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. However, the varying ELR may obscure certain characteristics of the intrinsic loss landscape structure. 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 regime has unique features and reflects specific properties of the intrinsic loss landscape, some of which have strong parallels with previous research on both regular and scale-invariant neural networks training. Finally, we demonstrate how the discovered regimes are reflected in conventional training of normalized networks and how they can be leveraged to achieve better optima.

1 Introduction

Most modern neural network architectures contain some type of normalization layers, such as Batch Normalization (BN) [10] 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. However, the latter influences the optimization by changing the *effective learning rate* (ELR), i.e., the learning rate (LR) 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 [33, 9, 1, 38, 24, 26, 29, 35, 27]. 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 [27], destabilization [22, 24], or stabilization on some sphere [26, 35]. 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 loss landscape structure. Therefore, in this work, we are focused on the direction dynamics. To eliminate the influence of the changing norm on

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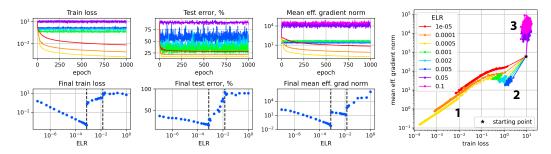


Figure 1: Three regimes of SI neural network training on the sphere: (1) convergence for the lowest ELRs, (2) chaotic equilibrium for medium ELRs, and (3) divergence for the highest ELRs. ConvNet on CIFAR-10. Dashed lines on scatter plots denote borders between the regimes.

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.

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 a sustained oscillating behavior of the loss around a certain value separated from both the global minimum and the random guess behavior. We call this regime a *chaotic equilibrium*, reminiscent of the equilibrium state reported in several previous works [26, 35]. The last regime (high ELRs) represents destabilized, diverged training associated with an excessively large optimization step size.

We analyze the underlying mechanisms behind each of these regimes on a toy example and conduct an extensive empirical study with neural networks trained on the sphere using projected stochastic gradient descent (SGD). We point out the main features of each regime and study how they relate to each other and what peculiarities of the optimization dynamics and intrinsic structure of the loss landscape they reveal. Our findings both reconfirmed some of the previous beliefs, like that training with larger (E)LR generally ends up in better optima, or that high-sharpness zones are present in the optimization trajectory, and introduced novel insights, like that different (E)LRs of the first regime even with the same initialization and batch ordering actually lead to distinguishable minima with different sharpness/generalization profiles depending on the specific (E)LR value, or that the high-sharpness zones are responsible for the boundary between the first and the second regimes and have close ties with the Double Descent phenomenon. Finally, we demonstrate how our results are reflected in conventional neural network training and suggest several practical implications that help achieve optimal solutions in terms of sharpness and generalization.

Our code is available at https://github.com/tipt0p/three_regimes_on_the_sphere.

2 Background and related work

As mentioned in the introduction, for every function $F(\theta)$ optimized w.r.t. its parameters θ we can separate the dynamics of the parameters direction $\theta/\|\theta\|$ from the dynamics of their norm $\|\theta\|$. If the function $F(\theta)$ is scale-invariant, i.e., $F(c\theta) = F(\theta)$, $\forall c > 0$, the former is the only factor that determines the value of the function, since $F(\theta/\|\theta\|) = F(\theta)$. However, even though the SI function's value does not depend on the parameters norm, the latter greatly influences its gradients: $\nabla F(c\theta) = \nabla F(\theta)/c$, $\forall c > 0$ and thus the optimization speed. This argument can be equivalently reformulated in terms of how the norm dynamics control the direction dynamics' speed via the notion of effective learning rate. For the standard (S)GD optimization, ELR is defined as the learning rate 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 [29].

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 [33, 38, 24, 26, 35, 27].

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 [22, 24], while others have argued that, on the contrary, the equilibrium state is eventually reached, i.e., ELR becomes stable after some time [33, 4, 26, 20, 35]. Recently, Lobacheva et al. [27] 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 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 previous scattered deep learning work. We note that similar experiments were conducted by, e.g., Arora et al. [1] and Lobacheva et al. [27] 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, similar to 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 $F(\theta)$ of a vector parameter $\theta \in \mathbb{R}^P$ that can be divided into n groups: $\theta = (\theta_1, \dots, \theta_n)$, where each $\theta_i \in \mathbb{R}^{p_i}$ 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 a 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 θ is scale-invariant too.

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

$$\min_{\boldsymbol{\theta} \in \mathcal{S}^{P-1}(\rho)} F(\boldsymbol{\theta}), \tag{1}$$

where $S^{P-1}(\rho) = \{\theta \in \mathbb{R}^P : \|\theta\| = \rho\}$. We do that using the projected gradient descent method with a fixed learning rate η :

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

Of course, since the function is scale-invariant w.r.t. each individual group θ_i , we could optimize it on the product of n independent spheres \mathcal{S}^{p_i-1} 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 for n spheres) or overconstrained the problem (one learning rate for all n spheres). We also argue that constraining the total parameters norm is much more natural and closer to the standard neural networks training with weight decay (see discussion in Appendix A.1).

We now define the notions of *effective gradient* and *effective learning rate* for each SI group θ_i . Effective gradient is the gradient w.r.t. θ_i measured at the same point but with the group θ_i projected on its unit sphere, i.e., at point $\tilde{\theta} = (\theta_1, \dots, \theta_i/\rho_i, \dots, \theta_n)$, where $\rho_i \equiv ||\theta_i||$. Due to scale

invariance w.r.t. θ_i , the function's value is equal at both points θ and $\hat{\theta}$ 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. θ_i : $\tilde{g}_i = g_i \rho_i$, where $g_i \equiv \|\nabla_{\theta_i} F(\theta)\|$. Effective learning rate $\tilde{\eta}_i$ is the learning rate required to make a gradient step w.r.t. θ_i equivalent to the original but started from the point $\tilde{\theta}$. It is known from the previous literature on scale-invariant functions [29, 35, 27] that ELR for the group θ_i equals $\tilde{\eta}_i = \eta/\rho_i^2$. We also define the total effective gradient norm $\tilde{g} = g\rho$, where $g \equiv \|\nabla_{\theta} F(\theta)\|$, 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:²

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

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 θ_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:

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

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

This function has also been used in previous works to visually demonstrate various properties of general scale-invariant functions [26, 27]. 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:

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

where $\mathbf{x} = (x_1, \dots, x_n)$, $\mathbf{y} = (y_1, \dots, y_n)$, and each $\alpha_i > 0$ is a fixed positive coefficient. In this function, there are n groups of SI parameters: $(x_i, y_i), i = 1, \dots, n$. 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 $\mathbf{\theta} = (\mathbf{x}, \mathbf{y}) = ((x_1, y_1), \dots, (x_n, y_n)), P = 2n, \rho = 1$ into equations (1) and (2).

Now we would like to study the behavior of optimization of F(x, 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 Appendix A.3, answers this question.

²See the derivation of this and the following equations of this section in Appendix A.2.

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(x, y) can converge to the minimum only when its ELR stays below $1/\alpha_i$ 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:

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

What if the total ELR exceeds that threshold? The first regime cannot be observed: convergence becomes impossible, since at least one of the individual ELRs exceeds its convergence threshold value, according to eq. (3). By Proposition 1 the value of the corresponding subfunction is separated from zero by some quantity depending on its ELR. This means that the total function value, and therefore the total effective gradient, is also nonvanishing (we give a more formal argument in Appendix A.4). 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 stabilize 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:

$$\tilde{\eta}_i^* \equiv \frac{\tilde{\eta} \sum_{j=1}^n \alpha_j}{\alpha_i}.$$
(9)

Due to the negative feedback principle of eq. (5), the system will naturally tend towards this state when ESS values are non-negligible. Note that, in contrast, in the first regime, ESS values decay too rapidly due to convergence, and the model may fail 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 the optimization dynamics will resemble a random walk. 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 $\tilde{\eta}<1/7\approx0.143$, 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 Appendix A.5, we 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 the optimization is too unstable to distinguish any equilibration.

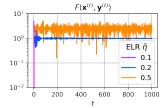


Figure 2: Function values evolution during optimization of the function (7) using three different ELRs corresponding to the three optimization regimes, respectively.

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 on CIFAR-10 [18] and CIFAR-100 [19] datasets. Both networks are in the implementation of Lobacheva et al. [27] and we train them by optimizing cross-entropy loss using stochastic gradient descent with batch size 128 for 1000 epochs. In Appendix O, we also show that three training regimes may be observed for other neural architectures, such as multilayer perceptron and Transformer [34].

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. [27]. We fix the non-scale-invariant weights, i.e., we use zero shift and unit scale 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: $\{10^{-k}, 2 \cdot 10^{-k}, 5 \cdot 10^{-k}\}_{k=0}^{7}$, which more than covers the values of ELR usually encountered during training of regular networks. We also used a more fine grained ELR grid closer to the boundaries between the regimes. In Section 6, we investigate how the observed training regimes transfer to more practical scenarios. We train networks in the whole parameter space with a fixed learning rate and weight decay as in Lobacheva et al. [27], Wan et al. [35]. 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 for 200 epochs. More details can be found in Appendix C.

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 E 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 this 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 [13, 37, 32] (see Appendix B). 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 D.

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 reach regions with very low training loss 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. Also, training with different ELRs results in solutions with different sharpness (mean norm of stochastic effective gradients) and generalization (test error): higher ELRs lead to less sharp solution with better generalization. Similar results are well known in the literature [13, 36, 23, 30, 15, 21, 6, 3, 31, 12, 8], i.e., training neural networks using larger learning rates typically results in flatter and better generalizing optima. Furthermore, we discovered that the optima achieved after training with different ELRs not only vary in sharpness and generalization but also reside in different basins, i.e., there is a significant loss barrier on the linear interpolation between them (see Appendix I for more details).

The value of ELR affects not only the rate of convergence and the properties of the final solution; it may have an effect on 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 of the first regime in Figure 3, left. For the lowest ELRs the trajectories coincide, but the training is too 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 as parallel lines.

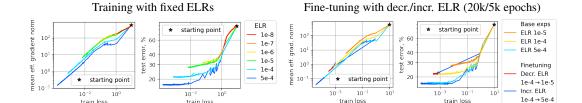


Figure 3: First training regime, ConvNet on CIFAR-10. Left: training with fixed ELRs converge to the regions with different sharpness and generalization profiles. Right: fine-tuning with decreased ELR stays on the same trajectory, while fine-tuning with increased ELR jumps out and converges to a flatter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

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 conditioning of the optimization trajectory [15, 6, 12, 8].

The parallelism of the trajectories in the low-loss region is particularly interesting and leads us to the following question: do the basins to which training with different ELRs converges have different *overall* sharpness and generalization profiles? That is, can we hypothesize that all solutions reachable with SGD in a given basin have similar sharpness and generalization at the same training loss? To answer that, we take a solution achieved with a specific ELR and fine-tune it with lower and higher ELR values (see Figure 3, right). Fine-tuning with a lower ELR stays in the same basin and continues to move along the same trajectory as the pre-trained model, hence no sharper sub-minima can be found inside the flat basin. Fine-tuning with a higher ELR also maintains the same trajectory at first but jumps out of the low-loss region after a while and converges to a new basin with a profile attributed to that higher ELR. That means that the initial basin is too sharp for the higher ELR to converge. The results are consistent for different ELR values, see Appendix H; we also provide results on linear connectivity of pre-trained and fine-tuned solutions in 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 small ELRs, the trajectories coincide and optimization converges to the sharpest available basin. Increasing ELR results in flatter optima, but at some value the 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 of 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 loss level. We observe 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 the stabilization of individual ELRs. In Figure 4 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 dashed 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.

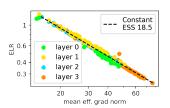
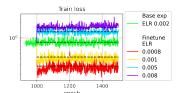


Figure 4: Equilibration of individual ESS values in the second regime. ConvNet on CIFAR-10.

In the second regime, the optimization localizes a certain region in the loss landscape and "hops along its walls". For moderate ELRs, this region is locally convex in the sense that the loss on the linear path

Fine-tuning with second regime ELRs

Fine-tuning with first regime ELRs (2k epochs)



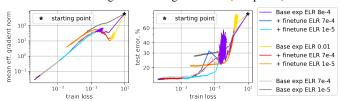


Figure 5: Second training regime, ConvNet on CIFAR-10. Left: fine-tuning with a different second regime ELR results in the training loss level corresponding to the new ELR value (such levels for all considered ELRs are depicted with dashed lines). Right: fine-tuning with first regime ELR from the low second regime ELR always results in flattest possible solutions, while from higher starting ELRs, solutions of various sharpness can be reached.

between different checkpoints from the same trajectory is convex and generally much lower than at its edges. However, for the highest ELRs, the dynamics become more chaotic and distinguished barriers may appear on the linear path. We provide the corresponding plots in Appendix K. Each ELR of the second regime determines its own loss level — the height at which the optimization "hops". Changing the ELR value during training appropriately changes the training dynamics: increasing/decreasing the ELR directly leads to the trajectory with a loss level corresponding to the new ELR value (see Figure 5, left). This significantly distinguishes the second regime from the first, where fine-tuning with a different ELR does not affect the learning trajectory, unless the new ELR is too large, in which case the optimization suddenly jumps out of the basin.

Now, what if we fine-tune 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 L). Fine-tuning the models, pre-trained with low second regime ELRs, using any first regime ELR converges to basins with the sharpness/generalization profile attributed to the maximum ELR in the first regime. For larger second regime ELRs, fine-tuning results in a variety of trajectories depending on the chosen ELR of the first regime. That means that training with low second regime ELRs discovers regions containing only flat minima. Meanwhile, regions discovered with high ELRs contain optima of different sharpness. Moreover, fine-tuning from these regions results in 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). We call it the third, *divergent training regime*. We explicitly compare the third regime with random walk in Appendix M.

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 encounter 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

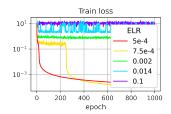


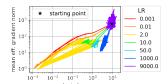
Figure 6: Three regimes and transitions between them, ConvNet on CIFAR-10.

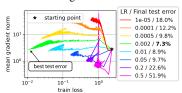
line) results in the chaotic equilibrium, when the loss is stabilized near a certain value, which is lower the lower the ELR. For ELR values between the highest ELRs of the first regime and the lowest ones of the second regime (yellow line), we can witness a sudden change from equilibrium behavior to 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 [14, 15, 21, 12, 8]. In the

SI networks in the whole space

Training with fixed LRs

Training with cosine LR schedule





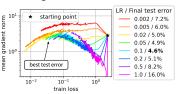


Figure 7: Training regimes in standard training. Left: training of SI networks in the whole parameter space with weight decay, ConvNet on CIFAR-10. Middle and right: conventional training with fixed LRs and cosine LR schedules, ResNet-18 on CIFAR-10. Results for other dataset-architecture pairs are presented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

gradient norm vs. training loss diagram in Figure 1, we can observe 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 G, we discuss the relationship between this transition and the epoch-wise double descent of the test error [28]: 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.

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 and what clues they can give to achieve a good minimum in terms of sharpness and generalization. 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. [27] 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 (the yellow trajectory for LR = 2.0). On the other hand, experiments of Li et al. [26] and Wan et al. [35] with fixed LRs demonstrate that the equilibrium state is reached, which we can observe in the second training regime.

Now, let us consider conventional neural networks training, which implies optimization of all network's weights (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 the non-scale-invariant parameters, and so training with very high LR values results in NaN values in the loss, since the weights of the last layer can become large enough to lead to numerical overflows. 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 F, 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 (< 0.01) passes the region with the highest sharpness along the trajectory and starts converging to a flatter region, while training with higher LRs (≥ 0.01) gets stuck in the high-sharpness zone. The former can be attributed to the first training regime, and the latter to the second one. Note that, in accordance with Section 5, the best test accuracy is achieved with the largest LR of the first regime.

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 a low LR (≤ 0.02), optimization is carried out all or

almost all the time with LRs of the first regime, 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 a 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 converge 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 [23, 11].

7 Conclusion and Discussion

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. They uncover multiple properties of the intrinsic loss landscape of scale-invariant neural networks: some are related to diverse previous results in deep learning, and some appear as novel. We showed that these regimes are present in conventional neural network training as well and can provide intuition on how to achieve better optima.

Possible future directions Speaking about the potential prospects for further research, three directions can be distinguished. First, it would be interesting to develop more solid and general theoretical groundings for the observed phenomena. For instance, a closer look at the negative feedback principle in eq. (5) could potentially shed more light on the ESS/ELR dynamics in the first and second regimes compared to the current decay vs. alignment dichotomy and maybe better explain occasional transitions from the second to the first regime for certain ELRs in Section 5.3. Second, the analysis could be extended to other tasks, architectures, and especially optimizers like Adam [16], which can be challenging due to their indirect impact on the effective direction and effective learning rate in SI models [29]. Third, it is very tempting to investigate other potential practical implications of the three regimes for conventional training. The analysis of various LR schedules from the perspective of the discovered training regimes is intriguing and might help in designing more efficient and more explainable LR schedules. For example, from our experiments we observe that decreasing (E)LR in the first regime during training does not influence the final solution but only slows down the convergence; at the same time, for the optimal final performance, optimization should run through the low second regime (E)LRs, which allows to achieve basins containing solutions with the best sharpness/generalization properties.

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 [20]. 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] URL at the end of Introduction.
 - (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section 4 and Appendix C.
 - (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 E
 - (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 C.
- 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
 - (a) If your work uses existing assets, did you cite the creators? [Yes] See Section 4.
 - (b) Did you mention the license of the assets? [Yes] See Appendix C. 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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A Theory

In this section, we provide proofs and additional details for Section 3.

A.1 Norm constraint: total vs. individual

In this section, we will give additional arguments in favor of our choice of constraining the total norm, rather than each individual SI group. Consider a more general formulation than (1), where we relax the condition on fixing the total norm strictly at ρ :

$$\begin{cases}
\min_{\boldsymbol{\theta} \in \mathbb{R}^P} F(\boldsymbol{\theta}) \\
\|\boldsymbol{\theta}\|^2 \le \rho^2.
\end{cases}$$
(10)

Arora et al. [1] show that after a gradient step, the norm of SI parameters can only increase. That means that if we solved the problem (10) using the projected gradient descent method starting from $\theta^{(0)}: \|\theta^{(0)}\| = \rho$, we would end up with the same algorithm, as presented in eq. (2), because we would project θ onto $S(\rho)$ at each iteration. Thus, this relaxation does not any significantly vary the setup considered in the main text.

The Lagrangian function associated with (10) is

$$\mathcal{L}(\boldsymbol{\theta}, \lambda) = F(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|^2 - \lambda \rho^2, \ \lambda \ge 0. \tag{11}$$

Minimizing (11) w.r.t. θ is equivalent to standard training with L_2 regularizer or, in the case of gradient descent, applying weight decay with coefficient λ in the optimizer. This is a perfectly normal procedure when training machine learning models.

If we, however, tried putting constraints on each individual SI group norm, we would end up with the following optimization problem:

$$\begin{cases} F(\boldsymbol{\theta}) \to \min_{\boldsymbol{\theta} \in \mathbb{R}^P} \\ \|\boldsymbol{\theta}_i\|^2 \le \rho_i^2, \ i = 1, \dots, n, \end{cases}$$
 (12)

which yields the following Lagrangian function:

$$\mathcal{L}(\boldsymbol{\theta}, \lambda_1, \dots, \lambda_n) = F(\boldsymbol{\theta}) + \sum_{i=1}^n \lambda_i \|\boldsymbol{\theta}_i\|^2 - \sum_{i=1}^n \lambda_i \rho_i^2, \ \lambda_i \ge 0, \ i = 1, \dots, n.$$
 (13)

Now, minimizing (13) w.r.t. θ would imply setting n separate weight decay coefficients λ_i (one for each SI group), which has much less to do with actual practice.

A.2 Derivations for Section 3.1

We begin with a formal derivation of the formulas in Section 3.1. We remind that we consider a function $F(\theta)$ whose parameters can be split into n SI groups: $\theta = (\theta_1, \dots, \theta_n)$. We solve an optimization problem (1) with projected gradient descent (2). For each SI group θ_i we denote its norm as $\rho_i \equiv \|\theta_i\|$, its effective gradient norm as $\tilde{g}_i = g_i \rho_i$, where $g_i \equiv \|\nabla_{\theta_i} F(\theta)\|$, and its ELR as $\tilde{\eta}_i = \eta/\rho_i^2$. Similarly, for the whole parameters vector θ we define $\tilde{g} = g\rho$, where $g \equiv \|\nabla_{\theta} F(\theta)\|$, and $\tilde{\eta} = \eta/\rho^2$.

Equation (3) can be directly obtained from the basic constraint on the total parameters norm:

$$\sum_{i=1}^{n} \rho_i^2 = \rho^2 \implies \sum_{i=1}^{n} \frac{1}{\tilde{\eta}_i} = \sum_{i=1}^{n} \frac{\rho_i^2}{\eta} = \frac{\rho^2}{\eta} = \frac{1}{\tilde{\eta}}.$$
 (14)

Equation (4) expresses the total squared ESS value as a weighted average of squared individual ESS values and can be obtained the following way:

$$(\tilde{\eta}\tilde{g})^2 = \tilde{\eta}\eta g^2 = \{g^2 = \sum_{i=1}^n g_i^2\} = \tilde{\eta}\sum_{i=1}^n \eta g_i^2 = \tilde{\eta}\sum_{i=1}^n \tilde{\eta}_i \tilde{g}_i^2 = \sum_{i=1}^n \omega_i (\tilde{\eta}_i \tilde{g}_i)^2, \ \omega_i \equiv \frac{\tilde{\eta}}{\tilde{\eta}_i}.$$
(15)

Note that from eq. (3) it follows that $\sum_{i=1}^{n} \omega_i = 1$, i.e., the rightmost expression of eq. (15) is indeed a convex combination of squared individual ESS values with weights $\omega_i \propto \frac{1}{\bar{\eta}_i}$.

Finally, the update rule for ELRs (5) in process (2) can be obtained from a similar expression for the parameters norm updates:

$$(\rho_{i}^{(t+1)})^{2} = \frac{\left\|\boldsymbol{\theta}_{i}^{(t)} + \eta \nabla_{\boldsymbol{\theta}_{i}} F(\boldsymbol{\theta})^{(t)}\right\|^{2}}{\left\|\boldsymbol{\theta}^{(t)} + \eta \nabla_{\boldsymbol{\theta}} F(\boldsymbol{\theta})^{(t)}\right\|^{2}} \rho^{2} = \left\{ \langle \boldsymbol{\theta}_{i}, \nabla_{\boldsymbol{\theta}_{i}} F(\boldsymbol{\theta}) \rangle = 0 \text{ [24]} \right\} =$$

$$= \frac{(\rho_{i}^{(t)})^{2} + \eta^{2} g_{i}^{2}}{1 + (\tilde{\eta} \tilde{q}^{(t)})^{2}} = (\rho_{i}^{(t)})^{2} \frac{1 + (\tilde{\eta}_{i}^{(t)} \tilde{g}_{i}^{(t)})^{2}}{1 + (\tilde{\eta} \tilde{q}^{(t)})^{2}}. \quad (16)$$

A.3 Proof of Proposition 1

Now, we accurately formulate and prove Proposition 1.

Proposition 2 Consider a SI function $f_{\alpha}(x,y) = \alpha \frac{x^2}{x^2+y^2}$. Let it be optimized using projected gradient descent (2) with learning rate $\eta \equiv \tilde{\eta}$ on the unit sphere starting from a point $(x^{(0)}, y^{(0)})$ such that $x^{(0)} \neq 0$ and $y^{(0)} \neq 0$. Then the following results hold:

- 1. $\tilde{\eta} < \frac{1}{\alpha}$ is a sufficient condition for linear convergence of the function to zero (global minimum);
- 2. $\tilde{\eta} > \frac{1}{\alpha}$ is a sufficient condition for the function to stabilize at value $\frac{1}{2} \left(\alpha \frac{1}{\tilde{\eta}} \right)$.

Remark 1 If $\tilde{\eta} = \frac{1}{\alpha}$, the convergence to the minimum is still preserved, although it may not be as stable, so we omit this case as degenerate.

Remark 2 The above formulation allegedly lacks the third (divergent) regime. We draw the line between the second and the third regimes by comparing them with random guess quality (see Appendix M): the third regime is much more reminiscent of the random walk behavior than the second one (chaos \gg equilibrium). Using the same criterion, we may notice that in the limit of $\tilde{\eta} \to \infty$ the value of the function $f_{\alpha}(x,y)$ around which optimization "stabilizes" is $\frac{\alpha}{2}$ corresponding to the expected value of the function given that input points are randomly sampled on the sphere, which totally accords with our intuition.

Proof. To study the convergence properties of $f_{\alpha}(x,y)$, note first that it depends only on the x/y ratio, which we denote as $r \equiv x/y$:

$$f_{\alpha}(x,y) = \alpha \frac{x^2}{x^2 + y^2} = \alpha \frac{r^2}{1 + r^2}.$$
 (17)

That allows us to conclude that $f(x^{(t)},y^{(t)})\underset{t\to\infty}{\longrightarrow} 0 \iff r^{(t)}\underset{t\to\infty}{\longrightarrow} 0$, thus studying the convergence of f_{α} to the minimum is equivalent to studying the convergence of r to zero. The gradient of the function is

$$\nabla f_{\alpha}(x,y) = \frac{2\alpha xy}{(x^2 + y^2)^2} [y, -x]^T.$$
 (18)

That induces the following update rule for r (note that $(x^{(t)})^2 + (y^{(t)})^2 = 1$):

$$r^{(t+1)} = \frac{x^{(t+1)}}{y^{(t+1)}} = \frac{x^{(t)} - 2\alpha\tilde{\eta}x^{(t)}(y^{(t)})^2}{y^{(t)} + 2\alpha\tilde{\eta}(x^{(t)})^2y^{(t)}} = \frac{x^{(t)}}{y^{(t)}} \left(1 - \frac{2\alpha\tilde{\eta}}{1 + 2\alpha\tilde{\eta}(x^{(t)})^2}\right) = r^{(t)} \left(1 - \frac{2\alpha\tilde{\eta}}{1 + 2\alpha\tilde{\eta}(r^{(t)})^2/(1 + (r^{(t)})^2)}\right). \quad (19)$$

Ultimately, we get the following expression for the next absolute value of r:

$$|r^{(t+1)}| = \kappa^{(t)}|r^{(t)}|, \ \kappa^{(t)} \equiv \left|1 - \frac{2\alpha\tilde{\eta}}{1 + 2\alpha\tilde{\eta}(r^{(t)})^2/(1 + (r^{(t)})^2)}\right|. \tag{20}$$

Now, we prove the first statement. If $\tilde{\eta} < \frac{1}{\alpha}$, then

$$0 < \frac{2\alpha\tilde{\eta}}{1 + 2\alpha\tilde{\eta}} < \frac{2\alpha\tilde{\eta}}{1 + 2\alpha\tilde{\eta}(r^{(t)})^2/(1 + (r^{(t)})^2)} < 2\alpha\tilde{\eta} < 2, \tag{21}$$

from which we obtain that $\kappa^{(t)} < 1$ in eq. (20), which implies linear convergence of r to zero.

For the second statement, based on eq. (21), one can obtain that

$$\kappa^{(t)} > 1 \iff \frac{2\alpha\tilde{\eta}}{1 + 2\alpha\tilde{\eta}(r^{(t)})^2/(1 + (r^{(t)})^2)} > 2 \iff \frac{(r^{(t)})^2}{(1 + (r^{(t)})^2)} < \frac{\alpha\tilde{\eta} - 1}{2\alpha\tilde{\eta}} \iff \\ \iff (r^{(t)})^2 < (r^*)^2 \equiv \frac{\alpha\tilde{\eta} - 1}{\alpha\tilde{\eta} + 1}. \quad (22)$$

That essentially means that r^2 must stabilize at level $(r^*)^2$ since otherwise, if $(r^{(t)})^2 < (r^*)^2$, $\kappa^{(t)} > 1$ and the sequence begins to increase, and if $(r^{(t)})^2 > (r^*)^2$, $\kappa^{(t)} < 1$ and the sequence is decreasing. Finally, note that the level $(r^*)^2$ from eq. (22) corresponds to the function's value $\frac{1}{2} \left(\alpha - \frac{1}{\tilde{\eta}} \right)$ due to eq. (17).

A.4 More formally on the results of Section 3.2

In this section, we provide a more formal argument on the results of Section 3.2.

Minimization of function (7) on the unit sphere can be represented as a separable optimization problem with a single uniform constraint on the parameters norm:

$$\begin{cases}
F(\boldsymbol{x}, \boldsymbol{y}) \to \min_{\boldsymbol{x}, \boldsymbol{y}} \\
\|\boldsymbol{x}\|^2 + \|\boldsymbol{y}\|^2 = 1
\end{cases}
\iff
\begin{cases}
\alpha_i f(x_i, y_i) \to \min_{x_i, y_i}, i = 1, \dots, n \\
\sum_{i=1}^n x_i^2 + y_i^2 = 1.
\end{cases}$$
(23)

According to the results of Section 3.1, solving it with the projected gradient method (2) with a fixed total ELR $\tilde{\eta}$ would be similar to running n projected gradient methods for each subfunction $\alpha_i f(x_i, y_i)$ with varying individual ELRs $\tilde{\eta}_i$, related by eq. (3). Proposition 1 states that for each subfunction to converge, its individual ELR $\tilde{\eta}_i$ must remain below the $\frac{1}{\alpha_i}$ threshold or, equivalently,

$$\frac{1}{\tilde{\eta}_i} > \alpha_i. \tag{24}$$

If the first regime condition (8) is fulfilled, then $\frac{1}{\tilde{\eta}} = \sum_{i=1}^{n} \frac{1}{\tilde{\eta}_i} > \sum_{i=1}^{n} \alpha_i$, and thus there is enough capacity to satisfy condition (24) for each subfunction and successfully converge to the minimum.

If, conversely, $\tilde{\eta} > \frac{1}{\sum_{i=1}^n \alpha_i}$, then at each iteration at least one of the individual ELRs exceeds its convergence threshold: $\tilde{\eta}_i > \frac{1}{\alpha_i}$. Due to Proposition 1, that subfunction's value will tend to stabilize at $\frac{1}{2} \left(\alpha_i - \frac{1}{\tilde{\eta}_i} \right)$. Generalizing that argument, at any moment each subfunction with individual ELR $\tilde{\eta}_i$ tends to $\max \left\{ 0, \frac{1}{2} \left(\alpha_i - \frac{1}{\tilde{\eta}_i} \right) \right\}$, and thus the whole function $F(\boldsymbol{x}, \boldsymbol{y})$ tends to their sum:

$$\sum_{i=1}^{n} \max \left\{ 0, \frac{1}{2} \left(\alpha_i - \frac{1}{\tilde{\eta}_i} \right) \right\} \ge \frac{1}{2} \sum_{i=1}^{n} \left(\alpha_i - \frac{1}{\tilde{\eta}_i} \right) = \frac{1}{2} \left(\sum_{i=1}^{n} \alpha_i - \frac{1}{\tilde{\eta}} \right) > 0.$$
 (25)

That means that in the second regime the function value is pushed away from zero towards some positive value at every iteration. The same applies to its gradient, from what we conclude that the total effective step size is also nonvanishing. That implies that the dynamics (5) work in the "undamped" regime, i.e., the squared effective step size values in the expression cannot be neglected. As stated in the main text, the only way for such dynamics to stabilize is to equalize the ESS values.

In Proposition 1, we prove that once ELR $\tilde{\eta}$ is larger than the $\frac{1}{\alpha}$ threshold, the function $f_{\alpha}(x,y)$ is stabilized at $\frac{1}{2}\left(\alpha-\frac{1}{\tilde{\eta}}\right)$. In the proof (see Proposition 2), we show that it follows from the stabilization of the $r^2\equiv x^2/y^2$ ratio at $(r^*)^2\equiv \frac{\alpha\tilde{\eta}-1}{\alpha\tilde{\eta}+1}$. Using eq. (18), it can be shown that the squared effective gradient norm of $f_{\alpha}(x,y)$ equals

$$\tilde{g}_{\alpha}^{2} \equiv \|\nabla f_{\alpha}(x,y)\|^{2} (x^{2} + y^{2}) = 4\alpha^{2} \frac{x^{2}y^{2}}{(x^{2} + y^{2})^{2}} = 4\alpha^{2} \frac{r^{2}}{(1+r^{2})^{2}}.$$
 (26)

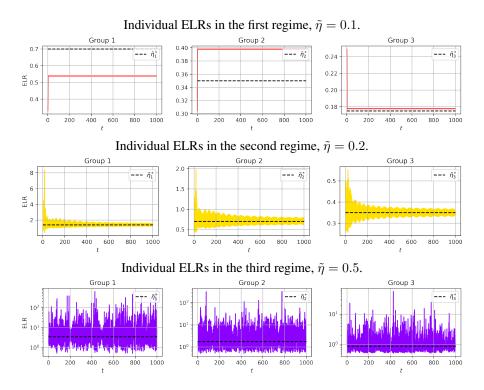


Figure 8: Individual ELRs from the experiment at the end of Section 3.2 in three regimes.

Now, substituting $(r^*)^2$ for r^2 in eq. (26) results in $\alpha^2 - \frac{1}{\tilde{\eta}^2}$, and thus the corresponding squared ESS value is $\alpha^2 \tilde{\eta}^2 - 1$. In the chaotic equilibrium state, when all the individual ESS values are equal, we obtain the following system of equations for individual ELRs:

$$\begin{cases} \alpha_i^2 \tilde{\eta}_i^2 - 1 = \alpha_j^2 \tilde{\eta}_j^2 - 1, \ i \neq j \\ \sum_{i=1}^n \frac{1}{\tilde{\eta}_i} = \frac{1}{\tilde{\eta}}. \end{cases}$$
 (27)

Eq. (9) solves the above system and hence represents the ideal equilibrium values that stabilize the dynamics (5) for the function F(x, y). Indeed, we verify in the experiment that individual ELRs in average equal (9) in the second regime (see below).

A.5 Additional plots for the example in Section 3.2

Here we provide additional plots depicting the behavior of individual ELRs in the toy example at the end of Section 3.2. Figure 8 illustrates the plots. Each row corresponds to a certain total ELR value (regime), each column corresponds to a certain SI parameters group. We can see that in the first regime, individual ELRs stabilize long before reaching their equilibrium limit (9) since ESS values quickly decay to zero and dynamics (5) begin to fade. In the second regime, individual ELR values closely match (in average by iterations) their corresponding equilibrium values, as the theory predicts. Finally, the third regime shows very chaotic behavior and no stabilization is visible.

B Sharpness measures

In our experiments, we use the averaged over mini-batches norm of the (effective) stochastic gradient as a measure of both local loss sharpness and optimization step length. While the second application appears obvious due to the nature of gradient optimization, we would like to provide more details on the first point.

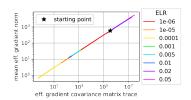
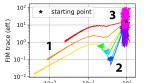


Figure 9: Mean gradient norm (28) vs. gradient covariance trace (29) during training. The two measures very strongly correlate. ConvNet, CIFAR-10.



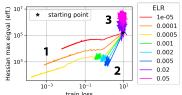


Figure 10: Training loss vs. sharpness measure diagrams with respect to different sharpness measures: Fisher Information Matrix trace (left) and maximum eigenvalue of Hessian (right). ConvNet on CIFAR-10.

Basically, we measure the following value:³

$$\mathbb{E}_{\mathcal{B}} \left\| \nabla L_{\mathcal{B}}(\boldsymbol{\theta}) \right\|, \tag{28}$$

where $L_{\mathcal{B}}(\theta)$ denotes the loss on the mini-batch \mathcal{B} and expectation is taken over the mini-batches, and we additionally multiply it by the parameters norm $\|\theta\|$ in the effective case. Expression (28) resembles the formula of the stochastic gradient covariance matrix trace:

$$\operatorname{Tr}\left(\mathbb{E}_{\mathcal{B}}\nabla L_{\mathcal{B}}(\boldsymbol{\theta})\nabla L_{\mathcal{B}}(\boldsymbol{\theta})^{T}\right) = \mathbb{E}_{\mathcal{B}}\left\|\nabla L_{\mathcal{B}}(\boldsymbol{\theta})\right\|^{2}.$$
(29)

The covariance matrix is known to be correlated with the loss Hessian matrix and the Fisher Information Matrix [32], and thus its trace can be regarded as a universal and easy-to-calculate measure of sharpness. Note that eq. (28) and eq. (29) are identical up to taking the square of the norm under expectation. Empirically, we find that these measures are highly correlated, which could be explained by a low variance of gradient norms across mini-batches (see Figure 9). We also consider other common sharpness measures and provide training loss vs. effective Fisher Information Matrix (FIM) trace and training loss vs. effective Hessian largest eigenvalue diagrams in Figure 10 that demonstrate the same pattern as in our main diagram in Figure 1.

C Experimental details

Datasets and architectures. We conduct experiments with a simple 3-layer BN convolutional neural network (ConvNet) and a ResNet-18, on CIFAR-10 [18] and CIFAR-100 [19] datasets. We use the implementation of both architectures available at https://github.com/tiptOp/periodic_behavior_bn_wd. In this implementation, additional BN layers are inserted in Resnet-18 to make the majority of neural network weights scale-invariant. CIFAR datasets are distributed under the MIT license, and the code is under Apache-2.0 License.

We use the standard PyTorch initialization for all layers. ConvNet contains an input convolutional layer with k filters followed by BN and ReLU non-linearity, then three blocks of convolution + BN + ReLU + maxpool with 2k/4k/8k filters in convolutional layers, respectively, and then maxpool + output linear layer. For ConvNet, we use width factor k=32 for all experiments on CIFAR-10 (except Appendix F, where we vary network width), and k=64 for all experiments on CIFAR-100 (the dataset is too complex for ConvNet with width factor 32 to reach low training loss and clearly depict the first training regime). In the case of SI ResNet (Appendix D and Appendix N), we use width factor of 32 for both datasets, while for conventional training (Section 6 and Appendix N) we use ResNet of standard width (width factor 64).

Most of the experiments are conducted with the scale-invariant modifications of both architectures obtained using the approach of Lobacheva et al. [27]. All non-scale-invariant weights, i.e., BN affine parameters and the last layer's parameters, are fixed. For BN layers, zero shift and unit scale parameters are used. The bias vector of the last layer is fixed at random initialization, while the weight matrix is fixed at rescaled random initialization (its norm equals 10).

Training. We train all networks using SGD with a batch size of 128. For training in the whole parameter space we use weight decay of 1e-4/5e-4 for ConvNet/ResNet-18. In the experiments with

³In the effective case, we measure this and other metrics on the unit sphere.

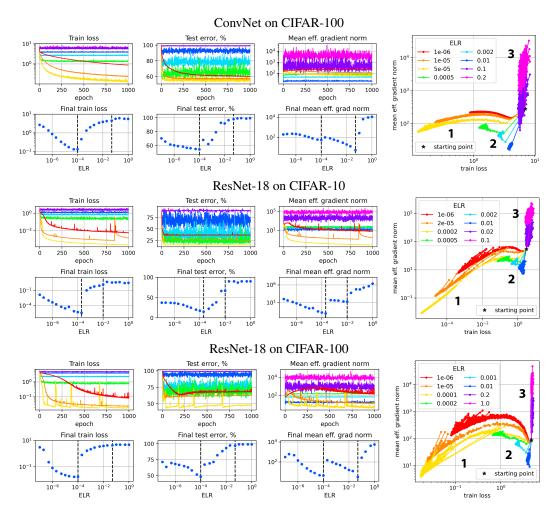


Figure 11: Three regimes of SI neural network training on the sphere. (1) convergence for the lowest ELRs, (2) chaotic equilibrium for medium ELRs, and (3) divergence for the highest ELRs. Dashed lines on scatter plots denote borders between the regimes.

momentum, we use the momentum of 0.9, in experiments with cosine LR schedule we train models for 200 epochs. In the experiments with data augmentation, we use standard CIFAR augmentations: random crop (size: 32, padding: 4) and random horizontal flip. All models were trained on NVidia Tesla V100 or NVidia GeForce GTX 1080. Obtaining the results reported in the paper took approximately 10K GPU hours. In all experiments we log all metrics after each epoch, computing train loss and its gradients by making an additional pass through the training dataset.

D Three regimes of training on the sphere

In this section, we provide the overview plots for other dataset-architecture pairs complementary to Figure 1 in the main text (see Figure 11). Three training regimes are present for all dataset-architecture pairs. Also, we observe periodic behavior of training dynamics in some ResNet-18 plots, even though we train our models on the fixed sphere. This is very reminiscent of the results of Lobacheva et al. [27], as they also observed periodic behavior when trained SI models in the whole parameters space using weight decay. Lobacheva et al. [27] showed that these sudden jumps in training loss are due to the norm of the scale-invariant parameters becoming too low. We hypothesize that similar reasons may cause periodic behavior in our case, since in relatively complex models such as ResNet, some groups of SI parameters may also come too close to the origin even at a fixed total norm, resulting in an explosion of gradients with respect to those groups.

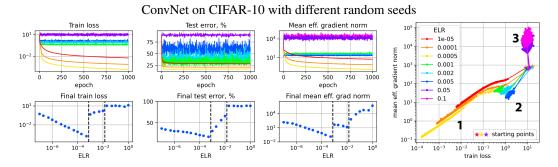


Figure 12: Three regimes of SI neural network training on the sphere with different random seed for each run (each ELR). The figure reproduces Figure 1 in the main text, including axes and the range of ELRs.

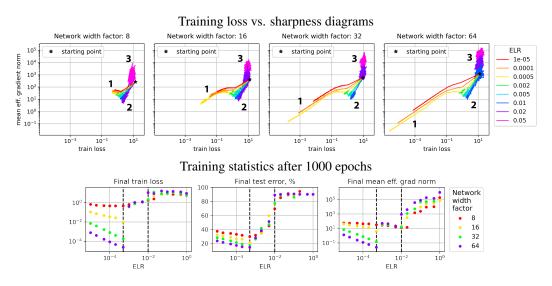


Figure 13: Three training regimes on the sphere for SI neural networks of different width. ConvNet on CIFAR-10. Axes limits are the same in each plot of the first line for convenient comparison. Dashed lines on scatter plots denote borders between the regimes for the networks of width factor 32, that we use in the rest of the paper.

E Three regimes: different random seeds

In this appendix, we provide plots analogous to Figure 1 in the main text but when each experiment is run with its own random seed, i.e., different runs (different ELRs) have different random initialization and mini-batch order during optimization. We report the results in Figure 12. It can be seen that the illustration is very similar to Figure 1, thus our findings withstand the randomness of optimization.

F Three regimes: different network sizes and data augmentation

In this section, we provide additional experiments about the dependence of the three regimes manifestation on the network size and data complexity.

In Figure 13, we demonstrate the diagrams of training loss vs. sharpness along with final training statistics, when we vary the network size (ConvNet of different width on CIFAR-10). We see that the difference between the regimes becomes much more noticeable for larger models. The smallest models (width factor 8) may not even show clear signs of transition to the first regime, i.e., convergence, and the border between the first two regimes becomes vague (see the scatter plots for the training loss and gradients). We can also notice that the second regime appears very similar for

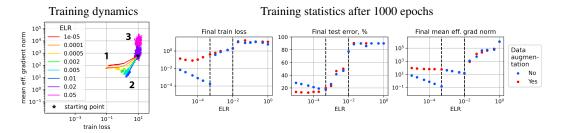


Figure 14: Three training regimes on the sphere for SI neural networks with data augmentation. ConvNet on CIFAR-10. Axes limits are the same as Figure 13 for convenient comparison. Dashed lines on scatter plots denote borders between the regimes for training without data augmentation, that we use in the rest of the paper.

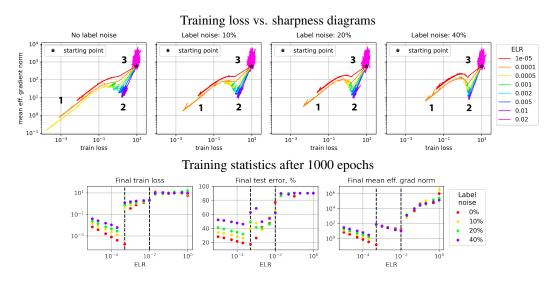


Figure 15: Three training regimes on the sphere for SI neural networks on data with different levels of label noise. ConvNet on CIFAR-10. Axes limits are the same in each plot of the first line for convenient comparison. Dashed lines on scatter plots denote borders between the regimes for training without label noise, that we use in the rest of the paper.

all network sizes, especially on the scatter plots, however, the transition between the second and third regimes happens at lower ELRs for wider networks.

Figure 14 shows the corresponding plots for ConvNet on CIFAR-10 with data augmentation. In scatter plots we provide the results for the same dataset-architecture pair without data augmentation for comparison. We observe that making dataset more complex, e.g., by turning data augmentation on, leads to a similar behavior in terms of the training loss and gradients norm as using a smaller neural network on the original dataset.

G Transition between regimes 1/2 and the double descent

Nakkiran et al. [28] discovered that deep learning models, especially when trained with noisy labels, can undergo the double descent behavior of the test error during training (epoch-wise Double Descent), and the effect becomes more noticeable the more noise is added to the training data. We replicate this setup and repeat our experiments with added label noise, i.e., we randomly select a portion of training objects and independently set their labels to the noise sampled from the uniform distribution over the classes. Figure 15 demonstrates the results for varying portion of corrupted labels. Note that the more noise is added to the training data, the clearer the sharpness peak becomes at the transition point between the first two regimes.

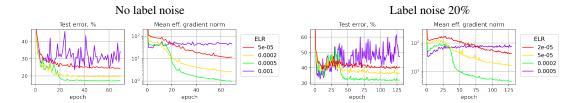


Figure 16: The first epochs of training without label noise (left) and with 20% label noise (right). Double descent behavior is observed both in test error and sharpness, ConvNet on CIFAR-10.

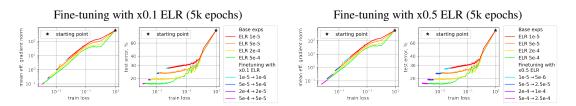


Figure 17: First training regime. Fine-tuning with decreased ELR maintains the same trajectory regardless of the initial and final ELR. ConvNet on CIFAR-10.

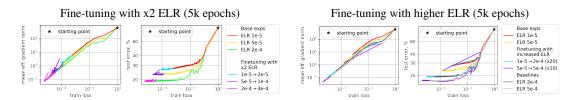


Figure 18: First training regime. Fine-tuning with a slightly increased ELR maintains the same trajectory, while with a substantially increased ELR, the training destabilizes and converges to a flatter region. ConvNet on CIFAR-10.

In Figure 16, we additionally plot the first epochs of training without label noise (left) and with 20% label noise (right). With label noise, we can clearly see that in the first regime both test error and sharpness demonstrate the double descent behavior and peak approximately at the same time. Without label noise, these peaks are not that apparent, but they also exist. At higher ELR values in the first regime, the double descent becomes more distinct, but as soon as we enter the second regime, the second descent disappears and the model gets stuck at the peak.

H First regime: fine-tuning with increased or decreased ELR

In this section, we provide additional results with decreased/increased ELR fine-tuning in the first regime. In Figure 17, we consider a wider range of initial ELR values when decreasing ELR. Sharpness and generalization profiles always maintain the same trajectory confirming that SGD cannot reach a sharper region after converging to the basin in the first regime.

Figure 18, left shows that basins in the first regime are also tolerant to fine-tuning with slightly increased ELR, except for the fact that the trajectories become more noisy. A greater increase in ELR (Figure 18, right) leads to destabilization and subsequent convergence to a new flatter region with sharpness/generalization profile corresponding to that of the final ELR value.

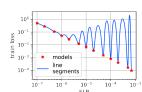
I First regime: linear mode connectivity

In this appendix, we provide additional plots on the linear mode connectivity in the first regime.

The optima achieved after learning with different ELRs not only vary in sharpness and generalization but also reside in different basins even if training starts from the same initialization and uses the

Training with constant ELR

Fine-tuning with increased/decreased ELR



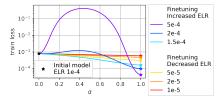


Figure 19: First training regime. Left: solutions achieved with different ELRs are not linearly connected. Right: the pre-trained and fine-tuned solutions are linearly connected for lower and moderately higher ELRs and not for significantly larger ELRs. ConvNet on CIFAR-10.

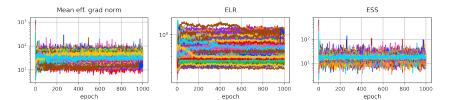


Figure 20: Individual mean effective gradient norms, ELRs, and ESS values of all SI parameters groups in the model by iterations. Stabilization of all metrics is observed; ESS values tend to cluster around the same value. ConvNet on CIFAR-10; total ELR is 0.001.

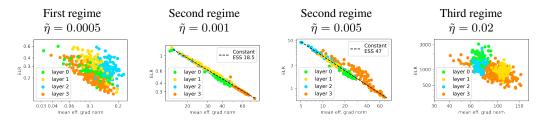


Figure 21: Individual ELRs and mean effective gradient norms of all SI parameters groups in the model (averaged over the last 200 epochs) for different total ELR values. Individual ESS equilibration is distinct in the second regime (note the dashed line). ConvNet on CIFAR-10.

same order of batches. In Figure 19, left, we check the linear connectivity of solutions achieved with different ELRs in the first regime. For each pair of neighboring ELRs, we connect the corresponding final weights with a linear path and plot the training loss along it. The results show that the solutions that converged to a low-loss region indeed lie in different basins, as there exist barriers of high loss between them.

Fine-tuning with a lower ELR does not change the basin sharpness/generalization profile, while a larger ELR may result in jumping out and converging to a new basin with its own profile. In Figure 19, right, we provide results on linear connectivity of pre-trained and fine-tuned solutions in the first regime. We can notice that the training loss is monotonically decreasing along a linear path connecting the pre-trained and the fine-tuned solution for lower and moderately higher ELR values. In contrast, for significantly larger ELRs, the linear segment has a noticeable barrier; moreover, we observe it only for the ELRs that lead to a jump in the training trajectory. This confirms our intuition that decreasing ELR maintains the same basin, while increasing ELR may result in a different one.

J Second regime: equilibration

In this section, we provide additional plots for Figure 5, left in the main text. In Figure 20 we give additional plots demonstrating that individual metrics (effective gradient norms, ELRs, and ESS values) for each SI parameters group in the network stabilize by iterations. Note also that ESS values tend to cluster around the same value, which is the main feature of the second regime.

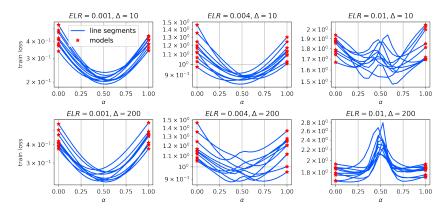


Figure 22: Second training regime. Linear connectivity of different checkpoints from the same training trajectory: small ELRs show locally convex loss, while large ELRs depict much more hilly landscape. Δ denotes the time difference (in epochs) between the connected checkpoints. ConvNet on CIFAR-10.

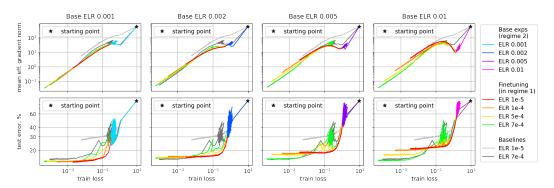


Figure 23: Second training regime. Fine-tuning with decreased ELR either keeps the same trajectory (for the lowest initial ELRs) or results in separate trajectories depending on the final ELR value (for the highest initial ELRs). ConvNet on CIFAR-10; fine-tuning for 2k epochs.

In Figure 21, we provide plots similar to Figure 5, left in the main text for other total ELR values. No equilibration of individual ESS values is observed neither in the first nor in the third regime, while in the second regime they accurately align (especially for the low ELRs of the second regime).

K Second regime: connecting checkpoints

In this appendix, we present the plots on linear connectivity of different checkpoints of the same trajectory in the second regime. From a given training trajectory obtained with a second regime ELR, we take several checkpoints and linearly connect them with the corresponding checkpoints obtained after Δ epochs. Figure 22 shows the loss behavior along these linear segments for several ELR and Δ values. We can notice that for small and moderate ELRs the training loss is almost convex and significantly lower in the middle of the segment than at its edges, which reinforces the "hopping along the walls" view on the second regime. For the highest ELRs of the second regime (especially when Δ is large), the loss is highly non-convex, indicating the more chaotic behavior of the optimization dynamics.

L Second regime: fine-tuning with first regime ELR

In this section, we provide an extensive comparison of fine-tuning results with lower ELRs starting from the second regime. As shown in Figure 23, top, the fine-tuning trajectories gradually tend to separate as the initial ELR increases (plots from left to right). In extreme cases, we have either

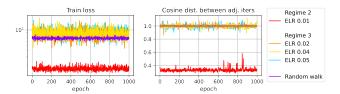


Figure 24: Random walk vs. the third regime dynamics. Cosine distance between weights on adjacent iterations (right) shows similarity between random walk and the third regime, while the training loss (left) shows difference. As a baseline, we show the largest ELR from the second regime. ConvNet on CIFAR-10.

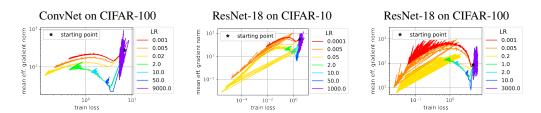


Figure 25: Three training regimes when training SI networks in the whole parameter space with weight decay.

convergence of all trajectories to the same wide optimum (lowest initial ELR 0.001), or a set of different trajectories covering the entire range of the first regime sharpness profiles (highest initial ELR 0.01). Therefore, we conclude that regions obtained with high second regime ELRs contain a rich spectrum of optima of various sharpness.

Figure 23, bottom, reveals the discrepancy between sharpness and generalization. For instance, while the fine-tuning trajectories starting from the highest ELR of the second regime closely match the baseline trajectories of the first regime in terms of sharpness range, the range of test errors achieved is much narrower than that of the baselines.

M Third regime: comparison with random walk

In this section, we compare the third regime dynamics with random walk (RW). For random walk dynamics, we train our model in the third regime but use a Gaussian random vector instead of a real gradient and appropriately scale its length to replicate the respective step size of a regular training. We found that the dynamics of RW corresponding to different ELRs in the third regime turn out to be very similar, therefore we show only one line for RW in Figure 24. We can see from Figure 24, right that the weights on adjacent iterations appear to be uncorrelated both in the third regime and in the RW case. This behavior substantially differs from the second regime, where the weights have relatively large correlation. Figure 24, left, demonstrates the difference between RW and the third regime: RW performs as a lower bound for the training loss achieved in the third regime.

N Three regimes in standard training

In this appendix, we present additional results for other dataset-architecture pairs complementary to Figure 7 in the main text.

When training SI networks in the whole parameter space using weight decay, we also observe the three regimes (Figure 25 supplements Figure 7, left). We note that ResNet-18 models demonstrate a periodic behavior in accordance with the results of Lobacheva et al. [27].

In the experiments with conventional training only first two regimes are present (Figure 26 supplements Figure 7, right). The regimes appear more distinguishable for ResNet-18 than for ConvNet (e.g., Figure 26, top right vs. bottom left), probably due to the fact that ResNet-18 is a significantly larger model. In the experiments with fixed LR, the best test accuracy is achieved at the largest

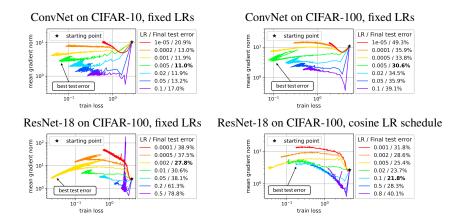


Figure 26: Training regimes in conventional training with fixed LRs and cosine LR schedules.

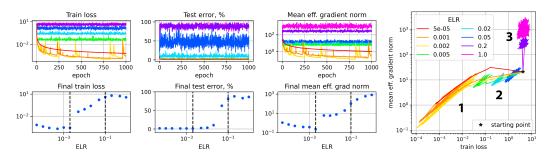


Figure 27: Training of fully-scale-invariant MLP on MNIST: all three training regimes are present.

LR of the first regime. We also conduct the experiment with cosine LR schedule for ResNet-18 on CIFAR-100 (see Figure 26, bottom right). As stated in the main text, the best performing models with cosine LR schedule correspond to the medium initial LR when both the first and second regimes are passed during the optimization.

O Additional experiments on other architectures and datasets

Most of our experiments include typical image classification tasks (CIFAR-10 and CIFAR-100) solved using convolutional architectures (ConvNet and ResNet-18). In this appendix, we present the results concerning the three training regimes obtained for other architectures and datasets: multilayer perceptron (MLP) on MNIST [7] and Transformer [34] on the AG NEWS dataset [39].

We train MLP on MNIST using the same setting as in the majority of our experiments, i.e., we make the network fully scale-invariant and optimize it on the sphere using projected SGD with a fixed ELR. We consider the following MLP architecture: a fully-connected neural network with two hidden layers of size 300 and 100, respectively. We use ReLU activation and add BN after both hidden linear layers. We made this network fully scale-invariant in accordance with Appendix C.

For the MLP on MNIST, which is shown in Figure 27, we can observe the same division on the three regimes: convergence to a minimum, chaotic equilibrium at some non-trivial loss level, and about random guess behavior. Some runs in the first regime exhibit a periodic behavior similar to the one observed with ResNet-18 in Appendix D due to similar reasons. We have also conducted experiments with MLP on the CIFAR-10 dataset but do not include them here, since the architecture appeared to be too simple to reach low loss values and adequately depict all three regimes (see Appendix F for a discussion of this issue).

In addition, we conducted an experiment in a domain other than computer vision in order to be more objective in our conclusions. We trained a Transformer neural network on the AG News classification dataset using standard SGD with weight decay of 1e-3, momentum of 0.9, and a constant learning

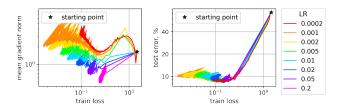


Figure 28: Conventional training of Transformer on the AG News. Results are similar to conventional training of ResNet-18 on CIFAR-10 in Section 6: the first two regimes can be clearly distinguished.

rate. For this dataset we used the encoder-only Transformer with $N=1, d_{model}=32, h=1$. We slightly modified the original architecture to make it more scale-invariant (similar to the modifications we made in ResNet architecture): we add a LayerNorm [2] after each fully-connected layer in feedforward sub-layers. Note that even after these changes the architecture is still not fully scale-invariant; making the Transformer architecture fully scale-invariant can be rather non-trivial [25], and we leave it for future work.

Sharpness/generalization vs. training loss diagrams for the Transformer on AG News are presented in Figure 28. The results are very reminiscent of the conventional training of ResNet-18 from Section 6. We can clearly observe the first two regimes on the diagram, while the third regime training quickly leads to NaNs. There is, however, a peculiar difference from the computer vision setting in a sense that the best achieved test error can be observed for LR values from both the first and the second regimes. We attribute this to overfitting of the model to the dataset.