GRADIENT-BASED OPTIMIZATION IS NOT NECESSARY FOR GENERALIZATION IN NEURAL NETWORKS

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ABSTRACT

It is commonly believed that the implicit regularization of optimizers is needed for neural networks to generalize in the overparameterized regime. In this paper, we observe experimentally that this implicit regularization behavior is *generic*, i.e. it does not depend strongly on the choice of optimizer. We demonstrate this by training neural networks using several gradient-free optimizers, which do not benefit from properties that are often attributed to gradient-based optimizers. This includes a guess-and-check optimizer that generates uniformly random parameter vectors until finding one that happens to achieve perfect train accuracy, and a zeroth-order Pattern Search optimizer that uses no gradient computations. In the low sample and few-shot regimes, where zeroth order optimizers are most tractable, we find that these non-gradient optimizers achieve test accuracy comparable to SGD.

1 INTRODUCTION

The impressive generalization of deep neural networks continues to defy conventional wisdom, where overparameterization relative to the number of data points is thought to hurt model performance. From the perspective of classical learning theory, using measures such as Rademacher complexity and VC dimension, as we increase the complexity of a model class, the generalization performance of learned models is more likely to deteriorate. However, in the case of deep learning models, we observe the exact opposite phenomenon – as we increase the number of model parameters, the performance continues to improve. This is particularly surprising since deep neural networks were shown to easily fit random labels in the overparameterized regime (Zhang et al., 2017). This combination of empirical and theoretical pointers lead to a large gap in our understanding of deep learning, which has sparked significant interest into studying various forms of implicit bias that could explain generalization phenomena.

Perhaps the most widely-held hypothesis posits that gradient-based optimization gives rise to implicit bias in the final learned network leading to better generalization (Arora et al., 2019; Advani et al., 2020; Liu et al., 2020; Galanti & Poggio, 2022). For example, (Arora et al., 2019) showed that deep matrix factorization, which can be viewed as a highly simplified neural network, is biased towards solutions with low rank when trained with gradient flow. Indeed, (Galanti & Poggio, 2022) shows theoretically and empirically that stochastic gradient descent (SGD) with a small batch size can implicitly bias neural networks towards matrices of low rank. A related concept was used by (Liu et al., 2020) to show that gradient agreement between examples is indicative of generalization in the learned model.

In this paper, we empirically examine the hypothesis that gradient dynamics is a necessary source of implicit bias for neural networks. Our investigation is based on a comparison of several zeroth order optimizers, which require no gradient computations, with the performance of SGD. We focus our studies on the small sample regime where zeroth order optimizations are tractable. Interestingly, we find that all the gradient-free optimizers we try generalize well compared to SGD in a variety of settings including MNIST (LeCun et al., 2010), CIFAR-10 (Krizhevsky, 2009), and few-shot problems (Bertinetto et al., 2019; Vinyals et al., 2016).

Even though we use fewer samples in our experiments compared to standard settings, this low-data regime highlights the role of model bias, where the generalization behavior of neural networks is particularly intriguing. The model we test has more than $10,000$ parameters, but it has to generalize with fewer than $1,000$ training samples. Without implicit bias, such a feat is nearly impossible in realistic use cases like the ones we consider. Our work shows empirically that generalization does

not require the implicit regularization of gradient dynamics, at least in the low-data regime. It is still an open question whether gradient dynamics play a larger role in other regimes, e.g., where more data is available.

We need to caution that we are not claiming that gradient dynamics have no effect on generalization, as it has been clearly shown both theoretically and empirically that it has a regularizing effect (Arora et al., 2019; Galanti & Poggio, 2022). Instead, we argue that the implicit regularization of gradient dynamics is only secondary to the observed generalization performance of neural networks, at least in the low-data regimes we study.

The observations in this paper supports the *volume hypothesis* for generalization: The implicit bias of neural network may arise from the volume disparity of different basins in the loss landscape, with good hypothesis classes occupying larger volumes. The conjecture is empirically supported by the observation that even a "guess & check algorithm," which randomly samples solutions from parameter space until one is found with low training error, can generalize well. The success of this optimizer strongly suggests that generalizing minima occupy a much larger volume than poorly generalizing minima in neural loss functions, and that this volume disparity alone is enough to explain generalization in the low-shot regime.

Finally, we use a simple quadratic regression model to illustrate how overparameterization may help increase volume of a certain hypothesis class and thus implicitly bias the learned function towards good minima, regardless of the choice of optimizer.

2 Related Work

The capability of highly overparametrized neural networks to generalize remains a puzzling topic of theoretical investigations. Despite their high model complexity and lack of strong regularization, neural networks do not overfit to badly generalizing solutions. From a classical perspective, this is surprising. Bad global solutions do exist (Zhang et al., 2017; Huang et al., 2020), yet usual training routines that optimize neural networks with stochastic gradient descent never find such worst-case solutions. This has led a flurry of work re-characterizing and investigating the source of the generalization ability of neural networks. In the following we highlight a few angles.

High-Dimensional Optimization Before reviewing the literature on gradient dynamics, we want to review the underlying reasons why gradient-based (first-order) optimization is so central to deep neural networks: The core reasons for this is often dubbed the *curse of dimensionality*: For arbitrary optimization problems (with minimal conditions, i.e. (Noll, 2014)) a first-order optimizer will converge to a local minimal solution in polynomial time in the worst-case, independent of the dimensionality of the problem. However, a zeroth order algorithm without gradient information will have to, in the worst-case, evaluate a number of queries that increases exponentially with the dimensionality of the problem, even for smooth, convex optimization problems (Nesterov, 2004). However as we will discuss, neural networks are far from a worst-case scenario, given that many solutions exist due to the inter-connectedness of minimas in neural networks.

Gradient Dynamics Here we briefly review literature that argues gradient descent as the main implicit bias for generalization of neural networks. In Liu et al. (2020), they argue that deep networks generalize well because of the large agreement of gradients among training examples using a quantity called gradient signal to noise ratio (GSNR). They found both empirically and theoretically that a large GSNR would lead to better generalization and that deep networks induce a large GSNR during training, leading to better generalization. Arora et al. (2019) show that the dynamics of gradient-based optimization induce implicit bias that is stronger than typical norm-based bias in the setting of deep matrix factorization, and raise the question whether implicit biases can be induced from first-order optimization that cannot be captured by any explicit regularization. Advani et al. (2020) argues that in the overparameterized regime, the gradient dynamics prevent learning from happening in certain subset of weights, which effectively works as implicit regularization. A recent paper by (Galanti & Poggio, 2022) proves that SGD trained networks have a low rank implicit bias and hypothesizes that such an implicit bias may be the source of superior generalization for deep neural networks.

Non-gradient Based Explanation of Implicit Bias Several works have tried to explain the generalization behavior of neural networks with non-gradient based implicit regularization. Neyshabur

et al. (2015) argues weight norms to be the main measure of capacity control that allows neural networks to generalize. Keskar et al. (2016) suggests that flatness in the parameter space corresponds to simpler functions, thus allowing neural networks to generalize. However, Dinh et al. (2017) later show that when the flatness measure is not scale-invariant, sharp solutions can generalize just as well with appropriate rescaling of the network parameters. Valle-Perez et al. (2018) argue that the parameter-function map is exponentially biased towards simple functions. Rahaman et al. (2019) shows that neural networks are biased toward low frequency functions that vary globally without local fluctuation. Among all works that try to explain neural network generalization, most recent works argue gradient descent or stochastic gradient descent as the main implicit bias of neural network training that allows deep overparameterized networks to generalize.

Volume and Bayesian Modeling From a Bayesian perspective, flat minima of the loss surface are highly represented in the Bayesian model average, especially when they contain functional diversity (Wilson & Izmailov, 2020). The size of a posterior peak has also been connected to Occam factors indicating that they represent simpler solutions which are more compressible and generalize well (MacKay et al., 2003). Smith & Le (2017) studies generalization behavior of overparameterized linear models where they find that the Bayesian evidence or marginal likelihood, which is connected to generalization, strongly favors flat minima. A line of work on PAC-Bayes generalization bounds, which is related to compressibility and the Bayesian evidence, uses compressibility to guarantee generalization and finds the flat minima are more compressible as they yield more bits back from the KL-divergence term in the bound (Dziugaite & Roy, 2017). In contrast to these works, our findings focus not on why flat minima generalize well but rather demonstrate that we can find them with or without gradient-based optimization.

Similar Lines of Inquiry Mingard et al. (2021) empirically show that when sampling from wide networks conditioned on the training set, the sampled models behave similarly to finite width networks trained with SGD. They approximate the posterior with Neural Network Gaussian Process, which is not exact in finite width networks. Geiping et al. (2022) show that full batch gradient descent, when coupled with explicit regularization can perform comparably to model trained with SGD, thus bringing into question the importance of SGD for generalization. Similar in spirit, we argue that SGD and all gradient-based optimizers are not the main source of generalization behavior of neural networks.

3 THE MYSTERY OF GENERALIZATION WITH OVERPARAMETERIZATION

In this section, we illustrate how the complexity of a hypothesis class increases with the number of parameters in the context of a simple classification problem. Specifically, we increase the number of hidden units of a two layer neural network and showcase the increasing complexity of the model class. Despite this increased complexity, SGD often consistently finds good classifiers. Then, we proceed to show that a similar generalization behavior can be achieved without any gradient dynamics.

We begin with a toy classification problem defined over two classes where the data distribution is a wedge "Λ" with a vertical margin separating the two classes (see Figure 1). Throughout this section, our training and testing data consist of 11 points and 5 points, respectively, each sampled uniformly at random.

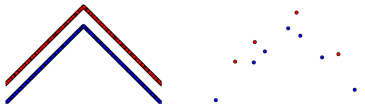


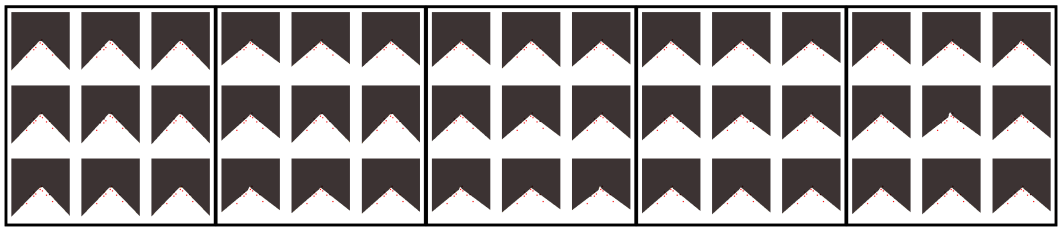
Figure 1: On the left, we have the true underlying distribution of the toy problem. On the left, we have the sampled training data.

3.1 OVERPARAMETERIZATION INCREASES MODEL COMPLEXITY

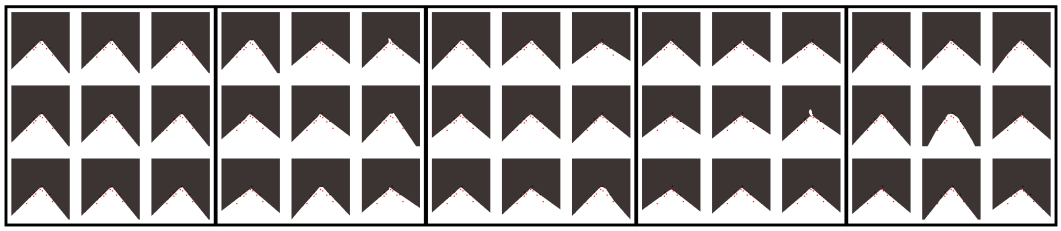
To illustrate how the model complexity increases with number of parameters, we first poison a model by minimizing the loss on the training data while maximizing the loss on the testing data. Given we only examine cases where the model (trained by SGD) achieves 100% training accuracy, this represents the worst-case decision boundary for the unpoisoned loss. As we increase the number of hidden units from 2 to 20, the decision boundary becomes much more ill-behaved (see Figure 2a). When the hypothesis class is restricted to 2 hidden units (the left most plots in Figure 2a), the model can only fit the data by using a single kink in the decision boundary, so it has to trade off either

Figure 2: In this figure, we show that even though the model becomes much more expressive as we increase the number of parameters, as shown in the possible decision boundaries of the poisoned network of various sizes, *both SGD and Guess & Check produce decision boundaries that are relatively stable* as we increase the number of parameters. From left to right, we have decision boundaries produced by 2, 4, 10, 15, 20 hidden units single layer neural networks with different training methods. For each (training method, model size) pair, we show 9 randomly sampled decision boundaries of the trained network. We showed even more samples of the decision boundaries in Appendix A

(a) Decision boundaries of a poisoned neural network



(b) Decision boundaries of SGD trained models



(c) Decision boundaries of Guess & Check trained models

fitting the training examples to 100% accuracy or performing badly on the poison objective. Given that the model fits training data, it has to perform well on testing data. This is consistent with the under-parameterized regime and with classical learning theory.

As we increase the model size, the model class now contains strange decision boundaries that can fit training data while performing poorly on the testing data. From the perspective of classical learning theory, we would expect models with 20 hidden units to perform much worse than the model with 2 hidden units. Surprisingly, even though more complicated decision boundaries are available as we increase the model size, we never see such boundaries when optimizing the (unpoisoned) training objective with SGD. For example, in Figure 2b, as we increase the number of hidden units, the decision boundary remains relatively consistent. Given that both the weird and nice decision boundaries exist in the model class, it is natural to ask what biases the learned network towards good vs. bad optima.

Due to the consistent behavior of SGD trained networks in the overparameterized regime, it is only reasonable that people started investigating gradient dynamics as a source of implicit regularization (Galanti & Poggio, 2022; Arora et al., 2019; Advani et al., 2020; Liu et al., 2020). However, we show below that, rather surprisingly, we can obtain similar generalization behavior on the toy problem by using a Guess & Check algorithm that is completely free of gradient dynamics.

3.2 Generalizing on toy problem without gradients

In our toy setting, we find that generalization is surprisingly generic with respect to the dynamics of optimizers. To avoid using optimizers with the same inductive biases as gradient methods, we experiment with Guess & Check: we repeatedly sample parameters until a model achieves 100%

training accuracy with train loss below a certain threshold. Unlike other optimizers, we do not use any gradient information, and we also do not take any iterative steps. Surprisingly, even with Guess & Check, we often end up with a well-behaving decision boundary like the one that we trained with regular SGD see Figure 2c.

From the simple two class toy problem, we can see clearly that Guess & Check solutions already endow the learned model with a very strong implicit bias that does not originate from gradient dynamics. In the next section, we extend a similar analysis to common datasets such as MNIST & CIFAR10 to see whether this observation continues to hold in more practical settings.

4 EXPERIMENTS

4.1 NON-GRADIENT BASED OPTIMIZERS

In our experiments, we test three different non-gradient based optimizers: Guess & Check, Pattern Search, and Greedy Random Search on varying scales of MNIST & CIFAR-10 and on different architectures. Here, we explain each optimizer.

4.1.1 GUESS & CHECK

Under the Guess & Check algorithm, we randomly draw a parameter vector uniformly from $[-1, 1]$ and independently for each parameter. If the randomly sampled model achieves 100% training accuracy and achieves training loss below a certain threshold, then the model is kept and the optimizer terminates.

With this optimizer, the likelihood that a set of solutions are selected is exactly proportional to the volume of solutions in parameter space. If a model generalizes well when trained with Guess & Check, then we know that solutions which generalize well have large volume among low-loss parameters. We do want to make a distinction between flat solutions (Keskar et al., 2016) and solutions with large volumes. It is possible that a collection of solutions has a very large volume, but is not itself a flat basin by containing many small volume regions that have large volume in aggregate.

When we train with Guess & Check, we can also be confident that gradient based implicit regularization plays no role in the final performance. In Appendix C, we also show that the results do no differ materially when using a different sampling interval.

Naïve guess-and-check suffers from the problem that the cost of interpolating the training data becomes exponentially expensive as the number of training examples or classes increase, so we have restricted experiments with Guess & Check to smaller sample sizes.

4.1.2 LOCAL NON-GRADIENT BASED OPTIMIZER

Due to the difficulty of scaling Guess & Check algorithm to large problems, we explore two alternative non-gradient based optimizers, Pattern Search and Random Greedy Search, that work for bigger datasets. Like SGD, both approaches update the model using a local search and may have biases that originate from factors other than volume alone. The success of Pattern Search and Random Greedy demonstrates that gradients are not *strictly* needed to observe implicit regularization, but we caution that they may exploit regularization properties of local search that are also exploited by SGD.

Pattern Search Pattern Search randomly selects a parameter in the model and takes a step of fixed size that is randomly chosen to be either positive or negative, if the model achieves lower loss after taking the step, then the parameter is accepted as the new starting point. If Pattern Search fails to find a step that decreases the loss after going through all the parameters, then the step size is decreased by a constant factor. We repeat this procedure until a solution is found that achieves 100% training accuracy. In our experiments, we use a starting radius of 1, and we decrease the radius by a factor of 2 when it fails to find a descent direction.

Random Greedy Search Random Greedy Search adds Gaussian noise to the initial parameter vector with standard deviation of σ. If the noised solution improves training loss, then the noised solution is accepted as a new starting point. If no solution is found after a fixed number of steps, then σ is decreased by a chosen factor before the search continues. Again, we repeat this procedure

Table 2: On the two class MNIST problem, G&C performs comparably to SGD across different train loss level and number of samples. This shows us that despite the large number of parameters, G&C solutions are implicitly regularized. To show that the degree of generalization of G&C is indeed substantial, we train an additional linear model, which has a much more restricted hypothesis class, but has on average 10% worse generalization performance. The empty cells correspond to linear models where we could not find solutions with 100% training accuracy. We also show the estimated standard deviations of the averages computed over 175 random data split and training seeds. For most cells, the standard deviation is less than 1%.

Sample Count	**Arch**	**Optimizer**	**Best Test Acc** (0.3, 0.35)	**Train Loss** (0.35, 0.4)	(0.4, 0.45)	(0.45, 0.5)	(0.5, 0.55)	(0.55, 0.6)	(0.6, 0.65)	
32	LeNet	G&C	93.02%±0.27%	93.02%±0.27%	92.39%±0.29%	90.59%±0.34%	89.18%±0.38%	87.22%±0.43%	86.23%±0.44%	83.15%±0.51%
	LeNet	SGD	**94.04%±0.25%**	-	-	94.04%±0.25%	93.49%±0.28%	92.54%±0.28%	91.63%±0.33%	88.60%±0.35%
	Linear	SGD	84.75%±0.47%	84.75%±0.47%	82.69%±0.43%	81.24%±0.44%	79.04%±3.14%	78.94%±4.74%	-	-
16	LeNet	G&C	89.21%±0.47%	89.21%±0.47%	87.01%±0.50%	85.18%±0.56%	84.69%±0.54%	81.91%±0.62%	78.61%±0.65%	75.37%±0.63%
	LeNet	SGD	**91.24%±0.40%**	91.24%±0.40%	90.87%±0.41%	90.84%±0.38%	88.77%±0.48%	87.93%±0.48%	86.98%±0.47%	83.90%±0.49%
	Linear	SGD	80.68%±0.55%	80.68%±0.55%	78.50%±0.56%	75.69%±0.60%	72.09%±0.56%	67.16%±0.67%	69.51%±3.40%	-
8	LeNet	G&C	83.05%±0.67%	83.05%±0.67%	80.72%±0.75%	78.23%±0.81%	78.05%±0.72%	76.40%±0.79%	70.76%±0.74%	67.48%±0.78%
	LeNet	SGD	**84.82%±0.63%**	83.63%±0.63%	84.82%±0.63%	82.62%±0.74%	81.85%±0.72%	79.70%±0.70%	79.74%±0.63%	76.51%±0.71%
	Linear	SGD	74.29%±0.72%	74.29%±0.72%	71.72%±0.75%	67.79%±0.69%	67.36%±0.76%	63.46%±0.75%	58.65%±0.79%	54.87%±0.75%
4	LeNet	G&C	76.28%±0.90%	76.28%±0.90%	73.93%±0.92%	72.63%±0.86%	70.89%±0.90%	68.27%±0.83%	65.63%±0.92%	62.38%±0.91%
	LeNet	SGD	**77.35%±0.81%**	77.35%±0.81%	75.01%±0.85%	75.61%±0.83%	73.95%±0.85%	73.28%±0.85%	69.15%±0.84%	67.65%±0.84%
	Linear	SGD	65.12%±0.81%	65.12%±0.81%	61.94%±0.82%	62.14%±0.78%	58.11%±0.88%	57.21%±0.91%	55.38%±0.88%	53.60%±0.83%
2	LeNet	G&C	66.89%±1.04%	66.89%±1.04%	65.87%±1.05%	64.03%±0.92%	62.81%±0.90%	61.02%±0.84%	59.90%±0.91%	56.82%±0.95%
	LeNet	SGD	**69.67%±0.98%**	69.67%±0.98%	67.11%±0.93%	64.94%±0.95%	63.42%±0.87%	64.38%±0.88%	63.82%±0.89%	62.33%±0.87%
	Linear	SGD	58.93%±0.94%	58.93%±0.94%	58.45%±0.92%	56.59%±0.89%	54.11%±0.91%	54.21%±0.87%	53.13%±0.93%	51.59%±0.89%

until a parameter is found that achieves 100% training accuracy. In our experiment, we start the procedure with $\sigma = 1$. If we fail to find a perturbation that decreases loss after 30000 random steps, then we decrease σ by a factor of 2.

4.2 Results on 2-Class CIFAR-10/MNIST

In this section, we apply the Guess & Check algorithm on a conventional LeNet model on MNIST (LeCun et al., 2010) and CIFAR-10 (Krizhevsky, 2009). Due to the exponential time complexity of the Guess & Check algorithm, we stick with 2-class problems with fewer than 32 total training samples. To enable fair comparisons between G&C and SGD optimized models, we compare the performance of the models across different train loss levels after the the model's weights have been normalized. This is crucial for a fair comparison because it has been observed that lower loss level corresponds to better generalization even after train accuracy has reached 100%.

MNIST # Samples	Val. Acc.	CIFAR # Samples	Val. Acc.
32	0%	24	0%
16	0%	16	0%
8	0%	8	0%
4	0%	4	0%
2	0%	2	0%

Table 1: Comparing poisoned validation error. In this table, we attempt to fit the training data of various sizes while poisoning the LeNet with the wrong validation labels. We find that the LeNet that we use is of sufficient capacity that it can completely fit the training data while failing to classify the validaiton set.

We find that given the same loss level and number of samples, Guess & Check performs comparably to SGD, especially at lower loss levels. In the case of CIFAR-10, Guess & Check even outperforms SGD solutions by a substantial margin. This result is made even more interesting given that the models are capable of pathological overfitting: they are able to completely misclassify the validation set while achieving 100% training accuracy (see Table 1).

To illustrate how well G&C performs, we also train a linear model on MNIST for comparison. Even though the hypothesis class is now restricted to only linear solutions, a significantly smaller hypothesis class compared to LeNet, the linear model still underperforms the Guess & Check solution on LeNet by more than 10% in many cases. Note that, despite being convex, solutions of the linear problem vary because we use SGD and apply early stopping when the desired loss level is achieved.

Even though the number of samples is small, we do note that this regime highlights the effects of overparametrization. For example, in our LeNet for MNIST, we have 11074 parameters, which is orders of magnitude larger than the number of examples. Yet the model continues to generalize well relative to SGD, showing us that the large volume of the good solution set is on its own enough to bias the optimizer towards favorable generalization.

Even though the generalization performance is similar between the SGD and G&C solutions, we do note that the test accuracies are not exactly the same between models trained with both methods, implying that SGD may have additional bias that G&C does not take into account. However, our main argument is that optimizer-specific bias is not needed to explain generalization, and may not even

Table 3: On the two class CIFAR10 problem, G&C performs comparably to SGD across different training losses and numbers of samples. This shows us that, despite the large number of parameters, G&C solutions are implicitly regularized. We do note that G&C in this low data regime consistently performs better than SGD though. We computed the standard deviation over 75 random data splits and training seeds.

Sample Count	**Optimizer**	**Best Test Acc**	**Train Loss** (0.55, 0.57)	(0.57, 0.59)	(0.59, 0.61)	(0.61, 0.63)	(0.63, 0.65)	(0.65, 0.67)
24	G&C	**66.59%±0.74%**	66.59%±0.74%	65.91%±0.80%	64.09%±0.96%	61.08%±0.89%	59.33%±0.88%	57.18%±0.89%
	SGD	63.16%±0.87%	63.16%±0.87%	62.02%±0.84%	60.74%±0.73%	58.21%±0.75%	57.62%±0.69%	56.24%±0.55%
16	G&C	**61.10%±0.98%**	61.10%±0.98%	59.54%±0.98%	59.21%±0.90%	57.53%±0.86%	57.71%±0.81%	55.06%±0.70%
	SGD	58.98%±0.69%	58.58%±0.77%	58.98%±0.69%	57.86%±0.79%	57.11%±0.61%	56.77%±0.62%	53.90%±0.50%
8	G&C	**57.17%±0.94%**	54.39%±0.80%	53.99%±0.76%	57.17%±0.94%	54.61%±0.68%	52.66%±0.66%	52.82%±0.62%
	SGD	56.76%±0.71%	56.76%±0.71%	55.02%±0.62%	54.79%±0.72%	54.62%±0.68%	53.39%±0.66%	53.53%±0.55%
4	G&C	**55.51%±0.84%**	55.51%±0.84%	53.59%±0.96%	52.78%±0.82%	52.30%±0.67%	52.38%±0.63%	54.07%±0.72%
	SGD	53.75%±0.62%	53.49%±0.68%	52.14%±0.51%	53.75%±0.62%	51.53%±0.63%	52.18%±0.66%	50.44%±0.55%
2	G&C	**52.39%±0.67%**	51.66%±0.74%	52.39%±0.67%	52.00%±0.60%	51.37%±0.56%	50.01%±0.71%	50.66%±0.62%
	SGD	51.98%±0.59%	51.93%±0.66%	51.39%±0.47%	51.98%±0.59%	51.16%±0.48%	50.65%±0.45%	50.05%±0.43%

Table 4: In this table, we trained the same LeNet, but with more examples and more classes. We found that the generalization performance is still fairly similar between SGD and alternative zeroth order optimizers that do not use any gradient information. The empty cells indicate the the experiment has timed out, and we failed to find models achieving 100% training accuracy within a reasonable time limit.

	Sample Count	1000	500	300	100
MNIST	SGD	93.46%±0.11%	90.15%±0.22%	**87.48%±0.26%**	**78.67%±0.51%**
	Pattern Search	**93.68%±0.12%**	90.33%±0.12%	87.26%±0.30%	78.43%±0.46%
	Random Greedy	93.34%±0.08%	**90.35%±0.10%**	87.33%±0.21%	78.51%±0.50%
CIFAR-10	SGD	**36.01%±0.25%**	29.91%±0.31%	**25.88%±0.34%**	**19.86%±0.27%**
	Pattern Search	-	**30.00%±0.69%**	25.04%±0.66%	18.70%±1.22%
	Random Greedy	34.44%±0.54%	27.06%±0.75%	24.04%±0.58%	16.80%±0.13%

be the primary cause of generalization behavior; in our experiments here, the bulk of generalization can be explained by the geometry of the loss landscape.

4.3 Results on 10-class CIFAR-10/MNIST

In this section, we evaluate the importance of gradient based optimizers in the setting where more classes are involved. However, the Guess & Check algorithm is no longer feasible due to the exponential time complexity. Instead of Guess & Check, we employ Pattern Search and Greedy Random Search to evaluate the dependence of generalization on gradient based optimizers. Again, we find that these non-gradient based optimizers offer similar levels of generalization benefits as SGD despite not using any gradient information at all.

In Table 4, we see that Greedy Random Search and Pattern Search both generalize comparably to SGD. The average performance difference is only 0.9% across different sample sizes, datasets, and optimizer combinations. In several cases, Pattern Search even performs better than SGD. Even though 0.9% may seem large when viewed from the perspective of achieving state-of-the-art accuracy, we note that a performance difference of 0.9% is within the margin that can be expected from hyperparameter tuning, and that we have not tuned either of the zeroth order optimizers, and yet they still achieve a comparable level of generalization to SGD.

4.4 Few-Shot Learning with ResNets

In this section, we evaluate the importance of gradient-based optimizers in the few-shot setting where we can evaluate the importance of gradient-based optimization on an industrial-scale model. For the most part, we find that non-gradient based optimizer Pattern Search performs comparably to SGD in the 1-shot setting.

Few-shot learning is usually used to test the ability of models to generalize to unseen tasks given limited training examples. This is a perfect evaluation task for our hypothesis for the following reasons: First, in few-shot learning, we only use 1 or 5 training images per class during the evaluation stage which makes zeroth order optimization possible. Second, few-shot learners usually utilize a

Table 6: We show that when we increase the number of polynomial terms p, the likelihood that a Guess & Check solution is close to the true linear model becomes higher. In other words, we have increased the likelihood of linear solutions relative to higher order polynomial solutions in the parameter space by overparameterization.

k	-2			-1			1			2		
degree of polynomial p	1	2	3	1	2	3	1	2	3	1	2	3
$P(\lvert b-k\rvert < \tau_{thres} \mid loss < \tau_{loss})$	8.70%	50.07%	61.67%	31.90%	61.86%	64.69%	31.92%	61.85%	64.69%	11.54%	50.10%	61.68%

pre-trained feature extractor on the base classes, and only learn a new classification head by SGD or other solvers such as SVM and ridge regression (Lee et al., 2019; Bertinetto et al., 2019) given the unseen tasks. This setting limits the dimension of learnable parameters, thus making training deeper networks such as ResNet possible with these non-gradient based optimizers. Finally, although we only attempt to learn a single layer, due to the few training examples (1 or 5 per class), we will still have an overparameterized model which is the setting we are interested in.

We evaluate the effectiveness of non-gradient based optimizers on CIFAR-FS (Bertinetto et al., 2019)and mini-ImageNet (Vinyals et al., 2016) with ResNet-12, a commonly used architecture in the few-shot classification literature. During the training stage, we pre-train a feature extractor on the base classes and evaluate the generalization on unseen tasks via 1-shot-5-way episodes, where each episode is a 5-way classification problem and each class contains 1 training image. During the evaluation stage, given the unseen episodes and pre-trained feature extractor, we learn a new classification head with a specific optimizer and evaluate the performance on the testing images. We compare the testing accuracy on 600 different episodes between SGD, and Pattern Search in Table 5. For Pattern Search, instead of stopping optimization immediately after fitting all the training examples, we keep updating the model until t steps, where we set $t = 3000$ for both CIFAR-FS and mini-ImageNet. As showed in Table 5, Pattern Search always outperforms SGD by a large margin, i.e., over 2% for both CIFAR-FS and mini-ImageNet, which suggests that gradient-based optimizers are not necessary for generalization in the few-shot setting.

Table 5: 1-shot-5-way classification performance on both CIFAR-FS and mini-ImageNet with ResNet-12 backbone. We provide mean test accuracy over 600 episodes and the one standard error. Compared to SGD, Pattern Search can always achieve better performance by a large margin.

Optimizer	CIFAR-FS	mini-ImageNet
SGD	68.35 ± 0.46	55.76 ± 0.42
Pattern Search	$\mathbf{70.25 \pm 0.45}$	$\mathbf{58.53 \pm 0.41}$

5 Toy Example: Volume and Simplicity Bias

In this section, we use a toy quadratic regression problem to illustrate one mechanism by which overparameterization can implicitly bias learned functions towards a particular hypothesis class by increasing its volume. Here, we define volume explicitly as the likelihood that a family of hypotheses is selected by G&C. At the end, we also show that volume may explain simplicity bias previously observed in Shah et al. (2020).

We consider toy problems with just two training examples, x_1, y_1 and x_2, y_2. The goal is to regress the points with a polynomial model of the form $f(x; \mathbf{a}, b, c) = \sum_{i=1}^{p} a_i x^p + bx + c$, which is parameterized by $\mathbf{a}$, b and c and where p represent the maximum power of the polynomial. Since we have only two data points, but many parameters, this problem is under determined. This is where bias, whether implicit or explicit, becomes very important for generalization.

One way of adding inductive bias is by simply applying a regularizer to the parameters. For example, if we believe the model is most likely a linear function, then we can apply a square penalty to a. However, most neural networks continue to generalize exceedingly well without explicit regularization, so we are more interested in an alternative way of enforcing such bias.

Here, we propose another way of biasing the network towards linear solutions. We can do so by increasing the number of terms associated with the linear term. The intuition is that as we use more linear terms, we artificially create more volume corresponding to near-linear functions. As opposed to using the original parameterization, we can overparameterize the original function as follows:

$$f(x; \mathbf{a}, \mathbf{b}, c) = \epsilon_{poly} \sum_{i=1}^{p} a_i x^p + \epsilon_{linear} \sum_{i=1}^{p} b_i x + c. \tag{1}$$

If $a_1, a_2, ...a_p, b_0, b_1, ..., b_p, c$ are Gaussian with the same standard deviation, we can show empirically that an expression with more terms associated with the first degree monomial, x, will have a stronger bias towards near-linear models. We test this on a data generating distribution of $y = kx$ where k is the term that we are trying to learn. We let $x_1 = -0.2$, $x_2 = 1$, $\epsilon_{poly} = 0.01$, $\epsilon_{linear} = 0.4$, and then we generate the corresponding regression label with different k. We then train the regression model with Guess & Check where a model is only accepted if the MSE loss is lower than $\tau_{loss} = 0.02$. To understand whether Guess & Check is biased towards linear functions, we can estimate the probability that a linear model close to the original $y = kx$ is selected. Specifically, we can evaluate the following,

$$\mathbb{P}\left(|\epsilon_{linear}\sum_i b_i - k| < \tau_{thresh} \middle| \sum_{j=1}^{2}(f(x_j) - y_j)^2 < \tau_{loss}\right), \tag{2}$$

which is the probability of finding a linear model where $b = \epsilon_{linear}\sum_i b_i$ is no more than τ_{thresh} from the true parameter k. Here, we set $\tau_{thresh} = 0.1$

In Table 6, we see that as we increase the number of polynomial terms, the Guess & Check solution becomes more biased towards the ground truth linear function even though the size of the hypothesis class has increased. This toy example shows that it is possible for over-parameterization to impact bias, although neural networks likely rely on more complex mechanisms.

5.1 Simplicity bias may originate from the volume bias as opposed to SGD

While we have mostly measured bias in terms of generalization in this paper, we think it is a promising future direction to quantify whether other forms of bias can be attributed to the volume hypothesis instead. One example is simplicity bias, where trained neural networks strongly prefer linear decision boundaries compared to robust ones. We provide a toy illustration on why this may be attributed to the volume hypothesis, but leave further exploration of this as future work.

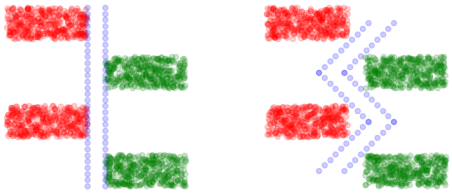


Figure 3: The volume of the decision boundary on the left as measured by G&C is 10^{-4} whereas the volume of the robust/complex decision boundary has volume smaller than 10^{-10}. The large volume disparity may explain trained network's strong preference for the linear solution.

Consider the following example: a trained neural network on the slab dataset ignores the more complex y-axis, as shown on the left of Figure 3, and uses a linear decision boundary drawn along the x-axis only as opposed to the robust decision boundary shown on the right of Figure 3. While Shah et al. (2020) has attributed the simplicity bias in this example to SGD, we found that the simplicity bias may simply originate from the large disparity in volumes between the linear and robust functions in the loss landscape. In fact, when we used G&C to measure the volume of the two respective decision boundaries in the parameter space, we found that the linear decision boundary has volume that is 6 orders of magnitude larger than that of the robust decision boundary. Specifically, we estimate the volume of the solution by taking the reciprocal of the number of guesses before a solution is obtained. The volume disparity may explain why the simple decision boundary is strongly preferred compared to the alternative.

6 Conclusion

In this paper, we empirically show that gradient-based implicit regularization of training dynamics is not required for generalization. Instead, we consider non-gradient optimizers that lack gradient dynamics, yet still perform well. The strong performance of gradient-free optimizers, in particular Guess & Check, strongly suggests that the disparate volume of good and bad hypothesis classes is the main implicit bias that enables these optimizers to succeed. Finally, we observe that redundancy in parameters can increase the volume of simple or well-generalizing solutions. For future work, we think more critically examining the role of volume in neural network's bias will be a fruitful and interesting direction.

7 REPRODUCIBILITY STATEMENT

We ran all the experiments with prespecified random seeds, so all of the tables will be reproducible by running the respective scripts in our included code base.

REFERENCES

Madhu S. Advani, Andrew M. Saxe, and Haim Sompolinsky. High-dimensional dynamics of generalization error in neural networks. *Neural Networks*, 132:428–446, 2020. ISSN 0893-6080. doi: https://doi.org/10.1016/j.neunet.2020.08.022. URL https://www.sciencedirect.com/science/article/pii/S0893608020303117.

Sanjeev Arora, Nadav Cohen, Wei Hu, and Yuping Luo. Implicit regularization in deep matrix factorization. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper/2019/file/c0c783b5fc0d7d808f1d14a6e9c8280d-Paper.pdf.

Luca Bertinetto, Joao F. Henriques, Philip Torr, and Andrea Vedaldi. Meta-learning with differentiable closed-form solvers. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=HyxnZh0ct7.

Laurent Dinh, Razvan Pascanu, Samy Bengio, and Yoshua Bengio. Sharp minima can generalize for deep nets. In Doina Precup and Yee Whye Teh (eds.), *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pp. 1019–1028. PMLR, 06–11 Aug 2017. URL https://proceedings.mlr.press/v70/dinh17b.html.

Gintare Karolina Dziugaite and Daniel M. Roy. Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data. *CoRR*, abs/1703.11008, 2017. URL https://arxiv.org/abs/1703.11008.

Tomer Galanti and Tomaso Poggio. Sgd noise and implicit low-rank bias in deep neural networks. 03/2022 2022. URL https://cbmm.mit.edu/publications/sgd-noise-and-implicit-low-rank-bias-deep-neural-networks.

Jonas Geiping, Micah Goldblum, Phil Pope, Michael Moeller, and Tom Goldstein. Stochastic training is not necessary for generalization. In *International Conference on Learning Representations*, 2022. URL https://openreview.net/forum?id=ZBESeIUB5k.

W. Ronny Huang, Zeyad Emam, Micah Goldblum, Liam Fowl, Justin K. Terry, Furong Huang, and Tom Goldstein. Understanding Generalization through Visualizations. *arXiv:1906.03291 [cs, stat]*, November 2020. URL http://arxiv.org/abs/1906.03291.

Nitish Shirish Keskar, Dheevatsa Mudigere, Jorge Nocedal, Mikhail Smelyanskiy, and Ping Tak Peter Tang. On large-batch training for deep learning: Generalization gap and sharp minima. *CoRR*, abs/1609.04836, 2016. URL http://arxiv.org/abs/1609.04836.

Alex Krizhevsky. Learning multiple layers of features from tiny images. Technical report, 2009.

Yann LeCun, Corinna Cortes, and CJ Burges. Mnist handwritten digit database. *ATT Labs [Online]. Available: http://yann.lecun.com/exdb/mnist*, 2, 2010.

Kwonjoon Lee, Subhransu Maji, Avinash Ravichandran, and Stefano Soatto. Meta-learning with differentiable convex optimization. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 10657–10665, 2019.

Jinlong Liu, Yunzhi Bai, Guoqing Jiang, Ting Chen, and Huayan Wang. Understanding why neural networks generalize well through gsnr of parameters. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=HyevIJStwH.

David JC MacKay, David JC Mac Kay, et al. *Information theory, inference and learning algorithms*. Cambridge university press, 2003.

Chris Mingard, Guillermo Valle-Pérez, Joar Skalse, and Ard A. Louis. Is sgd a bayesian sampler? well, almost. *Journal of Machine Learning Research*, 22(79):1–64, 2021. URL http://jmlr.org/papers/v22/20-676.html.

Yurii Nesterov. *Introductory Lectures on Convex Optimization*, volume 87 of *Applied Optimization*. Springer US, Boston, MA, 2004. ISBN 978-1-4613-4691-3 978-1-4419-8853-9. URL http://link.springer.com/10.1007/978-1-4419-8853-9.

Behnam Neyshabur, Ryota Tomioka, and Nathan Srebro. Norm-based capacity control in neural networks. In *Conference on Learning Theory*, pp. 1376–1401. PMLR, 2015.

Dominikus Noll. Convergence of non-smooth descent methods using the Kurdyka–\Lojasiewicz inequality. *Journal of Optimization Theory and Applications*, 160(2):553–572, 2014. URL http://link.springer.com/article/10.1007/s10957-013-0391-8.

Nasim Rahaman, Aristide Baratin, Devansh Arpit, Felix Draxler, Min Lin, Fred Hamprecht, Yoshua Bengio, and Aaron Courville. On the spectral bias of neural networks. In *International Conference on Machine Learning*, pp. 5301–5310. PMLR, 2019.

Harshay Shah, Kaustav Tamuly, Aditi Raghunathan, Prateek Jain, and Praneeth Netrapalli. The pitfalls of simplicity bias in neural networks. *Advances in Neural Information Processing Systems*, 33:9573–9585, 2020.

Samuel L Smith and Quoc V Le. A bayesian perspective on generalization and stochastic gradient descent. *arXiv preprint arXiv:1710.06451*, 2017.

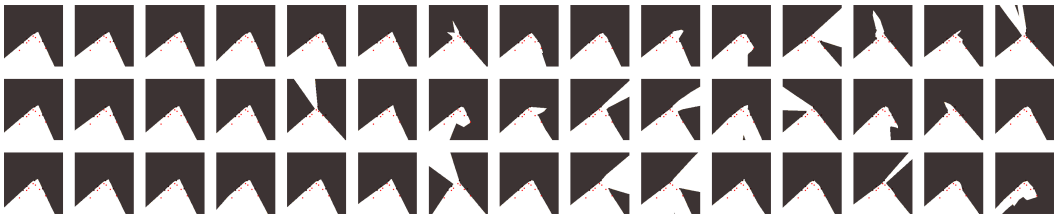
Guillermo Valle-Perez, Chico Q Camargo, and Ard A Louis. Deep learning generalizes because the parameter-function map is biased towards simple functions. *arXiv preprint arXiv:1805.08522*, 2018.

Oriol Vinyals, Charles Blundell, Timothy P. Lillicrap, Koray Kavukcuoglu, and Daan Wierstra. Matching networks for one shot learning. *CoRR*, abs/1606.04080, 2016. URL http://arxiv.org/abs/1606.04080.

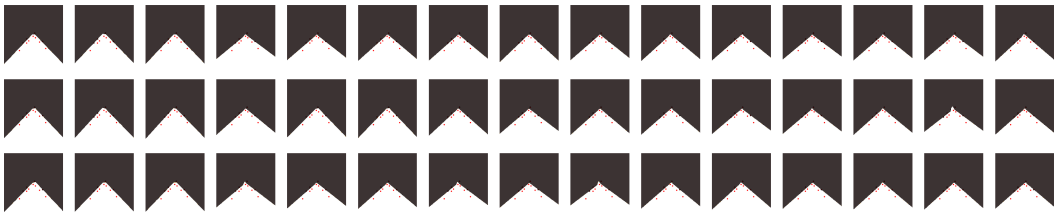
Andrew G Wilson and Pavel Izmailov. Bayesian deep learning and a probabilistic perspective of generalization. *Advances in neural information processing systems*, 33:4697–4708, 2020.

Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning requires rethinking generalization. *International Conference on Learning Representations (ICLR) 2017*, 2017. URL https://openreview.net/forum?id=Sy8gdB9xx.

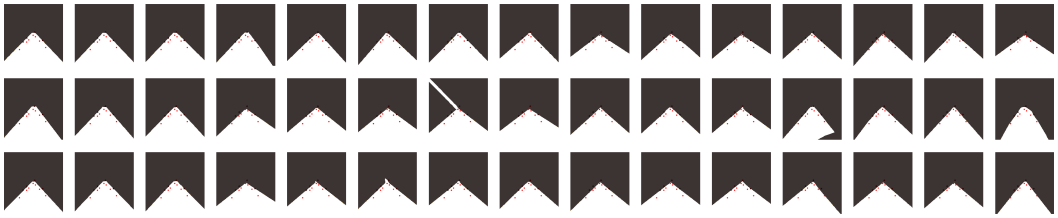
A ADDITIONAL EXPERIMENTS FOR TOY EXAMPLES



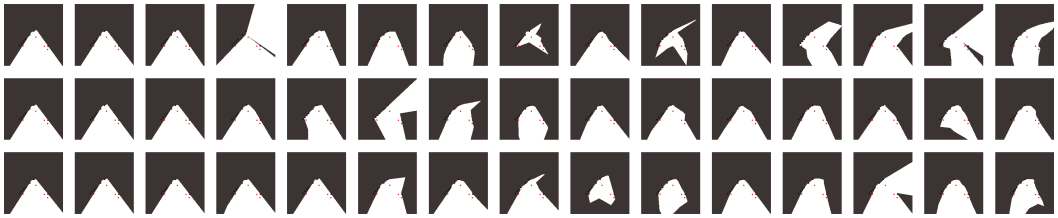
(a) Decision boundaries of a poisoned neural network - seed 0



(b) Decision boundaries of SGD trained models - seed 0



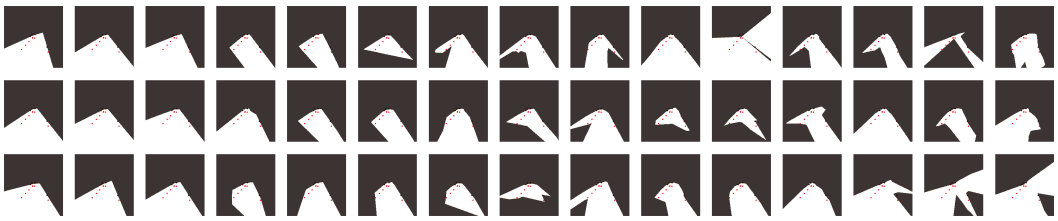
(c) Decision boundaries of Guess & Check trained models - seed 0



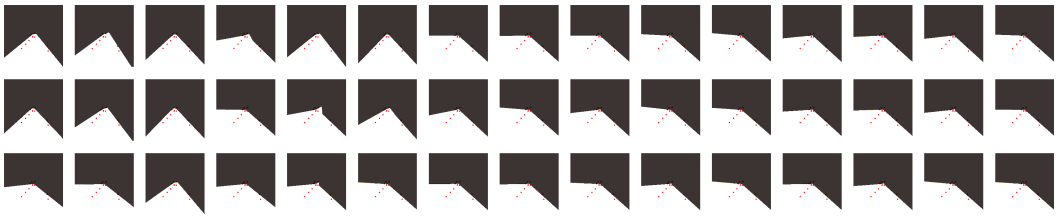
(a) Decision boundaries of a poisoned neural network - seed 1

(b) Decision boundaries of SGD trained models - seed 1

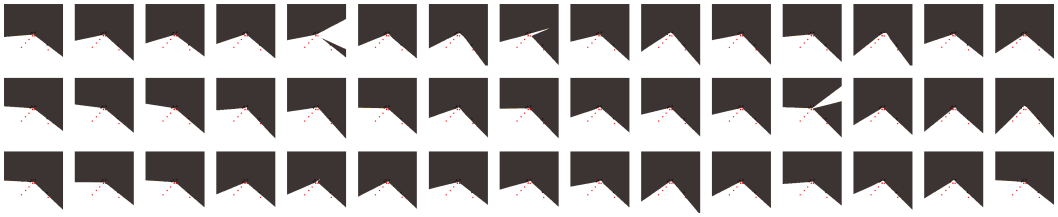
(c) Decision boundaries of Guess & Check trained models - seed 1



(a) Decision boundaries of a poisoned neural network - seed 2

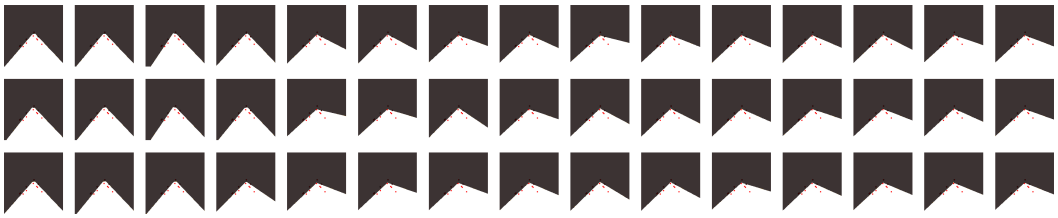


(b) Decision boundaries of SGD trained models - seed 2

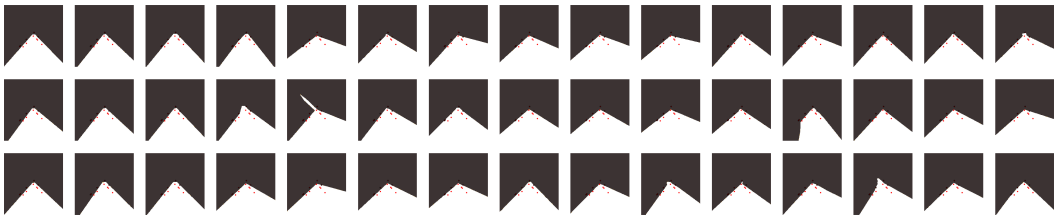


(c) Decision boundaries of Guess & Check trained models - seed 2

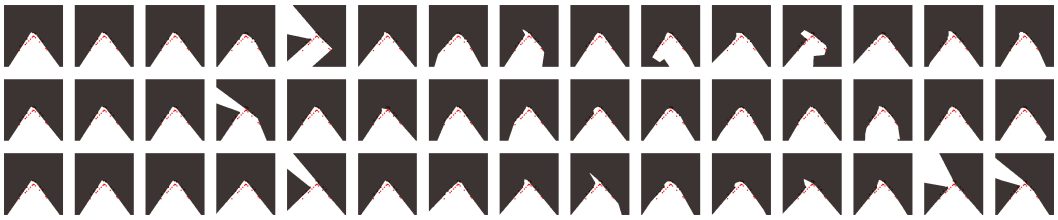
(a) Decision boundaries of a poisoned neural network - seed 3



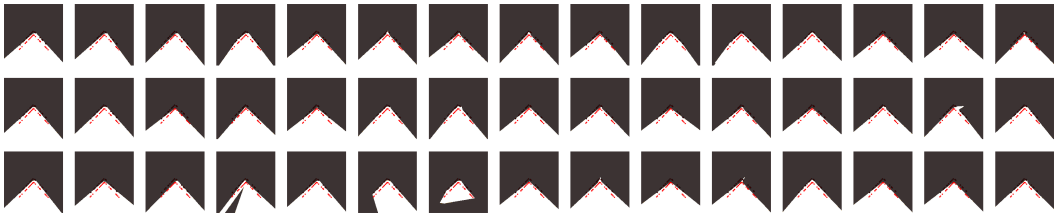
(b) Decision boundaries of SGD trained models - seed 3



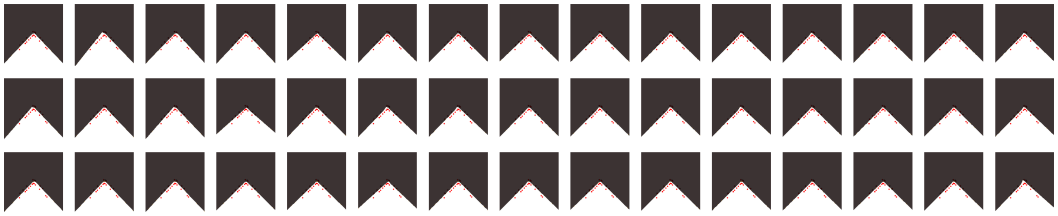
(c) Decision boundaries of Guess & Check trained models - seed 3



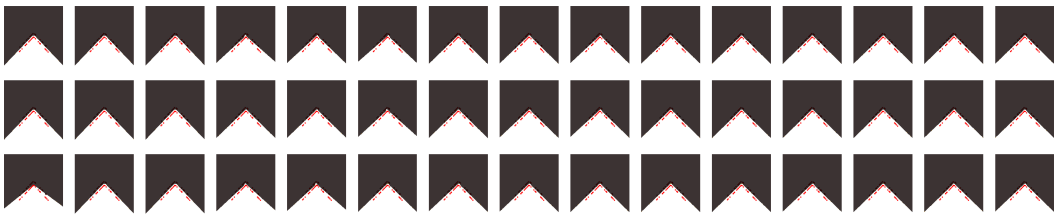
(a) Decision boundaries of a poisoned neural network 32 samples



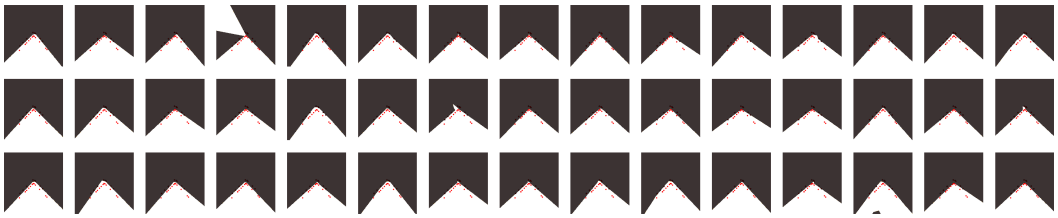
(b) Decision boundaries of a poisoned neural network 64 samples



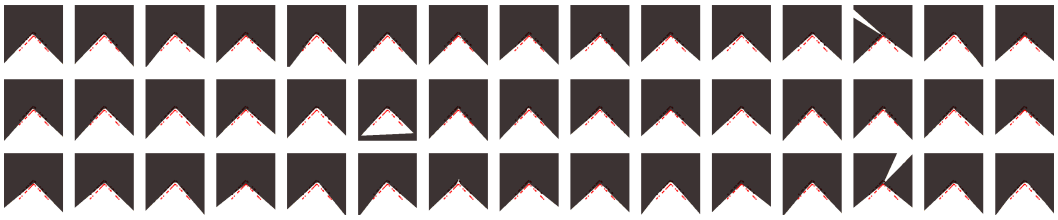
(c) Decision boundaries of SGD trained models 32 samples



(d) Decision boundaries of SGD trained models 64 samples



(e) Decision boundaries of Guess & Check trained models 32 samples



(f) Decision boundaries of Guess & Check trained models 64 samples

Figure 8: Decision boundaries as we increase the number of samples

B How does G&C behave as we scale up the model?

width	Loss Level (0.3, 0.35)	(0.35, 0.4)	(0.4, 0.45)	(0.45, 0.5)	(0.5, 0.55)	(0.55, 0.6)	(0.6, 0.65)
1	n/a	n/a	n/a	n/a	n/a	92.11%±1.35%	93.44%±n/a
0.9	n/a	n/a	n/a	n/a	90.89%±n/a	86.33%±6.81%	90.90%±3.03%
0.8	n/a	n/a	93.34%±n/a	83.89%±8.97%	87.71%±n/a	93.29%±n/a	81.94%±7.35%
0.7	97.73%±n/a	96.32%±n/a	95.20%±0.42%	92.30%±1.21%	86.10%±6.24%	80.59%±2.96%	87.37%±n/a
0.6	91.20%±1.40%	89.66%±1.88%	87.76%±2.22%	85.45%±2.07%	83.64%±2.78%	82.76%±3.33%	79.43%±3.06%
0.5	89.21%±0.47%	87.01%±0.50%	85.18%±0.56%	84.69%±0.54%	81.91%±0.62%	78.61%±0.65%	75.37%±0.63%
0.4	85.82%±0.53%	83.78%±0.61%	81.43%±0.61%	79.63%±0.65%	77.50%±0.64%	75.98%±0.66%	72.30%±0.77%
0.3	79.55%±0.60%	79.13%±0.60%	76.63%±0.72%	75.43%±0.63%	74.22%±0.66%	72.28%±0.72%	71.75%±0.67%
0.2	77.39%±0.56%	76.08%±0.63%	74.70%±0.56%	73.40%±0.60%	71.84%±0.60%	69.66%±0.64%	68.49%±0.58%

Table 7: Performance of G&C on MNIST with 16 samples as we scale up the model. The n/a indicates that a model has not been found for the cell.

In Table 7, we see that as we increase the width of the model, the validation accuracy increases. This is a surprising observation because as we increase the size of the model class, the performance of the model actually becomes better as opposed to worse, directly contradicting generalization theories based on model capacity.

C Influence of Sampling Range for Guess & Check Optimizer

	L2 Norm	Loss Level (0.3, 0.35)	(0.35, 0.4)	(0.4, 0.45)	(0.45, 0.5)	(0.5, 0.55)	(0.55, 0.6)	(0.6, 0.65)
Uniform (-1,1)	60	**93.02%**	**92.39%**	90.59%	89.18%	87.22%	86.23%	**83.15%**
Uniform (-2,2)	120	92.52%	90.16%	89.06%	**89.89%**	87.89%	85.17%	82.17%
Uniform (-5,5)	300	92.79%	92.04%	**91.18%**	87.59%	87.16%	86.42%	82.40%
Sphere	100	92.87%	92.20%	89.79%	89.84%	**87.91%**	**86.70%**	82.81%

Table 8: Comparing performance of models given different sampling methods on MNIST with 24 samples. We tested uniform sampling between (-2, 2) and (-5, 5). We also tested sampling from a sphere with L2 norm of 100. For the most part, we found that the sampling range does not materially change the performance of the model.

	L2 Norm	Loss Level (0.55, 0.57)	(0.57, 0.59)	(0.59, 0.61)	(0.61, 0.63)	(0.63, 0.65)	(0.65, 0.67)
Uniform (-1,1)	60	66.59%	**65.91%**	64.09%	61.08%	59.33%	57.18%
Uniform (-2,2)	120	65.93%	65.14%	**64.93%**	61.31%	**61.85%**	57.22%
Uniform (-5,5)	300	**67.63%**	61.69%	63.63%	**62.19%**	60.33%	58.41%
Sphere	100	61.81%	64.31%	59.30%	62.01%	56.72%	**60.77%**

Table 9: Comparing performance of models given different sampling methods on CIFAR with 36 samples. We tested uniform sampling between (-2, 2) and (-5, 5). We also tested sampling from a sphere with L2 norm of 100. For the most part, we found that the sampling range does not materially change the performance of the model.