Piecewise convexity of artificial neural networks

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Abstract

Although artificial neural networks have shown great promise in applications including computer vision and speech recognition, there remains considerable practical and theoretical difficulty in optimizing their parameters. The seemingly unreasonable success of gradient descent methods in minimizing these non-convex functions remains poorly understood. In this work we offer some theoretical guarantees for networks with piecewise affine activation functions, which have in recent years become the norm. We prove three main results. Firstly, that the network is piecewise convex as a function of the input data. Secondly, that the network, considered as a function of the parameters in a single layer, all others held constant, is again piecewise convex. Finally, that the network as a function of all its parameters is piecewise multi-convex, a generalization of biconvexity. From here we characterize the local minima and stationary points of the training objective, showing that they minimize certain subsets of the parameter space. We then analyze the performance of two optimization algorithms on multi-convex problems: gradient descent, and a method which repeatedly solves a number of convex sub-problems. We prove necessary convergence conditions for the first algorithm and both necessary and sufficient conditions for the second, after introducing regularization to the objective. Finally, we remark on the remaining difficulty of the global optimization problem. Under the squared error objective, we show that by varying the training data. a single rectifier neuron admits local minima arbitrarily far apart, both in objective value and parameter space.

Index terms— convex analysis; gradient descent; optimization; machine learning; neural networks; convergence

1. Introduction

Artificial neural networks are currently considered the state of the art in applications ranging from image classification, to speech recognition and even machine translation. However, little is understood about the process by which they are trained for supervised learning tasks. The problem of optimizing their parameters is an active area both practical and theoretical research. Despite considerable sensitivity to initialization and choice of hyperparameters, neural networks often achieve compelling results after optimization by gradient descent methods. Due to the nonconvexity and massive parameter space of these functions, it is poorly understood how these sub-optimal methods have proven so successful. Indeed, training a certain kind of neural network is known to be NP-Complete, making it difficult to provide any worst-case training guarantees [1]. Much recent work has attempted to reconcile these differences between theory and practice [2, 3].

This article attempts a modest step towards understanding the dynamics of the training procedure. We establish three main convexity results for a certain class of neural network, which is the current the state of the art. First, that the objective is piecewise convex as a function of the input data, with parameters fixed, which corresponds to the behavior at test time. Second, that the objective is again piecewise convex as a function of the parameters of a single layer, with the input data and all other parameters held constant. Third, that the training objective function, for which all parameters are variable but the input data is fixed, is piecewise multi-convex. That is, it is a continuous function which can be represented by a finite number of multi-convex functions, each active on a multi-convex parameter set. This generalizes the notion of biconvexity found in the optimization literature to piecewise functions and arbitrary index sets [4]. To prove these results, we require two main restrictions on the definition of a neural network: that its layers are piecewise affine functions, and that its objective function is convex and continuously differentiable. Our definition includes many contemporary use cases, such as least squares or logistic regression on a convolutional neural network with rectified linear unit (ReLU) activation functions and either max- or mean-pooling. In recent years these networks have mostly supplanted the classic sigmoid type, except in the case of recurrent networks [5]. We make no assumptions about the training data, so our results apply to the current state of the art in many practical scenarios.

Piecewise multi-convexity allows us to characterize the extrema of the training objective. As in the case of biconvex functions, stationary points and local minima are guaranteed optimality on larger sets than we would have for general smooth functions. Specifically, these points are partial minima when restricted to the relevant piece. That is, they are points for which no decrease can be made in the training objective without simultaneously varying the parameters across multiple layers, or crossing the boundary into a different piece of the function. Unlike global minima, we show that partial minima are reliably found by the optimization algorithms used in current practice.

Finally, we provide some guarantees for solving general multi-convex optimization problems by various algorithms. First we analyze gradient descent, proving necessary convergence conditions. We show that every point to which gradient descent converges is a piecewise partial minimum, excepting some boundary conditions. To prove stronger results, we define a different optimization procedure breaking each parameter update into a number of convex sub-problems. For this procedure, we show both necessary and sufficient conditions for convergence to a piecewise partial minimum. Interestingly, adding regularization to the training objective is all that is needed to prove necessary conditions. Similar results have been independently established for many kinds of optimization problems, including bilinear and biconvex optimization, and in machine learning the special case of linear autoencoders [6, 4, 7]. Our analysis extends existing results on alternating convex optimization to the case of arbitrary index sets, and general multi-convex point sets, which is needed for neural networks. We admit biconvex problems, and therefore linear autoencoders, as a special case.

Despite these results, we find that it is difficult to pass from partial to global optimality results. Unlike the encouraging case of linear autoencoders, we show that a single rectifier neuron, under the squared error objective, admits arbitrarily poor local minima. This suggests that much work remains to be done in understanding how sub-optimal methods can succeed with neural networks. Still, piecewise multi-convex functions are in some senses easier to minimize than the general class of smooth functions, for which none of our previous guarantees can be made. We hope that our characterization of neural networks could contribute to a better understanding of these important machine learning systems.

2. Preliminary material

We begin with some preliminary definitions and basic results concerning continuous piecewise functions.

Definition 2.1. Let $g_1, g_2, ..., g_N$ be continuous functions from $\mathbb{R}^n \to \mathbb{R}$. A continuous piecewise function f has a finite number of closed, connected sets $S_1, S_2, ..., S_M$ covering \mathbb{R}^n such that for each k we have $f(\mathbf{x}) = g_k(\mathbf{x})$ for all $\mathbf{x} \in S_k$. The set S_k is called a **piece** of f, and the function g_k is called **active** on S_k .

More specific definitions follow by restricting the functions g. A continuous piecewise affine function has $g_k(\mathbf{x}) = \mathbf{a}^T \mathbf{x} + b$ where $\mathbf{a} \in \mathbb{R}^n$ and $b \in \mathbb{R}$. A continuous piecewise convex function has g_k convex, with S_k convex as well.

Note that this definition of piecewise convexity differs from that found in the convex optimization literature, which focuses on *convex* piecewise convex functions, i.e. maxima of convex functions [8]. Note also that we do not claim a unique representation in terms of active functions g_k and pieces S_k , only that there exists at least one such representation.

Before proceeding, we shall extend definition 2.1 to functions of multidimensional codomain for the affine case.

Definition 2.2. A function $f : \mathbb{R}^m \to \mathbb{R}^n$, and let $f_k : \mathbb{R}^m \to \mathbb{R}$ denote the k^{th} component of f. Then f is continuous piecewise affine if each f_k is.

Choose some piece S_k from each f_k and let $S = \bigcap_{k=1}^n S_k$, with $S \neq \emptyset$. Then S is a piece of f, on which we have $f(\mathbf{x}) = A\mathbf{x} + \mathbf{b}$ for some $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$.

First, we prove an intuitive statement about the geometry of the pieces of continuous piecewise affine functions.

Theorem 2.3. Let $f : \mathbb{R}^m \to \mathbb{R}^n$ be continuous piecewise affine. Then f admits a representation in which every piece is a convex polytope.

Proof. Let $f_k : \mathbb{R}^m \to \mathbb{R}$ denote the k^{th} component of f. Now, f_k can be written in closed form as a max-min polynomial [9]. That is, f_k is the maximum of minima of its active functions. Now, for the minimum of two affine functions we have

$$\min(g_i, g_j) = \min(\boldsymbol{a}_i^T \boldsymbol{x} + b_i, \boldsymbol{a}_j^T \boldsymbol{x} + b_j).$$
(1)

This function has two pieces divided by the hyperplane $(\boldsymbol{a}_i^T - \boldsymbol{a}_j^T)\boldsymbol{x} + b_i - b_j = 0$. The same can be said of $\max(g_i, g_j)$. Thus the pieces of f_k are intersections of half-spaces, which are just convex polytopes. Since the pieces of f are intersections of the pieces of f_k , they are convex polytopes as well.

See figure 5 in section 8 for an example of this result on a specific neural network. Our next result concerns the composition of piecewise functions, which is essential for the later sections.

Theorem 2.4. Let $g : \mathbb{R}^m \to \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}$ be continuous piecewise affine. Then so is $f \circ g$.

Proof. To establish continuity, note that the composition of continuous functions is continuous.

Let S be a piece of g and T a piece of f such that $S \cap g^{-1}(T) \neq \emptyset$, where $g^{-1}(T)$ denotes the inverse image of T. By theorem 2.3, we can choose S and T to be convex polytopes. Since g is affine, $g^{-1}(T)$ is closed and convex [10]. Thus $S \cap g^{-1}(T)$ is a closed, convex set on which we can write

$$f(\boldsymbol{x}) = \boldsymbol{a}^T \boldsymbol{x} + b$$
(2)
$$g(\boldsymbol{x}) = C\boldsymbol{x} + \boldsymbol{d}.$$

Thus

$$f \circ g(\boldsymbol{x}) = \boldsymbol{a}^T C \boldsymbol{x} + \boldsymbol{a}^T \boldsymbol{d} + b \tag{3}$$

which is an affine function.

Now, consider the finite set of all such pieces $S \cap g^{-1}(T)$. The union of $g^{-1}(T)$ over all pieces T is just \mathbb{R}^n , as is the union of all pieces S. Thus we have

$$\bigcup_{S} \bigcup_{T} \left(S \cap g^{-1}(T) \right) = \bigcup_{S} \left(S \cap \bigcup_{T} g^{-1}(T) \right)$$
$$= \bigcup_{S} \left(S \cap \mathbb{R}^{n} \right)$$
$$= \mathbb{R}^{n}.$$

Thus $f \circ g$ is piecewise affine on \mathbb{R}^n .

We now turn to continuous piecewise convex functions, of which continuous piecewise affine functions are a subset.

Theorem 2.5. Let $g : \mathbb{R}^m \to \mathbb{R}^n$ be a continuous piecewise affine function, and $h : \mathbb{R}^n \to \mathbb{R}$ a convex function. Then $f = h \circ g$ is continuous piecewise convex.

Proof. On each piece S of g we can write

$$f(\boldsymbol{x}) = h(A\boldsymbol{x} + \boldsymbol{b}). \tag{4}$$

This function is convex, as it is the composition of a convex and an affine function [10]. Furthermore, S is convex by theorem 2.3. This establishes piecewise convexity by the proof of theorem 2.4.

Our final theorem concerns the arithmetic mean of continuous piecewise convex functions, which is essential for the analysis of neural networks.

Theorem 2.6. Let $f_1, f_2, ..., f_N$ be continuous piecewise convex functions. Then so is their arithmetic mean $(1/N) \sum_{i=1}^N f_i(\boldsymbol{x})$.

The proof takes the form of two lemmas.

Lemma 2.7. Let f_1 and f_2 be a pair of continuous piecewise convex functions on \mathbb{R}^n . Then so is $f_1 + f_2$.

Proof. Let S_1 be a piece of f_1 , and S_2 a piece of f_2 , with $S_1 \cap S_2 \neq \emptyset$. Note that the sum of convex functions is convex [11]. Thus $f_1 + f_2$ is convex on $S_1 \cap S_2$. Furthermore, $S_1 \cap S_2$ is convex because it is an intersection of convex sets [11]. Since this holds for all pieces of f_1 and f_2 , we have that $f_1 + f_2$ is continuous piecewise convex on \mathbb{R}^n .

Lemma 2.8. Let $\alpha > 0$, and let f be a continuous piecewise convex function. Then so is αf .

Proof. The continuous function αf is convex on every piece of f.

Having established that continuous piecewise convexity is closed under addition and positive scalar multiplication, we can see that it is closed under the arithmetic mean, which is just the composition of these two operations.

3. Neural networks

In this work, we define a neural network to be a composition of functions of two kinds: a convex continuously differentiable objective (or loss) function h, and continuous piecewise affine functions $g_1, g_2, ..., g_N$, constituting the Nlayers. Furthermore, the outermost function must be h, so that we have

$$f = h \circ g_N \circ g_{N-1} \circ \dots \circ g_1 \tag{5}$$

where f denotes the entire network. This definition is not as restrictive as it may seem upon first glance. For example, it is easily verified that the rectified linear unit (ReLU) neuron is continuous piecewise affine, as we have

$$g(\boldsymbol{x}) = \max(\boldsymbol{0}, A\boldsymbol{x} + \boldsymbol{b}), \tag{6}$$

where the maximum is taken pointwise. It can be shown that maxima and minima of affine functions are piecewise affine [9]. This includes the convolutional variant, in which A is a Toeplitz matrix. Similarly, max pooling is continuous piecewise linear, while mean pooling is simply linear. Furthermore, many of the objective functions commonly seen in machine learning are convex and continuously differentiable, as in least squares and logistic regression. Thus this seemingly restrictive class of neural networks actually encompasses the current state of the art.

By theorem 2.4, the composition of all layers $g = g_N \circ g_{N-1} \circ ... \circ g_1$ is continuous piecewise affine. Therefore, a neural network is ultimately the composition of a continuous convex function with a single continuous piecewise affine function. Thus by theorem 2.5 the network is continuous piecewise convex. Figure 1 provides a visualization of this result for the example network

$$f(x,y) = \left(2 - \left[[x-y]_{+} - [x+y]_{+} + 1\right]_{+}\right)^{2}, \tag{7}$$

where $[x]_{+} = \max(x, 0)$. For clarity, this is just the two-layer ReLU network

$$f(x,y,z) = \left(z - \left[a_5\left[a_1x + a_2y\right]_+ + a_6\left[a_3x + a_4y\right]_+ + b_1\right]_+\right)^2 \tag{8}$$

with the squared error objective and a single data point ((x, y), z), setting z = 2and $a_2 = a_6 = -1$, with all other parameters set to 1.

Before proceeding further, we must define a special kind of differentiability for piecewise continuous functions, and show that this holds for neural networks.

Definition 3.1. Let f be piecewise continuous. We say that f is **piecewise** continuously differentiable if each active function g is continuously differentiable.

To see that neural networks are piecewise continuously differentiable, note that the objective h is continuously differentiable, as are the affine active functions of the layers. Thus their composition is continuously differentiable. It follows that non-differentiable points are found only on the boundaries between pieces.

4. Network parameters of a single layer

In the previous section we have defined neural networks as functions of labeled data. These are the functions relevant during testing, where parameters are constant and data is variable. In this section, we extend these results to the



Figure 1: The neural network of equation 7, on the unit square. Although f is not convex on \mathbb{R}^2 , it is convex in each piece, and each piece is a convex set.

case where data is constant and parameters are variable, which is the function to optimized during training. For example, consider the familiar equation

$$f = (ax + b - y)^2 \tag{9}$$

with parameters (a, b) and data (x, y). During testing, we hold (a, b) constant, and consider f as a function of the data (x, y). During training, we hold (x, y)constant and consider f as a function of the parameters (a, b). This is what we mean when we say that a network is being "considered as a function of its parameters¹." This leads us to an additional stipulation on our definition of a neural network. That is, each layer must be piecewise affine *as a function of its parameters* as well. This is easily verified for all of the layer types previously mentioned. For example, with the ReLU neuron we have

$$f(A, \mathbf{b}) = [A\mathbf{x} + \mathbf{b}]_{+} \tag{10}$$

so for $(A\mathbf{x} + \mathbf{b})_k \geq 0$ we have that the k^{th} component of f is linear in (A, \mathbf{b}) , while for $(A\mathbf{x} + \mathbf{b})_k < 0$ it is constant. To see this, we can re-arrange the elements of A into a column vector \mathbf{a} , in row-major order, so that we have

$$A\boldsymbol{x} + \boldsymbol{b} = \begin{pmatrix} \boldsymbol{x}^{T} & \boldsymbol{0}^{T} & \dots & \dots & \boldsymbol{0}^{T} & \boldsymbol{1}^{T} \\ \boldsymbol{0}^{T} & \boldsymbol{x}^{T} & \boldsymbol{0}^{T} & \dots & \boldsymbol{0}^{T} & \boldsymbol{1}^{T} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \boldsymbol{0}^{T} & \dots & \dots & \boldsymbol{0}^{T} & \boldsymbol{x}^{T} & \boldsymbol{1}^{T} \end{pmatrix} \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix}.$$
(11)

¹This is made rigorous by taking cross-sections of point sets in section 5.

In section 3 we have said that a neural network, considered as a function of its input data, is convex and continuously differentiable on each piece. Now, a neural network need *not* be piecewise convex as a function of the entirety of its parameters². However, we can regain piecewise convexity by considering it only as a function of the parameters in a single layer, all others held constant.

Theorem 4.1. A neural network f is continuous piecewise convex and piecewise continuously differentiable as a function of the parameters in a single layer.

Proof. For the time being, assume the input data consists of a single point \boldsymbol{x} . By definition f is the composition of a convex objective h and layers $g_1, g_2, ..., g_N$, with g_1 a function of \boldsymbol{x} . Let $f_m(\boldsymbol{x})$ denote the network f considered as a function of the parameters of layer g_m , all others held constant. Now, the layers $g_{m-1} \circ g_{m-2} \circ ... \circ g_1$ are constant with respect to the parameters of g_m , so we can write $\boldsymbol{y} = g_{m-1} \circ g_{m-2} \circ ... \circ g_1(\boldsymbol{x})$. Thus on each piece of g_m we have

$$g_m = A\boldsymbol{y} + \boldsymbol{b}.\tag{12}$$

By definition g_m is a continuous piecewise affine function of its parameters. Since \boldsymbol{y} is constant, we have that $\tilde{g}_m = g_m \circ g_{m-1} \circ \ldots \circ g_1$ is a continuous piecewise affine function of the parameters of g_m . Now, by theorem 2.4 we have that $g = g_N \circ g_{N-1} \circ \ldots \circ \tilde{g}_m$ is a continuous piecewise affine function of the parameters of g_m . Thus by theorem 2.5, f_m is continuous piecewise convex.

To establish piecewise continuous differentiability, recall that affine functions are continuously differentiable, as is h.

Having established the theorem for the case of a single data point, consider the case where we have multiple data points, denoted $\{\boldsymbol{x}_k\}_{k=1}^M$. Now, by theorem 2.6 the arithmetic mean $(1/M)\sum_{k=1}^M f_m(\boldsymbol{x}_k)$ is continuous piecewise convex. Furthermore, the arithmetic mean preserves piecewise continuous differentiability. Thus these results hold for the mean value of the network over the dataset.

We conclude this section with a simple remark which will be useful in later sections. Let f_m be a neural network, considered as a function of the parameters of the m^{th} layer, and let S be a piece of f_m . Then the optimization problem

minimize
$$f_m(\boldsymbol{x})$$

subject to $\boldsymbol{x} \in S$ (13)

is convex.

²To see this, consider the following two-layer network: h(x) = x, $g_2(x) = ax$, and $g_1(x) = bx$. For $f = h \circ g_2 \circ g_1$ we have f(x) = abx. Now fix the input as x = 1. Considered as a function of its parameters, this is f(a, b) = ab, which is decidedly not convex.

5. Network parameters of multiple layers

In the previous section we analyzed the convexity properties of neural networks when optimizing the parameters of a single layer, all others held constant. Now we are ready to extend these results to the ultimate goal of simultaneously optimizing all network parameters. Although not convex, the problem has a special convex substructure that we can exploit in proving future results. We begin by defining this substructure for point sets and functions.

Definition 5.1. Let $S \subseteq \mathbb{R}^n$, let $I \subset \{1, 2, ..., n\}$, and let $x \in S$. The set

$$S_I(\boldsymbol{x}) = \{ \boldsymbol{y} \in S : (\boldsymbol{y}_k = \boldsymbol{x}_k)_{k \notin I} \}$$
(14)

is the cross-section of S intersecting x with respect to I.

In other words, $S_I(\boldsymbol{x})$ is the subset of S for which every point is equal to \boldsymbol{x} in the components not indexed by I. Note that this differs from the typical definition, which is the intersection of a set with a hyperplane. For example, $\mathbb{R}^3_{\{1\}}(\mathbf{0})$ is the *x*-axis, whereas $\mathbb{R}^3_{\{1,2\}}(\mathbf{0})$ is the *xy*-plane. Note also that cross-sections are not unique, for example $\mathbb{R}^3_{\{1,2\}}(0,0,0) = \mathbb{R}^3_{\{1,2\}}(1,2,0)$. In this case the first two components of the cross section are irrelevant, but we will maintain them for notational convenience. We can now apply this concept to functions on \mathbb{R}^n .

Definition 5.2. Let $S \subseteq \mathbb{R}^n$, let $f : S \to \mathbb{R}$ and let \mathcal{I} be a collection of sets covering $\{1, 2, ..., n\}$. We say that f is **multi-convex** with respect to \mathcal{I} if f is convex when restricted to the cross section $S_I(\mathbf{x})$, for all $\mathbf{x} \in S$ and $I \in \mathcal{I}$.

This formalizes the notion of restricting a non-convex function to a variable subset on which it is convex, as in section 4 when a neural network was restricted to the parameters of a single layer. For example, let f(x, y, z) = xy + z, and let $I_1 = \{1, 3\}$, and $I_2 = \{2, 3\}$. Then $f_1(x, y_0, z)$ is a convex function of (x, z)with y fixed at y_0 . Similarly, $f_2(x_0, y, z)$ is a convex function of (y, z) with x fixed at x_0 . Thus f is multi-convex with respect to $\mathcal{I} = \{I_1, I_2\}$. To fully define a multi-convex optimization problem, we introduce a similar concept for point sets.

Definition 5.3. Let $S \subseteq \mathbb{R}^n$ and let \mathcal{I} be a collection of sets covering $\{1, 2, ..., n\}$. We say that S is **multi-convex** with respect to \mathcal{I} if the cross-section $S_I(\mathbf{x})$ is convex for all $\mathbf{x} \in S$ and $I \in \mathcal{I}$.

This generalizes the notion of biconvexity found in the optimization literature [4]. From here, we can extend definition 2.1 to multi-convex functions. However, we will drop the topological restrictions on the pieces of our function, since multi-convex sets need not be connected.

Definition 5.4. Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuous function. We say that f is **continuous piecewise multi-convex** if each there exists a collection of multi-convex functions $g_1, g_2, ..., g_N$ and multi-convex sets $S_1, S_2, ..., S_N$ covering

 \mathbb{R}^n such that for each k we have $f(\mathbf{x}) = g_k(\mathbf{x})$ for all $\mathbf{x} \in S_k$. Next, let $h : \mathbb{R}^m \to \mathbb{R}^n$. Then, h is continuous piecewise multi-convex so long as each component is, as in definition 2.2.

From this definition, it is easily verified that a continuous piecewise multiconvex function $f : \mathbb{R}^m \to \mathbb{R}^n$ admits a representation where all pieces are multi-convex, as in the proof of theorem 2.3.

Before we can extend the results of section 4 to multiple layers, we must add one final constraint on the definition of a neural network. That is, each of the layers must be continuous piecewise multi-convex, considered as functions of both the parameters and the input. Again, this is easily verified for the all of the layer types previously mentioned. We have already shown they are piecewise convex on each cross-section, taking our index sets to separate the parameters from the input data. It only remains to show that the number of pieces is finite. The only layer which merits consideration is the ReLU, which we can see from equation 10 consists of two pieces for each component: the "dead" or constant region, with $(Ax)_j + b_j < 0$, and its compliment. With *n* components we have at most 2^n pieces, corresponding to binary assignments of "dead" or "alive" for each component.

Having said that each layer is continuous piecewise multi-convex, we can extend these results to the whole network.

Theorem 5.5. Let f be a neural network, and let \mathcal{I} be a collection of index sets, one for the parameters of each layer of f. Then f is continuous piecewise multi-convex with respect to \mathcal{I} .

We begin the proof with a lemma for more general multi-convex functions.

Lemma 5.6. Let $X \subseteq \mathbb{R}^n$, $Y \subseteq \mathbb{R}^m$, and let $g: X \to Z$ and $f: Z \times Y \to \mathbb{R}^n$ be continuous piecewise multi-convex, g with respect to a collection of index sets \mathcal{G} , and f with respect to $\mathcal{F} = \{I_Z, I_Y\}$, where I_Z indexes the variables in Z, and I_Y the variables in Y. Then $h(\mathbf{x}, \mathbf{y}) = f(g(\mathbf{x}), \mathbf{y})$ is continuous piecewise multi-convex with respect to $\mathcal{H} = \mathcal{G} \cup \{I_Y\}$.

Proof. Let G be a piece of g, let F be a piece of f and let $H = \{(x, y) : x \in G, (g(x), y) \in F\}$, with F chosen so that $H \neq \emptyset$. Clearly h is multiconvex on H with respect to \mathcal{H} . It remains to show that H is a multi-convex set. Now, let $(x, y) \in H$ and we shall show that the cross-sections are convex. First, for any $I_X \in \mathcal{G}$ we have $H_{I_X}(x, y) = G_{I_X}(x) \times \{y\}$. Similarly, we have $H_{I_Y}(x, y) = \{x\} \times \{y : (z, y) \in F_{I_Y}(g(x), y)\}$. These sets are convex, as they are the Cartesian products of convex sets [11]. Finally, as in the proof of theorem 2.4, we can cover $X \times Y$ with the finite collection of all such pieces H, taken over all G and F.

Our next lemma extends theorem 2.6 to multi-convex functions.

Lemma 5.7. Let \mathcal{I} be a collection of sets covering $\{1, 2, ..., n\}$, and let $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}$ be continuous piecewise multi-convex with respect to \mathcal{I} . Then so is f + g.

Proof. Let F be a piece of f and G be a piece of g with $x \in F \cap G$. Then for all $I \in \mathcal{I}$, $(F \cap G)_I(\mathbf{x}) = F_I(\mathbf{x}) \cap G_I(\mathbf{x})$, a convex set on which f + g is convex. Thus f + q is continuous piecewise multi-convex, where the pieces of f + q are the intersections of pieces of f and g.

We can now prove the theorem.

Proof. For the moment, assume we have only a single data point. Now, let g_1 and g_2 denote layers of f, with parameters $\theta_1 \in \mathbb{R}^m$, $\theta_2 \in \mathbb{R}^n$. Since g_1 and g_2 are continuous piecewise multi-convex functions of their parameters and input, we can write the two-layer sub-network as $h = f(q_1(\theta_1), \theta_2)$. By repeatedly applying lemma 5.6, the whole network is multi-convex on a finite number of sets covering the input and parameter space.

Now we extend the theorem to the whole dataset, where each data point defines a continuous piecewise multi-convex function f_k . By lemma 5.7, the arithmetic mean $(1/N) \sum_{k=1}^{N} f_k$ is continuous piecewise multi-convex.

In the coming sections, we shall see that multi-convexity allows us to give certain guarantees about the convergence of various optimization algorithms. But first, we shall prove some basic results independent of the optimization procedure. These results were summarized by Gorksi et al. for the case of biconvex differentiable functions [4]. Here we extend them to piecewise functions and arbitrary index sets. First we define a special type of minimum relevant for multi-convex functions.

Definition 5.8. Let $f : S \to \mathbb{R}$ and let \mathcal{I} be a collection of sets covering $\{1, 2, ..., n\}$. We say that \mathbf{x}_0 is a **partial minimum** of f with respect to \mathcal{I} if $f(\boldsymbol{x}_0) \leq f(\boldsymbol{x}) \text{ for all } \boldsymbol{x} \in \bigcup_{I \in \mathcal{I}} S_I(\boldsymbol{x}_0).$

In other words, \boldsymbol{x}_0 is a partial minimum of f with respect to \mathcal{I} if it minimizes f on every cross-section of S intersecting x_0 , as shown in figure 2. By convexity, these points are intimately related to the stationary points of f.

Theorem 5.9. Let $\mathcal{I} = \{I_1, I_2, ..., I_m\}$ be a collection of sets covering $\{1, 2, ..., n\}$, let $f: \mathbb{R}^n \to \mathbb{R}$ be continuous piecewise multi-convex with respect to \mathcal{I} , and let $\nabla f(\mathbf{x}_0) = \mathbf{0}$. Then \mathbf{x}_0 is a partial minimum of f on every piece containing \mathbf{x}_0 .

Proof. Let S be a piece of f containing \boldsymbol{x}_0 , let $I \in \mathcal{I}$, and let $S_I(\boldsymbol{x}_0)$ denote the relevant cross-section of S. We know f is convex on $S_I(\boldsymbol{x}_0)$, and since $\nabla f(\boldsymbol{x}_0) = \boldsymbol{0}$, we have that \boldsymbol{x}_0 minimizes f on this convex set. Since this holds for all $I \in \mathcal{I}$, \boldsymbol{x}_0 is a partial minimum of f on S.

It is clear that multi-convexity provides a wealth of results concerning partial minima, while piecewise multi-convexity restricts those results to a subset of the domain. Less obvious is that partial minima of smooth multi-convex functions



Figure 2: Cross-sections of a biconvex set.

need not be local minima. An example was pointed out by a reviewer of this work, that the biconvex function f(x, y) = xy has a partial minimum at the origin which is not a local minimum. However, the converse is easily verified, even in the absence of differentiability.

Theorem 5.10. Let \mathcal{I} be a collection of sets covering $\{1, 2, ..., n\}$, let $f : \mathbb{R}^n \to \mathbb{R}$ be continuous piecewise multi-convex with respect to \mathcal{I} , and let \mathbf{x}_0 be a local minimum on some piece S of f. Then \mathbf{x}_0 is a partial minimum on S.

Proof. The proof is essentially the same as that of theorem 5.9.

We have seen that for multi-convex functions there is a close relationship between stationary points, local minima and partial minima. For these functions, infinitesimal results concerning derivatives and local minima can be extended to larger sets. However, we make no guarantees about global minima. The good news is that, unlike global minima, we shall see that we can easily solve for partial minima.

6. Gradient descent

In the realm of non-convex optimization, also called global optimization, methods can be divided into two groups: those which can certifiably find a global minimum, and those which cannot. In the former group we sacrifice speed, in the latter correctness. This work focuses on algorithms of the latter kind, called local or sub-optimal methods, as only this type is used in practice for deep neural networks. In particular, the most common methods are variants of gradient descent, where the gradient of the network with respect its parameters is computed by a procedure called backpropagation. Since its explanation is often obscured by jargon, we shall provide a simple summary here.

Backpropagation is nothing but the chain rule applied to the layers of a network. Splitting the network into two functions $f = u \circ v$, where $u : \mathbb{R}^n \to \mathbb{R}$, and $v : \mathbb{R}^m \to \mathbb{R}^n$, we have

$$\nabla f = \nabla u \mathcal{D} v \tag{15}$$

where \mathcal{D} denotes the Jacobian operator. Note that here the parameters of u are considered fixed, whereas the parameters of v are variable and the input data is fixed. Thus ∇f is the gradient of f with respect to the parameters of v, if it exists. The special observation is that we can proceed from the top layer of the neural network g_N to the bottom g_1 , with $u = g_N \circ g_{N-1} \circ \ldots \circ g_{m+1}$, and $v = g_m$, each time computing the gradient of f with respect to the parameters of g_m . In this way, we need only store the vector ∇u and the matrix $\mathcal{D}v$ can be forgotten at each step. This is known as the "backward pass," which allows for efficient computation of the gradient of a neural network with respect to its parameters. A similar algorithm computes the value of $g_{m-1} \circ g_{m-2} \circ \ldots \circ g_1$ as a function of the input data, which is often needed to evaluate $\mathcal{D}v$. First we compute and store g_1 as a function of the input data, then $g_2 \circ g_1$, and so on until we have f. This is known as the "forward pass." After one forward and one backward pass, we have computed ∇f with respect to all the network parameters.

Having computed ∇f , we can update the parameters by gradient descent, defined as follows.

Definition 6.1. Let $S \subset \mathbb{R}^n$, and $f : S \to \mathbb{R}$ be partial differentiable, with $x_0 \in S$. Then gradient descent on f is the sequence $\{x_k\}_{k=0}^{\infty}$ defined by

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha_k \nabla f(\boldsymbol{x}_k) \tag{16}$$

where $\alpha_k > 0$ is called the **step size** or "learning rate." In this work we shall make the additional assumption that $\sum_{k=0}^{\infty} a_k = \infty$.

Variants of this basic procedure are preferred in practice because their computational cost scales well with the number of network parameters. There are many different ways to choose the step size, but our assumption that $\sum_{k=0}^{\infty} a_k = \infty$ covers what is usually done with deep neural networks. Note that we have not defined what happens if $\boldsymbol{x}_k \notin S$. Since we are ultimately interested in neural networks on \mathbb{R}^n , we can ignore this case and say that the sequence diverges. Gradient descent is not guaranteed to converge to a global minimum for all differentiable functions. However, it is natural to ask to which points it can converge. This brings us to a basic but important result.

Theorem 6.2. Let $f : \mathbb{R}^n \to \mathbb{R}$, and let $\{x_k\}_{k=0}^{\infty}$ result from gradient descent on f with $\lim_{k\to\infty} x_k = x^*$, and f continuously differentiable at x^* . Then $\nabla f(x^*) = \mathbf{0}$.

Proof. First, we have

$$\boldsymbol{x}^* = \boldsymbol{x}_0 - \sum_{k=0}^{\infty} \alpha_k \nabla f(\boldsymbol{x}_k).$$
(17)

Assume for the sake of contradiction that for the j^{th} partial derivative we have $|\partial f(\boldsymbol{x}^*)/\partial(\boldsymbol{x})_j| > 0$. Now, pick some ε such that $0 < \varepsilon < |\partial f(\boldsymbol{x}^*)/\partial(\boldsymbol{x})_j|$, and by continuous differentiability, there is some $\delta > 0$ such that for all \boldsymbol{x} , $\|\boldsymbol{x}^* - \boldsymbol{x}\|_2 < \delta$ implies $\|\nabla f(\boldsymbol{x}^*) - \nabla f(\boldsymbol{x})\|_2 < \varepsilon$. Now, there must be some K such that for all $k \geq K$ we have $\|\boldsymbol{x}^* - \boldsymbol{x}_k\|_2 < \delta$, so that $\partial f(\boldsymbol{x}_k)/\partial(\boldsymbol{x})_j$ does not change sign. Then we can write

$$\sum_{k=K}^{\infty} \alpha_k \frac{\partial f(\boldsymbol{x}_k)}{\partial (\boldsymbol{x})_j} \bigg| = \sum_{k=K}^{\infty} \alpha_k \left| \frac{\partial f(\boldsymbol{x}_k)}{\partial (\boldsymbol{x})_j} \right|$$
$$\geq \sum_{k=K}^{\infty} \alpha_k \left(\left| \frac{\partial f(\boldsymbol{x}^*)}{\partial (\boldsymbol{x})_j} \right| - \varepsilon \right)$$
$$= \infty.$$

But this contradicts the fact that \boldsymbol{x}_k converges. Thus $\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$.

In the convex optimization literature, this simple result is sometimes stated in connection with Zangwill's much more general convergence theorem [12, 13]. Note, however, that unlike Zangwill we state necessary, rather than sufficient conditions for convergence. While many similar results are known, it is difficult to strictly weaken the conditions of theorem 6.2. For example, if we relax the condition that α_k is not summable, and take f(x) = x, then x_k will always converge to a non-stationary point. Similarly, if we relax the constraint that f is continuously differentiable, taking f(x) = |x| and a_k decreasing monotonically to zero, we will always converge to the origin, which is not differentiable. Furthermore, if we have f(x) = |x| with α_k constant, then x_k will not converge for almost all x_0 . It is possible to prove much stronger necessary and sufficient conditions for gradient descent, but these results require additional assumptions about the step size policy as well as the function to be minimized, and possibly even the initialization \mathbf{x}_0 [14].

It is worth discussing f(x) = |x| in greater detail, since this is a piecewise affine function and thus of interest in our investigation of neural networks. While we have said its only convergence point is not differentiable, it remains subdifferentiable, and convergence results are known for subgradient descent [13]. In this work we shall not make use of subgradients, instead considering descent on a piecewise continuously differentiable function, where the pieces are $x \leq 0$ and $x \geq 0$. Although theorem 6.2 does not apply to this function, the relevant results hold anyways. That is, x = 0 is minimal on some piece of f, a result which extends to any continuous piecewise convex function, as any saddle point is guaranteed to minimize some piece.

Here we should note one way in which this analysis fails in practice. So far we have assumed the gradient ∇f is precisely known. In practice, it is often prohibitively expensive to compute the average gradient over large datasets. Instead we take random subsamples, in a procedure known as *stochastic* gradient descent. We will not analyze its properties here, as current results on the topic impose additional restrictions on the objective function and step size, or require different definitions of convergence [15, 16, 17]. Restricting ourselves to the true gradient ∇f allows us to provide simple proofs applying to an extensive class of neural networks.

We are now ready to generalize these results to neural networks. There is a slight ambiguity in that the boundary points between pieces need not be differentiable, nor even sub-differentiable. Since we are interested only in necessary conditions, we will say that gradient descent diverges when $\nabla f(\boldsymbol{x}_k)$ does not exist. However, our next theorem can at least handle non-differentiable limit points.

Theorem 6.3. Let $\mathcal{I} = \{I_1, I_2, ..., I_m\}$ be a collection of sets covering $\{1, 2, ..., n\}$, let $f : \mathbb{R}^n \to \mathbb{R}$ be continuous piecewise multi-convex with respect to \mathcal{I} , and piecewise continuously differentiable. Then, let $\{x_k\}_{k=0}^{\infty}$ result from gradient descent on f, with $\lim_{k\to\infty} x_k = x^*$, such that either

- 1. f is continuously differentiable at x^* , or
- 2. there is some piece S of f and some K > 0 such that $\boldsymbol{x}_k \in S^{\circ}$ for all $k \geq K$.

Then x^* is a partial minimum of f on every piece containing x^* .

Proof. If the first condition holds, the result follows directly from theorems 6.2 and 5.9. If the second condition holds, then $\{\boldsymbol{x}_k\}_{k=K}^{\infty}$ is a convergent gradient descent sequence on g, the active function of f on S. Since g is continuously differentiable on \mathbb{R}^n , the first condition holds for g. Since $f|_S = g|_S$, \boldsymbol{x}^* is a partial minimum of $f|_S$ as well.

The first condition of theorem 6.3 holds for every point in the interior of a piece, and some boundary points. The second condition extends these results to non-differentiable boundary points so long as gradient descent is eventually confined to a single piece of the function. For example, consider the continuous piecewise convex function $f(x) = \min(x, x^4)$ as shown in figure 3. When we converge to x = 0 from the piece [0, 1], it is as if we were converging on the smooth function $g(x) = x^4$. This example also illustrates an important caveat regarding boundary points: although x = 0 is an extremum of f on [0, 1], it is not an extremum on \mathbb{R} .

7. Iterated convex optimization

Although the previous section contained some powerful results, theorem 6.3 suffers from two main weaknesses, that it is a necessary condition and that it requires extra care at non-differentiable points. It is difficult to overcome these limitations with gradient descent. Instead, we shall define a different optimization technique, from which necessary and sufficient convergence results follow, regardless of differentiability.



Figure 3: Example of a piecewise convex function. The point x = 0 minimizes the function on the piece [0, 1].

Iterated convex optimization splits a non-convex optimization problem into a number of convex sub-problems, solving the sub-problems in each iteration. For a neural network, we have shown that the problem of optimizing the parameters of a single layer, all others held constant, is piecewise convex. Thus, restricting ourselves to a given piece yields a convex optimization problem. In this section, we show that these convex sub-problems can be solved repeatedly, converging to a piecewise partial optimum.

Definition 7.1. Let $\mathcal{I} = \{I_1, I_2, ..., I_m\}$ be a collection of sets covering $\{1, 2, ..., n\}$, and let $S \subseteq \mathbb{R}^n$ and $f : S \to \mathbb{R}$ be multi-convex with respect to \mathcal{I} . Then **iterated** convex optimization is any sequence where \mathbf{x}_k is a solution to the optimization problem

minimize
$$f(\boldsymbol{y})$$
 (18)
subject to $\boldsymbol{y} \in \bigcup_{I \in \mathcal{I}} S_I(\boldsymbol{x}_{k-1})$

with $\boldsymbol{x}_0 \in S$.

We call this iterated convex optimization because problem 18 can be divided into convex sub-problems

minimize
$$f(\boldsymbol{y})$$
 (19)
subject to $\boldsymbol{y} \in S_I(\boldsymbol{x}_{k-1}).$

for each $I \in \mathcal{I}$. In this work, we assume the convex sub-problems are solvable, without delving into specific solution techniques. Methods for alternating between solvable sub-problems have been studied by many authors, for many different types of sub-problems [6]. In the context of machine learning, the same results have been developed for the special case of linear autoencoders [7]. Still, extra care must be taken in extending these results to arbitrary index sets. The key is that \boldsymbol{x}_k is not updated until all sub-problems have been solved, so that each iteration consists of solving m convex sub-problems. This is equivalent to the usual alternating convex optimization for biconvex functions, where \mathcal{I} consists of two sets, but not for general multi-convex functions.

Some basic convergence results follow immediately from the solvability of problem 18. First, note that \mathbf{x}_{k-1} is a feasible point, so we have $f(\mathbf{x}_k) \leq f(\mathbf{x}_{k-1})$. This implies that $\lim_{k\to\infty} f(\mathbf{x}_k)$ exists, so long as f is bounded below. However, this does not imply the existence of $\lim_{k\to\infty} \mathbf{x}_k$. See Gorski et al. for an example of a biconvex function on which \mathbf{x}_k diverges [4]. To prove stronger convergence results, we introduce regularization to the objective.

Theorem 7.2. Let \mathcal{I} be a collection of sets covering $\{1, 2, ..., n\}$, and let $S \subseteq \mathbb{R}^n$ and $f: S \to \mathbb{R}$ be multi-convex with respect to \mathcal{I} . Next, let $\inf f > -\infty$, and let $g(\boldsymbol{x}) = f(\boldsymbol{x}) + \lambda ||\boldsymbol{x}||$, where $\lambda > 0$ and $||\boldsymbol{x}||$ is a convex norm. Finally, let $\{\boldsymbol{x}_k\}_{k=0}^{\infty}$ result from iterated convex optimization of g. Then \boldsymbol{x}_k has at least one convergent subsequence, in the topology induced by the metric $d(\boldsymbol{x}, \boldsymbol{y}) = ||\boldsymbol{x} - \boldsymbol{y}||$.

Proof. From lemma 2.7, g is multi-convex, so we are allowed iterated convex optimization. Now, if $\inf f + \lambda || \boldsymbol{x} || > g(\boldsymbol{x}_0)$ we have that $g(\boldsymbol{x}) > g(\boldsymbol{x}_0)$. Thus $g(\boldsymbol{x}) > g(\boldsymbol{x}_0)$ whenever $|| \boldsymbol{x} || > (g(\boldsymbol{x}_0) - \inf f) / \lambda$. Since $g(\boldsymbol{x}_k)$ is a non-increasing sequence, we have that $|| \boldsymbol{x}_k || \le (g(\boldsymbol{x}_0) - \inf f) / \lambda$. Equivalently, \boldsymbol{x}_k lies in the set $A = \{ \boldsymbol{x} : || \boldsymbol{x} || \le (g(\boldsymbol{x}_0) - \inf f) / \lambda \}$. Since $|| \boldsymbol{x} ||$ is continuous, A is closed and bounded, and thus it is compact. Then, by the Bolzano-Weierstrauss theorem, \boldsymbol{x}_k has at least one convergent subsequence [18].

In theorem 7.2, the function g is called the **regularized** version of f. In practice, regularization often makes a non-convex optimization problem easier to solve, and can reduce over-fitting. The theorem shows that iterated convex optimization on a regularized function always has at least one convergent subsequence. Next, we shall establish some rather strong properties of the limits of these subsequences.

Theorem 7.3. Let \mathcal{I} be a collection of sets covering $\{1, 2, ..., n\}$, and let $S \subseteq \mathbb{R}^n$ and $f: S \to \mathbb{R}$ be multi-convex with respect to \mathcal{I} . Next, let $\{\boldsymbol{x}_k\}_{k=0}^{\infty}$ result from iterated convex optimization of f. Then the limit of every convergent subsequence is a partial minimum on S° with respect to \mathcal{I} , in the topology induced by the metric $d(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|$ for some norm $\|\boldsymbol{x}\|$. Furthermore, if $\{\boldsymbol{x}_{m_k}\}_{k=1}^{\infty}$ and $\{\boldsymbol{x}_{n_k}\}_{k=1}^{\infty}$ are convergent subsequences, then $\lim_{k\to\infty} f(\boldsymbol{x}_{m_k}) = \lim_{k\to\infty} f(\boldsymbol{x}_{n_k})$.

Proof. Let \mathbf{x}_{n_k} denote a subsequence of \mathbf{x}_k with $\mathbf{x}^* = \lim_{n \to \infty} \mathbf{x}_{n_k}$. Now, assume for the sake of contradiction that \mathbf{x}^* is not a partial minimum on int Swith respect to \mathcal{I} . Then there is some $I \in \mathcal{I}$ and some $\mathbf{x}' \in S_I(\mathbf{x}^*)$ with $\mathbf{x}' \in S^\circ$ such that $f(\mathbf{x}') < f(\mathbf{x}^*)$. Now, f is continuous at \mathbf{x}' , so there must be some $\delta > 0$ such that for all $\mathbf{x} \in S$, $\|\mathbf{x} - \mathbf{x}'\| < \delta$ implies $|f(\mathbf{x}) - f(\mathbf{x}')| < f(\mathbf{x}^*) - f(\mathbf{x}')$. Furthermore, since \mathbf{x}' is an interior point, there must be some open ball $B \subset S$ of radius r centered at \mathbf{x}' , as shown in figure 4. Now, there must be some Ksuch that $\|\mathbf{x}_{n_K} - \mathbf{x}^*\| < \min(\delta, r)$. Then, let $\tilde{\mathbf{x}} = \mathbf{x}_{n_K} + \mathbf{x}' - \mathbf{x}^*$, and since



Figure 4: Illustration of the proof of theorem 7.3. Note the cross-sections of the biconvex set S.

 $\|\tilde{\boldsymbol{x}}-\boldsymbol{x}'\| < r$, we know that $\tilde{\boldsymbol{x}} \in B$, and thus $\tilde{\boldsymbol{x}} \in S_I(\boldsymbol{x}_{n_K})$. Finally, $\|\tilde{\boldsymbol{x}}-\boldsymbol{x}'\| < \delta$, so we have $f(\tilde{\boldsymbol{x}}) < f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}_{n_K+1})$, which contradicts the fact that \boldsymbol{x}_{n_K+1} minimizes g over a set containing $\tilde{\boldsymbol{x}}$. Thus \boldsymbol{x}^* is a partial minimum on S^{o} with respect to \mathcal{I} .

Finally, let $\{\boldsymbol{x}_{m_k}\}_{k=1}^{\infty}$ and $\{\boldsymbol{x}_{n_k}\}_{k=1}^{\infty}$ be two convergent subsequences of \boldsymbol{x}_k , with $\lim_{k\to\infty} \{\boldsymbol{x}_{m_k}\} = \boldsymbol{x}_m^*$ and $\lim_{k\to\infty} \{\boldsymbol{x}_{n_k}\} = \boldsymbol{x}_n^*$, and assume for the sake of contradiction that $f(\boldsymbol{x}_m^*) > f(\boldsymbol{x}_n^*)$. Then by continuity, there is some Ksuch that $f(\boldsymbol{x}_{n_K}) < f(\boldsymbol{x}_m^*)$. But this contradicts the fact that $f(\boldsymbol{x}_k)$ is nonincreasing. Thus $f(\boldsymbol{x}_m^*) = f(\boldsymbol{x}_n^*)$.

The previous theorem is an extension of results reviewed in Gorski et al. to arbitrary index sets [4]. While Gorski et al. explicitly constrain the domain to a compact biconvex set, we show that regularization guarantees x_k cannot escape a certain compact set, establishing the necessary condition for convergence. Furthermore, our results hold for general multi-convex sets, while the earlier result is restricted to Cartesian products of compact sets.

These results for iterated convex optimization are considerably stronger than what we have shown for gradient descent. While any bounded sequence in \mathbb{R}^n has a convergent subsequence, and we can guarantee boundedness for some variants of gradient descent, we cannot normally say much about the limits of subsequences. For iterated convex optimization, we have shown that the limit of any subsequence is a partial minimum, and all limits of subsequences are equal in objective value. For all practical purposes, this is just as good as saying that the original sequence converges to partial minimum.

8. Global optimization

Although we have provided necessary and sufficient conditions for convergence of various optimization algorithms on neural networks, the points of convergence need only minimize cross-sections of pieces of the domain. Of course we would prefer results relating the points of convergence to global minima of the training objective. In this section we illustrate the difficulty of establishing such results, even for the simplest of neural networks.

In recent years much work has been devoted to providing theoretical explanations for the empirical success of deep neural networks, a full accounting of which is beyond the scope of this article. In order to simplify the problem, many authors have studied *linear* neural networks, in which the layers have the form $g(\mathbf{x}) = A\mathbf{x}$, where A is the parameter matrix. With multiple layers this is clearly a linear function of the output, but not of the parameters. As a special case of piecewise affine functions, our previous results suffice to show that these networks are multi-convex as functions of their parameters. This was proven for the special case of linear autoencoders by Baldi and Lu [7].

Many authors have claimed that linear neural networks contain no "bad" local minima, i.e. every local minimum is a global minimum [2, 3]. This is especially evident in the study of linear autoencoders, which were shown to admit many points of inflection, but only a single strict minimum [7]. While powerful, this claim does not apply to the networks seen in practice. To see this, consider the dataset $D = \{(0, 1/2), (-1, \alpha), (1, 2\alpha)\}$ consisting of three (x, y) pairs, parameterized by $\alpha > 1$. Note that the dataset has zero mean and unit variance in the x variable, which is common practice in machine learning. However, we do not take zero mean in the y variable, as the model we shall adopt is non-negative.

Next, consider the simple neural network

$$f(a,b) = \sum_{(x,y)\in D} \left(y - [ax+b]_+\right)^2$$

$$= \left(\frac{1}{2} - [b]_+\right)^2 + \left(\alpha - [b-a]_+\right)^2 + \left(2\alpha - [b+a]_+\right)^2.$$
(20)

This is the squared error of a single ReLU neuron, parameterized by $(a, b) \in \mathbb{R}^2$. We have chosen this simplest of all networks because we can solve for the local minima in closed form, and show they are indeed very bad. First, note that fis a continuous piecewise convex function of six pieces, realized by dividing the plane along the line ax + b = 0 for each $x \in D$, as shown in figure 5. Now, for all but one of the pieces, the ReLU is "dead" for at least one of the three data points, i.e. ax + b < 0. On these pieces, at least one of the three terms of equation 20 is constant. The remaining terms are minimized when y = ax + b, represented by the three dashed lines in figure 5. There are exactly three points where two of these lines intersect, and we can easily show that two of them are strict local minima. Specifically, the point $(a_1, b_1) = (1/2 - \alpha, 1/2)$ minimizes the first two terms of equation 20, while $(a_2, b_2) = (2\alpha - 1/2, 1/2)$ minimizes the first and last term. In each case, the remaining term is constant over the piece containing the point of intersection. Thus these points are strict global minima on their respective pieces, and strict local minima on \mathbb{R}^2 . Furthermore, we can compute $f(a_1, b_1) = 4\alpha^2$ and $f(a_2, b_2) = \alpha^2$. This gives

$$\lim_{\alpha \to \infty} a_1 = -\infty,$$
$$\lim_{\alpha \to \infty} a_2 = +\infty,$$

and

$$\lim_{n \to \infty} \left(f(a_1, b_1) - f(a_2, b_2) \right) = \infty.$$
(21)

Now, it might be objected that we are not permitted to take $\alpha \to \infty$ if we require that the *y* variable has unit variance. However, these same limits can be achieved with variance tending to unity by adding $\lfloor \alpha \rfloor$ instances of the point $(1, 2\alpha)$ to our dataset. Thus even under fairly stringent requirements we can construct a dataset yielding arbitrarily bad local minima, both in the parameter space and the objective value. This provides some weak justification for the empirical observation that success in deep learning depends greatly on the data at hand.

We have shown that the results concerning local minima in linear networks do not extend to the nonlinear case. Ultimately this should not be a surprise, as with linear networks the problem can be relaxed to linear regression on a convex objective. That is, the composition of all linear layers $g(\boldsymbol{x}) = A_1 A_2 \dots A_n \boldsymbol{x}$ is equivalent to the function $f(\boldsymbol{x}) = A\boldsymbol{x}$ for some matrix A, and under our previous assumptions the problem of finding the optimal A is convex. Furthermore, it is easily shown that the number of parameters in the relaxed problem is polynomial in the number of original parameters. Since the relaxed problem fits the data at least as well as the original, it is not surprising that the original problem is computationally tractable.

This simple example was merely meant to illustrate the difficulty of establishing results for *every* local minimum of *every* neural network. Since training a certain kind of network is known to be NP-Complete, it is difficult to give any guarantees about worst-case global behavior [1]. We have made no claims, however, about probabilistic behavior on the average practical dataset, nor have we ruled out the effects of more specialized networks, such as very deep ones.

9. Conclusion

We showed that a common class of neural networks is piecewise convex in each layer, with all other parameters fixed. We extended this to a theory of a piecewise multi-convex functions, showing that the training objective function can be represented by a finite number of multi-convex functions, each active on a multi-convex parameter set. From here we derived various results concerning the extrema and stationary points of piecewise multi-convex functions. We established convergence conditions for both gradient descent and iterated convex optimization on this class of functions, showing they converge to piecewise partial minima. Similar results are likely to hold for a variety of other optimization



Figure 5: Parameter space of the neural network from equation 20, with pieces divided by the bold black lines. The points (a_1, b_1) and (a_2, b_2) are local minima, which can be made arbitrarily far apart by varying the dataset.

algorithms, especially those guaranteed to converge at stationary points or local minima.

We have witnessed the utility of multi-convexity in proving convergence results for various optimization algorithms. However, this property may be of practical use as well. Better understanding of the training objective could lead to the development of faster or more reliable optimization methods, heuristic or otherwise. These results may provide some insight into the practical success of sub-optimal algorithms on neural networks. However, we have also seen that local optimality results do not extend to global optimality as they do for linear autoencoders. Clearly there is much left to discover about how, or even if we can optimize deep, nonlinear neural networks.

Acknowledgments

The author would like to thank Mihir Mongia for his helpful comments in preparing this manuscript.

Funding

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

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