frac{\mu_*}{L^2} \) is upper bounded by \( 2^d \cdot \frac{r_W - 2 \mu_1 (1 - \gamma \mu_*)}{c_X} \cdot \frac{\mathcal{L}(X)}{\mathcal{L}(W)} \) when \( c_X \leq r_W \) and is zero otherwise.

**Proof.** Due to \( \mu_* \)-OPSC property of the landscape over \( \mathbb{R}^d \setminus X, \) as long as \( x_t \notin X, \) we have

\[
\|x_{t+1} - x_*\|^2_2 = \|x_t - \gamma \nabla f(x_t) - x_*\|^2_2
\]

\[
= \|x_t - x_*\|^2_2 - 2\gamma \langle \nabla f(x_t), x_t - x_* \rangle + \gamma^2 \|\nabla f(x_t)\|^2_2
\]

\[
\leq (1 - 2\gamma \mu_* + \gamma^2 L^2)\|x_t - x_*\|^2_2
\]

\[
\leq (1 - \gamma (2\mu_* - \gamma L^2))\|x_t - x_*\|^2_2
\]

\[
\leq (1 - \gamma \mu_*)\|x_t - x_*\|^2_2,
\]

where the last inequality holds because \( \gamma \leq \frac{\mu_*}{L^2}. \) Hence, if \( x_t \notin X \) for \( t \in [T - 1], \) we have

\[
\|x_T - x_*\|^2_2 \leq (1 - \gamma \mu_*)^T\|x_1 - x_*\|^2_2
\]

\[
\leq (1 - \gamma \mu_*)^T r_W.
\]

Let \( T_0 := \frac{\log_2 \frac{r_W}{c_X}}{\log_2 (1 - \gamma \mu_*)}. \) For \( T > T_0, \) we have

\[
\|x_T - x_*\|^2_2 \leq (1 - \gamma \mu_*)c_X < c_X,
\]

which means \( x_T \notin X. \) Therefore, if GD does not reach any point in \( X \) in the first \( T_0 \) steps, it will not reach any point in \( X \) afterwards neither. Therefore, the probability of encountering any point in \( X \) is the same as the probability of encountering such points in the first \( T_0 \) steps. According to Theorem 1, this value is bounded as:

\[
2^{(T_0+1)d} \cdot \frac{\mathcal{L}(X)}{\mathcal{L}(W)} = 2^d \cdot \frac{c_X}{r_W} \frac{d}{\log_2 (1 - \gamma \mu_*)} \cdot \frac{\mathcal{L}(X)}{\mathcal{L}(W)}
\]

\[
= 2^d \cdot \frac{r_W - \frac{d}{\log_2 (1 - \gamma \mu_*)}}{c_X} \cdot \frac{\mathcal{L}(X)}{\mathcal{L}(W)}.
\]
D Proof of Theorem 2

Theorem. Let $f$ be a function that is $L_{global}$-smooth and consider running GD with learning rate $\gamma$ randomly initialized over a set $W$ with $\mathcal{L}(W) > 0$. Let $M$ be a set with diameter $r$, containing a local minimum $x^t$ and define $P(M) := \{x \notin M \mid \|x - x^t\|_2 \leq r \sqrt{\gamma^2L^2_{global} - 3}\}$ to be the set surrounding $M$. Assume $f$ is $L < L_{global}$-smooth and $\mu*$-OPSC over $P(M)$ with respect to a (global) minimum $x_*$ that is sufficiently far from $M$, formally, $\|x_* - x^t\|_2 \geq r \cdot \frac{1 + \sqrt{(\gamma^2L^2_{global} - 3)\left(1 - \gamma\mu_*\right)}}{1 - \sqrt{1 - \gamma\mu_*}}$. Finally, assume $f$ is $\mu^*$-OPSC with respect to $x^t$ over $M$ where $\mu^* > \frac{2L^2}{\mu_*}$. Then, using a suitable learning rate $\frac{2}{\mu^*} < \gamma \leq \frac{\mu_*}{\mu}$, if GD reaches a point $M$, it will escape $M$ and reach a point with distance to $x_*$ of less than $\|x^t - x_*\| - r$ almost surely.

Proof. Let $t$ be the smallest step where $x_t \in M$. Using Corollary 1, $x_t \neq x^t$ almost surely. Therefore $\|x_t - x^t\| > 0$. Since $\gamma > \frac{2}{\mu^*}$, we have

$$
\|x_{t+1} - x^t\|_2^2 = \|x_t - \gamma \nabla f(x_t) - x^t\|_2^2 \\
= \|x_t - x^t\|_2^2 - 2\gamma \langle \nabla f(x_t), x_t - x^t \rangle + \gamma^2 \|\nabla f(x_t)\|_2^2 \\
\geq \|x_t - x^t\|_2^2 - 2\gamma \|\nabla f(x_t)\|_2 \|x_t - x^t\|_2 + \gamma^2 \|\nabla f(x_t)\|_2^2 \\
= \|x_t - x^t\|_2^2 + \gamma \|\nabla f(x_t)\|_2 \|\nabla f(x_t)\|_2 \|x_t - x^t\|_2 - 2\|x_t - x^t\|_2^2 \\
\geq \|x_t - x^t\|_2^2 + \gamma \|\nabla f(x_t)\|_2 \|x_t - x^t\|_2 - 2\|x_t - x^t\|_2^2 \\
\geq \|x_t - x^t\|_2^2 + \gamma \mu_* \|x_t - x^t\|_2 - 2\|x_t - x^t\|_2^2 \\
\geq (2\gamma\mu_* - 3)\|x_t - x^t\|_2^2.
$$

Therefore, the distance to $x^t$ grows at least with the rate $2\gamma\mu_* - 3 > 0$. Hence, GD is guaranteed to reach a point $x_{t+k}$ outside $M$ for some $k > 0$. If $\|x_{t+k} - x_*\| \leq \|x^t - x_*\| - r$, we are done. Otherwise, we verify that this condition holds for $x_{t+k+1}$.

First note that

$$
\|x_{t+k+1} - x^t\|_2^2 = \|x_{t+k-1} - \gamma \nabla f(x_{t+k-1}) - x^t\|_2^2 \\
= \|x_{t+k-1} - x^t\|_2^2 - 2\gamma \langle \nabla f(x_{t+k-1}), x_{t+k-1} - x^t \rangle + \gamma^2 \|\nabla f(x_{t+k-1})\|_2^2 \\
\leq \|x_{t+k-1} - x^t\|_2^2 + \gamma^2 \|\nabla f(x_{t+k-1})\|_2^2 \\
\leq r^2(1 - 2\gamma\mu_* + \gamma^2L^2_{global}) \\
\leq r^2(\gamma^2L^2_{global} - 3),
$$

where the last inequality holds because $\gamma > \frac{2}{\mu^*}$.

$$
\|x_{t+k+1} - x_*\|_2^2 = \|x_{t+k} - \gamma \nabla f(x_{t+k}) - x_*\|_2^2 \\
= \|x_{t+k} - x_*\|_2^2 - 2\gamma \langle \nabla f(x_{t+k}), x_{t+k} - x_* \rangle + \gamma^2 \|\nabla f(x_{t+k})\|_2^2 \\
\leq \|x_{t+k} - x_*\|_2^2 - 2\gamma\mu_* + \gamma^2L^2 \\
\leq \|x_{t+k} - x_*\|_2^2(1 - \gamma\mu_*),
$$

where in the last inequality we used $\gamma \leq \frac{\mu_*}{\mu^*}$. We can now write

$$
\|x_{t+k+1} - x_*\|_2 \leq \left(\|x^t - x_*\|_2 + \|x_{t+k} - x^t\|_2\right)\sqrt{1 - \gamma\mu_*} \\
\leq \left(\|x^t - x_*\|_2 + r\sqrt{\gamma^2L^2_{global} - 3}\right)\sqrt{1 - \gamma\mu_*}.
$$
Given the lower bound on distance $\|x^\dagger - x^*_\|$ we have

$$r(\sqrt{(\gamma^2 L_{\text{global}}^2 - 3)(1 - \gamma \mu^*_\star)} + 1) \leq \|x^\dagger - x^*_\|_2(1 - \sqrt{1 - \gamma \mu^*_\star}).$$

This yields

$$\|x_{t+\delta+1} - x^*_\|_2 \leq \|x^\dagger - x^*_\|_2 - r,$$

completing the proof.

**E Function for Toy Example**

$$f(x) := \begin{cases} 
-1600(x - 2.5)^5 - 2000(x - 2.5)^4 + 800(x - 2.5)^3 + 1020(x - 2.5)^2 & 2 \leq x \leq 3, \\
1411.2 \times (1 - 10^4(x - 8.4)) & 8.4 \leq x \leq 8.40001, \\
0 & 8.40001 \leq x \leq 8.59999, \\
1479.2 \times (10^4(x - 8.6) + 1) & 8.59999 \leq x \leq 8.6, \\
20x^2 & \text{otherwise}. 
\end{cases}$$

**F Results of Stopping Repeats from Different Epochs**

In Section 4.1, we explained that at the end of training we stop using the same batch for $k$ steps and train in the standard way (each batch used just once) for additional 10 epochs. This was done to make sure the model that is used to obtain the accuracy on the test data is not overfitted on one batch which might be more likely to happen at the end of the training. In this section, we also experiment with stopping repeats, i.e. using the same batch for $k$ steps, earlier in the training. The result is plotted in Figure 8. No significant improvement is observed.

![Figure 8: Plot of test accuracy when we stop using the same batch several times (doing repeats) at different epochs. It can be clearly observed that the stopping epoch does not affect the final accuracy and the gap with the case of GD with a large learning rate can be clearly observed.](image)

**G Experiments on CIFAR100**

In order to make sure our results extend to other scenarios, we repeat the experiments in Section 4.1 on CIFAR100 and observe a similar behavior. The accuracy on the train and test datasets during training are plotted in Figure 9.
Figure 9: Comparison between performance of SGD with different learning rates on CIFAR100. Repeating batches is turned off at epoch 200 and 10 additional epochs are performed (green). For the experiment with 2000 epochs (orange), the plot is normalized to 200 epochs. For more explanations refer to Figure 6 and Section 4.1.

Additional References

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