Bad Global Minima Exist and SGD Can Reach Them

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Abstract

Several recent works have aimed to explain why severely overparameterized models, generalize well when trained by Stochastic Gradient Descent (SGD). The emergent consensus explanation has two parts: the first is that there are "no bad local minima," while the second is that SGD performs implicit regularization by having a bias towards low complexity models. We revisit both of these ideas in the context of image classification with common deep neural network architectures. Our first finding is that there exist bad *global* minima, *i.e.*, models that fit the training set perfectly, yet have poor generalization. Our second finding is that given only *unlabeled* training data, we can easily construct initializations that will cause SGD to quickly converge to such bad global minima that exhibit a test accuracy degradation of up to 40% compared to training from a random initialization. Finally, we show that regularization seems to provide SGD with an escape route: once heuristics such as data augmentation are used, starting from a complex model (adversarial initialization) has no effect on the test accuracy.

1 Introduction

In [1] it was shown that several popular deep neural network architectures for image classification have enough capacity to perfectly memorize the CIFAR10 training set. That is, they can achieve zero training error, even after the training examples are relabeled with uniformly random labels. Moreover, such memorizing models are not even hard to find; they are reached by standard training methods such as stochastic gradient descent (SGD) in about as much time as it takes to train with the correct labels. It would stand to reason that since these architectures have enough capacity to "fit anything," models derived by fitting the correctly labeled data, *i.e.*, "yet another anything," would fail to generalize. Yet, miraculously, they do not: models trained by SGD on even severly overparameterized architectures generalize spectacularly. Following recent work [2, 3, 4, 5, 6, 7], our study is motivated by the desire to shed some light onto this miracle which stands at the center of the recent machine learning revolution.

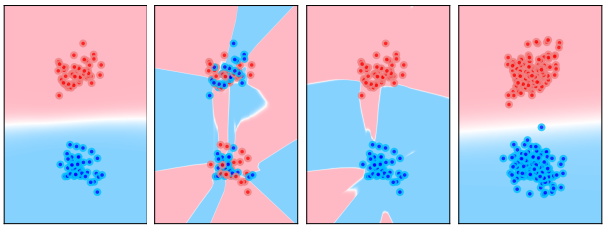
When the training set is labeled randomly, all models that minimize the corresponding loss function are equivalent in terms of generalization, in the sense that, we expect none of them to generalize. The first question we ask is: when the true labels are used, are *all* models that minimize the loss function equivalent in terms of generalization, or are some better than others? We show that not all global minima are created equal: there exist bad *global* minima, *i.e.*, global minima that generalize poorly.

The existence of bad global minima implies that the optimization method used for training, *i.e.*, to select among the (near-)global minima, has germane effect on generalization. In practice, SGD appears to avoid bad global minima, as different models produced by SGD from independent random initializations tend to all generalize equally well, a phenomenon attributed to an inherent bias of the algorithm to converge to models of low complexity [8, 9, 10, 11, 12, 13]. This brings about our second question: does SGD deserve all the credit for avoiding bad global minima, or are there also other factors at play? More concretely, can we initialize SGD so that it ends up at a bad global minimum? Of course, since we can always start SGD *at* a bad global minimum, our question has a trivial positive answer as stated. We show that initializations that cause SGD to converge to bad

global minima can be constructed given only *unlabeled* training data, *i.e.*, without any idea of the true loss landscape.

The fact that we can construct adversarial initializations without knowledge of the loss landscape suggests that these initializations correspond to models whose *inherently undesirable* characteristics persist, at least partially, in the trained models that perfectly fit the training examples with correct labels. Such a priori undesirability justifies a priori preference of some models over others, *i.e.*, regularization. In particular, if a regularization term makes an adversarial initialization appear a far worse model than before, this correspondingly incentivizes SGD to move away from it, a tendency amplified by the use of momentum during optimization. This is precisely what we find in our experiments: adding regularization and momentum allows SGD to overcome our adversarial initializations and end up at good global minima. In other words, in penalizing inherent characteristics of models, it appears that regularization plays a role beyond that of distinguishing between different models that fit the data equally well: it affects training dynamics, making good models easier to find, perhaps by making bad models more evidently bad.

A Sketch of the Phenomenon Consider training a two-layer, fully-connected, neural network for a binary classification task, where the training data are sampled from two identical, well-separated 2-dimensional Gaussians. Each class comprises 50 samples, while the network has 100 hidden units in each layer and uses ReLU activations. In Figure 1, we show the decision boundary of the model reached by training with SGD with a batch size of 10 until 100% accuracy is reached under the following four settings: 1) True labels, random initialization; 2) Random labels, random initialization; 3) True labels, initialization at the model in Fig. 1(b) (reached after training under setting 2); 4) Same as setting 3, but with data augmentation, l_2 regularization, and momentum[1]



(a) Setting 1 (b) Setting 2 (c) Setting 3 (d) Setting 4

Figure 1: The decision boundary of the model reached by SGD in Settings 1–4, respectively.

Figure 1(a) shows that from a random initialization, SGD converges to a model with near max margin, which may attributed to its implicit bias. Figure 1(b) shows that when fitting random labels, the decision margin becomes extremely complex and has miniscule margin. Figure 1(c) shows that when SGD is initialized at such an extremely complex model, it converges to a "nearby" model whose decision boundary is unnatural and has small margin. Finally, in Figure 1(d), we see that when data augmentation, regularization and momentum are added, SGD escapes the bad initialization and again reaches a model with a max margin decision boundary.

In the next section, we show that the phenomenon sketched above in a toy setting persists in state-of-the-art-neural network architectures over real data sets. We specifically examine VGG16, ResNet18, ResNet50, and DenseNet40, when trained on CIFAR, CINIC, and a restricted version of ImageNet. We consistently observe the following: 1) bad global minima exist; 2) initializations that cause SGD to converge to them can be easily derived given only unlabeled training data; 3) each of data augmentation, regularization, and momentum help SGD avoid reaching bad global minima by allowing the model to escape far away from such adversarial initializations.

2 Experimental Setup, Findings and Observed Phenomena

Datasets and Architectures We ran experiments on the CIFAR [14] data set (including both CIFAR10 and CIFAR100), CINIC10 [15] and a resized Restricted ImageNet [16]. We train on them four models: VGG16 [17], ResNet18 and ResNet50 [18] and DenseNet40 [19].

Implementation and Reproducibility We run our experiments on PyTorch 3.0. Our figures, models, and all results can be reproduced using the code available at an anonymized git repository.

Training methods We consider state-of-the-art (SOTA) SGD training and vanilla SGD training. The former corresponds to SGD with ℓ_2-regularization, data augmentation (random crops and flips), and momentum. The latter to SGD without any of these features.

[1]Data augmentation was performed by replicating each training point twice and adding Gaussian noise.

Initialization We consider two kinds of initialization: random and adversarial. For random initializations we use the PyTorch default. To create an adversarial initialization, we train the model on an augmented version of the original training dataset in which we have labeled every example uniformly at random.

Algorithm 1 Adversarial initialization

Input: Original training dataset S; Replication factor R; Noise factor N
$C = \emptyset$
for every image $x \in S$ **do**
  for i from 1 to R **do**
    $x_i \leftarrow$ zero-out a random subset comprising $N\%$ of the pixels in x
    $y_i \leftarrow$ Uniformly random label
    Add (x_i, y_i) to C
Train the architecture to 100% accuracy on C from a random initialization using vanilla SGD
Output: The weight vector of the architecture when training ends

Hyperparameters For CIFAR, CINIC10, and Restricted ImageNet, we use batch size 128, while the momentum term is set to 0.9 when it is used. When we use ℓ_2 regularization, the regularization parameter is $5 \cdot 10^{-4}$ for CIFAR and Restricted ImageNet and 10^{-4} for CINIC10. We use the following learning rate schedule for CIFAR: 0.1 for epochs 1 to 150, 0.01 for epoch 151 to 250, and 0.001 for epochs 251 to 350. We use the following learning rate schedules for CINIC and Restricted ImageNet: 0.1 epochs 1 to 150, 0.01 for epoch 151 to 225, and 0.001 for epochs 226 to 300. The CIFAR training set consists of 50k data points and the test set consists of 10k data points. The CINIC10 training set consists of 90k data points and the test set consists of 90k data points. The Restricted ImageNet training set consists of approximately 123k data points and the test set consists of 4.8k data poitns.

2.1 Findings and Observed Phenomena

The motivation behind our adversarial initialization comes from our expectation that memorizing random labels will consume some of the learning capacity of the network, and potentially reduce the positive effects of overparametrization. Furthermore, as seen in our toy example in Section 1, adversarial initialization tends to encourage SGD towards extremely complex decision boundaries, *i.e.*, decision regions that look surprising given the expectation of an implicit SGD bias toward simplicity. We first report the test error curves for our 16 setups (4 data sets and 4 models), followed by the impact of the replication parameter R on the test error.

Our main observations as taken from the figures below and our experimental data are as follows:

1. Vanilla SGD with random initialization reaches 100% training accuracy for all models and data sets tested, which is consistent with [1].
2. Vanilla SGD with adversarial initialization suffers up to a 40% test accuracy degradation compared to random initialization. That is, SGD models that are near global optima can have a difference of up to 40% in test accuracy: not all training global optima are equally good.
3. SOTA SGD with explicit regularization, converges to the same test error from random vs. adversarial initialization.

Test accuracy Our most important findings are the test accuracy curves shown in Figure 2, showing the test accuracy convergence during training. We see that the test accuracy of adversarially initialized vanilla SGD flattens out significantly below the corresponding accuracy under a random initialization, even though both methods achieve 100% training accuracy. The test error degradation can be up to 40% on CIFAR100, while for DenseNet the test degradation is comparatively smaller.

At the same time, we see that the detrimental effect of adversarial initialization vanishes once we use data augmentation, momentum, and ℓ_2 regularization. This demonstrates that by also changing the optimization landscape *far* from good models, regularization plays a role that has not received much attention, namely effecting the *dynamics* of the search for good models.

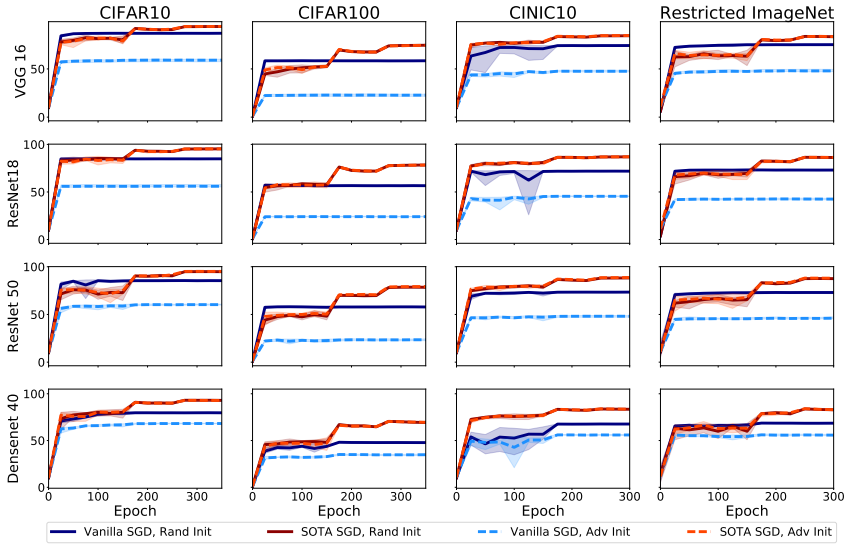


Figure 2: Test accuracy (%) vs number of epochs on CIFAR, CINIC10 and Restricted ImageNet on all four neural network models.

The Effect of the Replication Factor R on Test Error Here, we report the test accuracy effect of the replication factor R, *i.e.*, the number of randomly labeled augmentations that are applied to each point during adversarial initialization. In Figure 3, we plot the test accuracy performance for all networks we tested as a function of the number of the randomly labeled augmentations R. When we vary R we observe that SOTA SGD essentially achieves the same test error, while the test performance of vanilla SGD degrades, initially fast, and then slower for larger R.

We would like to note that although it would be interesting to make R even bigger, the time needed to generate the adversarial initializer grows proportional to R, as it requires training a data set (of size proportional to R) to full accuracy.

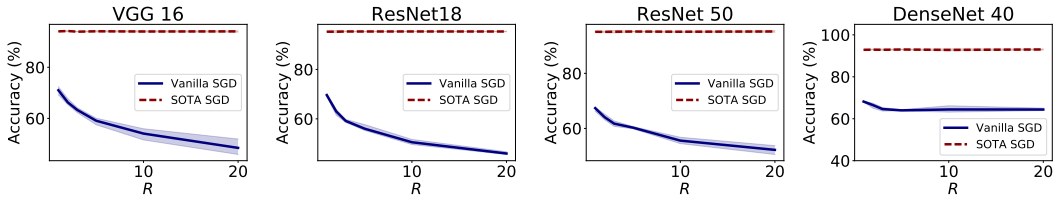


Figure 3: The effect of R on CIFAR10, the zero-out ratio is fixed to 10%. Clearly, increasing R causes vanilla SGD to suffer more. In contrast, SOTA SGD is always unaffected.

3 Conclusion

In this work, we show that not only bad *global* minima exist, *i.e.*, models that fit the training set perfectly, yet have poor generalization but, moreover, that these bad global minima are attractive to SGD even from initializations constructed from *unlabeled* data. We also demonstrate empirically that regularization rescues SGD from these adversarial initializations.

We believe that the main value of our work is in pointing out the role played by regularization in enabling SGD to escape from our adversarial initializations. Not because we consider such initializations particularly important in and of themselves, but because the phenomenon observed highlights the role of regularization in altering the dynamics of the search for good models. In other words, while the typical view of regularization is as a way to distinguish between good models (by minimizing risk), our work shows that the alteration of the optimization landscape induced by regularization is highly relevant even *very far* from good models. In that sense, we view the value of our work as an invitation for further work on this seemingly germane but largely unexplored point.

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