ON THE ORIGIN OF IMPLICIT REGULARIZATION IN STOCHASTIC GRADIENT DESCENT

Anonymous authors
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ABSTRACT

In the limit of vanishing learning rates, stochastic gradient descent (SGD) follows the path of gradient flow on the full batch loss function. However larger learning rates often achieve higher test accuracies, and this generalization benefit is not explained by convergence bounds, since it arises even for large compute budgets. To help interpret this phenomenon we prove that, for small but finite learning rates, the SGD iterates still stay close to the path of gradient flow *but on a modified loss*. This modified loss is composed of the full batch loss function and an implicit regularizer, which penalizes the mean euclidean norms of the minibatch gradients. Under reasonable assumptions, when the batch size is small, the scale of the implicit regularization term is proportional to the ratio of the learning rate to the batch size. We verify empirically that explicitly including the implicit regularizer in the loss function can enhance the test accuracy when the learning rate is small.

1 INTRODUCTION

In the limit of vanishing learning rates, stochastic gradient descent with minibatch gradients (SGD) follows the path of gradient flow on the full batch loss (Yaida, 2018). However in deep networks, SGD often achieves higher test accuracies when the learning rate is moderately large (LeCun et al., 2012; Keskar et al., 2016; Li et al., 2019). This generalization benefit is not explained by convergence rate bounds for SGD (Ma et al., 2017; Zhang et al., 2019), because it arises even for large compute budgets for which smaller learning rates achieve lower training losses (Smith et al., 2020).

In a recent work, Barrett & Dherin (2020) analyzed the influence of finite learning rates on the iterates of full batch gradient descent (GD). Their approach is inspired by *backward error analysis*, a method for the numerical analysis of ordinary differential equation (ODE) solvers (Hairer et al., 2006). The key insight of backward error analysis is that we can describe the bias introduced when integrating an ODE with finite step sizes by introducing an ancillary *modified flow*. This modified flow is derived to ensure that discrete iterates on the original ODE lie on the path of the continuous solution to the modified flow. Using this technique, the authors show that if the learning rate ϵ is not too large, the iterates of GD lie close to the path of gradient flow on a modified loss $\tilde{C}_{GD}(\omega) = C(\omega)+(\epsilon/4)||\nabla C(\omega)||^2$. This modified loss is composed of the full batch loss $C(\omega)$, and an implicit regularizer penalizing the squared gradient norm, whose scale is proportional to the learning rate.

However these results hold only for full batch GD, while in practice the use of SGD with minibatch gradients is ubiquitous. In this work, we devise an alternative approach to backward error analysis, which accounts for the correlations between minibatch gradients during one epoch of training. Using this novel approach, we prove that for small finite learning rates, the mean SGD iterate after one epoch, averaged over all possible sequences of minibatches, lies close to the path of gradient flow on a second modified loss $\tilde{C}_{SGD}(\omega)$, which we define in equation 1. This new modified loss is also composed of the full batch loss function and an implicit regularizer. However the structure of the implicit regularizers for GD and SGD differ, and their modified losses can have different local minima. Our analysis assumes that each training example is sampled once per epoch, in line with best practice (Bottou, 2012; Haochen & Sra, 2019). We confirm empirically that explicitly including the implicit regularization term of SGD in the training loss can enhance the test accuracy when the learning rate is small. Finally, we prove that if the batch size is small and the gradients are sufficiently diverse, then the expected magnitude of the implicit regularization term of SGD is proportional to the ratio of the learning rate to the batch size (Goyal et al., 2017; Smith et al., 2017).

We note that many previous authors have sought to explain the generalization benefit of SGD using an analogy between SGD and stochastic differential equations (SDEs) (Mandt et al., 2017; Smith & Le, 2017; Jastrzębski et al., 2017; Chaudhari & Soatto, 2018). However this SDE analogy assumes that each minibatch is randomly sampled from the full dataset, which implies that some examples will be sampled multiple times in one epoch. Furthermore, the most common SDE analogy holds only for vanishing learning rates (Yaida, 2018) and therefore misses the generalization benefits of finite learning rates which we identify in this work. An important exception is Li et al. (2017), who applied backward error analysis to identify a modified SDE that holds when the learning rate is finite. However this work still relies on the assumption that minibatches are sampled randomly. It also focused on the convergence rate, and did not discuss the performance of SGD on the test set.

Main Result. We now introduce our main result. We define the cost function over parameters ω as $C(\omega) = (1/N)\sum_{j=1}^{N} C_j(\omega)$, which is the mean of the per-example costs $C_j(\omega)$, where N denotes the training set size. Gradient flow follows the ODE $\dot{\omega} = -\nabla C(\omega)$, while gradient descent computes discrete updates $\omega_{i+1} = \omega_i - \epsilon \nabla C(\omega_i)$, where ϵ is the learning rate. For simplicity, we assume that the batch size B perfectly splits the training set such that $N\%B = 0$, where $\%$ denotes the modulo operation, and for convenience we define the number of batches per epoch $m = N/B$. We can therefore re-write the cost function as a sum over minibatches $C(\omega) = (1/m)\sum_{k=0}^{m-1} \hat{C}_k(\omega)$, where the minibatch cost $\hat{C}_k(\omega) = (1/B)\sum_{j=kB+1}^{kB+B} C_j(\omega)$. In order to guarantee that we sample each example precisely once per epoch, we define SGD by the discrete update $\omega_{i+1} = \omega_i - \epsilon \nabla \hat{C}_{i\%m}(\omega_i)$.

Informally, our main result is as follows. The mean iterate of SGD with a small but finite learning rate ϵ, averaged over all possible random shuffles of the batch indices, stays close to the path of gradient flow on a modified loss $\dot{\omega} = -\nabla \widetilde{C}_{SGD}(\omega)$, where the modified loss $\widetilde{C}_{SGD}$ is given by:

$$\widetilde{C}_{SGD}(\omega) = C(\omega) + \frac{\epsilon}{4m} \sum_{k=0}^{m-1} ||\nabla \hat{C}_k(\omega)||^2. \tag{1}$$

The modified loss $\widetilde{C}_{SGD}(\omega)$ is composed of the *original loss* $C(\omega)$ and an *implicit regularizer* $C_{reg}(\omega) = (1/4m)\sum_{k=0}^{m-1} ||\nabla \hat{C}_k(\omega)||^2$. The scale of this implicit regularization term is proportional to the learning rate ϵ, and it penalizes the mean euclidean norm of the gradient evaluated on a batch of B examples. To help us compare the modified losses of GD and SGD, we can expand,

$$\widetilde{C}_{SGD}(\omega) = C(\omega) + \frac{\epsilon}{4}||\nabla C(\omega)||^2 + \frac{\epsilon}{4m} \sum_{i=0}^{m-1} ||\nabla \hat{C}_i(\omega) - \nabla C(\omega)||^2. \tag{2}$$

In the limit $B \to N$, we identify the modified loss of gradient descent, $\widetilde{C}_{GD} = C(\omega) + (\epsilon/4)||\nabla C(\omega)||^2$ (Barrett & Dherin, 2020), which penalizes "sharp regions" where the norm of the full-batch gradient ($||\nabla C(\omega)||^2$) is large. However, as shown by equation 2, the modified loss of SGD penalizes both sharp regions where the full-batch gradient is large, and "non-uniform" regions where the norms of the errors in the minibatch gradients ($||\nabla \hat{C}(\omega) - \nabla C(\omega)||^2$) are large (Wu et al., 2018). Although local minima of $C(\omega)$ are local minima of $\widetilde{C}_{GD}(\omega)$, local minima of $C(\omega)$ may not be local minima of $\widetilde{C}_{SGD}(\omega)$, and vice-versa. Therefore, while GD with small finite learning rates converges to local minima of the original loss $C(\omega)$, the same may not be true for the averaged values of the SGD iterates. However GD and SGD share the same global minima on over-parameterized models which can interpolate the training set (Ma et al., 2017). We verify in our experiments that the implicit regularizer can enhance the test accuracy of models trained with SGD.

Paper structure. In section 2, we derive our main result (equation 1), and we confirm empirically that we can close the generalization gap between small and large learning rates by including the implicit regularizer explicitly in the loss function. In section 3, we confirm equation 1 satisfies the linear scaling rule between learning rate and batch size (Goyal et al., 2017). In section 4, we provide additional experiments that challenge the prevailing view that the generalization benefit of small batch SGD arises from the temperature of an associated SDE (Mandt et al., 2017; Park et al., 2019).

2 A Backward Error Analysis of Stochastic Gradient Descent

Backward error analysis has great potential to clarify the role of finite learning rates, and to help identify the implicit biases of different optimizers. We therefore give a detailed introduction to the core methodology in section 2.1, before deriving our main result in section 2.2. In section 2.3, we confirm empirically that the implicit regularizer enhances the test accuracy of deep networks.

2.1 AN INTRODUCTION TO BACKWARD ERROR ANALYSIS

In numerical analysis, we often wish to integrate ODEs of the form $\dot{\omega} = f(\omega)$. This system usually cannot be solved analytically, forcing us to simulate the continuous flow with discrete updates, like the Euler step $\omega(t+\epsilon) \approx \omega(t) + \epsilon f(\omega(t))$. However discrete steps introduce approximation error when the step size ϵ is finite. To account for this we introduce a modified flow $\dot{\omega} = \widetilde{f}(\omega)$, where,

$$\widetilde{f}(\omega) = f(\omega) + \epsilon f_1(\omega) + \epsilon^2 f_2(\omega) + \dots . \tag{3}$$

The modified flow of $\widetilde{f}(\omega)$ is equal to the original flow of $f(\omega)$ when $\epsilon \to 0$, but it differs from the original flow if ϵ is finite. The goal of backward error analysis is to choose the correction terms $f_i(\omega)$ such that the iterates obtained from discrete updates on the original flow with finite step sizes lie on the path taken by the continuous solution to the modified flow with vanishing step sizes.

The standard derivation of backward error analysis begins by taking a Taylor expansion in ϵ of the solution to the modified flow $\omega(t+\epsilon)$. We obtain the derivatives of $\omega(t+\epsilon)$ recursively using the modified flow equation $\dot{\omega} = \widetilde{f}(\omega)$ (see Hairer et al. (2006)), and we identify the correction terms $f_i(\omega)$ by ensuring this Taylor expansion matches the discrete update (e.g., $\omega_{t+1} = \omega_t + \epsilon f(\omega_t)$) for all powers of ϵ. However, this approach does not clarify *why* these correction terms arise. To build our intuition for the origin of the corrections terms, and to clarify how we might apply this analysis to SGD, we take a different approach. First, we will identify the path taken by the continuous modified flow by considering the combined influence of an infinite number of discrete steps with vanishing learning rate, and then we will compare this continuous path to either a single step of GD or a single epoch of SGD. First, imagine taking n Euler steps on the modified flow $\widetilde{f}(\omega)$ with step size α,

$$\begin{aligned}
\omega_{t+n} &= \omega_t + \alpha\widetilde{f}(\omega_t) + \alpha\widetilde{f}(\omega_{t+1}) + \alpha\widetilde{f}(\omega_{t+2}) + \dots && (4)\\
&= \omega_t + \alpha\widetilde{f}(\omega_t) + \alpha\widetilde{f}(\omega_t + \alpha\widetilde{f}(\omega_t)) + \alpha\widetilde{f}(\omega_t + \alpha\widetilde{f}(\omega_t) + \alpha\widetilde{f}(\omega_t + \alpha\widetilde{f}(\omega_t))) + \dots && (5)\\
&= \omega_t + n\alpha\widetilde{f}(\omega_t) + (n/2)(n-1)\alpha^2\nabla\widetilde{f}(\omega_t)\widetilde{f}(\omega_t) + O(n^3\alpha^3). && (6)
\end{aligned}$$

We arrived at equation 6 by taking the Taylor expansion of $\widetilde{f}$ and then counting the number of terms of type $\nabla\widetilde{f}(\omega_t)\widetilde{f}(\omega_t)$ using the formula for an arithmetic series. Note that we assume $\nabla\widetilde{f}$ exists. Next, to ensure ω_{t+n} in equation 6 coincides with the solution $\omega(t+\epsilon)$ of the continuous modified flow $\dot{\omega} = \widetilde{f}(\omega)$ for small but finite ϵ, we let the number of steps $n \to \infty$ while setting $\alpha = \epsilon/n$,

$$\begin{aligned}
\omega(t+\epsilon) &= \omega(t) + \epsilon\widetilde{f}(\omega(t)) + (\epsilon^2/2)\nabla\widetilde{f}(\omega(t))\widetilde{f}(\omega(t)) + O(\epsilon^3) && (7)\\
&= \omega(t) + \epsilon f(\omega(t)) + \epsilon^2\left(f_1(\omega(t)) + (1/2)\nabla f(\omega(t))f(\omega(t))\right) + O(\epsilon^3). && (8)
\end{aligned}$$

We have replaced $\widetilde{f}(\omega)$ with its definition from equation 3. As we will see below, equation 8 is the key component of backward error analysis, which describes the path taken when integrating the continuous modified flow $\widetilde{f}(\omega)$ with vanishing learning rates over a discrete time step of length ϵ.

Gradient descent: As a simple example, we will now derive the first order correction $f_1(\omega)$ of the modified flow for GD. First, we recall that the discrete updates obey $\omega_{i+1} = \omega_i - \epsilon\nabla C(\omega_i)$, and we therefore fix $f(\omega) = -\nabla C(\omega)$. In order to ensure that the continuous modified flow coincides with this discrete update, we need all terms at $O(\epsilon^2)$ and above in equation 8 to vanish. At order ϵ^2, this implies that $f_1(\omega) + (1/2)\nabla\nabla C(\omega)\nabla C(\omega) = 0$, which yields the first order correction,

$$f_1(\omega) = -(1/2)\nabla\nabla C(\omega)\nabla C(\omega) = -(1/4)\nabla\left(||\nabla C(\omega)||^2\right). \tag{9}$$

We conclude that, if the learning rate ϵ is sufficiently small such that we can neglect higher order terms in equation 3, then the discrete steps of GD lie on the path of the following continuous ODE,

$$\begin{aligned}
\dot{\omega} &= -\nabla C(\omega) - (\epsilon/4)\nabla\left(||\nabla C(\omega)||^2\right) + O(\epsilon^2) && (10)\\
&= -\nabla\widetilde{C}_{GD}(\omega) + O(\epsilon^2). && (11)
\end{aligned}$$

Equation 11 corresponds to gradient flow on the modified loss, $\widetilde{C}_{GD}(\omega) = C(\omega) + (\epsilon/4)||\nabla C(\omega)||^2$.

2.2 BACKWARD ERROR ANALYSIS AND STOCHASTIC GRADIENT DESCENT

We now derive our main result (equation 1). As described in the introduction, we assume $N\%B = 0$, where N is the training set size, B is the batch size, and $\%$ denotes the modulo operation. The

number of updates per epoch $m = N/B$, and the minibatch costs $\hat{C}_k(\omega) = (1/B)\sum_{j=kB+1}^{kB+B} C_j(\omega)$. SGD with constant learning rates obeys $\omega_{i+1} = \omega_i - \epsilon\nabla\hat{C}_{i\%m}(\omega_i)$. It is standard practice to shuffle the dataset once per epoch, but this step does not affect our analysis and we omit it for brevity. In equation 6 above we derived the influence of n Euler steps on the flow $\widetilde{f}(\omega)$ with step size α. Following a similar approach, we now derive the influence of m SGD updates with learning rate ϵ,

$$\begin{aligned}
\omega_m &= \omega_0 - \epsilon\nabla\hat{C}_0(\omega_0) - \epsilon\nabla\hat{C}_1(\omega_1) - \epsilon\nabla\hat{C}_2(\omega_2) - ... && (12)\\
&= \omega_0 - \epsilon\sum_{j=0}^{m-1}\nabla\hat{C}_j(\omega_0) + \epsilon^2\sum_{j=0}^{m-1}\sum_{k<j}\nabla\nabla\hat{C}_j(\omega_0)\nabla\hat{C}_k(\omega_0) + O(m^3\epsilon^3) && (13)\\
&= \omega_0 - m\epsilon\nabla C(\omega_0) + \epsilon^2\xi(\omega_0) + O(m^3\epsilon^3). && (14)
\end{aligned}$$

The error in equation 14 is $O(m^3\epsilon^3)$ since there are $O(m^3)$ terms in the Taylor expansion proportional to ϵ^3. Notice that a single epoch of SGD is equivalent to a single GD update with learning rate $m\epsilon$ up to first order in ϵ. Remarkably, this implies that when the learning rate is sufficiently small, there is no noise in the iterates of SGD after completing one epoch. For clarity, this observation arises because we require that each training example is sampled once per epoch. However the second order correction $\xi(\omega) = \sum_{j=0}^{m-1}\sum_{k<j}\nabla\nabla\hat{C}_j(\omega)\nabla\hat{C}_k(\omega)$ does not appear in the GD update, and it is a random variable that depends on the order of the mini-batches. In order to identify the bias introduced by SGD, we will evaluate the mean correction $\mathbb{E}(\hat{\xi})$, where we take the expectation across all possible sequences of the (non-overlapping) mini-batches $\{\hat{C}_0, \hat{C}_1, ..., \hat{C}_{m-1}\}$. Note that we hold the composition of the batches fixed, averaging only over their order. We conclude that,

$$\begin{aligned}
\mathbb{E}(\xi(\omega)) &= \frac{1}{2}\left(\sum_{j=0}^{m-1}\sum_{k\neq j}\nabla\nabla\hat{C}_j(\omega)\nabla\hat{C}_k(\omega)\right) && (15)\\
&= \frac{m^2}{2}\nabla\nabla C(\omega)\nabla C(\omega) - \frac{1}{2}\sum_{j=0}^{m-1}\nabla\nabla\hat{C}_j\nabla\hat{C}_j && (16)\\
&= \frac{m^2}{4}\nabla\left(||\nabla C(\omega)||^2 - \frac{1}{m^2}\sum_{j=0}^{m-1}||\nabla\hat{C}_j(\omega)||^2\right). && (17)
\end{aligned}$$

For clarity, in equation 15 we exploit the fact that every sequence of batches has a corresponding sequence in reverse order. Combining equations 14 and 17, we conclude that after one epoch,

$$\begin{aligned}
\mathbb{E}(\omega_m) &= \omega_0 - m\epsilon\nabla C(\omega_0)\\
&+ \frac{m^2\epsilon^2}{4}\nabla\left(||\nabla C(\omega_0)||^2 - (1/m^2)\sum_{j=0}^{m-1}||\nabla\hat{C}_j(\omega_0)||^2\right) + O(m^3\epsilon^3). && (18)
\end{aligned}$$

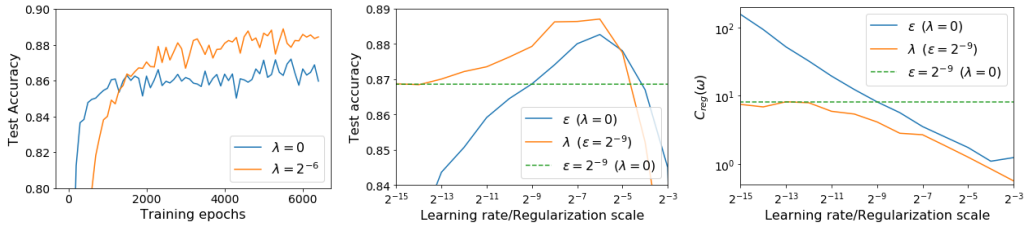
Having identified the expected value of the SGD iterate after one epoch $\mathbb{E}(\omega_m)$ (for small but finite learning rates), we can now use this expression to identify the corresponding modified flow. First, we set $f(\omega) = -\nabla C(\omega)$, $t = 0$, $\omega(0) = \omega_0$, and let $\epsilon \to m\epsilon$ in equations 3 and 8 to obtain,

$$\omega(m\epsilon) = \omega_0 - m\epsilon\nabla C(\omega_0) + m^2\epsilon^2\left(f_1(\omega_0) + (1/4)\nabla||\nabla C(\omega_0)||^2\right) + O(m^3\epsilon^3). \quad (19)$$

Next, we equate equations 18 and 19 by setting $\omega(m\epsilon) = \mathbb{E}(\omega_m)$. We immediately identify the first order correction to the modified flow $f_1(\omega) = -(1/(4m^2))\nabla\sum_{j=0}^{m-1}||\nabla\hat{C}_j(\omega)||^2$. We therefore conclude that, after one epoch, the expected SGD iterate $\mathbb{E}(\omega_m) = \omega(m\epsilon) + O(m^3\epsilon^3)$, where $\omega(0) = \omega_0$ and $\dot{\omega} = -\nabla C(\omega) + m\epsilon f_1(\omega)$. Simplifying, we conclude $\dot{\omega} = -\nabla\widetilde{C}_{SGD}(\omega)$, where,

$$\widetilde{C}_{SGD}(\omega) = C(\omega) + (\epsilon/4m)\sum_{k=0}^{m-1}||\nabla\hat{C}_k(\omega)||^2. \quad (20)$$

Equation 20 is identical to equation 1, and this completes the proof of our main result. We emphasize that $\widetilde{C}_{SGD}$ assumes a fixed set of minibatches $\{\hat{C}_0, \hat{C}_1, ..., \hat{C}_{m-1}\}$. We will evaluate the expected modified loss after shuffling the dataset and sampling a new set of minibatches in section 3. Additionally, our analysis assumes $m\epsilon = N\epsilon/B$ is small. Higher order contributions to the modified flow may therefore have a significant influence if the ratio of the learning rate to the batch size is large. We also note that to achieve the highest test accuracies, practitioners usually decay the learning rate during training. Under this scheme, the modified loss will change as training proceeds. However it is widely thought that the generalization benefit of SGD arises from the use of large learning rates early in training (Smith et al., 2017; Li et al., 2019; Lewkowycz et al., 2020), and popular learning rate schedules usually hold the learning rate constant or approximately constant for several epochs. Finally, we emphasize that our primary goal in this work is to study the influence of finite learning rates on training. The implicit regularization term may not be beneficial in all models and datasets.



(a) (b) (c)

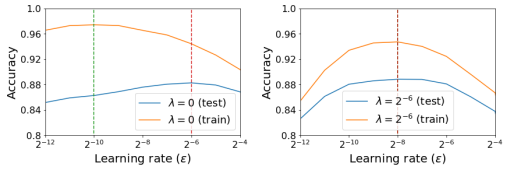
Figure 1: (a) Explicitly including the implicit regularizer in the loss improves the test accuracy when training with small learning rates. (b) The optimal regularization coefficient $\lambda_{opt} = 2^{-6}$ is equal to the optimal learning rate $\epsilon_{opt} = 2^{-6}$. (c) Increasing either the learning rate ϵ or the regularization coefficient λ reduces the value of the implicit regularization term $C_{reg}(\omega)$ at the end of training.

2.3 An Empirical Evaluation of the Modified Loss

In order to confirm that the modified loss $\widetilde{C}_{SGD}(\omega)$ can help explain why large learning rates enhance generalization, we now verify empirically that the implicit regularizer inherent in constant learning rate SGD, $C_{reg}(\omega) = (1/4m)\sum_{k=0}^{m-1} ||\nabla \hat{C}_k(\omega)||^2$, can enhance the test accuracy of deep networks. To this end, we train the same model with two different (explicit) loss functions. The first loss function $C(\omega)$ represents the original loss, while the second $C_{mod}(\omega) = C(\omega) + \lambda C_{reg}(\omega)$ is obtained from the modified loss $\widetilde{C}_{SGD}(\omega)$ by replacing the learning rate ϵ with an explicit regularization coefficient λ. Notice that $C_{mod}(\omega) = (1/m)\sum_{k=0}^{m-1}\left(\hat{C}_k(\omega) + (\lambda/4)||\nabla \hat{C}_k(\omega)||^2\right)$, which ensures that it is straightforward to minimize the modified loss $C_{mod}(\omega)$ with minibatch gradients. Since the implicit regularization term $C_{reg}(\omega)$ is expensive to differentiate (typically 5-10x overhead), we consider a 10-1 Wide-ResNet model (Zagoruyko & Komodakis, 2016) for classification on CIFAR-10. To ensure close agreement with our theoretical analysis, we train without batch normalization using SkipInit initialization (De & Smith, 2020). We train for 6400 epochs at batch size 32 without any learning rate decay using SGD without Momentum. We use standard data augmentation including crops and random flips, and we use weight decay with L_2 coefficient 5×10^{-4}.

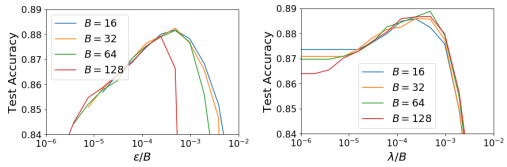
In figure 1(a), we compare two training runs, one minimizing the modified loss $C_{mod}(\omega)$ with $\lambda = 2^{-6}$, and one minimizing the original loss $C(\omega)$. For both runs we use a small constant learning rate $\epsilon = 2^{-9}$. As expected, the regularized training run achieves significantly higher test accuracies late in training. This confirms that the implicit regularizer, which arises as a consequence of using SGD with finite learning rates, can also enhance the test accuracy if it is included explicitly in the loss. In figure 1(b), we provide the test accuracy for a range of regularization strengths λ (orange line). We provide the mean test accuracy of the best 5 out of 7 training runs at each regularization strength, and for each run we take the highest test accuracy achieved during the entire training run. We use a fixed learning rate $\epsilon = 2^{-9}$ for all λ. For comparison, we also provide the test accuracy achieved with the original loss $C(\omega)$ for a range of learning rates ϵ (blue line). In both cases, the test accuracy rises initially, before falling for large regularization strengths or large learning rates. The optimal regularization strength on the modified loss $\lambda_{opt} = 2^{-6}$ is equal to the optimal learning rate on the original loss $\epsilon_{opt} = 2^{-6}$, consistent with our theoretical analysis. Meanwhile when $\lambda \to 0$ the performance of the modified loss approaches the performance of the original loss at $\epsilon = 2^{-9}$ (dotted green line). We provide the corresponding training accuracies in appendix C. Finally, in figure 1(c), we provide the values of the implicit regularizer $C_{reg}(\omega)$ at the end of training. As predicted by our analysis, training with larger learning rates reduces the value of the implicit regularization term.

In figure 2, we take the same 10-1 Wide-ResNet model and provide the mean training and test accuracies achieved at a range of learning rates for two regularization coefficients (following the experimental protocol above). In figure 2(a), we train on the original loss $C(\omega)$ ($\lambda = 0$), while in figure 2(b), we train on the modified loss $C_{mod}(\omega)$ with regularization coefficient $\lambda = 2^{-6}$. From figure 2(a), when $\lambda = 0$ there is a clear generalization benefit to large learning rates, as the learning rate that maximizes test accuracy (2^{-6}) is 16 times larger than the learning rate that maximizes training accuracy (2^{-10}). However in figure 2(b) with $\lambda = 2^{-6}$, the learning rates that maximize the test and training accuracies are equal (2^{-8}). This suggests that when we include the implicit regularizer explicitly in the loss, the generalization benefit of large learning rates is diminished.



(a) (b)

Figure 2: (a) There is a clear generalization benefit to large learning rates when training on the original loss $C(\omega)$ with $\lambda = 0$. (b) When we include the implicit regularizer explicitly in $C_{mod}(\omega)$ and set $\lambda = 2^{-6}$, the generalization benefit of large learning rates is diminished.



(a) (b)

Figure 3: (a) Different batch sizes achieve the same test accuracy if the ratio of the learning rate to the batch size (ϵ/B) is constant and B is not too large. (b) The test accuracy is independent of the batch size if the ratio of the regularization coefficient to the batch size (λ/B) is constant.

3 Implicit Regularization and the Batch Size

In section 2.2, we derived the modified loss (equations 1 and 2) by considering the expected SGD iterate after one epoch. We held the composition of the batches fixed, averaging only over the order in which the batches are seen. This choice helped make clear how to explicitly include the implicit regularizer in the loss function in section 2.3. However, in order to clarify how the implicit regularizer term depends on the batch size, we now evaluate the expected modified loss after randomly shuffling the dataset and sampling a new set of m non-overlapping minibatches $\{\hat{C}_0, \hat{C}_1, ..., \hat{C}_{m-1}\}$. Since the minibatch losses $\hat{C}_i(\omega)$ are all identically distributed by symmetry, we conclude that,

$$\mathbb{E}(\widetilde{C}_{SGD}(\omega)) = C(\omega) + (\epsilon/4)||\nabla C(\omega)||^2 + (\epsilon/4)\mathbb{E}(||\nabla \hat{C}(\omega) - \nabla C(\omega)||^2), \tag{21}$$

where $\hat{C}(\omega)$ denotes a batch of B non-overlapping examples, drawn randomly from the full dataset. To simplify equation 21, we prove in appendix A that $\mathbb{E}(||\nabla \hat{C}(\omega) - \nabla C(\omega)||^2) = \frac{(N-B)}{(N-1)}\frac{\Gamma(\omega)}{B}$, where $\Gamma(\omega) = (1/N)\sum_{i=1}^{N} ||\nabla C_i(\omega) - \nabla C(\omega)||^2$. Finally we assume $N \gg B \geq 1$ to obtain,

$$\mathbb{E}(\widetilde{C}_{SGD}(\omega)) = C(\omega) + (\epsilon/4)\,||\nabla C(\omega)||^2 + (\epsilon/4B)\,\Gamma(\omega). \tag{22}$$

Notice that we have not assumed the gradients are Gaussian distributed (Simsekli et al., 2019). Equation 22 shows that the implicit regularization term of SGD has two contributions. The first term is proportional to the learning rate ϵ, and it penalizes the norm of the full batch gradient. The second term is proportional to the ratio of the learning rate to the batch size ϵ/B, and it penalizes the trace of the covariance matrix of the per-example gradients, defined by $\Gamma(\omega)$. To interpret this result, we assume the gradients are diverse, such that $\Gamma(\omega) \gg ||\nabla C(\omega)||^2$. Therefore, when the batch size is small, the second term above will dominate. In this limit, two different batch sizes will experience the same implicit regularization if the ratio of the learning rate to the batch size is constant.

To verify this claim, in figure 3 we plot the mean test accuracies achieved on a 10-1 Wide-ResNet, trained on CIFAR-10 with a constant learning rate, for a range of learning rates ϵ, regularization coefficients λ and batch sizes B. As expected, in figure 3(a), training on the original loss $C(\omega)$ for 6400 epochs, we see that different batch sizes achieve similar test accuracies so long as the ratio ϵ/B is constant and the batch size is not too large. We note that this linear scaling rule is well known and has been observed in prior work (Goyal et al., 2017; Smith & Le, 2017; Jastrzębski et al., 2017; Zhang et al., 2019). To confirm that this behaviour is consistent with the modified loss, in figure 3(b) we fix the learning rate $\epsilon = 2^{-9}$ and train on $C_{mod}(\omega)$ at a range of regularization strengths λ for 10 million steps. As expected, different batch sizes achieve similar test accuracy so long as the ratio λ/B is constant. We note that this phenomenon would break down for very large batch sizes.

For very large batch sizes, the first implicit regularization term in equation 22 will dominate, the linear scaling rule breaks down, and the bias of SGD is similar to the bias of GD. We expect the optimal learning rate to be independent of the batch size in this limit, as observed by McCandlish et al. (2018) and Smith et al. (2020). Previous theoretical work on convergence bounds also predicted a transition between a small batch regime where the optimal learning rate $\epsilon \propto B$ and a large batch regime where the optimal learning rate is constant (Ma et al., 2017; Zhang et al., 2019). However these analyses identify the learning rate that minimizes the training loss. Our analysis compliments these claims by explaining why similar conclusions hold when maximizing the test accuracy.

4 FINITE LEARNING RATES AND STOCHASTIC DIFFERENTIAL EQUATIONS

In the previous two sections, we argued that the use of finite learning rates and small batch sizes introduces implicit regularization, which can enhance the test accuracy of deep networks. We analyzed this effect using backward error analysis (Hairer et al., 2006; Li et al., 2017; Barrett & Dherin, 2020), but many previous papers have argued that this effect can be understood by interpreting small batch SGD as the discretization of an SDE (Mandt et al., 2017; Smith & Le, 2017; Jastrzębski et al., 2017; Park et al., 2019). In this section, we compare this popular perspective with our main results from sections 2 and 3. To briefly recap, in the SDE analogy a single gradient update is given by $\omega_{i+1} = \omega_i - \epsilon \nabla \hat{C}(\omega_i)$, where $\hat{C}$ denotes a random batch of B non-overlapping training examples. Notice that in the SDE analogy, since examples are drawn randomly from the full dataset, there is no guarantee that each training example is sampled once per epoch. Assuming $N \gg B \gg 1$ and that the gradients are not heavy tailed, the central limit theorem is applied to model the noise in an update by a Gaussian noise source ξ whose covariance is inversely proportional to the batch size:

$$\omega_{i+1} = \omega_i - \epsilon\big(\nabla C(\omega_i) + \xi_i/\sqrt{B}\big) \quad = \quad \omega_i - \epsilon \nabla C(\omega_i) + \sqrt{\epsilon T}\xi_i. \tag{23}$$

This assumes $\mathbb{E}(\xi_i) = 0$ and $\mathbb{E}(\xi_i \xi_j^T) = F(\omega)\delta_{ij}$, where $F(\omega)$ is the covariance matrix of the per example gradients, and we define the "temperature" $T = \epsilon/B$. The SDE analogy notes that equation 23 is identical to the Euler discretization of an SDE with step size ϵ and temperature T (Gardiner et al., 1985). Therefore one might expect the SGD iterates to remain close to this underlying SDE in the limit of small learning rates ($\epsilon \to 0$). In this limit, the temperature defines the influence of mini-batching on the dynamics, and it is therefore often assumed that the temperature also governs the generalization benefit of SGD (Smith & Le, 2017; Jastrzębski et al., 2017; Park et al., 2019).

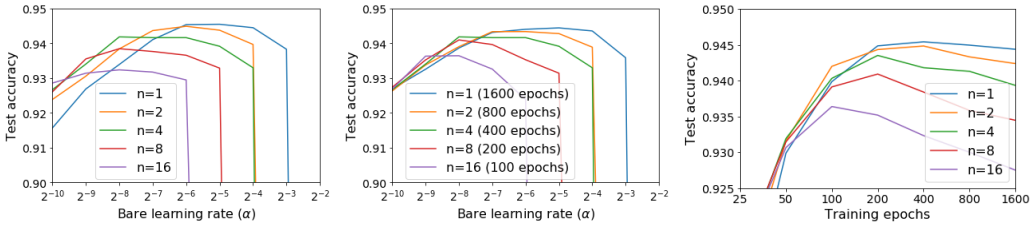
However this conclusion from the SDE analogy is inconsistent with our analysis in section 2. To see this, note that in section 2 we assumed that each training example is sampled once per epoch, as recommended by practitioners (Bottou, 2012), and showed that under this assumption there is *no noise* in the dynamics of SGD up to first order in ϵ after one epoch of training. The SDE analogy therefore relies on the assumption that minibatches are sampled randomly from the full dataset. Furthermore, SGD only converges to the underlying SDE when the learning rate $\epsilon \to 0$, but in this limit the temperature $T \to 0$ and SGD converges to gradient flow (Yaida, 2018). We must use a finite learning rate to preserve a finite temperature, but at any finite learning rate the distributions of the SGD iterates and the underlying SDE may differ. We now provide empirical evidence to support our contention that the generalization benefit of SGD arises from finite learning rates, not the temperature of an associated stochastic process. First, we introduce a modified SGD update rule:

n-step SGD: *Apply n gradient descent updates sequentially on the same minibatch with bare learning rate α, effective learning rate $\epsilon = n\alpha$ and batch size B. Sample the next minibatch and repeat.*

To analyze n-step SGD, we compute the combined influence of n updates on the same minibatch:

$$\begin{aligned} \omega_{i+1} &= \omega_i - \alpha \nabla \hat{C}(\omega_i) - \alpha \nabla \hat{C}(\omega_i - \alpha \nabla \hat{C}(\omega_i)) + ... && (24) \\ &= \omega_i - n\alpha \nabla \hat{C}(\omega_i) + O(n^2\alpha^2) && (25) \\ &= \omega_i - \epsilon \nabla C(\omega_i) + \sqrt{\epsilon T}\xi_i + O(\epsilon^2). && (26) \end{aligned}$$

Equations 23 and 26 are identical up to first order in ϵ but they differ at $O(\epsilon^2)$ and above. Therefore, if minibatches are randomly sampled from the full dataset, then the dynamics of standard SGD and n-step SGD should remain close to the same underlying SDE in the limit $\epsilon \to 0$, but their dynamics will differ when the learning rate is finite. We conclude that if the dynamics of SGD is close to the continuum limit of the associated SDE, then standard SGD and n-step SGD ought to achieve similar test accuracies after the same number of training epochs. However if, as we argued in section 2, the generalization benefit of SGD arises from finite learning rate corrections at $O(\epsilon^2)$ and above, then we should expect the performance of standard SGD and n-step SGD to differ. For completeness, we provide a backward error analysis of n-step SGD in appendix B. In line with section 2 (and best practice), we assume each training example is sampled once per epoch. We find that after one epoch, the expected n-step SGD iterate $\mathbb{E}(\omega_m) = \omega(m\epsilon) + O(m^3\epsilon^3)$, where $\omega(0) = \omega_0$, $\dot{\omega} = -\nabla \widetilde{C}_{nSGD}(\omega)$ and $\widetilde{C}_{nSGD}(\omega) = C(\omega) + (\epsilon/4mn)\sum_{i=0}^{m-1} ||\nabla C_i(\omega)||^2$. The scale of the implicit regularizer is proportional to ϵ/n, which implies that the implicit regularization is suppressed as n increases if we hold ϵ constant. As expected, we recover equation 1 when $n = 1$.



(a) (b) (c)

Figure 4: (a) When training for 400 epochs, smaller values of n achieve higher test accuracies and are stable at larger bare learning rates α. (b) Similar conclusions hold when training for a fixed number of updates. (c) We show the test accuracy at the optimal learning rate for a range of epoch budgets. Smaller values of n achieve higher test accuracy and also benefit from larger epoch budgets.

In figure 4(a), we plot the performance of n-step SGD at a range of bare learning rates α, when training a 16-4 Wide-ResNet on CIFAR-10 for 400 epochs using SkipInit (De & Smith, 2020) at batch size 64. Each example is sampled once per epoch. One of our goals in this section is to confirm whether our theoretical insights are relevant in practical training setups. We therefore introduce a learning rate schedule, whereby we hold the learning rate constant for the first half of training, before decaying the learning rate by a factor of 2 every remaining tenth of training. We also apply dropout before the softmax with drop probability 0.5, and we provide the mean test accuracy of the best 5 out of 7 training runs for each value of α. The optimal test accuracy drops from 94.5% when $n = 1$ (standard SGD) to 93.2% when $n = 16$. This occurs even though all values of n perform the same number of training epochs, indicating that 16-step SGD performed 16 times more gradient updates. These results provide strong evidence to suggest that the generalization benefit of SGD may not be controlled by the temperature of an associated SDE, but instead arises from the implicit regularization associated with finite learning rates. When we increase n we reduce the largest stable bare learning rate α, and this suppresses the implicit regularization, which reduces the test accuracy.

We verify in figure 4(b) that similar conclusions arise if we hold the number of parameter updates fixed (such that the number of training epochs is inversely proportional to n). The test accuracy is independent of n when the learning rate is small, while smaller values of n are stable at larger learning rates, enabling higher test accuracies. Finally we confirm in figure 4(c) that the test accuracy degrades as n increases even if one also identifies the optimal epoch budget for each value of n.

5 Discussion

Many authors have observed that large learning rates (Li et al., 2019; Lewkowycz et al., 2020), and small batch sizes (Keskar et al., 2016; Smith et al., 2020), can enhance generalization. Most theoretical work has sought to explain this by observing that increasing the learning rate, or reducing the batch size, increases the variance of the SGD iterates (Smith & Le, 2017; Jastrzębski et al., 2017; Chaudhari & Soatto, 2018). We take a different approach, and note that when the learning rate is finite, the SGD iterates are also biased (Roberts, 2018). Backward error analysis (Hairer et al., 2006; Li et al., 2017; Barrett & Dherin, 2020) provides a powerful tool which computes how this bias accumulates over multiple parameter updates. Although this work focused on GD and SGD, we anticipate that backward error analysis could also be used to clarify the role of finite learning rates in adaptive optimizers like Adam (Kingma & Ba, 2014) or Natural Gradient Descent (Amari, 1998).

Analyses of SGD often assume the examples in each minibatch are drawn randomly from the full dataset (Mandt et al., 2017; Li et al., 2017), rather than requiring that each example is sampled once per epoch, as recommended in practice (Bottou, 2012). Our analysis shows that this assumption has important consequences when the learning rate ϵ is small (but still finite). If one assumes that batches are drawn randomly from the full dataset, then the dynamics of SGD will exhibit variance at $O(\epsilon)$, while the bias of SGD arises at $O(\epsilon^2)$. However if we ensure each example is drawn once per epoch, then SGD only exhibits variance at $O(\epsilon^2)$ or higher. Our theoretical analysis and our experiments both suggest that the generalization benefit of SGD primarily arises from bias, not variance. However, in this work, we have only considered terms at $O(\epsilon^2)$ and below. Higher order terms may also play a significant role in the training dynamics for many architectures and datasets.

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A THE EXPECTED NORM OF A MINIBATCH GRADIENT

To keep the notation clean, we define $X_i = (\nabla C_i(\omega) - \nabla C(\omega))$. We also recall for clarity that the expectation value $\mathbb{E}(...)$ is taken over all possible random shuffles of the indices i. Therefore,

$$\begin{aligned}
\mathbb{E}(||(\nabla \hat{C}(\omega) - \nabla C(\omega))||^2) &= \frac{1}{B^2}\mathbb{E}(\sum_{i=1}^{B}\sum_{j=1}^{B} X_i \cdot X_j) && (27)\\
&= \frac{B}{B^2}\mathbb{E}(X_i \cdot X_i) + \frac{B(B-1)}{B^2}\mathbb{E}(X_i \cdot X_{j\neq i}) && (28)\\
&= \frac{1}{NB}\sum_{i=1}^{N} X_i \cdot X_i + \frac{(B-1)}{B}\frac{1}{N(N-1)}\sum_{i=1}^{N}\sum_{j\neq i} X_i \cdot X_j && (29)\\
&= \frac{1}{NB}\sum_{i=1}^{N} X_i \cdot X_i + \frac{(B-1)}{BN(N-1)}\sum_{i=1}^{N}\sum_{j=1}^{N} \left(X_i \cdot X_j(1-\delta_{ij})\right).
\end{aligned}$$

Note that we obtain equation 28 by counting the number of diagonal and off-diagonal terms in the sum in equation 27. Next, we recall that $\sum_{i=1}^{N} X_i = \sum_{i=1}^{N}(\nabla C_i(\omega) - \nabla C(\omega)) = 0$. Therefore,

$$\begin{aligned}
\mathbb{E}(||(\nabla \hat{C}(\omega) - \nabla C(\omega))||^2) &= \frac{1}{NB}\sum_{i=1}^{N} X_i \cdot X_i - \frac{(B-1)}{BN(N-1)}\sum_{i=1}^{N} X_i \cdot X_i && (30)\\
&= \frac{1}{NB}\left(1 - \frac{(B-1)}{(N-1)}\right)\sum_{i=1}^{N} X_i \cdot X_i && (31)\\
&= \frac{(N-B)}{(N-1)}\frac{\Gamma(\omega)}{B}, && (32)
\end{aligned}$$

where $\Gamma(\omega) = (1/N)\sum_{i=1}^{N} X_i \cdot X_i = (1/N)\sum_{i=1}^{N} ||\nabla C_i(\omega) - \nabla C(\omega)||^2$. We can immediately identify $\Gamma(\omega)$ as the trace of the empirical covariance matrix of the per-example gradients.

B A BACKWARD ERROR ANALYSIS FOR N-STEP SGD

Under n-step SGD, we apply n gradient descent updates on the same minibatch with bare learning rate α and batch size B. After n updates, we sample the next minibatch and repeat. For convenience, we define the effective learning rate $\epsilon = n\alpha$. After one minibatch (n parameter updates),

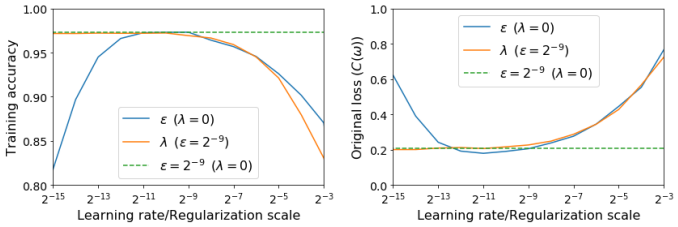
$$\begin{aligned}
\omega_{i+1} &= \omega_i - \alpha\nabla\hat{C}_i(\omega_i) - \alpha\nabla\hat{C}_i(\omega_i - \alpha\nabla\hat{C}_i(\omega_i)) + ... && (33)\\
&= \omega_i - n\alpha\nabla\hat{C}_i(\omega_i) + (n/2)(n-1)\alpha^2\nabla\nabla\hat{C}_i(\omega_i)\nabla\hat{C}_i(\omega_i) + O(n^3\alpha^3) && (34)\\
&= \omega_i - \epsilon\nabla\hat{C}_i(\omega_i) + (1/4)(1-1/n)\epsilon^2\nabla\left(||\nabla\hat{C}_i(\omega_i)||^2\right) + O(\epsilon^3). && (35)
\end{aligned}$$

After one epoch (including terms up to second order in ϵ),

$$\begin{aligned}
\omega_m = \omega_0 \quad &- \quad \epsilon\nabla\hat{C}_0(\omega_0) + (1/4)(1-1/n)\epsilon^2\nabla\left(||\nabla\hat{C}_0(\omega_0)||^2\right)\\
&- \quad \epsilon\nabla\hat{C}_1(\omega_1) + (1/4)(1-1/n)\epsilon^2\nabla\left(||\nabla\hat{C}_1(\omega_1)||^2\right)\\
&- \quad ...\\
&- \quad \epsilon\nabla\hat{C}_{m-1}(\omega_{m-1}) + (1/4)(1-1/n)\epsilon^2\nabla\left(||\nabla\hat{C}_{m-1}(\omega_{m-1})||^2\right) + O(\epsilon^3). \quad (36)
\end{aligned}$$

To simplify this expression, we note that $\omega_{i+1} = \omega_i - \epsilon\nabla\hat{C}_i(\omega_i) + O(\epsilon^2)$. We can therefore re-use our earlier analysis from section 2.2 of the main text (see equation 13 for comparison) to obtain,

$$\begin{aligned}
\omega_m &= \omega_0 - m\epsilon\nabla C(\omega_0) + \epsilon^2\sum_{j=0}^{m-1}\sum_{k<j}\nabla\nabla\hat{C}_j(\omega_0)\nabla\hat{C}_k(\omega_0)\\
&\quad + (1/4)(1-1/n)\epsilon^2\sum_{i=0}^{m-1}\nabla\left(||\nabla\hat{C}_i(\omega_0)||^2\right) + O(\epsilon^3). && (37)
\end{aligned}$$



(a) (b)

Figure 5: (a) When training on the original loss $C(\omega)$, the training accuracy achieved within 6400 epochs is maximized when the learning rate $\epsilon = 2^{-9}$. Smaller learning rates have not yet converged, while larger learning rates reach a plateau. When training on the modified loss $C_{mod}(\omega)$ with fixed learning rate $\epsilon = 2^{-9}$ and regularization coefficient λ, we achieve high training accuracies when λ is small, but are unable to achieve high training accuracies when λ is large. (b) We plot the value of the original loss $C(\omega)$ at the end of training. Remarkably, the training losses achieved when training on the original loss with a large learning rate are similar to the training losses achieved when training on the modified loss with small learning rate ($\epsilon = 2^{-9}$) and a large regularization coefficient λ.

Taking the expectation over all possible batch orderings (see equations 15 to 18), we obtain,

$$\mathbb{E}(\omega_m) = \omega_0 - m\epsilon\nabla C(\omega_0) + \frac{m^2\epsilon^2}{4}\nabla\left(||\nabla C(\omega_0)||^2 - \frac{1}{m^2 n}\sum_{i=0}^{m-1}||\nabla\hat{C}_i(\omega_0)||^2\right) + O(m^3\epsilon^3). \quad (38)$$

Fixing $f(\omega) = -\nabla C(\omega)$ and equating equation 38 with the continuous modified flow in equation 19 by setting $\mathbb{E}(\omega_m) = \omega(m\epsilon)$, we identify the modified flow $\dot{\omega} = -\nabla\widetilde{C}_{nSGD} + O(m^2\epsilon^2)$, where,

$$\widetilde{C}_{nSGD}(\omega) = C(\omega) + \frac{\epsilon}{4mn}\sum_{i=0}^{m-1}||\nabla\hat{C}_i(\omega)||^2. \quad (39)$$

Comparing equation 39 to equation 1, we note that the modified losses of SGD and n-step SGD coincide when $n = 1$. However for n-step SGD when $n > 1$, the strength of the implicit regularization term is proportional to the scale of the bare learning rate $\alpha = \epsilon/n$, not the effective learning rate ϵ.

C TRAINING LOSSES

In figure 1(b) of section 2.3 in the main text, we compared the test accuracies achieved when training on the original loss $C(\omega)$ at a range of learning rates ϵ, to the test accuracies achieved when training on the modified loss $C_{mod}(\omega)$ at fixed learning rate $\epsilon = 2^{-9}$ and a range of regularization coefficients λ. For completeness, in figure 5, we provide the corresponding training accuracies, as well as the final values of the original loss $C(\omega)$. Remarkably, large learning rates and large regularization coefficients achieve similar training accuracies and similar original losses. This suggests that the implicit regularization term in the modified loss of SGD ($\widetilde{C}_{SGD}(\omega)$) may help explain why the training accuracies and losses often exhibit plateaus when training with large learning rates.