Training Scale-Invariant Neural Networks on the Sphere Can Happen in Three Regimes

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Abstract

A fundamental property of deep learning normalization techniques, such as batch normalization, is making the pre-normalization parameters scale invariant. The intrinsic domain of such parameters is the unit sphere, and therefore their gradient optimization dynamics can be represented via spherical optimization with varying effective learning rate (ELR), which was studied previously. In this work, we investigate the properties of training scale-invariant neural networks directly on the sphere using a fixed ELR. We discover three regimes of such training depending on the ELR value: convergence, chaotic equilibrium, and divergence. We study these regimes in detail both on a theoretical examination of a toy example and on a thorough empirical analysis of real scale-invariant deep learning models. Each of the regimes possesses its own unique features and has strong parallels with previous research on both general and specific scale-invariant neural networks training. Finally, we demonstrate how the discovered regimes are reflected in the conventional training of normalized networks.

1 Introduction

Most modern neural network architectures contain some type of normalization layers, such as Batch Normalization (BN) [9] or Layer Normalization [2]. Normalization makes networks partially *scale-invariant* (SI), i.e., multiplication of their parameters preceding the normalization layers by a positive scalar does not change the model's output. In general, the training dynamics of model parameters can be viewed from two perspectives: the *direction dynamics*, i.e., the dynamics of the projection of the parameters onto the unit sphere, and the *norm dynamics*. For SI neural networks, the former seems to be more important since the direction alone determines the output of the scale-invariant function. Nevertheless, the latter influences the optimization by changing the *effective learning rate* (ELR), i.e., the learning rate a scale-invariant model would have if it were optimized on the unit sphere.

Many works have studied the effect of scale invariance on training dynamics through the prism of norm or, equivalently, ELR dynamics [28, 8, 1, 32, 21, 22, 25, 29, 23]. They discovered that during standard training with weight decay the ELR can change in a non-trivial way and lead to different optimization dynamics: periodic behavior [23], destabilization [19, 21], or stabilization on some sphere [22, 29]. However, considering only the ELR dynamics is not enough for a comprehensive study of the specifics of training normalized neural networks. In particular, the impact of the varying ELR on training may obscure certain important properties of SI neural networks intrinsic domain, i.e., the unit sphere, thus narrowing our intuition about the general loss landscape structure. Therefore, in this work, we are focused on the direction dynamics. To eliminate the influence of the changing norm on training, we fix the total norm of all scale-invariant parameters of the normalized neural network and train it with a constant effective learning rate on the sphere.

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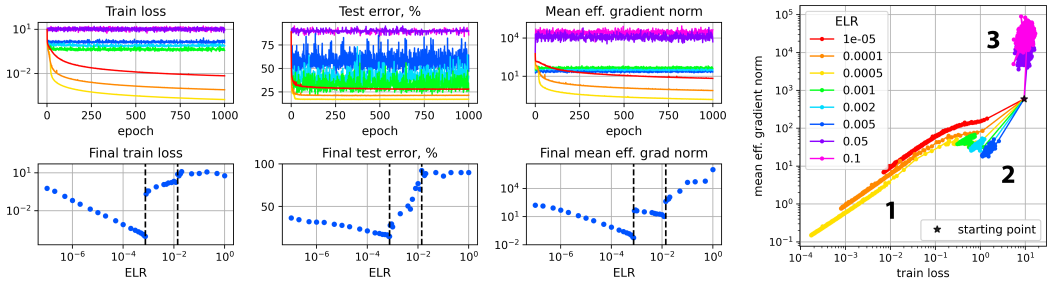

Figure 1: Three regimes of SI neural network training on the sphere: (1) convergence for the lowest ELRs, (2) chaotic equilibrium for medium ELRs, and (3) divergence for the highest ELRs. ConvNet on CIFAR-10. Dashed lines on scatter plots denote borders between the regimes.

We discover three regimes of such an optimization procedure depending on the ELR value (see Figure 1). The first regime (small ELRs) can be considered as a typical convergence to a minimum with monotonically decaying training loss. The second one (medium ELRs) demonstrates an oscillating behavior of the loss around a certain value separated from both the global minimum and random guess behavior. We call this regime a *chaotic equilibrium*, reminiscent of the equilibrium state reported in several previous works [22, 29]. The last regime (high ELRs) represents destabilized, diverged training associated with an excessively large optimization step size.

We thoroughly investigate the three regimes of training SI neural networks on the sphere. We analyze the underlying mechanisms behind each of these regimes on a model example and conduct an extensive empirical study with neural networks trained on the sphere. We also provide connections between the three regimes and prior work on neural networks training, both general and scale-invariant specific, and demonstrate how they are manifested in the conventional neural networks training.

2 Background and related work

As mentioned in the introduction, for every function $F(\boldsymbol{\theta})$ optimized w.r.t. its parameters $\boldsymbol{\theta}$ we can separate the dynamics of the parameters direction $\boldsymbol{\theta}/\|\boldsymbol{\theta}\|$ from the dynamics of their norm $\|\boldsymbol{\theta}\|$. If the function $F(\boldsymbol{\theta})$ is scale-invariant, i.e., $F(c\boldsymbol{\theta}) = F(\boldsymbol{\theta}),\ \forall c > 0$, the former is the only factor that determines the evolution of the function, since $F(\boldsymbol{\theta}/\|\boldsymbol{\theta}\|) = F(\boldsymbol{\theta})$. However, even though the SI function's value does not depend on the parameters norm, the latter greatly influences its gradients: $\nabla F(c\boldsymbol{\theta}) = \nabla F(\boldsymbol{\theta})/c,\ \forall c > 0$ and thus the optimization speed. This argument can be equivalently reformulated in terms of how the norm dynamics control the direction dynamics' pace via the notion of effective learning rate. For the standard (S)GD optimization, ELR is defined as the learning rate (LR) divided by the squared parameters norm, and it represents how the learning rate should be adapted to mimic the same direction dynamics if the function were optimized directly on the unit sphere [25].

Most of the previous work has dealt with the implications of using normalization in neural networks, i.e., making them (partially) scale-invariant, from the perspective of the ELR dynamics. For example, Arora et al. [1] study the convergence properties of batch normalized neural networks and explain why they allow much higher learning rates compared to their non-BN counterparts. Many works have also focused on training scale-invariant neural networks with weight decay [28, 32, 21, 22, 29, 23]. They all discovered the non-trivial dynamics of ELR induced by the interplay between normalization and weight decay but came to different conclusions. Some studies have reported training instability caused by this interplay [19, 21], while others have argued that, on the contrary, the equilibrium state is eventually reached, i.e., ELR becomes stable after some time [28, 4, 22, 17, 29]. Recently, Lobacheva et al. [23] demonstrated that training with weight decay and constant LR may experience regular periodic behavior for a practical range of LRs.

However, while all of these works mainly study the direction dynamics with varying rate, they lack exploring the properties of optimization of SI models with a *fixed* effective learning rate. Decoupling the direction dynamics from the changing norm effects could reveal particular features of the intrinsic domain of scale-invariant neural networks that were potentially obscured by the dynamical ELR. To cope with it, we optimize our models directly on the sphere using projected stochastic gradient

descent (SGD) with a constant learning rate, which is equivalent to fixing the ELR. Our method reveals some interesting results about SI neural networks and allows to draw parallels with scattered previous deep learning work. We note that similar experiments were conducted by, e.g., Arora et al. [1] and Lobacheva et al. [23] to highlight certain features of standard training when ELR is dynamical. Also, Cho and Lee [5] optimized scale-invariant parameters in normalized neural networks directly on their intrinsic domain using Riemannian gradient descent, but they proposed an optimization method rather than investigating the properties of such training.

3 Theoretical analysis

To explain the observed behavior, we proceed with the theoretical analysis of scale-invariant functions optimization with a fixed effective learning rate. At first, we derive several important general properties of such a process that will help to clarify some of its empirical aspects. Then we consider a concrete example of a function with multiple scale-invariant parameter groups, alike normalized neural networks, and study its convergence depending on the ELR value to shed more light on the prime causes of the three regimes. We provide all formal derivations and proofs in Appendix A.

3.1 General properties

We begin with an analysis of common features of all SI functions optimization with a fixed learning rate on the sphere. For that, consider a function $F(\boldsymbol{\theta})$ of a vector parameter $\boldsymbol{\theta} \in \mathbb{R}^P$ that can be divided into n groups: $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_n)$, where each $\boldsymbol{\theta}_i \in \mathbb{R}^{p_i}$ and $\sum_{i=1}^n p_i = P$. We say that each of these groups is scale-invariant, i.e., we can multiply it by a positive scalar value, with the others fixed, and the output of the function does not change. This is typical for neural networks with multiple normalized layers: each of these layers (and even each column/filter in each layer) is scale-invariant. Naturally, if a function is scale-invariant w.r.t. several parameter groups, it is also scale-invariant w.r.t. their union, therefore the whole vector $\boldsymbol{\theta}$ is scale-invariant too.

Since scale-invariant functions are effectively defined on the sphere, we try to minimize $F(\boldsymbol{\theta})$ on the sphere of radius ρ:

$$\begin{cases} F(\boldsymbol{\theta}) \to \min_{\boldsymbol{\theta} \in \mathbb{R}^P} \\ \|\boldsymbol{\theta}\| = \rho. \end{cases} \tag{1}$$

We do that using the projected gradient descent method with a fixed learning rate η:

$$\begin{cases} \hat{\boldsymbol{\theta}}^{(t)} \leftarrow \boldsymbol{\theta}^{(t)} - \eta \nabla F(\boldsymbol{\theta}^{(t)}), \\ \boldsymbol{\theta}^{(t+1)} \leftarrow \hat{\boldsymbol{\theta}}^{(t)} \cdot \frac{\rho}{\left\|\hat{\boldsymbol{\theta}}^{(t)}\right\|}. \end{cases} \tag{2}$$

Of course, since the function is scale-invariant w.r.t. each group $\boldsymbol{\theta}_i$, we could optimize it on the product of n independent spheres instead of the single mutual sphere, as we do in eq. (1). However, that would either require introducing too many hyperparameters in the model (n different learning rates) or overconstrainted the problem (one learning rate for all spheres). We also argue that constraining the total parameters norm is much more natural and closer to the standard neural networks training (see discussion in Appendix B).

We now define the notions of *effective gradient* and *effective learning rate* for each SI group $\boldsymbol{\theta}_i$. Effective gradient is the gradient w.r.t. $\boldsymbol{\theta}_i$ measured at the same point but with the group $\boldsymbol{\theta}_i$ projected on its unit sphere, i.e., at point $\tilde{\boldsymbol{\theta}} = (\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_i/\rho_i, \dots, \boldsymbol{\theta}_n)$, where $\rho_i \equiv \|\boldsymbol{\theta}_i\|$. Due to scale invariance w.r.t. $\boldsymbol{\theta}_i$, the function's value is equal at both points $\boldsymbol{\theta}$ and $\tilde{\boldsymbol{\theta}}$ but, as discussed earlier, the norm of the effective gradient, which we denote as $\tilde{g}_i$, is ρ_i times the norm of the regular gradient w.r.t. $\boldsymbol{\theta}_i$: $\tilde{g}_i = g_i \rho_i$, where $g_i \equiv \|\nabla_{\boldsymbol{\theta}_i} F(\boldsymbol{\theta})\|$. Effective learning rate $\tilde{\eta}_i$ is the learning rate required to make a gradient step w.r.t. $\boldsymbol{\theta}_i$ equivalent to the original but started from the point $\tilde{\boldsymbol{\theta}}$. It is known from the previous literature on scale-invariant functions [25, 29, 23] that ELR for the group $\boldsymbol{\theta}_i$ equals $\tilde{\eta}_i = \eta/\rho_i^2$. We also define the total effective gradient norm $\tilde{g} = \rho g$, where $g \equiv \|\nabla_{\boldsymbol{\theta}} F(\boldsymbol{\theta})\|$, and the total ELR $\tilde{\eta} = \eta/\rho^2$, *which is fixed in the considered setup*.

From the constraint on the total norm $\sum_{i=1}^{n} \rho_i^2 = \rho^2$ we obtain the following fundamental equation relating the ELRs of individual SI groups to the total ELR value:

$$\sum_{i=1}^{n} \frac{1}{\tilde{\eta}_i} = \frac{1}{\tilde{\eta}}. \tag{3}$$

Another important notion is the *effective step size* (ESS) which is the product of the effective gradient length by the effective learning rate: $\tilde{\eta}_i \tilde{g}_i$. This value defines how far we effectively move the scale-invariant parameters $\boldsymbol{\theta}_i$ after one gradient step. It can be shown that the total squared ESS can be expressed as a convex combination of squared ESS values of individual SI groups:

$$(\tilde{\eta}\tilde{g})^2 = \sum_{i=1}^{n} \omega_i (\tilde{\eta}_i \tilde{g}_i)^2, \ \sum_{i=1}^{n} \omega_i = 1, \ \omega_i \propto \frac{1}{\tilde{\eta}_i}. \tag{4}$$

The process (2) and eq. 3 yield the following update rule for each group's individual ELR:

$$\tilde{\eta}_i^{(t+1)} \leftarrow \tilde{\eta}_i^{(t)} \frac{1 + (\tilde{\eta}\tilde{g}^{(t)})^2}{1 + (\tilde{\eta}_i^{(t)} \tilde{g}_i^{(t)})^2}, \tag{5}$$

from what follows that *for a given SI group the higher (lower) the ESS at the current iteration, the lower (higher) the ELR becomes after it*. Since, by definition, ESS and ELR values are highly correlated, we conclude that at each iteration the largest ELRs tend to become smaller and vice versa. This "negative feedback" principle becomes very important in distinguishing between the three regimes of optimization.

3.2 Explaining the regimes

To provide a clear and easy-to-follow explanation of the differences between the three regimes of training on the sphere, we construct a simple yet illustrative example of a function with several groups of SI parameters and analyze its optimization properties depending on the total ELR value.

The simplest working example of a scale-invariant function is the following one:

$$f(x, y) = \frac{x^2}{x^2 + y^2}, \ x, y \in \mathbb{R} \setminus \{0\}. \tag{6}$$

This function has also been used in previous works to visually demonstrate various properties of general scale-invariant functions [22, 23]. Based on it, we develop an elucidative example of a function that contains more than one group of scale-invariant parameters — just as real multilayer normalized neural networks do. For that, we take a conical combination of $n > 1$ functions (6) each depending on its own pair of variables:

$$F(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{n} \alpha_i f(x_i, y_i) = \sum_{i=1}^{n} \alpha_i \frac{x_i^2}{x_i^2 + y_i^2}, \tag{7}$$

where $\boldsymbol{x} = (x_1, \ldots, x_n)$, $\boldsymbol{y} = (y_1, \ldots, y_n)$, and each $\alpha_i > 0$ is a fixed positive coefficient. In this function, there are n groups of SI parameters: $(x_i, y_i), i = 1, \ldots, n$. In accordance with the setup described previously, we intend to optimize this function on the unit sphere using the projected gradient descent method with a fixed (effective) learning rate, i.e., we plug $\boldsymbol{\theta} = (\boldsymbol{x}, \boldsymbol{y}) = ((x_1, y_1), \ldots, (x_n, y_n))$, $P = 2n$, $\rho = 1$ into equations (1) and (2).

Now we would like to study the behavior of optimization of $F(\boldsymbol{x}, \boldsymbol{y})$ on the unit sphere depending on the learning rate value η, which equals to the total ELR $\tilde{\eta}$ due to $\rho = 1$. But first we need to dwell on the convergence properties of each of its subfunctions $\alpha_i f(x_i, y_i)$. The next proposition, which we rigorously formulate and prove in the appendix, answers this question.

Proposition 1 *For the SI function $f_\alpha(x, y) = \alpha \frac{x^2}{x^2+y^2}$ minimized with ELR $\tilde{\eta}$:*

1. *if $\tilde{\eta} < \frac{1}{\alpha}$, it linearly converges to zero, i.e., its global minimum;*
2. *if $\tilde{\eta} > \frac{1}{\alpha}$, it stabilizes at value $\frac{1}{2}\left(\alpha - \frac{1}{\tilde{\eta}}\right)$.*

Knowing that each of the subfunctions of $F(\boldsymbol{x}, \boldsymbol{y})$ can converge to the minimum only when its ELR stays below the $1/\alpha_i$ value and considering the fundamental constraint on ELRs (3), we state that *the first regime (convergence)* is only possible when the total ELR is below a certain threshold:

$$\tilde{\eta} < \frac{1}{\sum_{i=1}^{n} \alpha_i}. \tag{8}$$

If the total ELR exceeds that threshold, the overall convergence is impossible, since at least one of individual ELRs must exceed its convergence threshold value. By Proposition 1, the value of each such subfunction is also separated from the minimum (zero) by some quantity depending on its ELR. This means that the total function value, and therefore the total effective gradient, is also non-vanishing (we give a more formal argument in the appendix). This brings us to the "undamped" dynamics of ELRs (5), where the effective step sizes do not tend to zero. In that case, *the dynamics stabilizes only when all the ESS values become equal*, which is possible if and only if each individual ELR $\tilde{\eta}_i$ takes its corresponding *equilibrium* value:

$$\tilde{\eta}_i^* \equiv \frac{\tilde{\eta} \sum_{i=1}^{d} \alpha_i}{\alpha_i}. \tag{9}$$

Due to the negative feedback principle of eq. (5), the system will naturally tend towards this state. Note that, in contrast, in the first regime ESS values decay too rapidly, and the model may not have enough time to reach equilibrium. In sum, when the total ELR exceeds the convergence threshold and each individual ELR (in average) equals its equilibrium value corresponding to the equalized ESS, the optimization process enters *the second regime, i.e., the chaotic equilibrium*. Finally, if the total ELR is set too high, the chaos will dominate equilibration, and in that case we observe *the third regime, or divergence*.

In Figure 2, we plot the evolution of the function (7) during optimization on the unit sphere with three different effective learning rates. We set $n = 3$, $\alpha_i = 2^i$, $i = 0, 1, 2$, and start from a point randomly selected on the 6-dimensional unit sphere. In this case, the threshold condition (8) becomes $\tilde{\eta} < 1/7 \approx 0.143$, and thus we select three ELRs corresponding to the three optimization regimes, respectively: 0.1, 0.2, and 0.5. The lines on the plot directly demonstrate the anticipated behavior: the smallest ELR leads to a fast decay of the function's value, the medium one makes the function stabilize around a certain level, and the largest ELR depicts the most chaotic behavior. In the appendix, we also provide plots of the individual ELRs dynamics that show that in the chaotic equilibrium $\tilde{\eta}_i$ in average by iterations closely match the predicted values (9), while in the first regime they are not reached due to quick convergence, and in the third one the optimization is too unstable to distinguish any equilibration.

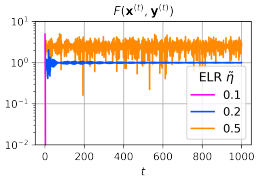

Figure 2: Function values evolution during optimization of the function (7) using three different ELRs corresponding to the three optimization regimes, respectively.

4 Experimental setup

After discussing the theoretical substantiation of the different regimes of learning on the sphere in the case of a simple SI function, let us move on to an empirical analysis of the learning dynamics of neural networks equipped with Batch Normalization. We conduct experiments with a simple 3-layer BN convolutional neural network (ConvNet) and a ResNet-18[1] on CIFAR-10 [15] and CIFAR-100 [16] datasets. We train all networks by optimizing cross-entropy loss using stochastic gradient descent with batch size 128 for 1000 epochs.

In Section 5, we analyze the training regimes of fully scale-invariant neural networks, trained on the sphere with a fixed ELR. To obtain fully scale-invariant versions of the networks we follow the same approach as in Lobacheva et al. [23]. We fix the non-scale-invariant weights, i.e., we use zero mean and unit variance in BN layers and freeze the weights of the last layer at random initialization with increased norm equal to 10. To train a network with ELR $\tilde{\eta}$, we fix the norm of the weights at the initial value ρ and use the projected SGD with a fixed learning rate $\eta = \tilde{\eta}\rho^2$. We consider a wide range of ELRs: $\{10^{-k}, 2 \cdot 10^{-k}, 5 \cdot 10^{-k}\}_{k=\overline{0,7}}$, with additional values close to the regime

[1] Both networks in the implementation of `https://github.com/tipt0p/periodic_behavior_bn_wd`.

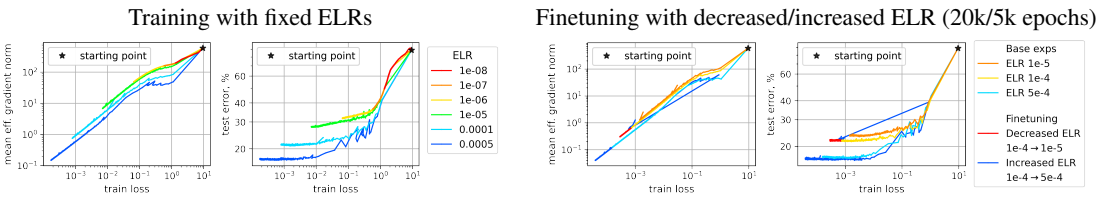

Figure 3: First training regime, ConvNet on CIFAR-10. Left: training with fixed ELRs converge to the regions with different sharpness and generalization profiles. Right: finetuning with decreased ELR stays on the same trajectory, while finetuning with increased ELR jumps out and converges to a flatter region. As baselines, we show training with the decreased/increased ELR from the initialization.

transitions. In Section 6, we investigate how the observed training regimes transfer to more practical scenarios. We train the networks in the whole parameter space, not only on the sphere, with a fixed learning rate and weight decay as in Lobacheva et al. [23], Wan et al. [29]. We use weight decay of $1e-4/5e-4$ for ConvNet / ResNet-18 in all the experiments and a range of LRs, specific for each scenario. In some experiments, we also use momentum of 0.9, standard CIFAR data augmentation, and cosine LR schedule of 200 epochs. More details can be found in Appendix D.

To make the experiments with different ELRs/LRs fully comparable, we train the networks from the same random initialization and with the same optimizer random seed. However, we show in Appendix F that the results are consistent if we vary both of them. For each visualization we choose the most representative subset of ELRs/LRs due to the difficulties of distinguishing between many noisy lines on the plots. At each training epoch, we log standard train / test statistics and the mean (over mini-batches) norm of the stochastic effective gradients for fully scale-invariant networks or the mean norm of the regular stochastic gradients in the case of standard networks. We choose the latter metric for the following two reasons. First, it can serve as a measure of sharpness of the minimum to which we converge in the first regime, since the mean stochastic gradient norm is strongly correlated with the trace of the gradient covariance matrix, which in turn is closely tied with the loss Hessian and the Fisher Information Matrix [12, 31, 27] (see Appendix C). Second, it represents the average (effective) step size up to multiplication by (E)LR and thus is also related to optimization dynamics.

5 Three regimes of training on the sphere

In this section, we investigate the three training regimes of fully scale-invariant neural networks, trained on the sphere with a fixed ELR. We first analyze the learning dynamics in each regime, including the properties of the resulting solutions and the loss landscape around them. After that, we discuss transitions between the regimes in more detail. We show the results for ConvNet on CIFAR-10, the results for other dataset-architecture pairs are consistent and presented in Appendix E.

5.1 Regime one: convergence

Training with the smallest ELRs results in the first training regime, which we call *the convergence regime*. As shown in Figure 1, optimization in this regime experiences a typical convergence behavior: after a number of epochs the model is able to achieve a very low training loss region and continues converging to the minimum. The speed of convergence depends on the ELR value — the higher the ELR, the faster the optimization, and the lower training loss is achieved after a fixed number of epochs. Training with different ELRs also results in solutions with different sharpness and generalization. We measure sharpness of a solution as the average norm of stochastic effective gradients at that point and generalization as its test error. Higher ELRs lead to less sharp solution with better generalization. Similar results are well known in the literature [12, 30, 20, 14, 18, 6, 3, 26, 11, 7]: training neural networks using larger learning rates typically results in flatter and better generalizing optima.

Furthermore, ELR not only influences the rate of convergence and the properties of the final solution but its local neighborhood and the whole training trajectory as well. To analyze the training trajectories independently from the training speed, we look at the evolution of sharpness and generalization vs. training loss during the optimization. We show the corresponding plots for different ELR values in the first regime in Figure 3, left. For the lowest ELRs the trajectories coincide, but the training is too

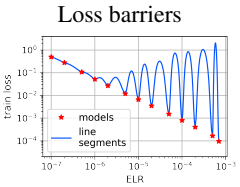

Figure 4: First training regime: solutions achieved with different ELRs are not linearly connected.

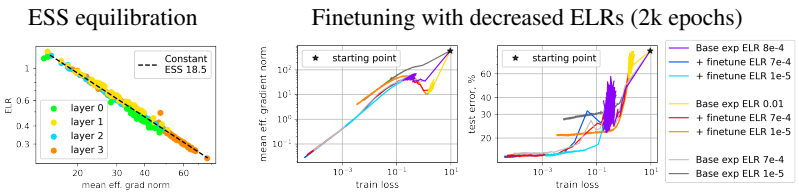

Figure 5: Second training regime, ConvNet on CIFAR-10. Left: equilibration of individual ESS values: we plot individual ELRs and effective gradient norms for different SI parameter groups (mean values over last 200 epochs); ELR = 0.001. Right: finetuning from the low second regime ELR always results in flattest possible solutions, while from higher starting ELRs, solutions of various sharpness can be reached.

slow to converge to the low-loss region. For the remaining values, as we increase ELR, we obtain a lower trajectory, and in the low-loss region trajectories of different ELRs appear like parallel lines. Such differences in trajectories show that training with a higher ELR not only results in a flatter final solution but also traverses less sharp regions the whole time: for any fixed value of the training loss, the point corresponding to a higher ELR has lower sharpness and better generalization. This is also consistent with recent results on the impact of higher learning rates on better optimization trajectory conditioning [14, 6, 11, 7].

The optima achieved after training with different ELRs not only vary in sharpness and generalization but also lie in different loss landscape regions even if optimization starts from the same initialization and uses the same order of batches. In Figure 4 we check whether the solutions achieved with different ELRs are linearly connected. For each pair of neighboring ELRs we connect the corresponding final weight vectors with a line segment and look at the training loss along this segment. The results show that the solutions that converged to a low-loss region lie in different basins and there exist barriers of high loss between them.

The resulting basins have different sharpness and generalization profiles, which are reflected as parallel lines in the low-loss region in Figure 3, left. Moreover, each basin has its own specific profile in a sense that SGD cannot find a solution with significantly different sharpness and generalization in that basin. To confirm that, we take a solution achieved with a specific ELR and finetune it with lower and higher ELR values (see Figure 3, right). Finetuning with lower ELR continues to move along the same trajectory as the initial experiment, hence there are no sharper sub-minima observed inside the flat basin. Finetuning with higher ELR also maintains the same trajectory at first but after some time jumps out of the low-loss region and converges to a new basin with a profile typical for higher ELRs. It means that the initial basin is too sharp for the higher ELR to converge. The results are consistent for different ELR values, see Appendix I.

As can be seen from Figure 3, left, the range of sharpness and generalization profiles reachable with the fixed ELR training in the first regime is limited. For low ELRs the trajectories coincide and optimization converges to the sharpest reachable basin. Increasing ELR results in flatter optima, but after some ELR optimization stops converging to low-loss regions and demonstrates the behavior of the second training regime, which we describe next.

5.2 Regimes two and three: chaotic equilibrium and divergence

A further increase in ELR in the first regime leads to a sharp switch to another regime, *the chaotic equilibrium*. Figure 1 shows that after a certain threshold ELR, the optimization is no longer able to reach low-loss regions and gets stuck at some level. We see that the effective gradients norm also stabilizes, and higher ELRs correspond to a higher loss but lower sharpness.

As we determined in Section 3.2, the second regime corresponds to the state when all individual effective step sizes become equal, which also leads to stabilization of individual ELRs. In Figure 5, left, we depict the values (averaged over last 200 epochs) of individual ELRs and effective gradient norms w.r.t. each SI parameters group of each layer of the neural network trained with $\tilde{\eta} = 10^{-3}$. We see that the effective step sizes (ELR times effective gradient norm) indeed concentrate around a certain equilibrium value denoted as a dotted black line on the plot. In Appendix J, we provide results

for other ELRs and additional plots demonstrating the stabilization of individual ELRs and effective gradient norms, which corroborates our definition of the second regime as the chaotic equilibrium.

Now, what if we finetune a model from the second regime with a smaller ELR corresponding to the first regime? As can be seen from Figure 5, right, the resulting optima highly depend on the starting ELR (more results in Appendix K). Finetuning networks, obtained with low second regime ELRs, with any first regime ELR converges to basins with the same sharpness/generalization profile that corresponds to the maximum ELR in the first regime. For larger second regime ELRs, however, finetuning results in a variety of trajectories depending on the chosen first regime ELR. It means that training with low second regime ELR resides in regions containing only flat optima. Meanwhile, basins obtained with high ELRs contain optima of different sharpness. Moreover, finetuning leads to the same range of sharpness/generalization profiles that was observed in the first regime.

For the highest considered ELR values, we observe the most unstable optimization behavior corresponding to the random guess accuracy (see Figure 1). This is the third, *divergent training regime*. We compare it with random walk in Appendix L.

5.3 Transitions between the regimes

In the end, we would like to discuss the connections between the three regimes and our global view of training on the sphere. In Figure 6, we plot the training loss for several ELR values that correspond to the three regimes and transitions between them. When the ELR is too high (purple line), the total ESS becomes so large that the model is unable to even detect any region in the parameters space with non-trivial quality, and we observe the third regime. With a smaller ELR (light blue line), the model starts occasionally hitting the edge of the region with a (relatively) low loss but then quickly escapes it and returns back to the random guess behavior; this could be attributed to the border regime between the second and the third regimes. Setting the ELR to an even smaller value (green line) results in the chaotic equilibrium, when the loss is stabilized near a certain value, which is lower the lower the ELR. For ELR values between the highest ELRs of the first regime and the lowest ones of the second regime (yellow line), we can witness a sudden change from equilibrium behavior to convergence. We conjecture that the major difference between the first and second optimization regimes and such a sharp transition between them, in particular, is due to the presence of zones of increased sharpness in the optimization trajectories of neural networks [13, 14, 18, 11, 7]. In the gradient norm vs. training loss diagram in Figure 1, we can see that the sharpness reaches its peak precisely at the transition point between the first two regimes; this leads us to a hypothesis that only training with sufficiently small ELR values allows getting through this bottleneck and enter the convergence regime. In Appendix H, we discuss the relationship between this transition and the epoch-wise double descent of the test error [24]: we discover that the sharpness peak correlates with the test error peak and also becomes much more noticeable at the presence of label noise in the training data. Finally, the smallest ELRs (orange line) correspond to a typical convergence to the optimum, i.e., the first regime, and the lower the ELR the sharper the minimum we converge to.

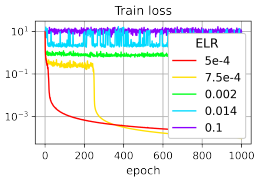

Figure 6: Three regimes and transitions between them, ConvNet on CIFAR-10.

6 Regimes in standard training

In this section, we study how different training regimes of SI neural networks on the sphere are represented in more practical scenarios. First, we experiment with training SI networks in a whole parameter space, where both direction and norm dynamics influence the optimization trajectory. We train SI networks with weight decay and vary LR instead of ELR. All three regimes are also present in such training (see Figure 7, left). We argue that the difference between the first and the second regimes explains why disparate results on training dynamics are reported in the literature. Lobacheva et al. [23] have discovered that SI neural networks experience convergence with periodic jumps during optimization. We observe the same behavior for high LR values in the first regime, where the trajectories periodically jump out of the low-loss region (see yellow trajectory for LR 2.0). On the other hand, experiments of Li et al. [22] and Wan et al. [29] with fixed LRs demonstrate that the equilibrium state is reached, which we also observe in the second training regime.

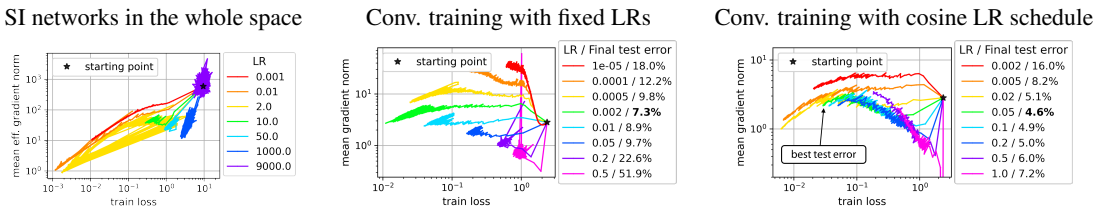

Figure 7: Training regimes in standard training. Left: training of SI networks in the whole parameter space with weight decay, ConvNet on CIFAR-10. Middle and right: conventional training with fixed LRs and cosine LR schedules , ResNet-18 on CIFAR-10. The results for other dataset-architecture pairs are presented in Appendix M.

Now, let us consider the conventional neural network training, which implies optimization of all network parameters, including the non-scale-invariant ones, in the entire parameter space with momentum and data augmentation. Here we use ResNet-18 network of standard size with weight decay and try both constant and the standard cosine LR schedule (see Figure 7, middle and right). In conventional training, only the first two training regimes are present because LR also affects non-scale-invariant parameters, and so training with very high LR values results in NaN values in the loss. The transition between the first two regimes is not as easy to locate, as in the previous experiments. All the training trajectories end up in regions with relatively high training loss, mainly because of the data augmentation, which makes the task much harder to learn and requires more time to converge to the low-loss region. Moreover, the task may become too hard for some models to achieve a low training loss at all. We show in Appendix G, that similar results are observed in case of training SI networks that are too small for the task in hand.

In the experiments with constant LRs, training with lower LRs passes the region with the highest sharpness along the trajectory and starts converging to a flatter region (LRs less then 0.01), while training with higher LRs gets stuck in the high-sharpness zone (LRs higher or equal to 0.01). The former may be assigned to the first training regime, and the latter to the second one. The best test accuracy is achieved for the highest LRs of the first regime, similarly to the results in Section 5.

In the experiments with cosine LR schedule, we decrease LR from some starting LR value to zero during 200 epochs of training. If we start with low LR (≤ 0.02), optimization happens with LRs of the first regime all or almost all time, and the first regime trajectory is observed. Moreover, for higher starting LRs, the solution with better sharpness profile and generalization is achieved. If we start with high LR (≥ 0.5), then most of the training is done with LRs of the second regime, and optimization does not have enough time with low LR values to converge to the low-loss region. The medium starting LR values are of the most interest here (between 0.02 and 0.5). In this case, training first has substantial time with gradually decreasing LRs of the second regime, which helps it to localize the region with the flattest optima, and then has just enough time with the first regime LRs to pass the high-sharpness zone and start converging to the minimum. With such training, solutions with better sharpening/generalization profiles are achieved, which is consistent with the results of Section 5.2 and the existing literature on pre-training with high LR values [20, 10].

7 Conclusion

In this work, we investigated the properties of training scale-invariant neural networks on the sphere using projected SGD. This method allowed us to study the intrinsic domain of SI models more accurately. We discovered three regimes of such training depending on the effective learning rate value: convergence, chaotic equilibrium, and divergence. We showed that these regimes are related to diverse previous results in deep learning and present in conventional neural network training as well.

Limitations and societal impact The main limitations of our work are applying a single optimization method on the sphere (projected SGD), experimenting only with BN networks as SI models, and considering only one of the symmetries that may conceal the actual properties of neural networks intrinsic domain [17]. To our knowledge, our work does not have any negative societal impact.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See the end of Section 7.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See the end of Section 7.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Section 3.
   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendix 3.

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Supplementary materials.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section‘4 and Appendix D.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We show that the described training regimes are consistent for different random seeds in Appendix F
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Appendix D.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
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   (b) Did you mention the license of the assets? [Yes] See Appendix D. CIFAR datasets are distributed under MIT license and code is under Apache-2.0 License license (we provide the link to the GitHub in Section 4.)
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