Continuous vs. Discrete Optimization of Deep Neural Networks

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Abstract

Existing analyses of optimization in deep learning are either continuous, focusing on (variants of) gradient flow, or discrete, directly treating (variants of) gradient descent. Gradient flow is amenable to theoretical analysis, but is stylized and disregards computational efficiency. The extent to which it represents gradient descent is an open question in deep learning theory. The current paper studies this question. Viewing gradient descent as an approximate numerical solution to the initial value problem of gradient flow, we find that the degree of approximation depends on the curvature along the latter's trajectory. We then show that over deep neural networks with homogeneous activations, gradient flow trajectories enjoy favorable curvature, suggesting they are well approximated by gradient descent. This finding allows us to translate an analysis of gradient flow over deep linear neural networks into a guarantee that gradient descent efficiently converges to global minimum *almost surely* under random initialization. Experiments suggest that over simple deep neural networks, gradient descent with conventional step size is indeed close to the continuous limit. We hypothesize that the theory of gradient flows will be central to unraveling mysteries behind deep learning.

1 Introduction

The success of deep neural networks is fueled by the mysterious properties of gradient-based optimization, namely, the ability of (variants of) gradient descent to minimize non-convex training objectives while exhibiting tendency towards solutions that generalize well. Vast efforts are being directed at mathematically analyzing this phenomenon, with existing results typically falling into one of two categories: *continuous* or *discrete*. Continuous analyses usually focus on gradient flow (or variants thereof), which corresponds to gradient descent (or variants thereof) with infinitesimally small step size. Compared to their discrete (positive step size) counterparts, continuous settings are oftentimes far more amenable to theoretical analysis (*e.g.* they admit use of the theory of differential equations), but on the other hand are stylized, and disregard the critical aspect of computational efficiency (number of steps required for convergence). Works analyzing gradient flow over deep neural networks either accept the latter shortcomings (see for example [44, 4, 41]), or attempt to reproduce part of the results via completely separate analysis of gradient descent (*cf.* [28, 17, 5]). The extent to which gradient flow represents gradient descent is an open question in the theory of deep learning.

The current paper formally studies the foregoing question. Viewing gradient descent as a numerical method for approximately solving the *initial value problem* corresponding to gradient flow, we turn to the literature on numerical analysis, and invoke a fundamental theorem concerning the approximation error. The theorem implies that in general, the match between gradient descent and gradient flow is determined by the curvature around the latter's trajectory. In particular, the "more convex" the trajectory, *i.e.* the larger the (possibly negative) eigenvalues of the Hessian along it are, the better the match will be. We show that when applied to deep neural networks (fully connected as well as convolutional) with homogeneous activations (*e.g.* linear, rectified linear or leaky rectified linear), gradient flow emanating from near-zero initialization (as commonly employed in practice) follows trajectories that are "roughly convex," in the sense that the minimal eigenvalue of the Hessian along

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them is far greater than in arbitrary points in space, particularly towards convergence. This implies that over deep neural networks, gradient descent with moderately small step size may in fact be close to its continuous limit, *i.e.* to gradient flow. We exemplify an application of this finding by translating an analysis of gradient flow over deep linear neural networks into a convergence guarantee for gradient descent. The guarantee we obtain is, to our knowledge, the first to ensure that a conventional gradient-based algorithm optimizing a deep (three or more layer) neural network of fixed (data-independent[a]) size efficiently converges[b] to global minimum *almost surely* under random (data-independent) near-zero initialization.

We corroborate our theoretical analysis through experiments with basic deep learning settings, which demonstrate that reducing the step size of gradient descent often leads to only slight changes in its trajectory. This suggest that, at least in some settings, central aspects of deep neural network optimization may indeed be captured by the continuous limit. We hypothesize that the vast bodies of knowledge on continuous dynamical systems, and gradient flow in particular (see, *e.g.*, [21, 3]), will pave way to unraveling mysteries behind deep learning.

1.1 Contributions

The main contributions of this work are: *(i)* we conduct the first formal study for the discrepancy between continuous and discrete optimization of deep neural networks; *(ii)* we demonstrate the use of *generic* mathematical machinery for translating a continuous non-convex convergence result into a discrete one; *(iii)* to our knowledge, the discrete result we obtain forms the first guarantee of random (data-independent) near-zero initialization *almost surely* leading a conventional gradient-based algorithm optimizing a deep (three or more layer) neural network of fixed (data-independent) size to efficiently convergence to global minimum; *(iv)* the fundamental theorem (from numerical analysis) we employ is seldom used in machine learning contexts and may be of independent interest; and *(v)* we provide empirical evidence suggesting that discrete optimization of simple deep neural networks is often close to the continuous limit.

1.2 Paper Organization

The remainder of the paper is organized as follows. Section 2 delivers preliminary background in numerical analysis, and in particular the fundamental theorem concerning numerical solution of initial value problems. Implications of the theorem on the role of curvature in determining the match between gradient flow and gradient descent are presented in Section 3. Section 4 shows that over deep neural networks, trajectories of gradient flow enjoy favorable curvature. An application of this finding for translating a convergence result from gradient flow to gradient descent is demonstrated in Section 5. Our experiments are presented in Section 6. Due to lack of space, we defer our review of related work to Appendix A, our conclusion to Appendix B, and nearly all proofs to Appendix L.

2 Preliminaries: Numerical Solution of Initial Value Problems

Let $d \in \mathbb{N}$. Given a function $\mathbf{g} : [0, \infty) \times \mathbb{R}^d \to \mathbb{R}^d$ (viewed as a time-dependent vector field) and a point $\boldsymbol{\theta}_s \in \mathbb{R}^d$, consider the *initial value problem*:

$$\boldsymbol{\theta}(0) = \boldsymbol{\theta}_s \quad , \quad \tfrac{d}{dt}\boldsymbol{\theta}(t) = \mathbf{g}(t, \boldsymbol{\theta}(t)) \ \text{ for } t \geq 0 \,. \tag{1}$$

The following result — an extension of the well known Picard-Lindelöf Theorem — provides conditions for the existence and uniqueness of a solution $\boldsymbol{\theta}(\cdot)$.

Theorem 1 (Existence-Uniqueness)**.** *Consider the initial value problem in Equation* (1)*, and suppose* $\mathbf{g}(\cdot)$ *is locally Lipschitz continuous. Then, there exists a solution* $\boldsymbol{\theta} : [0, t_e) \to \mathbb{R}^d$*, where either:* (i) $t_e = \infty$*; or* (ii) $t_e < \infty$ *and* $\lim_{t \nearrow t_e} \|\boldsymbol{\theta}(t)\|_2 = \infty$*. Moreover, the solution is unique in the sense that any other solution* $\boldsymbol{\theta}' : [0, t'_e) \to \mathbb{R}^d$ *must satisfy* $t'_e \leq t_e$ *and* $\forall t \in [0, t'_e) : \boldsymbol{\theta}'(t) = \boldsymbol{\theta}(t)$.

Proof. The theorem is a direct consequence of the results in Section 1.5 of [23].[c] □

It is typically the case that the solution to Equation (1) cannot be expressed in closed form, and a numerical approximation is sought after. Various numerical methods for approximately solving initial value problems have been developed over the years (see Chapter 12 in [50] for an introduction), of which the simplest is known as *Euler's method*. The latter is parameterized by a *step size* $\eta > 0$, and when applied to Equation (1) follows the recursive scheme:

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k + \eta \, \mathbf{g}(t_k, \boldsymbol{\theta}_k) \ \text{ for } k = 0, 1, 2, \ldots, \tag{2}$$

where $t_k := k\eta$ and the initial point $\boldsymbol{\theta}_0$ is typically set to $\boldsymbol{\theta}_s$. The motivation behind Euler's method is straightforward — a first order Taylor expansion of the exact solution $\boldsymbol{\theta}(\cdot)$ around time t_k yields:

$\boldsymbol{\theta}(t_{k+1}) = \boldsymbol{\theta}(t_k + \eta) \approx \boldsymbol{\theta}(t_k) + \eta \frac{d}{dt}\boldsymbol{\theta}(t_k) = \boldsymbol{\theta}(t_k) + \eta\, \mathbf{g}(t_k, \boldsymbol{\theta}(t_k))$, therefore if $\boldsymbol{\theta}(t_k)$ is well approximated by $\boldsymbol{\theta}_k$ we may expect $\boldsymbol{\theta}_{k+1}$ to resemble $\boldsymbol{\theta}(t_{k+1})$. The numerical solution produced by Euler's method may be viewed as a continuous polygonal curve:

$$\bar{\boldsymbol{\theta}} : [0, \infty) \to \mathbb{R}^d \ , \ \bar{\boldsymbol{\theta}}(0) = \boldsymbol{\theta}_0 \ , \ \tfrac{d}{dt}\bar{\boldsymbol{\theta}}(t) = \mathbf{g}(t_k, \boldsymbol{\theta}_k) \ \text{ for } t \in (t_k, t_{k+1}) \,,\, k = 0, 1, 2, \ldots \,. \tag{3}$$

The quality of the numerical solution then boils down to the distance between this curve and the exact solution, *i.e.* between $\bar{\boldsymbol{\theta}}(t)$ and $\boldsymbol{\theta}(t)$ for $t \geq 0$. Many efforts have been made to derive tight bounds for this distance. We provide below a modern result known as "Fundamental Theorem."

Theorem 2 (Fundamental Theorem)**.** *Consider the initial value problem in Equation* (1)*, and suppose* $\mathbf{g}(\cdot)$ *is continuously differentiable. Let* $\boldsymbol{\theta} : [0, t_e) \to \mathbb{R}^d$ *be the solution to this problem (see Theorem 1), and let* $\bar{\boldsymbol{\theta}} : [0, \infty) \to \mathbb{R}^d$ *be a continuous polygonal curve (Equation* (3)*) born from Euler's method (Equation* (2)*). For any* $t \in [0, t_e), \mathbf{q} \in \mathbb{R}^d$*, denote by* $J(t, \mathbf{q}) \in \mathbb{R}^{d,d}$ *the Jacobian of* $\mathbf{g}(\cdot)$ *with respect to its second argument at the point* $(t, \mathbf{q})$*, and by* $\lambda_{max}(t, \mathbf{q})$ *the maximal eigenvalue of* $\frac{1}{2}(J(t, \mathbf{q}) + J(t, \mathbf{q})^\top)$.[d] *Let* $m : [0, t_e) \to \mathbb{R}$ *be an integrable function satisfying* $\lambda_{max}(t, \mathbf{q}) \leq m(t)$ *for all* $t \in [0, t_e)$*,* $\mathbf{q} \in [\boldsymbol{\theta}(t), \bar{\boldsymbol{\theta}}(t)]$*, where* $[\boldsymbol{\theta}(t), \bar{\boldsymbol{\theta}}(t)]$ *stands for the line segment (in* $\mathbb{R}^d$*) between* $\boldsymbol{\theta}(t)$ *and* $\bar{\boldsymbol{\theta}}(t)$*. Let* $\delta : [0, t_e) \to \mathbb{R}_{\geq 0}$ *be an integrable function that meets* $\| \frac{d}{dt}\bar{\boldsymbol{\theta}}(t^+) - \mathbf{g}(t, \bar{\boldsymbol{\theta}}(t)) \|_2 \leq \delta(t)$ *for all* $t \in [0, t_e)$*, where* $\frac{d}{dt}\bar{\boldsymbol{\theta}}(t^+)$ *represents the right derivative of* $\bar{\boldsymbol{\theta}}(\cdot)$ *at time* t*. Denote* $\mu(t) := \int_0^t m(t')dt'$*. Then, for all* $t \in [0, t_e)$*:*

$$\|\boldsymbol{\theta}(t) - \bar{\boldsymbol{\theta}}(t)\|_2 \leq e^{\mu(t)} \Big(\|\boldsymbol{\theta}(0) - \bar{\boldsymbol{\theta}}(0)\|_2 + \textstyle\int_0^t e^{-\mu(t')} \delta(t') dt' \Big) \,. \tag{4}$$

Proof. The theorem is simply a restatement of Theorem 10.6 in [25]. □

3 Continuous vs. Discrete Optimization: Match Determined by Convexity

Let $f : \mathbb{R}^d \to \mathbb{R}$, where $d \in \mathbb{N}$, be a twice continuously differentiable function which we would like to minimize. Consider continuous optimization via *gradient flow* initialized at $\boldsymbol{\theta}_s \in \mathbb{R}^d$:

$$\boldsymbol{\theta}(0) = \boldsymbol{\theta}_s \quad , \quad \tfrac{d}{dt}\boldsymbol{\theta}(t) = -\nabla f(\boldsymbol{\theta}(t)) \ \text{ for } t \geq 0 \,. \tag{5}$$

This is a special case of the initial value problem presented in Equation (1).[e] By Theorem 1, it admits a unique solution $\boldsymbol{\theta} : [0, t_e) \to \mathbb{R}^d$, where either: *(i)* $t_e = \infty$; or *(ii)* $t_e < \infty$ and $\lim_{t \nearrow t_e} \|\boldsymbol{\theta}(t)\|_2 = \infty$. Numerically approximating this solution via Euler's method (Equation (2)) yields a discrete optimization algorithm which is no other than *gradient descent*:

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta\, \nabla f(\boldsymbol{\theta}_k) \ \text{ for } k = 0, 1, 2, \ldots, \tag{6}$$

where $\eta > 0$ is the chosen step size. We may thus invoke the Fundamental Theorem (Theorem 2) and obtain a bound on the distance between the trajectories of gradient flow and gradient descent.

Theorem 3. *Consider the trajectory of gradient flow (solution to Equation* (5)*)* $\boldsymbol{\theta} : [0, t_e) \to \mathbb{R}^d$*, and let* $\bar{t} \in (0, t_e)$ *and* $\epsilon > 0$*. Define* $\mathcal{D}_{\bar{t},\epsilon} := \bigcup_{t \in [0, \bar{t}]} \mathcal{B}_\epsilon(\boldsymbol{\theta}(t))$*, where* $\mathcal{B}_\epsilon(\boldsymbol{\theta}(t)) \subset \mathbb{R}^d$ *stands for the (closed) Euclidean ball of radius* ϵ *centered at* $\boldsymbol{\theta}(t)$*. Let* $\beta_{\bar{t},\epsilon}, \gamma_{\bar{t},\epsilon} > 0$ *be such that* $\sup_{\mathbf{q} \in \mathcal{D}_{\bar{t},\epsilon}} \|\nabla^2 f(\mathbf{q})\|_{spectral} \leq \beta_{\bar{t},\epsilon}$ *and* $\sup_{\mathbf{q} \in \mathcal{D}_{\bar{t},\epsilon}} \|\nabla f(\mathbf{q})\|_2 \leq \gamma_{\bar{t},\epsilon}$*. Let* $m : [0, \bar{t}] \to \mathbb{R}$ *be an integrable function satisfying* $-\lambda_{min}(\nabla^2 f(\mathbf{q})) \leq m(t)$ *for all* $t \in [0, \bar{t}]$*,* $\mathbf{q} \in \mathcal{B}_\epsilon(\boldsymbol{\theta}(t))$*, where* $\lambda_{min}(\nabla^2 f(\mathbf{q}))$ *stands for the minimal eigenvalue of* $\nabla^2 f(\mathbf{q})$*. Then, if the step size* $\eta > 0$ *chosen for gradient descent (Equation* (6)*) satisfies:*

$$\eta < \inf_{t \in (0, \bar{t}]} \big(\epsilon - e^{\int_0^t m(t')dt'} \|\boldsymbol{\theta}_0 - \boldsymbol{\theta}(0)\|_2 \big) \big(\beta_{\bar{t},\epsilon} \gamma_{\bar{t},\epsilon} \textstyle\int_0^t e^{\int_{t'}^t m(t'')dt''} dt' \big)^{-1} \,, \tag{7}$$

the first $\lfloor \bar{t}/\eta \rfloor$ *iterates of gradient descent will* ϵ*-approximate the trajectory of gradient flow up to time* $\bar{t}$*, i.e. we will have* $\|\boldsymbol{\theta}_k - \boldsymbol{\theta}(k\eta)\|_2 \leq \epsilon$ *for all* $k \in \{1, 2, \ldots, \lfloor \bar{t}/\eta \rfloor\}$*.*

Proof. The complete proof is provided in Subappendix L.2. □

Theorem 3 gives a sufficient condition — upper bound on step size η (Equation (7)) — for gradient descent to follow gradient flow up to a given time $\bar{t}$. The bound is inversely proportional to smoothness and Lipschitz constants ($\beta_{\bar{t},\epsilon}$ and $\gamma_{\bar{t},\epsilon}$ respectively), and more importantly, depends exponentially on the integral of $m(\cdot)$ along the gradient flow trajectory, where $m(\cdot)$ corresponds to minus the minimal eigenvalue of the Hessian. The smaller the integral of $m(\cdot)$, *i.e.* the larger (less negative or more positive) the minimal eigenvalue of the Hessian along the trajectory is, the more relaxed the bound will be. That is, *the "more convex" the objective function is along the trajectory of gradient flow, the better the match between that and gradient descent* is guaranteed to be.

Corollary 2 in Appendix C coarsely applies Theorem 3 by fixing $m(\cdot)$ to minus the minimal eigenvalue of the Hessian across the entire space. If $m(\cdot) \equiv m$ (now a constant) is negative, *i.e.* the objective

function $f(\cdot)$ is strongly convex, the upper bound on the step size η becomes constant, meaning it is independent of the time $\bar{t}$ until which gradient descent is required to follow gradient flow. If m is equal to zero, *i.e.* $f(\cdot)$ is (non-strongly) convex, the upper bound on η mildly tightens with $\bar{t}$, namely it scales as $1/\bar{t}$. If on the other hand m is positive, meaning $f(\cdot)$ is non-convex, the bound on η shrinks to zero (becoming more restrictive) exponentially fast as $\bar{t}$ grows. This suggests that as opposed to (strongly or non-strongly) convex objectives, over which gradient descent can easily be made to follow gradient flow, over non-convex objectives, in the worst case, gradient descent will immediately divert from gradient flow unless its step size is exponentially small. In Appendix E we present a simple example of such a worst case scenario. In this worst case, the minimal eigenvalue of the Hessian is bounded below and away from zero throughout the gradient flow trajectory. A question is then whether there are non-convex objectives in which the minimal eigenvalue of the Hessian along gradient flow trajectories is large enough for them to be followed by gradient descent. We will see that training losses of deep neural networks can meet this property.

4 Optimization of Deep Neural Networks is Roughly Convex

Section 3 has shown that the extent to which gradient descent matches gradient flow depends on "how convex" the objective function is along the latter's trajectory. More precisely, the larger (less negative or more positive) the minimal eigenvalue of the Hessian is around this trajectory, the longer gradient descent (with given step size) is guaranteed to follow it. In this section we establish that over training losses of deep neural networks (fully connected as well as convolutional) with homogeneous activations (*e.g.* linear, rectified linear or leaky rectified linear), when emanating from near-zero initialization (as commonly employed in practice), trajectories of gradient flow are "roughly convex," in the sense that the minimal eigenvalue of the Hessian around them is far greater than in arbitrary points in space, particularly towards convergence. This finding suggests that when optimizing deep neural networks, gradient descent may closely resemble gradient flow. We demonstrate an application of the finding in Section 5, translating an analysis of gradient flow over deep linear neural networks into a guarantee of efficient convergence to global minimum for gradient descent, which applies *almost surely* with respect to a random near-zero initialization.

4.1 Fully Connected Architectures

Consider the mappings realized by a fully connected neural network with depth $n \in \mathbb{N}_{\geq 2}$, input dimension $d_0 \in \mathbb{N}$, hidden widths $d_1, d_2, \ldots, d_{n-1} \in \mathbb{N}$, and output dimension $d_n \in \mathbb{N}$:

$$h_{\boldsymbol{\theta}} : \mathbb{R}^{d_0} \to \mathbb{R}^{d_n} \;\;,\;\; h_{\boldsymbol{\theta}}(\mathbf{x}) = W_n \, \sigma(W_{n-1} \, \sigma(W_{n-2} \cdots \sigma(W_1 \mathbf{x})) \cdots) \,, \tag{8}$$

where $W_j \in \mathbb{R}^{d_j, d_{j-1}}$, $j = 1, 2, \ldots, n$, are learned weight matrices, $\boldsymbol{\theta} \in \mathbb{R}^d$, with $d := \sum_{j=1}^{n} d_j d_{j-1}$, is their arrangement as a vector,[f] and $\sigma : \mathbb{R} \to \mathbb{R}$ is a predetermined activation function that operates element-wise when applied to a vector.[g] We assume that $\sigma(\cdot)$ is (positively) *homogeneous*, meaning $\sigma(cz) = c\,\sigma(z)$ for all $c \geq 0, z \in \mathbb{R}$. This allows for linear ($\sigma(z) = z$), as well as the commonly employed rectified linear ($\sigma(z) = \max\{z, 0\}$) and leaky rectified linear ($\sigma(z) = \max\{z, \alpha z\}$ for some $0 < \alpha < 1$) activations.

Let $\mathcal{Y}$ be a set of possible labels, and let $\mathcal{S} = \big((\mathbf{x}_i, y_i)\big)_{i=1}^{|\mathcal{S}|}$, with $\mathbf{x}_i \in \mathbb{R}^{d_0}, y_i \in \mathcal{Y}$ for $i = 1, 2, \ldots, |\mathcal{S}|$, be a sequence of labeled inputs. Given a loss function $\ell : \mathbb{R}^{d_n} \times \mathcal{Y} \to \mathbb{R}$ convex and twice continuously differentiable in its first argument (common choices include square, logistic and exponential losses), we learn the weights of the neural network by minimizing its *training loss* — average loss over elements of $\mathcal{S}$:

$$f : \mathbb{R}^d \to \mathbb{R} \;\;,\;\; f(\boldsymbol{\theta}) = \frac{1}{|\mathcal{S}|} \sum\nolimits_{i=1}^{|\mathcal{S}|} \ell(h_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i) \,. \tag{9}$$

Subsubsections 4.1.1 and 4.1.2 below show (for linear and non-linear activation functions, respectively) that although the minimal eigenvalue of $\nabla^2 f(\boldsymbol{\theta})$ (Hessian of training loss) — denoted $\lambda_{min}(\nabla^2 f(\boldsymbol{\theta}))$ — can in general be arbitrarily negative, along trajectories of gradient flow (which emanate from near-zero initialization) it is no less than moderately negative, becoming non-negative towards convergence. In light of Section 3, this suggests that over fully connected deep neural networks, gradient flow may lend itself to approximation by gradient descent — a prospect we confirm (for a case with linear activation) in Section 5.

4.1.1 Linear Activation

Assume that the activation function of the fully connected neural network (Equation (8)) is linear, *i.e.* $\sigma(z) = z$, and define the *end-to-end matrix*:

$$W_{n:1} := W_n W_{n-1} \cdots W_1 \in \mathbb{R}^{d_n, d_0} \,. \tag{10}$$

The mappings realized by the network can then be written as $h_{\boldsymbol{\theta}}(\mathbf{x}) = W_{n:1}\mathbf{x}$, and the training loss as $f(\boldsymbol{\theta}) = \phi(W_{n:1})$, where:

$$\phi : \mathbb{R}^{d_n,d_0} \to \mathbb{R} \ , \ \ \phi(W) = \tfrac{1}{|\mathcal{S}|}\sum\nolimits_{i=1}^{|\mathcal{S}|} \ell(W\mathbf{x}_i, y_i) \tag{11}$$

is convex and twice continuously differentiable. Lemma 1 below expresses $\nabla^2 f(\boldsymbol{\theta})$ in this case.

Lemma 1. *For any $\boldsymbol{\theta} \in \mathbb{R}^d$, regard $\nabla^2 f(\boldsymbol{\theta})$ not only as a (symmetric) matrix in $\mathbb{R}^{d,d}$, but also as a quadratic form $\nabla^2 f(\boldsymbol{\theta})[\,\cdot\,]$ that intakes a tuple $(\Delta W_1, \Delta W_2, \ldots, \Delta W_n) \in \mathbb{R}^{d_1,d_0} \times \mathbb{R}^{d_2,d_1} \times \cdots \times \mathbb{R}^{d_n,d_{n-1}}$, arranges it as a vector $\Delta\boldsymbol{\theta} \in \mathbb{R}^d$ (in correspondence with how weight matrices $W_1, W_2, \ldots, W_n$ are arranged to create $\boldsymbol{\theta}$), and returns $\Delta\boldsymbol{\theta}^\top \nabla^2 f(\boldsymbol{\theta})\, \Delta\boldsymbol{\theta} \in \mathbb{R}$. Similarly, for any $W \in \mathbb{R}^{d_n,d_0}$, regard $\nabla^2\phi(W)$ as a quadratic form $\nabla^2\phi(W)[\,\cdot\,]$ that intakes a matrix in $\mathbb{R}^{d_n,d_0}$ and returns a scalar (non-negative since $\phi(\cdot)$ is convex). Then, $\nabla^2 f(\boldsymbol{\theta})$ is given by:*

$$\begin{aligned}\nabla^2 f(\boldsymbol{\theta})\,[\Delta W_1, \Delta W_2, \ldots, \Delta W_n] &= \nabla^2\phi(W_{n:1})\big[\textstyle\sum_{j=1}^{n} W_{n:j+1}(\Delta W_j)W_{j-1:1}\big] \\ &+2\,\mathrm{Tr}\left(\nabla\phi(W_{n:1})^\top \textstyle\sum_{1\le j<j'\le n} W_{n:j'+1}(\Delta W_{j'})W_{j'-1:j+1}(\Delta W_j)W_{j-1:1}\right)\end{aligned} \tag{12}$$

where $W_{j':j}$, for any $j, j' \in \{1, 2, \ldots, n\}$, is defined as $W_{j'}W_{j'-1}\cdots W_j$ if $j \le j'$, and as an identity matrix (with size to be inferred by context) otherwise.

Proof. A sketch and the complete proof are provided in Subappendix L.3) □

The following proposition makes use of Lemma 1 to show that (under mild conditions) $\lambda_{min}(\nabla^2 f(\boldsymbol{\theta}))$ can be arbitrarily negative, *i.e.* $\inf_{\boldsymbol{\theta}\in\mathbb{R}^d} \lambda_{min}(\nabla^2 f(\boldsymbol{\theta})) = -\infty$.

Proposition 1. *Assume that the network is deep ($n \ge 3$), and that the zero mapping is not a global minimizer of the training loss (meaning $\nabla\phi(0) \neq 0$).*[h] *Then $\inf_{\boldsymbol{\theta}\in\mathbb{R}^d} \lambda_{min}(\nabla^2 f(\boldsymbol{\theta})) = -\infty$.*

Proof. A sketch and the complete proof are provided in Subappendix L.4. □

Building on Lemma 1, Lemma 2 below provides a lower bound on $\lambda_{min}(\nabla^2 f(\boldsymbol{\theta}))$.

Lemma 2. *For any $\boldsymbol{\theta} \in \mathbb{R}^d$:*

$$\lambda_{min}(\nabla^2 f(\boldsymbol{\theta})) \ge -2n\sqrt{\min\{d_0, d_n\}}\,\|\nabla\phi(W_{n:1})\|_{Frobenius} \max_{\substack{\mathcal{J}\subseteq\{1,2,\ldots,n\} \\ |\mathcal{J}|=n-2}} \prod_{j\in\mathcal{J}} \|W_j\|_{spectral}\,. \tag{13}$$

Proof. A sketch and the complete proof are provided in Subappendix L.5. □

Assuming the training loss is non-constant and the network is deep ($n \ge 3$), the infimum (over $\boldsymbol{\theta} \in \mathbb{R}^d$) of the lower bound in Equation (13) is minus infinity. In particular, if $\boldsymbol{\theta}$ is not a global minimizer ($\nabla\phi(W_{n:1}) \neq 0$) and at least $n-2$ of its weight matrices $W_1, W_2, \ldots, W_n$ are non-zero, then by rescaling the latter it is possible to take the lower bound to minus infinity while keeping the end-to-end matrix $W_{n:1}$ (and thus the input-output mapping $h_{\boldsymbol{\theta}}(\cdot)$ and the training loss value $f(\boldsymbol{\theta})$) intact. However, gradient flow over fully connected neural networks is known to maintain balance between weight matrices (when emanating from near-zero initialization) — see [17] — and so along its trajectories the lower bound in Equation (13) takes a much tighter form. This is formalized below.

Proposition 2. *If $\boldsymbol{\theta} \in \mathbb{R}^d$ resides on a trajectory of gradient flow (over $f(\cdot)$) initialized at some point $\boldsymbol{\theta}_s \in \mathbb{R}^d$, with $\|\boldsymbol{\theta}_s\|_2 \le \epsilon$ for some $\epsilon > 0$, then:*

$$\lambda_{min}(\nabla^2 f(\boldsymbol{\theta})) \ge -2n\sqrt{\min\{d_0, d_n\}}\,\|\nabla\phi(W_{n:1})\|_{Frobenius}\|W_{n:1}\|_{spectral}^{1-2/n} - c\,\epsilon^{1-2/n}, \tag{14}$$

where $c := 8n^2\sqrt{\min\{d_0, d_n\}}\,\|\nabla\phi(W_{n:1})\|_{Frobenius} \max\left\{1, \max\{\|W_j\|_{spectral}\}_{j=1}^{n}\right\}^{2n^2}$.

Proof. A sketch and the complete proof are provided in Subappendix L.6. □

The lower bound in Equation (14) primarily depends on the sizes (norms) of the end-to-end matrix $W_{n:1}$ and the gradient of the loss with respect to it, *i.e.* $\nabla\phi(W_{n:1})$ (see Equations (10) and (11)). Along a trajectory of gradient flow (over $f(\cdot)$) emanating from near-zero initialization, $W_{n:1}$ is initially small, and (since the loss $f(\boldsymbol{\theta}) = \phi(W_{n:1})$ is monotonically non-increasing) remains confined to sublevel sets of $\phi(\cdot)$ (which is convex) thereafter. $\nabla\phi(W_{n:1})$ on the other hand tends to zero upon convergence to global minimum. We conclude that the lower bound on $\lambda_{min}(\nabla^2 f(\boldsymbol{\theta}))$ in Equation (14) starts off slightly negative, and becomes non-negative (if and) as the trajectory approaches global minimum. By Section 3, this implies that gradient flow may lend itself to approximation by gradient descent. Indeed, Proposition 2 (with Lemmas 1 and 2) is used in Section 5 to translate an analysis of gradient flow into a guarantee of efficient convergence to global minimum for gradient descent.

4.1.2 Non-Linear Activation

When the (homogeneous) activation function of the fully connected neural network (Equation (8)) is non-linear, *i.e.* $\sigma(z) = \alpha\max\{z, 0\} - \bar{\alpha}\max\{-z, 0\}$ for some $\alpha, \bar{\alpha} \in \mathbb{R}$, $\alpha \neq \bar{\alpha}$, the training loss $f(\cdot)$

is (typically) not everywhere differentiable. It is however locally Lipschitz thus differentiable almost everywhere (see Theorem 9.1.2 in [10]). Moreover, as established by Proposition 10 in Appendix G, for almost every $\boldsymbol{\theta}' \in \mathbb{R}^d$ there exist diagonal matrices $D'_{i,j} \in \mathbb{R}^{d_j,d_j}$, $i = 1, 2, \ldots, |\mathcal{S}|$, $j = 1, 2, \ldots, n-1$, with diagonal elements in $\{\alpha, \bar{\alpha}\}$, such that $f(\cdot)$ coincides with the function:

$$\boldsymbol{\theta} \mapsto \tfrac{1}{|\mathcal{S}|} \sum\nolimits_{i=1}^{|\mathcal{S}|} \ell(W_n D'_{i,n-1} W_{n-1} D'_{i,n-2} W_{n-2} \cdots D'_{i,1} W_1 \mathbf{x}_i, y_i) \tag{15}$$

on an open region $\mathcal{D}_{\boldsymbol{\theta}'} \subseteq \mathbb{R}^d$ containing $\boldsymbol{\theta}'$, that is closed under positive rescaling of weight matrices (*i.e.* under $(W_1, W_2, \ldots, W_n) \mapsto (c_1 W_1, c_2 W_2, \ldots, c_n W_n)$ with $c_1, c_2, \ldots, c_n > 0$). The notion of gradient flow over a non-differentiable locally Lipschitz objective function is typically formalized via differential inclusion and Clarke subdifferentials (*cf.* [14, 13]). To our knowledge there exists no analogue of the Fundamental Theorem (Theorem 2) that applies to this formalization, thus we focus on (open) regions of the form $\mathcal{D}_{\boldsymbol{\theta}'}$, where $f(\cdot)$ is given by Equation (15) and in particular is twice continuously differentiable. On such regions the analysis of Section 3 applies, and since they constitute the entire weight space but a negligible (closed and zero measure) set, they can facilitate a "piecewise characterization" of the discrepancy between gradient flow and gradient descent.

Lemma 3 below expresses $\nabla^2 f(\boldsymbol{\theta})$ for $\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\theta}'}$.

Lemma 3. *Let $\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\theta}'}$. For $i \in \{1, 2, \ldots, |\mathcal{S}|\}$ and $j, j' \in \{1, 2, \ldots, n\}$ define $(D'_{i,*} W_*)_{j':j}$ to be the matrix $D'_{i,j'} W_{j'} D'_{i,j'-1} W_{j'-1} \cdots D'_{i,j} W_j$ (where by convention $D'_{i,n} \in \mathbb{R}^{d_n,d_n}$ stands for identity) if $j \leq j'$, and an identity matrix (with size to be inferred by context) otherwise. For $i \in \{1, 2, \ldots, |\mathcal{S}|\}$ let $\nabla \ell_i \in \mathbb{R}^{d_n}$ and $\nabla^2 \ell_i \in \mathbb{R}^{d_n,d_n}$ be the gradient and Hessian (respectively) of the loss $\ell(\cdot)$ at the point $\big((D'_{i,*} W_*)_{n:1} \mathbf{x}_i, y_i\big)$ with respect to its first argument. Then, regarding Hessians as quadratic forms (see Lemma 1), it holds that:*

$$\begin{aligned}\nabla^2 f(\boldsymbol{\theta})[\Delta W_1, \Delta W_2, \ldots, \Delta W_n] = \frac{1}{|\mathcal{S}|} \sum_{i=1}^{|\mathcal{S}|} \nabla^2 \ell_i \left[\sum_{j=1}^{n} (D'_{i,*} W_*)_{n:j+1} D'_{i,j} (\Delta W_j) (D'_{i,*} W_*)_{j\text{-}1:1} \mathbf{x}_i \right] \\ + \frac{2}{|\mathcal{S}|} \sum_{i=1}^{|\mathcal{S}|} \nabla \ell_i^\top \sum_{1 \leq j < j' \leq n} (D'_{i,*} W_*)_{n:j'+1} D'_{i,j'} (\Delta W_{j'}) (D'_{i,*} W_*)_{j'\text{-}1:j+1} D'_{i,j} (\Delta W_j) (D'_{i,*} W_*)_{j\text{-}1:1} \mathbf{x}_i \,.\end{aligned} \tag{16}$$

Proof. A sketch and the complete proof are provided in Subappendix L.7. □

The following proposition employs Lemma 3 to show that (under mild conditions) there exists $\boldsymbol{\theta} \in \mathbb{R}^d$ for which $\lambda_{min}(\nabla^2 f(\boldsymbol{\theta}))$ is arbitrarily negative.

Proposition 3. *Assume that:* (i) *the network is deep ($n \geq 3$); and* (ii) *the loss function $\ell(\cdot)$ and training set $\mathcal{S}$ are non-degenerate, in the sense that there exists a weight setting $\boldsymbol{\theta} \in \mathbb{R}^d$ for which $\sum_{i=1}^{|\mathcal{S}|} \nabla \ell(\mathbf{0}, y_i)^\top h_{\boldsymbol{\theta}}(\mathbf{x}_i) \neq 0$, where $\nabla \ell(\cdot)$ stands for the gradient of $\ell(\cdot)$ with respect to its first argument, and $h_{\boldsymbol{\theta}}(\cdot)$ is the input-output mapping realized by the network (Equation* (8))*.*[i] *Then, it holds that* $\inf_{\boldsymbol{\theta} \in \mathbb{R}^d \text{ s.t. } \nabla^2 f(\boldsymbol{\theta}) \text{ exists}} \lambda_{min}(\nabla^2 f(\boldsymbol{\theta})) = -\infty$.

Proof. A sketch and the complete proof are provided in Subappendix L.8. □

Relying on Lemma 3, Lemma 4 below provides a lower bound on $\lambda_{min}(\nabla^2 f(\boldsymbol{\theta}))$ for $\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\theta}'}$.

Lemma 4. *With the notations of Lemma 3, for any $\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\theta}'}$:*

$$\lambda_{min}(\nabla^2 f(\boldsymbol{\theta})) \geq -\max\{|\alpha|, |\bar{\alpha}|\}^{n-1} \frac{2n}{|\mathcal{S}|} \sum_{i=1}^{|\mathcal{S}|} \|\nabla \ell_i\|_2 \|\mathbf{x}_i\|_2 \max_{\substack{\mathcal{J} \subseteq \{1,2,\ldots,n\} \\ |\mathcal{J}| = n-2}} \prod_{j \in \mathcal{J}} \|W_j\|_{Frobenius} \,. \tag{17}$$

Proof. A sketch and the complete proof are provided in Subappendix L.9. □

The lower bound in Equation (17) is highly sensitive to the scales of the individual weight matrices. Specifically, if $\boldsymbol{\theta}$ does not perfectly fit all non-zero training inputs (meaning there exists $i \in \{1, 2, \ldots, |\mathcal{S}|\}$ for which $\nabla \ell_i \neq \mathbf{0}$ and $\mathbf{x}_i \neq \mathbf{0}$), and if at least $n-2$ of its weight matrices $W_1, W_2, \ldots, W_n$ are non-zero, then it is possible to rescale each W_j by $c_j > 0$, with $\prod_{j=1}^{n} c_j = 1$, such that the lower bound in Equation (17) becomes arbitrarily negative[j] despite the input-output mapping $h_{\boldsymbol{\theta}}(\cdot)$ (and thus the training loss value $f(\boldsymbol{\theta})$) remaining unchanged. Nevertheless, similarly to the case of linear activation (Subsubsection 4.1.1), we may employ the fact that (when emanating from near-zero initialization) gradient flow over fully connected neural networks maintains balance between weight matrices — *cf.* [17] — to show that along its trajectories, the lower bound in Equation (17) assumes a tighter form. This is done in Proposition 4 below.

Proposition 4. *If $\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\theta}'}$ resides on a trajectory of gradient flow (over $f(\cdot)$) initialized at some point $\boldsymbol{\theta}_s \in \mathbb{R}^d$, with $\|\boldsymbol{\theta}_s\|_2 \leq \epsilon$ for some $\epsilon > 0$, then, using the notations of Lemma 3:*

$$\lambda_{min}(\nabla^2 f(\boldsymbol{\theta})) \geq -\max\{|\alpha|, |\bar{\alpha}|\}^{n-1} \frac{2n}{|\mathcal{S}|} \sum_{i=1}^{|\mathcal{S}|} \|\nabla \ell_i\|_2 \|\mathbf{x}_i\|_2 \Big(\min_{j \in \{1,2,\ldots,n\}} \|W_j\|_{Frobenius} + \epsilon \Big)^{n-2} . \quad (18)$$

Proof. A sketch and the complete proof are provided in Subappendix L.10. □

The lower bound in Equation (18) primarily depends on the *minimal* size (Frobenius norm) of a weight matrix W_j, and on $\nabla \ell_1, \nabla \ell_2, \ldots, \nabla \ell_{|\mathcal{S}|}$ — gradients of the loss function with respect to the predictions over the training set. Along a trajectory of gradient flow (over $f(\cdot)$) emanating from near-zero initialization, $W_1, W_2, \ldots, W_n$ are initially small, and if a perfect fit of the training set is ultimately achieved, $\nabla \ell_1, \nabla \ell_2, \ldots, \nabla \ell_{|\mathcal{S}|}$ will converge to zero. Therefore, if not all weight matrices $W_1, W_2, \ldots, W_n$ become large along the trajectory, the lower bound on $\lambda_{min}(\nabla^2 f(\boldsymbol{\theta}))$ in Equation (18) will only be moderately negative before becoming non-negative (if and) as the trajectory approaches a perfect fit. By Section 3, this suggests that gradient flow may lend itself to approximation by gradient descent. For the case of linear activation (Subsubsection 4.1.1) such prospect is theoretically verified in Section 5. For the non-linear case we provide empirical corroboration in Section 6, deferring to future work a complete theoretical affirmation.

4.2 Convolutional Architectures

We account for convolutional neural networks by allowing for weight sharing and sparsity patterns to be imposed on the layers of the fully connected model analyzed in Subsection 4.1. Namely, we consider the exact same mappings as in Equation (8), but now, rather than being learned directly, the matrices $W_j \in \mathbb{R}^{d_j, d_{j-1}}$, $j = 1, 2, \ldots, n$, are determined by learned weight vectors $\mathbf{w}_j \in \mathbb{R}^{d'_j}$, with $d'_j \in \mathbb{N}$, $j = 1, 2, \ldots, n$, such that each entry of W_j is either fixed at zero or connected to a predetermined coordinate of $\mathbf{w}_j$ (with no repetition of coordinates within the same row). The weight setting $\boldsymbol{\theta} \in \mathbb{R}^d$ is then simply a concatenation of the weight vectors $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_n$, and its dimension is accordingly $d = \sum_{j=1}^{n} d'_j$. Our analysis for this model (which includes convolutional neural networks as a special case) is essentially the same as that presented for fully connected neural networks with non-linear activation (Subsubsection 4.1.2). In particular, we use the fact that even with weight sharing and sparsity patterns imposed on the layers of a fully connected neural network, gradient flow over the latter maintains balance between weights of different layers (when emanating from near-zero initialization) — *cf.* [17]. For the complete analysis see Appendix F.

5 Continuous Proof of Discrete Convergence for Deep Linear Networks

Section 3 invoked the Fundamental Theorem for numerical solution of initial value problems to show that in general, the extent to which gradient descent matches gradient flow is determined by how large (less negative or more positive) the minimal eigenvalue of the Hessian is along the latter's trajectory. Section 4 established that for training losses of deep neural networks, along trajectories of gradient flow emanating from near-zero initialization (as commonly employed in practice), the minimal eigenvalue of the Hessian is no less than moderately negative, becoming non-negative towards convergence. In this section we combine the two findings, translating an analysis of gradient flow over deep linear neural networks into a convergence guarantee for gradient descent. The guarantee we obtain is, to our knowledge, the first to ensure that a conventional gradient-based algorithm optimizing a deep (three or more layer) neural network of fixed (data-independent[a]) size efficiently converges[b] to global minimum *almost surely* under random (data-independent) near-zero initialization.

Deep (three or more layer) linear neural networks — fully connected neural networks with linear activation (see Subsection 4.1) — are perhaps the most common subject of theoretical study in the context of optimization in deep learning. Though trivial from an expressiveness point of view (realize only linear input-output mappings), they induce highly non-convex training losses, giving rise to highly non-trivial phenomena under gradient-based optimization. In recent years, various results concerning gradient flow over deep linear neural networks have been proven, most notably for the case of *balanced initialization* (see for example [44, 4, 31, 6, 41]). Under the notations of Subsection 4.1 (in particular with $W_1, W_2, \ldots, W_n$ standing for network weight matrices), balanced initialization means that when optimization commences:

$$W_{j+1}^{\top} W_{j+1} = W_j W_j^{\top} \text{ for } j = 1, 2, \ldots, n-1 . \quad (19)$$

The condition holds approximately with any near-zero initialization, and exactly when the following procedure (taken from [5]) is employed.

Procedure 1 (random balanced initialization)**.** *With a distribution $\mathcal{P}$ over d_n-by-d_0 matrices of rank at most $\min\{d_0, d_1, \ldots, d_n\}$, initialize $W_j \in \mathbb{R}^{d_j, d_{j-1}}$, $j = 1, 2, \ldots, n$, via following steps:*

(i) *sample* $A \sim \mathcal{P}$*;* (ii) *take singular value decomposition* $A = U\Sigma V^\top$*, where* $U \in \mathbb{R}^{d_n,\min\{d_0,d_n\}}$ *and* $V \in \mathbb{R}^{d_0,\min\{d_0,d_n\}}$ *have orthonormal columns, and* $\Sigma \in \mathbb{R}^{\min\{d_0,d_n\},\min\{d_0,d_n\}}$ *is diagonal and holds the singular values of* A*; and* (iii) *set* $W_n \simeq U\Sigma^{1/n}, W_{n-1} \simeq \Sigma^{1/n}, W_{n-2} \simeq \Sigma^{1/n}, \ldots, W_2 \simeq \Sigma^{1/n}, W_1 \simeq \Sigma^{1/n}V^\top$*, where "*$\simeq$*" stands for equality up to zero-valued padding.*

Compared to gradient flow, little is known about gradient descent when it comes to optimization of deep linear neural networks. Indeed, there are relatively few results along this line (*cf.* [9, 28, 5]), and these are typically highly specific, built upon technical proofs that are difficult to generalize. Being able to obtain results via translation of gradient flow analyses is thus of prime interest.

We focus in this section on deep linear neural networks trained for scalar regression per least-squares criterion. In the context of Subsection 4.1, this means that the activation function $\sigma(\cdot)$ is linear ($\sigma(z) = z$), the output dimension d_n is one, and the loss function $\ell(\cdot)$ is the square loss (*i.e.* $\mathcal{Y} = \mathbb{R}$ and $\ell(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$). We assume that training inputs are whitened, *i.e.* have been transformed such that their empirical (uncentered) covariance matrix $\Lambda_{xx} := \frac{1}{|\mathcal{S}|}\sum_{i=1}^{|\mathcal{S}|} \mathbf{x}_i\mathbf{x}_i^\top \in \mathbb{R}^{d_0,d_0}$ is equal to identity. A standard calculation (see Appendix I) shows that in this case the function $\phi(\cdot)$ defined by Equation (11) becomes $\phi(W) = \frac{1}{2}\|W - \Lambda_{yx}\|_{Frobenius}^2 + c$, where $\Lambda_{yx} := \frac{1}{|\mathcal{S}|}\sum_{i=1}^{|\mathcal{S}|} y_i\mathbf{x}_i^\top \in \mathbb{R}^{1,d_0}$ is the empirical (uncentered) cross-covariance matrix between training labels and inputs, and $c \in \mathbb{R}$ is a constant (independent of W). We may thus write the training loss $f(\cdot)$ (Equation (9)) as:

$$f(\boldsymbol{\theta}) \;=\; \tfrac{1}{2}\|W_{n:1} - \Lambda_{yx}\|_{Frobenius}^2 + c \;=\; \tfrac{1}{2}\|W_{n:1} - \Lambda_{yx}\|_{Frobenius}^2 + \min_{\mathbf{q}\in\mathbb{R}^d} f(\mathbf{q})\,, \tag{20}$$

where $W_{n:1} \in \mathbb{R}^{1,d_0}$ is the network's end-to-end matrix (Equation (10)). We disregard the degenerate case where $\Lambda_{yx} = 0$, *i.e.* where the zero mapping attains the global minimum, and assume that training labels are normalized (scaled) such that Λ_{yx} has unit length ($\|\Lambda_{yx}\|_{Frobenius} = 1$).

Proposition 5 below analyzes gradient flow over the training loss in Equation (20). Relying on a known characterization for the dynamics of the end-to-end matrix (*cf.* [4]), it establishes convergence to global minimum. Moreover, harnessing the results of Subsubsection 4.1.1, it derives a lower bound on (the integral of) the minimal eigenvalue of the Hessian around the gradient flow trajectory.

Proposition 5. *Consider minimization of the training loss* $f(\cdot)$ *in Equation* (20) *via gradient flow (Equation* (5)*) starting from initial point* $\boldsymbol{\theta}_s \in \mathbb{R}^d$ *that meets the balancedness condition (Equation* (19)*). Denote by* $W_{n:1,s}$ *the initial value of the end-to-end matrix (Equation* (10)*), and suppose that* $\|W_{n:1,s}\|_{Frobenius} \in (0, 0.2]$ *(initialization is small but non-zero). Assume that* $W_{n:1,s}$ *is not antiparallel to* Λ_{yx}*, i.e.* $\nu := \mathrm{Tr}(\Lambda_{yx}^\top W_{n:1,s})/\big(\|\Lambda_{yx}\|_{Frobenius}\|W_{n:1,s}\|_{Frobenius}\big) \neq -1$*. Then, the trajectory of gradient flow is defined over infinite time, and with* $\boldsymbol{\theta} : [0, \infty) \to \mathbb{R}^d$ *representing this trajectory, for any* $\bar{\epsilon} > 0$*, the following time* $\bar{t}$ *satisfies* $f(\boldsymbol{\theta}(\bar{t})) - \min_{\mathbf{q}\in\mathbb{R}^d} f(\mathbf{q}) \leq \bar{\epsilon}$*:*

$$\bar{t} = 2n\|W_{n:1,s}\|_{Frobenius}^{-1}\big(1.5\max\{1, \tfrac{1-\nu}{1+\nu}\}\big)^n \ln\Big(\tfrac{10n}{\bar{\epsilon}\|W_{n:1,s}\|_{Frobenius}}\max\{1, \tfrac{1-\nu}{1+\nu}\}\Big)\,. \tag{21}$$

Moreover, under the notations of Theorem 3, for any $t \in (0, \bar{t} + 1]$ *and* $\epsilon \in (0, \frac{1}{2n}]$ *with corresponding* $\mathcal{D}_{t,\epsilon}$ *(*ϵ*-neighborhood of gradient flow trajectory up to time* t*), we have the smoothness and Lipschitz constants* $\beta_{t,\epsilon} = 16n$ *and* $\gamma_{t,\epsilon} = 6\sqrt{n}$ *respectively, and the following (upper) bound on the integral of (minus) the minimal eigenvalue of the Hessian:*

$$\int_0^t m(t')dt' \leq \ln\Big(\big(\max\{1, \tfrac{1-\nu}{1+\nu}\}\big)^{6n} e^{10n} n^4 \|W_{n:1,s}\|_{Frobenius}^{-4}\Big) + \Big(\epsilon + \frac{n\big(\max\{1.5\cdot\frac{1-\nu}{1+\nu}\}\big)^n}{\|W_{n:1,s}\|_{Frobenius}}\epsilon^2\Big)\frac{80n^3\big(1.5\max\{1, \frac{1-\nu}{1+\nu}\}\big)^n}{\|W_{n:1,s}\|_{Frobenius}} \ln\Big(\frac{10n\max\{1, \frac{1-\nu}{1+\nu}\}}{\min\{1,\bar{\epsilon}\}\|W_{n:1,s}\|_{Frobenius}}\Big)\,. \tag{22}$$

Proof. A sketch and the complete proof are provided in Subappendix L.11. □

Plugging the gradient flow results of Proposition 5 into the generic Theorem 3 translates them to the following convergence guarantee for gradient descent.

Theorem 4. *Assume the same conditions as in Proposition 5, but with minimization via gradient descent (Equation* (6)*) instead of gradient flow.*[k] *Then, with* $\boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots$ *representing the iterates of gradient descent, for any* $\tilde{\epsilon} > 0$*, if the step size* η *meets:*

$$\eta \leq \left(\frac{20000n^{10}}{\sqrt{\tilde{\epsilon}}\|W_{n:1,s}\|_{Frobenius}^6}\big(\max\{1, \tfrac{1-\nu}{1+\nu}\}\big)^{8n} e^{13n}\Big(\ln\big(\tfrac{40n}{\tilde{\epsilon}\|W_{n:1,s}\|_{Frobenius}}\max\{1, \tfrac{1-\nu}{1+\nu}\}\big)\Big)^2\right)^{-1}, \tag{23}$$

it holds that $f(\boldsymbol{\theta}_k) - \min_{\mathbf{q}\in\mathbb{R}^d} f(\mathbf{q}) \leq \tilde{\epsilon}$*, where:*

$$k = \left\lfloor \frac{1}{\eta}\frac{2n}{\|W_{n:1,s}\|_{Frobenius}}\big(1.5\max\{1, \tfrac{1-\nu}{1+\nu}\}\big)^n \ln\Big(\tfrac{40n}{\tilde{\epsilon}\|W_{n:1,s}\|_{Frobenius}}\max\{1, \tfrac{1-\nu}{1+\nu}\}\Big)\right\rfloor\,. \tag{24}$$

Proof. A sketch and the complete proof are provided in Subappendix L.12. □

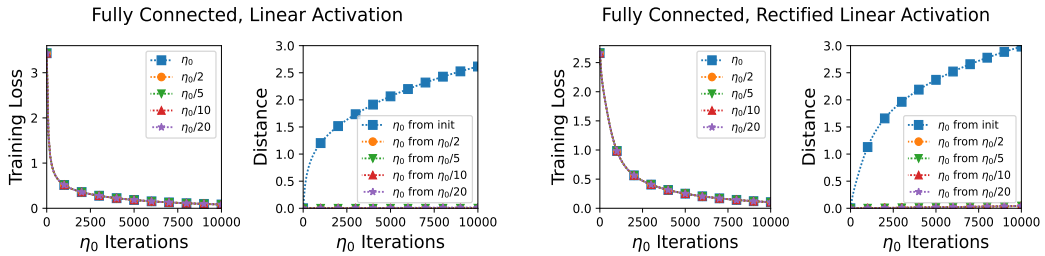

Figure 1: Over deep fully connected neural networks, trajectories of gradient descent with conventional step size barely change when the latter is reduced, suggesting they are close to the continuous limit, *i.e.* to trajectories of gradient flow. Presented results were obtained on fully connected neural networks as analyzed in Subsection 4.1, trained to classify MNIST handwritten digits (28-by-28 grayscale images, each labeled as an integer between 0 and 9 — *cf.* [32]). Networks had depth $n = 3$, input dimension $d_0 = 784$ (corresponding to $28 \cdot 28 = 784$ pixels), hidden widths $d_1 = d_2 = 50$ and output dimension $d_3 = 10$ (corresponding to ten possible labels). Training was based on gradient descent applied to cross-entropy loss with no regularization, starting from a near-zero point drawn from Xavier distribution (*cf.* [22]). Separately on each network, we compared runs differing only in the step size η. Specifically, with $\eta_0 = 0.001$ (standard choice of step size) and r ranging over $\{2, 5, 10, 20\}$, we compared, in terms of training loss value and location in weight space, every iteration of a run using $\eta = \eta_0$ to every r'th iteration of a run in which $\eta = \eta_0/r$. Left pair of plots reports results obtained on a network with linear activation ($\sigma(z) = z$), while right pair corresponds to a network with rectified linear activation ($\sigma(z) = \max\{z, 0\}$). In each pair, left plot displays training loss values, and right one shows (Euclidean) distances in weight space, namely, distance between initialization and run with $\eta = \eta_0$, alongside distances between the latter and runs having $\eta = \eta_0/r$ for different values of r. Horizontal axes represent time in units of $\eta = \eta_0$ iterations (meaning each time unit corresponds to r iterations of a run with $\eta = \eta_0/r$). Notice that the drift between runs with different step sizes is minor compared to the distance traveled. For further implementation details, and results of similar experiments on convolutional neural networks, see Appendix K.

Remark 1. *Theorem 3 — our generic tool for translating analyses between gradient flow and gradient descent — allows for the two to be initialized differently. Accordingly, the convergence guarantee of Theorem 4 may be extended to account for initialization which is not perfectly balanced, i.e. which satisfies Equation* (19) *only approximately. For details see Appendix J.*

Remark 2. *The convergence guarantee of Theorem 4 requires a number of iterates that scales exponentially with network depth* (n)*. [46] has proven that under mild conditions, for a deep linear neural network whose input, hidden and output dimensions are all equal to one (i.e.* $d_0 = d_1 = \cdots = d_n = 1$*), such exponential dependence on depth is unavoidable. We defer to future work the question of whether this also holds in the context of Theorem 4.*

Combining Theorem 4 with random balanced initialization (Procedure 1) yields what is, to our knowledge, the first guarantee of random (data-independent) near-zero initialization *almost surely* leading a conventional gradient-based algorithm to efficiently converge to global minimum when optimizing a deep (three or more layer) neural network of fixed (data-independent) size.

Corollary 1. *Consider minimization of the training loss* $f(\cdot)$ *in Equation* (20) *via gradient descent (Equation* (6)*) emanating from a random balanced initialization (Procedure 1) whose underlying distribution* $\mathcal{P}$ *is continuous and satisfies* $\Pr_{A\sim\mathcal{P}}\left[\|A\|_{Frobenius} \leq 0.2\right] = 1$*. Let* $W_{n:1,s}$ *and* ν *be as defined in Proposition 5. Then, almost surely with respect to (i.e. with probability one over) initialization, for any* $\tilde{\epsilon} > 0$*, if the step size* η *meets Equation* (23)*, the value of* $f(\cdot)$ *after* k *iterates will be within* $\tilde{\epsilon}$ *from global minimum, where* k *is given by Equation* (24)*.*

Proof. The complete proof is provided in Subappendix L.14. □

6 Experiments

In this section we corroborate our theory by presenting experiments suggesting that over simple deep neural networks, gradient descent with conventional step size is indeed close to the continuous limit, *i.e.* to gradient flow. Our experimental protocol is simple — on several deep neural networks classifying MNIST handwritten digits ([32]), we compare runs of gradient descent differing only in the step size η. Specifically, separately on each evaluated network, with $\eta_0 = 0.001$ (standard choice of step size) and r ranging over $\{2, 5, 10, 20\}$, we compare, in terms of training loss value and location in weight space, every iteration of a run using $\eta = \eta_0$ to every r'th iteration of a run in which $\eta = \eta_0/r$. Figure 1 reports the results obtained on fully connected neural networks (as analyzed in Subsection 4.1), with both linear and non-linear activation. As can be seen, reducing the step size η leads to only slight changes, suggesting that the trajectory of gradient descent with $\eta = \eta_0$ is already close to the continuous limit. Similar results obtained on convolutional neural networks (see Subsection 4.2 for corresponding analysis) are reported by Figure 3 in Subappendix K.1.

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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]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (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]
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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]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [N/A]
   (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]
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]
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   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A] There are no new assets other than our code (included in supplemental material).
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
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5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]