The duality structure gradient descent algorithm: analysis and applications to neural networks.

Thomas Flynn

Abstract The training of machine learning models is typically carried out using some form of gradient descent, often with great success. However, non-asymptotic analyses of first-order optimization algorithms typically employ a gradient smoothness assumption (formally, Lipschitz continuity of the gradient) that is too strong to be applicable in the case of deep neural networks. To address this, we propose an algorithm named duality structure gradient descent (DSGD) that is amenable to non-asymptotic performance analysis, under mild assumptions on the training set and network architecture. The algorithm can be viewed as a form of layer-wise coordinate descent, where at each iteration the algorithm chooses one layer of the network to update. The decision of what layer to update is done in a greedy fashion, based on a rigorous lower bound on the improvement of the objective function for each choice of layer. In the analysis, we bound the time required to reach approximate stationary points, in both the deterministic and stochastic settings. The convergence is measured in terms of a parameter-dependent family of norms that is derived from the network architecture and designed to confirm a smoothness-like property on the gradient of the training loss function. We empirically demonstrate the behavior of DSGD in several neural network training scenarios.

Keywords Stochastic optimization · Machine learning · Non-convex optimization

1 Introduction

Gradient descent and its variants are often used to train machine learning models, and these algorithms have led to impressive results in many different
applications. These include training neural networks for tasks such as representation learning [46, 32], image classification [22, 29], scene labeling [19], and multimodal signal processing [48], just to name a few. In each case, these systems employ some form gradient based optimization, and the algorithm settings must be carefully tuned to guarantee success. For example, choosing small step-sizes leads to slow optimization, and step-sizes that are too large result in unstable algorithm behavior. Therefore it would be useful to have a theory that provides a rule for the step-sizes and other settings that guarantees the success of optimization.

A common assumption in analyses of gradient descent for non-convex functions, some of which are reviewed below in Section 1.2, is Lipschitz continuity of the gradient of the objective function, or related criteria. This assumption, also termed “gradient smoothness” or simply “smoothness”, typically states that the objective function has a Lipschitz gradient. Assuming the function is twice continuously differentiable, this is equivalent to requiring that the second derivative is bounded. For example, if the objective has a Lipschitz continuous gradient, with Lipschitz constant $L$, then gradient descent with a step-size of $1/L$ is guaranteed to find approximate stationary points [40, Section 1.2.3]. However, it is doubtful that this approach to the analysis can be applied to multi-layer neural networks, since there are very simple neural network training problems where the objective function does not have a Lipschitz continuous gradient. In Section 2 we present an example problem of this type.

Our approach has three main components. The starting point is a layer-wise Lipschitz property that is satisfied by the neural network optimization objective. Motivated by this we design our algorithm to choose one layer of the network to update at each iteration, using a lower bound for the amount of function decrease that each choice of layer would yield. The second component is an analytical framework based on parameter-dependent norms that is used to prove the convergence of our algorithm, and that we believe may also be of general interest. Thirdly, the geometric point of view is not just a tool for analysis but offers flexibility, as a variety of algorithms with convergence guarantees can be described this way: by defining the search directions within each layer according to a possibly non-Euclidean norm one can generate a variety of different update rules, and these can all be accommodated in our analysis framework. Combining these three components leads to an optimization procedure that is provably convergent for a significant class of multi-layer neural network optimization problems. Note that the focus of this paper is mostly theoretical, and we do not explore practical variants of DSGD in depth in the present work. We now describe these three components in more detail.

*Layer-wise Lipschitz property* A network with no hidden layers presents a relatively straightforward optimization problem (under mild assumptions on the loss function). Typically, the resulting objective function has a Lipschitz continuous gradient; for instance, this follows from Proposition 4.3 by restricting to a network with a single layer. When multiple layers are connected in the typical feed-forward fashion, the result is a hierarchical system that as a whole
generally does not have a Lipschitz continuous gradient. This is rigorously established in Proposition 2.1 below. However, if we focus our attention to only one layer of the multi-layer network, then the task is somewhat simplified. Specifically, consider a neural network with the weight matrices ordered from input to output as $w_1, w_2, \ldots, w_L$. Then under mild assumptions, the magnitude of the second derivative (Hessian matrix) of the objective function restricted to the weights in layer $i$ can be bounded by a polynomial in the norms of the successive matrices $w_{i+1}, \ldots, w_L$, which is a sufficient for Lipschitz continuity of the gradient. This is formalized below in Proposition 4.3. This fact can be used to infer a lower bound on the function decrease that will happen when taking a gradient descent step on layer $i$. By computing this bound for each possible layer $i \in \{1, \ldots, L\}$ we can choose which update to perform using the greedy heuristic of picking the layer that maximizes the lower bound. The pseudocode for the procedure is presented in Algorithm 4.1 below.

**Duality Structure Gradient Descent** A widely used success criterion for non-convex optimization is that the algorithm yields a point where the Euclidean norm of the derivative of the objective is small. This is motivated by the fact that points where the derivative is zero are stationary points. It appears difficult to establish this sort of guarantee in the situation described above, where one layer at a time is updated according to a greedy criteria. However, the analysis becomes simpler if we are willing to adjust the geometric framework used to define convergence. In the geometry we introduce, the norm at each point in the parameter space is determined by the weights of the neural network, and the convergence criterion we use is that the algorithm generates a point with a small derivative as measured using the local norm.

Our analysis is based on a continuously varying family of norms that is designed in response to the structure of the neural network, taking into account our bound on the Lipschitz constants, and our greedy “maximum update” criterion. The family of norms encodes our algorithm in the sense that one step of the algorithm corresponds to taking a step in the steepest descent direction as defined by the family of norms. The steepest descent directions are computed by solving a secondary optimization problem at each iteration, in order to identify the layer maximizing the lower bound on the function decrease. Formally, a duality structure represents the solutions to these sub-problems.

**Intralayer update rules** A third component of our approach, which turns out to be key to obtaining an algorithm that is not only theoretically convergent but also effective in practice, is to consider the geometry within each layer of the weight matrices. Typically in first order gradient descent, the update direction is the vector of partial derivatives of the objective function. This can be motivated using Taylor’s theorem: if it is known that the spectral norm of the Hessian matrix of a given function $f$ is bounded by a constant $L$, then Taylor’s theorem provides a quadratic upper bound for the objective of the form $f(w - \Delta) \leq f(w) - \frac{\partial f}{\partial w}(w) \cdot \Delta + \frac{L}{2} \|\Delta\|_2^2$, and setting $\Delta = \frac{1}{L} \frac{\partial f}{\partial w}(w)$ results in a function decrease of magnitude at least $\frac{1}{2L} \|\frac{\partial f}{\partial w}(w)\|_2^2$. Using a different
norm when applying Taylor’s theorem results in a different quadratic upper bound, and a general theorem about gradient descent for arbitrary norms is stated in Proposition 4.4. The basic idea is that if $\| \cdot \|$ is an arbitrary norm and $L$ is a global bound on the norm of the bilinear maps $\frac{\partial^2 f}{\partial w^2}(w)$, as measured with respect to $\| \cdot \|$, then $f$ satisfies a quadratic bound of the form $f(w - \Delta) \leq f(w) - \frac{\partial f}{\partial w}(w) \cdot \Delta + \frac{L}{2} \| \Delta \|^2$. Using the notion of a duality map $\rho$ for the norm $\| \cdot \|$ (see Equation (4) for a formal definition), the update $\Delta = \frac{1}{L} \rho(\frac{\partial f}{\partial w}(w))$ leads to a decrease of magnitude at least $\frac{1}{2} L \| \frac{\partial f}{\partial w}(w) \|^2$. For example, when the argument $w$ has a matrix structure and $\| \cdot \|$ is the spectral norm, then the update direction is a spectrally-normalized version of the Euclidean gradient, in which the matrix of partial derivatives has its non-zero singular values set to unity, a fact that is recalled in Proposition 4.5 below. The choice of norm for the weights can be encoded in the overall family of norms, and each norm leads to a different provably convergent variant of the algorithm. In our experiments we considered update rules based on the matrix norms induced by $\| \cdot \|_q$ for $q = 1, 2, \infty$. Despite the possible complexity of the family of norms, the analysis is straightforward and mimics the standard proof of convergence for Euclidean gradient descent. In the resulting convergence theory, we study how quickly the norm of the gradient tends to zero, measured with respect to the local norms $\| \cdot \|_{w(t)}$. Roughly speaking, the quantity that is proved to tend to zero is $\| \frac{\partial f}{\partial w}(w(t)) \| / \rho(\| w(t) \|)$, where $\| w(t) \|$ is the norm of the network parameters and $\rho$ is a polynomial that depends on the architecture of the neural network. This is in contrast to the usual Euclidean non-asymptotic performance analysis, which tracks the gradient measured with respect to a fixed norm, that is, $\| \frac{\partial f}{\partial w}(w(t)) \|$. See Proposition 4.3 and the discussion following it for more details on how the local norms are defined in the case of neural networks. To finish this section, we would like to comment on the applicability of our results. We consider the case of multi-layer neural networks that use activation functions that are bounded and differentiable (up to 2nd order). This excludes neural networks with rectified linear units (ReLU), which constitute a popular class of models. The main reason for this is that ReLu units do not have second derivatives at every point in their domain, which is a requirement in our theory.

1.1 Outline

After reviewing some related work, in Section 2 we present an example of a neural network training problem where the objective function does not have bounded second derivatives. In Section 3 we introduce the abstract duality structure gradient descent (DGD) algorithms and the convergence analyses. The main result in this section is Theorem 3.5 concerning the expected number of iterations needed to reach an approximate stationary point in DGD. Corollaries 3.6 and 3.7 consider special cases, including batch gradient descent and that of a trivial family of norms, in the latter case recovering the known rates for standard stochastic gradient descent. In Section 4 we show how DGD may be
applied to neural networks with multiple hidden layers. The main results in this section are convergence analyses for the neural network training procedure presented in Algorithm 4.1, both in the deterministic case (Theorem 4.8) and a corresponding analysis for the mini-batch variant of the algorithm (Theorem 4.10). Numerical experiments on the MNIST, Fashion-MNIST, CIFAR-10, and SVHN benchmark data sets are presented in Section 5. We finish with a discussion in Section 6. Several proofs are deferred to an appendix.

1.2 Related work

There are a number of performance analyses of gradient descent for non-convex functions which utilize the assumption that one or more higher derivatives are bounded. Although we are specifically concerned with non-convex optimization, it is worth mentioning that \texttt{sgd} for convex functions is more well understood, and there are analyses that bypass the smoothness assumption [43, 39].

For non-convex optimization, gradient-descent using a step-size proportional to $1/L$ achieves a convergence guarantee on the order of $1/T$, where $T$ is the running time of the algorithm [40, Section 1.2.3]. Note the inverse relationship between the Lipschitz constant $L$ and the step-size $1/L$, which is characteristic of results that rely on a Lipschitz property of the gradient for non-asymptotic analysis. Most practical algorithms in machine learning are stochastic variants of gradient descent. The Randomized Stochastic Gradient (RSG) algorithm is one such example [21]. In RSG, a stochastic gradient update is run for $T$ steps, and then a random iterate is returned. In [21] it was proved that the expected squared-norm of the returned gradient tends to zero at rate of $1/\sqrt{T}$. Their assumptions include a Lipschitz gradient and uniformly bounded variance of gradient estimates.

A variety of other, more specialized algorithms have also been analyzed under the Lipschitz-gradient assumption. The Stochastic Variance Reduced Gradient (SVRG) algorithm combines features of deterministic and stochastic gradient descent, alternating between full gradient calculations and \texttt{sgd} iterations [25]. Notably, it was shown that SVRG for non-convex functions requires fewer gradient evaluations on average compared to RSG [3] [45]. The step-sizes follow a $1/L$ rule, and the variance assumptions are weaker compared to RSG. For machine learning on a large scale, distributed and decentralized algorithms become of interest. Decentralized \texttt{sgd} was analyzed in [34], leading to a $1/L$-type result for this setting.

Adaptive gradient methods, including Adagrad [18], RMSProp [49] and ADAM [27] define another important variant of gradient descent. These methods update learning rates on the fly based on the trajectory of observed (possibly stochastic) gradients. Convergence bounds for Adagrad-style updates in the context of non-convex functions have recently been derived [33, 50] [24]. A key difference between these adaptive gradient methods and our work, aside from the relaxation of the smoothness assumption that we pursue, is that in DSGD, gradients are scaled by the norm of the iterates, rather than the sum of the
norms of the gradients. High probability bounds for AdaGrad style algorithms have also been derived [26]. Another form of adaption is clipping, whereby updates are rescaled if their magnitude is too large. Convergence rates for Clipped GD and Clipped SGD have recently been derived in [54]. It was shown that Clipped GD converges for a broader class of functions than those having a Lipschitz gradient. However, it is not clear if their generalized smoothness condition holds in the setting of deep neural networks. Clipped SGD also admits convergence guarantees in the case of convex functions with rapidly growing subgradients, and weakly convex functions [38]. While the class of weakly convex functions includes those with a Lipschitz gradient, it is too restrictive to include neural networks with multiple layers.

One approach to extend the results on gradient descent is to augment or replace the assumption on the second derivative with an analogous assumption on third order derivatives. In an analysis of cubic regularization methods, Cartis et al. [11] proved a bound on the asymptotic rate of convergence for non-convex functions that have a Lipschitz-continuous Hessian. In a non-asymptotic analysis of a trust region algorithm in [13], convergence was shown to points that approximately satisfy a second order optimality condition, assuming a Lipschitz gradient and Lipschitz Hessian.

A natural question is whether these results can be generalized to exploit the Lipschitz properties of derivatives of arbitrary order. This question was taken up by Birgin et al. [8], where it is assumed that the derivative of order \( p \) is Lipschitz continuous, for arbitrary \( p \geq 1 \). They consider an algorithm that constructs a \( p + 1 \) degree polynomial majorizing the objective at each iteration, and the next iterate is obtained by approximately minimizing this polynomial. The algorithm in a sense generalizes first order gradient descent and well as cubic regularization methods. A remarkable feature of the analysis is that the convergence rate improves as \( p \) increases. Note that the trade off is that higher values of \( p \) lead to subproblems of minimizing potentially high degree multivariate polynomials.

Another approach to generalizing smoothness assumptions uses the concept of relative smoothness, defined by Lu et al. [37] and closely related to the condition \( LC \) proposed by Bauschke et al. [6]. Roughly speaking, a function \( f \) is defined to be relatively smooth relative to a reference function \( h \) if the Hessian of \( f \) is upper bounded by the Hessian of \( h \) (see Proposition 1.1 in [37].) In the optimization procedure, one solves sub-problems that involve the function \( h \) instead of \( f \), and if \( h \) is significantly simpler than \( f \) the procedure can be practical. A non-asymptotic convergence guarantee is established under an additional relative-convexity condition. We note that recent works have explored relative smoothness in non-convex [9] [7] and stochastic settings [16] [55]. Our work in this paper is also concerned with generalized gradient smoothness condition; however, there are two primary differences. Firstly, our primary assumption (Assumption 3.2) differs in that it does not require bounding the action of the Hessian on all possible update directions, but only in those directions relevant to the algorithm update steps (this is manifested by the presence of the duality mapping in the criterion). We posit that this enables
step-sizes that are less conservative. In addition, motivated by applications to neural networks, in our analysis of the stochastic settings we confirm that the minibatch gradients satisfy a generalized bound on the variance as well.

In this work we utilize the notion of a continuously varying family of norms in the convergence analysis of DSGD, ideas that are also used in variable metric methods [14, 15] and optimization on manifolds more generally. Notable instances of optimization on manifolds include optimizing over spaces of structured matrices [2], and parameterized probability distributions, as in information geometry [4]. In the context of neural networks, natural gradient approaches to optimization have been explored [30, 4], and recently Ollivier [44] considered some practical variants of the approach, while also extending it to networks with multiple hidden layers.

We note that several heuristics for step-size selection in the specific case of gradient descent for neural networks have been proposed, including [47, 18, 27], but the theoretical analyses in these works is limited to convex functions. Other heuristics include forcing Lipschitz continuity of the gradient by constraining the parameters to a bounded set, for instance using weight clipping, although this leads to the problem of how to choose an appropriate bounded region, and how to determine learning rate and other algorithm settings based on the size of this region. Finally, we point out that in certain cases one can establish that SGD converges to a local minimum, rather than a stationary point, given an initial point in a small enough neighborhood to such a minimum [20].

Table 1 Notation

| Symbol | Description |
|--------|-------------|
| \(f\)  | an objective function |
| \(f^*\) | a lower bound on values of \(f\) |
| \(w\)  | optimization variable |
| \(n\)  | dimension of parameter space |
| \(t\)  | iteration number |
| \(\mathcal{L}(\mathbb{R}^d, \mathbb{R})\) | the linear maps from \(\mathbb{R}^d\) to \(\mathbb{R}\) |
| \(\ell\) | an element in \(\mathcal{L}(\mathbb{R}^d, \mathbb{R})\) |
| \(\epsilon\) | step-size for optimization |
| \(\varphi(t)\) | an approximate derivative |
| \(\delta\) | error of a derivative estimate |
| \(L\)  | Lipschitz-type constant |
| \(K\)  | number of layers in a network |
| \(n_k\) | number of nodes in layer \(k\) |
| \(y_k\) | state of layer \(k\) of network |
| \(x\)  | input to network |
| \(z\)  | output target for a network |
| \(m\)  | number of items in a training set |
| \(f_i\) | loss function for training example \(i\) |
| \(\| \cdot \|\) | a norm |
| \(\| \cdot \|_w\) | norm depending on a parameter \(w\) |
| \(\rho\) | a duality map |
| \(\rho_w\) | duality map as a function of \(w\) |
| \(b\)  | batch size |
| \(B(t)\) | items in the batch at time \(t\) |
| \(r, v, s\) | functions used to bounds derivatives |
| \(J\)  | loss function used for network |
| \(\text{sgn}\) | \(\text{sgn}(x) = 1_{x \geq 0} - 1_{x < 0}\) |
| \(w_{1:k}\) | a subvector \(w_{1:k} = (w_1, \ldots, w_k)\) |

Notation The notation we will use is listed in Table 1.2. In addition, we will use the following definitions and conventions. Given two linear maps \(A_1 : Z \to U\) and \(A_2 : Z \to U\), the direct sum \(A_1 \oplus A_2\) is the linear map from \(Z \times Z\) to \(U \times U\) that maps a vector \((z_1, z_2)\) to \((A_1 z_1, A_2 z_2)\). \(C(x, y)\) is the result of applying bilinear map \(C\) to the vectors \(x, y\); in terms of components,
Diagonal of a bilinear map \( C : X \times Y \rightarrow Z \), is \( \| C \| = \sup_{\| x \|_X = 1} \sup_{\| y \|_Y = 1} \| C(u_1, u_2) \|_Z \). If \( \ell : \mathbb{R}^n \rightarrow \mathbb{R} \) is a linear functional, then we represent the value of \( \ell \) at the point \( u \in \mathbb{R}^n \) by \( \ell \cdot u \), following the notation used by Abraham et al. [1]. The derivative of a function \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \) at point \( x_0 \in \mathbb{R}^n \) is a linear map from \( \mathbb{R}^n \) to \( \mathbb{R}^m \), denoted by \( \frac{\partial f}{\partial x}(x_0) \). The result of applying this linear map to a vector \( u \in \mathbb{R}^n \) is a vector in \( \mathbb{R}^m \) denoted \( \frac{\partial f}{\partial x}(x_0) \cdot u \). The second derivative of a function \( f \) at \( x_0 \) is a bilinear map from \( \mathbb{R}^n \times \mathbb{R}^n \) to \( \mathbb{R}^m \), denoted by \( \frac{\partial^2 f}{\partial x^2}(x_0) \), and we use the notation \( \frac{\partial^2 f}{\partial x^2}(x_0) \cdot (u, v) \) to represent the \( \mathbb{R}^m \)-valued result of applying this bilinear map to the pair of vectors \( (u, v) \).

2 Motivating example

For completeness, this section details a simple neural network training problem where the gradient of the objective function does not have a Lipschitz gradient. Consider the network depicted in Figure 1. This network maps a real-valued input to a hidden layer with two nodes and produces a real-valued output. Suppose that the sigmoid activation function \( \sigma(u) = \frac{1}{1 + e^{-u}} \) is used, so that the function computed by the network is

\[
y(w_1, w_2, w_3, w_4; x) = \sigma(w_3 \sigma(w_1 x) + w_4 \sigma(w_2 x))
\]

Consider training the network to map the input \( x = 1 \) to the output 0, using a squared-error loss function. The optimization objective \( f : \mathbb{R}^4 \rightarrow \mathbb{R} \) will be

\[
f(w_1, w_2, w_3, w_4) = |y(w_1, w_2, w_3, w_4; 1)|^2.
\]

Proposition 2.1 establishes that \( f \) does not have bounded second derivatives, and hence cannot have a Lipschitz continuous gradient.

**Proposition 2.1** The function \( f \) defined in Equation (2) has unbounded second derivatives: \( \sup_{w \in \mathbb{R}^4} \| \frac{\partial^2 f}{\partial w^2}(w) \| = \infty \).

The proof is deferred to an appendix.

A consequence of this proposition is that analyses assuming the objective function has a Lipschitz gradient cannot be used to guarantee the convergence of gradient descent for this (and related) functions. Intuitively, when the parameters tend towards regions of space where the second derivative is larger, the steepest descent curve could be changing direction very quickly, and this means first-order methods may have to use ever smaller step-sizes to avoid over-stepping and increasing the objective function. Note our example can be extended to show that third and higher-order derivatives of the objective \( E \) are also not globally bounded, and therefore convergence analysis that shift the requirement of a derivative bounded onto such higher-order derivatives would also not be applicable. On the other hand, the DSGD algorithm introduced below allows us to prove convergence for a variety of neural network training scenarios, including the function (2). Finally, the negative conclusion in Proposition 2.1...
Fig. 1 The small network used as a motivating example in Section 2. We show that the training problem of mapping the input 1 to the output 0, using the logistic activation function and squared-error loss, leads to an objective where the gradient is not Lipschitz continuous.

does not mean that algorithms like stochastic gradient descent would fail in practice, but it does suggest that the theory would be needed to be extended in order analyze the convergence in the context of training neural networks.

3 Duality Structure Gradient Descent

We begin by assuming there is a user-defined family of norms parameterized by elements of the search space. The norm of a vector $u$ at parameter $w$ is denoted by $\|u\|_w$. The family of norms is subject to a continuity condition:

**Assumption 3.1** The function $(w, u) \mapsto \|u\|_w$ is continuous on $\mathbb{R}^n \times \mathbb{R}^n$.

Intuitively, the Assumption stipulates that two norms $\| \cdot \|_{w_1}$ and $\| \cdot \|_{w_2}$ should be similar if $w_1$ and $w_2$ are close. This implies that the family of norms defines a Finsler structure on the search space [17, Definition 27.5]. In the remainder we use the terminology “family of norms” to refer to any collection of norms satisfying Assumption 3.1. An example that the reader may keep in mind is $\|u\|_w = \frac{1}{1 + \|w\|_2^2} \|u\|_2$, where $\| \cdot \|_2$ is the standard Euclidean norm on $\mathbb{R}^n$.

The family of norms induces a norm on the dual space $L(\mathbb{R}^n, \mathbb{R})$ at each $w \in \mathbb{R}^n$; if $\ell \in L(\mathbb{R}^n, \mathbb{R})$ then

$$\|\ell\|_w = \sup_{\|u\|_w = 1} \ell \cdot u. \quad (3)$$

It is the case that for any family of norms the dual norm map $(w, \ell) \mapsto \|\ell\|_w$ is continuous on $\mathbb{R}^n \times L(\mathbb{R}^n, \mathbb{R})$. This follows from [17] Proposition 27.7.

A vector $u$ achieving the supremum in Equation (3) always exists, as it is the maximum of a continuous function over a compact set. We represent scaled versions of vectors achieving the supremum in (3) using a duality map:

**Definition 3.1** A duality map at $w$ is a function $\rho_w : L(\mathbb{R}^n, \mathbb{R}) \to \mathbb{R}^n$ such that for all $\ell \in L(\mathbb{R}^n, \mathbb{R})$,

$$\|\rho_w(\ell)\|_w = \|\ell\|_w, \quad (4a)$$
$$\ell \cdot \rho_w(\ell) = \|\ell\|_w^2. \quad (4b)$$
If the underlying norm $\| \cdot \|_w$ is an inner product norm, then it can be shown that there is a unique choice for the duality map at $w$. In detail, let $Q_w$ be the positive definite matrix such that $\| u \|_w = \sqrt{u \cdot (Q_w u)}$ for all vectors $u$. Then the duality map for this norm is $\rho_w(\ell) = Q_w^{-1} \ell$. However, in general there might be more than one choice for the duality map. For instance, consider the norm $\| \cdot \|_\infty$ on $\mathbb{R}^2$, and let $\ell$ be the linear functional $\ell(x_1, x_2) = x_1$. Then we could set $\rho_\infty(\ell)$ to be either of the vectors $(1, 1)$ or $(1, -1)$, and in both cases properties (4a), (4b) would be satisfied.

A duality structure assigns a duality map to each $w \in \mathbb{R}^n$:

**Definition 3.2** A duality structure is a function $\rho : \mathbb{R}^n \times \mathcal{L}(\mathbb{R}^n, \mathbb{R}) \to \mathbb{R}^n$ such that for all $w \in \mathbb{R}^n$, the function $\rho_w \in \mathcal{L}(\mathbb{R}^n, \mathbb{R})$ satisfies the two properties (4a) and (4b).

The simplest family of norms is the one that assigns the Euclidean norm to each parameter. In this situation the dual norm is also the Euclidean norm and the duality map at each point is simply the identity function. For the family of norms $\| u \|_\infty = (1 + \| u \|_2) \| u \|_2$, the reader may verify that a duality structure is $\rho_w(\ell) = \frac{1}{1+\| u \|_2^2} \ell$. Before continuing, let us consider a less trivial example.

**Example 3.1** Let $h : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$ be continuous. Consider the following family of norms on $\mathbb{R}^2$:

$$ \|(u, v)\|_{(x, y)} = \sqrt{1 + |h(y)| |u|} + \sqrt{1 + |g(x)| |v|}. $$

As the function $(x, y, u, v) \mapsto \|(u, v)\|_{(x, y)}$ is continuous, this family of norms is a well defined. Denoting a linear functional on $\mathbb{R}^2$ by $\ell = (\ell_1, \ell_2)$, it follows from Proposition 4.6 below that the dual norm is

$$ \|(\ell_1, \ell_2)\|_{(x, y)} = \max \left\{ \frac{|\ell_1|}{\sqrt{1 + |h(y)|}}, \frac{|\ell_2|}{\sqrt{1 + |g(x)|}} \right\}, $$

and a duality map is

$$ \rho_{(x, y)}(\ell_1, \ell_2) = \begin{cases} \left( \frac{\ell_1}{1 + |h(y)|}, 0 \right) & \text{if } \frac{|\ell_1|}{\sqrt{1 + |h(y)|}} \geq \frac{|\ell_2|}{\sqrt{1 + |g(x)|}}, \\ \left( 0, \frac{\ell_2}{1 + |g(x)|} \right) & \text{else}. \end{cases} $$

This concludes the example.

As the example of the norm $\| \cdot \|_\infty$ shows, there may be multiple duality structures that can be chosen for a family of norms. In this case, any one of them can be chosen without affecting the convergence bounds of the algorithms.

Given the definition of duality structure, we can now explain the steps of the DSGD algorithm, shown in Algorithm 3.1. Each iteration of this algorithm uses an estimate $g(t)$ of the derivative. The algorithm computes the duality map on this estimate, and the result serves as the update direction. A step-size $\epsilon(t)$ determines how far to go in this direction. Note that for a trivial family of norms ($\| \cdot \|_w = \| \cdot \|_2$ for all $w$), the algorithm reduces to standard SGD.
Our analysis seeks to bound the expected number of iterations until the algorithm generates an approximate stationary point for the function $f$, measured relative to the local norms. Formally, for $\gamma > 0$ we define the stopping time $\tau$ as the first time the gradient has a norm less than or equal to $\gamma$:

$$\tau = \inf \left\{ t \geq 1 \left| \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 \leq \gamma \right. \right\},$$

and the goal of our analysis is to find an upper bound for $E[\tau]$. In our definition of $\tau$, the magnitude of the gradient is measured relative to the local norms $\| \cdot \|_{w(t)}$. This criterion for success is a standard notion in the literature of optimization on manifolds (see Theorem 4 of [10], and Theorem 2 of [53].) Note that this stopping rule is not part of the algorithms described in this paper, but is an analytical tool to prove something about the behavior of the iterates generated by the algorithms.

Next, we describe the conditions on the function $f$ and the derivative estimates $g(t)$ that will be used in the convergence analysis. The conditions on the objective $f$ are that the function is differentiable and obeys a quadratic bound along each ray specified by the duality map.

**Assumption 3.2** The function $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable, bounded from below by $f^* \in \mathbb{R}$, and there is an $L \geq 0$ such that, for all $w \in \mathbb{R}^n$, all $\eta \in L(\mathbb{R}^n, \mathbb{R})$, and all $\epsilon \in \mathbb{R}$,

$$f(w + \epsilon \rho \cdot w(\eta)) - f(w) - \epsilon \frac{\partial f}{\partial w}(w) \cdot \rho \cdot w(\eta) \leq \frac{L}{2} \epsilon^2 \|\eta\|_{w}^2.$$ 

Note that when the family of norms is simply the Euclidean norm, $\| \cdot \|_{w} = \| \cdot \|_2$ for all $w$, then this condition, often called smoothness, is satisfied by functions that have a Lipschitz continuous gradient [40, Lemma 1.2.3]. While superficially appearing similar to the standard Lipschitz gradient assumption, by allowing for a family of norms in the definition (and also by involving the duality structure), a larger set of functions can be seen to satisfy the criteria, and hence this is assumption is strictly more general than the standard smoothness assumption. Most importantly for us, in Proposition 4.7 below, we show that Assumption 3.2 is satisfied for the empirical loss function of a deep neural network, by appropriate choice of the family of norms. This setting of course includes the simple network with two hidden nodes presented in Section 2, and we refer the reader to Proposition A.2 in the appendix which explicitly establishes Assumption 3.2 for the example of Section 2. Another function class that does not satisfy Euclidean smoothness but does satisfy Assumption 3.2 is given below in Example 3.2. Roughly speaking, if the family of norms is defined using a scalar function like $\| \cdot \|_{w} = g(x) \| \cdot \|$ for some underlying norm $\| \cdot \|$ and a real-valued function $g$, then the condition (3.2) can be interpreted as requiring that the 2nd derivative of $f$ grows slower than $g(x)^2$. Finally, this assumption can also be compared with condition A3 in [10], except it concerns the simple search space of $\mathbb{R}^n$, and it is adapted to use a a family of norms on Euclidean space instead of a Riemannian structure.
Algorithm 3.1: Duality structure gradient descent (DSGD)

1. **input:** Initial point $w(1) \in \mathbb{R}^n$ and step-size sequence $\epsilon(t)$.

2. **for** $t = 1, 2, \ldots$ **do**
   3. ▶ Obtain derivative estimate $g(t)$
   4. ▶ Compute the search direction $\Delta(t) = \rho_{w(t)}(g(t))$
   5. ▶ Update the parameter $w(t+1) = w(t) - \epsilon(t)\Delta(t)$

6. **end**

To begin the analysis of DSGD, we define the filtration $\{F(t)\}_{t=0,1,\ldots}$, where $F(0) = \sigma(w(1))$ and for $t \geq 1$, $F(t) = \sigma(w(1), g(1), g(2), \ldots, g(t))$. We assume that the derivative estimates $g(t)$ are unbiased, and have bounded variance relative to the family of norms:

**Assumption 3.3** For $t = 1, 2, \ldots$, define $\delta(t) = g(t) - \frac{\partial f}{\partial w}(w(t))$. The $\delta(t)$ must satisfy

$$
E[\delta(t) | F(t-1)] = 0, \quad (6a)
$$

$$
E[\|\delta(t)\|_w^2 | F(t-1)] \leq \sigma^2 < \infty. \quad (6b)
$$

When $\| \cdot \|_w = \| \cdot \|_2$ for all $w$, Equation (6b) states that, conditioned on past observations, the gradient estimates have uniformly bounded variance in the usual sense. In ML applications, the stochastic gradient is typically computed with respect to a random minibatch of examples. However, in the context of using SGD to train deep neural nets, it may be problematic to require the right hand side of (6b) be bounded uniformly over all $t$ and all $w(1)$, since, as we demonstrate in Proposition A.3 below, it is possible to construct training data sets for the neural network model of Section 2 such that the variance of the minibatch gradient estimator with unit batch-size is unbounded as a function of $\|w\|$. By allowing for a family of norms, Assumption 3.3 avoids this problem; as shown below in Lemma 4.9, the variance of mini-batch gradient estimator for DSGD is bounded relative to the appropriate family of norms.

Compared to the analysis of SGD in the Euclidean case (e.g., that of [21]), the analysis of DSGD is more involved because of the duality map, which may be a nonlinear function. This means that even if $g(t)$ is unbiased in the sense of Assumption 3.3, it may be the case that $E[\rho_{w(t)}(g(t))] \neq \rho_{w(t)}(\frac{\partial f}{\partial w}(w(t)))$. To address this, we quantify the bias in the update directions in terms of a convexity parameter of the family of norms, defined as follows:

**Definition 3.3** [12 Section 4.1] A family of norms $\| \cdot \|_w$ is 2-uniformly convex with parameter $c$ if there is a constant $c \geq 0$ satisfying, for all $w, x, y \in \mathbb{R}^n$,

$$
\left\| \frac{x + y}{2} \right\|_w^2 \leq \frac{1}{2} \|x\|_w^2 + \frac{1}{2} \|y\|_w^2 - \frac{c}{4} \|x - y\|_w^2. \quad (7)
$$
Equivalently, this definition states that the function \( x \mapsto \|x\|_w^2 \) is strongly convex with parameter \( 2c \), uniformly over \( w \). For example, if the family of norms is such that each \( \| \cdot \|_w \) is an inner product norm, then \( c = 1 \), while if \( \| \cdot \|_w = \| \cdot \|_p \) for some \( 1 < p < 2 \) we can take \( c = p - 1 \) [35, Proposition 3]. Note that Equation (7) always holds with \( c = 0 \), although positive values of \( c \) lead to better convergence rates, as we show below.

The following Lemma states bounds we shall use to relate bias and convexity:

**Lemma 3.4** Let \( \| \cdot \| \) be a norm on \( \mathbb{R}^n \) that is 2-uniformly convex with parameter \( c \), and let \( \rho \) be a corresponding duality map. If \( \delta \) is a \( \mathbb{R}^n \)-valued random variable such that \( E[\delta] = 0 \) then

\[
E[\ell \cdot \rho(\ell + \delta)] \geq \left( \frac{1 + c}{2} \right) \|\ell\|^2 - \left( \frac{1 - c}{2} \right) E[\|\delta\|^2], \quad (8a)
\]

\[
E[\|\ell + \delta\|^2] \leq (2 - c)\|\ell\|^2 + (2 - c^2) E[\|\delta\|^2]. \quad (8b)
\]

The proof of this lemma is in the appendix. Note that when \( \| \cdot \| \) is an inner product norm, the convexity coefficient is \( c = 1 \) and both relations in the lemma are qualities.

We can now proceed to our analysis of DSGD. This theorem gives some conditions on \( \epsilon \) and \( \gamma \) that guarantee finiteness of the expected amount of time to reach a \( \gamma \)-approximate stationary point.

**Theorem 3.5** Let Assumptions 3.2 and 3.3 hold, and suppose the family of norms has convexity parameter \( c \geq 0 \). Consider running Algorithm 3.1 using constant step-sizes \( \epsilon(t) := \epsilon > 0 \). Suppose that \( \gamma \) and \( \epsilon \) satisfy

\[
\gamma > \left( \frac{1 - c}{1 + c} \right) \sigma^2,
\]

\[
\epsilon < \frac{1}{L} \times \frac{(1 + c) \gamma - (1 - c) \sigma^2}{(2 - c) \gamma + (2 - c^2) \sigma^2}\]

Define \( G = f(w(1)) - f^* \). If \( \tau \) is defined as in Equation (5), then,

\[
E[\tau] \leq \frac{2G + (1 + c - Le(2 - c)) \gamma}{\epsilon (1 + c - Le(2 - c)) \gamma - \epsilon (Le(2 - c^2) + 1 - c) \sigma^2}. \quad (10)
\]

The proof of Theorem 3.5 is deferred to appendix. Let us consider some special cases of this result.

**Corollary 3.6** Under Assumptions 3.2 and 3.3, the following special cases of Theorem 3.5 hold:

1. (Standard SGD) Suppose \( \| \cdot \|_w = \| \cdot \|_2 \) for all \( w \), and let \( \rho_w(\ell) = \ell \). Then for any \( \gamma > 0 \), setting \( \epsilon = \frac{1}{L} \left( \frac{\gamma}{\gamma + \sigma^2} \right) \) leads to

\[
E[\tau] \leq \frac{2G L \sigma^2}{\gamma^2} + \frac{4L(G + \sigma^2)}{\gamma} + 8L.
\]
2. More generally, suppose $\| \cdot \|_w$ has parameter of convexity $c \geq 0$. Then for any $\gamma > \left(\frac{1-c}{1+\tau}\right) \sigma^2$, setting $\epsilon = \frac{1}{2L} \left(\frac{(1+c)\gamma-(1-c)\sigma^2}{(2-c)\gamma+(2-c)\sigma^2}\right)$ leads to

$$E[\tau] \leq \frac{8Lc(2-c)^2\sigma^2}{((1+c)\gamma+(1-c)c^2)^2} + \frac{8L(2-c^2)(G+c^2)}{(1+c)\gamma+(1-c)\sigma^2} + 8L(2-c).$$

Proof The claimed inequalities follow by plugging the given values of $\epsilon$ into Equation (10). The details are given in the appendix.

Note that the batch case, represented by $\sigma^2 = 0$, admits a simpler proof that avoids dependence on the convexity parameter, leading to the following:

**Corollary 3.7** Let Assumption 3.2 hold, and assume $g(t) = \frac{\partial f}{\partial w}(w(t))$. Then for any family of norms $\| \cdot \|_w$, if $\gamma = \frac{1}{T}$ then

$$\min_{1 \leq t \leq T} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_w^2 \leq \frac{2GL}{T}.$$  

Expressed using the stopping variable $\tau$, this says $\tau \leq \lceil 2GL/\gamma \rceil$. Furthermore, any accumulation point $w^*$ of the algorithm is a stationary point of $f$, meaning $\frac{\partial f}{\partial w}(w^*) = 0$.

Proof The proof closely follows that of Theorem 3.5 and the details are deferred to an appendix.

For the trivial family of norms that simply assigns the Euclidean norm to each point in the space, Algorithm 3.1 reduces to standard gradient descent and we recover the known $1/T$ convergence rate for GD (10). In the general case, the non-asymptotic performance guarantee concerns the quantities $\| \frac{\partial f}{\partial w}(w(t)) \|_w(t)$, where the gradient magnitude is measured relative to the local norms $w(t)$. We leave to future work the interesting question of under what conditions a relation can be established between the convergence of $\| \frac{\partial f}{\partial w}(w(t)) \|_w(t)$ and the convergence of $\| \frac{\partial f}{\partial w}(w(t)) \|$, where the norm is fixed.

The main application of Theorem 3.5 will come in the following section, where it is used to prove the convergence of a layer-wise training algorithm for neural networks (Theorems 4.8 and 10). For another example of an optimization problem where this theory applies, consider the following.

**Example 3.2** Consider applying DSGD to the function $f : \mathbb{R}^2 \to \mathbb{R}$ defined by $f(x,y) = g(x)h(y)$, where $g : \mathbb{R} \to \mathbb{R}$ and $h : \mathbb{R} \to \mathbb{R}$ are functions that have bounded second derivatives. For simplicity, assume that $\|g''\|_\infty \leq 1$ and $\|h''\|_\infty \leq 1$. Furthermore, assume that $\sup_{(x,y) \in \mathbb{R}^2} g(x)h(y) \geq f^*$ for some $f^* \in \mathbb{R}$ (for instance, this occurs if $g$ and $h$ are non-negative). The function $f$ need not have a Lipschitz continuous gradient, as the example of $g(x) = x^2$ and $h(y) = y^2$ demonstrates.

Let us denote pairs in $\mathbb{R}^2$ by $w = (x, y)$. Define the family of norms

$$\| (\delta x, \delta y) \|_w = \sqrt{1+|h(y)||\delta x|} + \sqrt{1+|g(x)||\delta y|}.$$
The dual norm and duality map are as previously defined in Example 3.1.

Let $\eta = (\eta_1, \eta_2)$ be any vector. If $\frac{\eta_1}{\sqrt{1 + |h(y)|}} \geq \frac{\eta_2}{\sqrt{1 + |g(x)|}}$, then $\|\eta\|_w = \frac{\|\eta\|}{\sqrt{1 + |h(y)|}}$ and $\rho(\eta) = \left( \frac{\eta_1}{\sqrt{1 + |h(y)|}}, 0 \right)$. Then, since the function $x \mapsto f(x, y)$ has a second derivative that is bounded by $|h(y)|$, we can apply a standard quadratic bound (Proposition 4.4) to conclude that

$$
\left| f(w + \epsilon \rho_w(\eta)) - f(w) - \epsilon \frac{\partial f}{\partial w}(w) \cdot \rho_w(\eta) \right| \leq \epsilon^2 \frac{1}{(1 + |h(y)|)^2} \frac{1}{2} |h(y)||\eta||^2
$$

$$
= \epsilon^2 \frac{|h(y)|}{1 + |h(y)|} \frac{1}{2} |\eta|^2_w
$$

$$
\leq \frac{\epsilon^2}{2} |\eta|^2_w.
$$

The case $\frac{\eta_1}{\sqrt{1 + |h(y)|}} < \frac{\eta_2}{\sqrt{1 + |g(x)|}}$ is similar. Hence Assumption 3.2 is satisfied.

According to Corollary 3.7, convergence will be guaranteed in batch DSGD with $\epsilon = 1$. In more details, in the first step (Line 4) the algorithm computes the duality map on the derivative $g(t) = \frac{\partial f}{\partial w}(w(t))$.

$$
\left| \frac{\partial f}{\partial x}(x(t), y(t)) \right| \geq \left| \frac{\partial f}{\partial y}(x(t), y(t)) \right| \geq \frac{1}{\sqrt{1 + |y(x(t))|}}
$$

(11)

then the update direction is $\Delta(t) = \left( \frac{\partial f}{\partial x}(x(t), y(t)) \frac{1}{\sqrt{1 + |y(x(t))|}}, 0 \right)$. In this case, at the next step (Line 5) the next point is computed by keeping $y$ the same ($y(t + 1) = y(t)$) and updating $x$ as $x(t + 1) = x(t) - \epsilon \frac{\partial f}{\partial x}(x(t), y(t)) \frac{1}{1 + |h(y)|}$. If (11) does not hold, then $y$ is updated instead: $x(t + 1) = x(t)$ and $y(t + 1) = y(t) - \epsilon \frac{\partial f}{\partial y}(x(t), y(t)) \frac{1}{1 + |g(x(t))|}$. The resulting convergence guarantee associated with the algorithm is that

$$
\max \left\{ \left| \frac{\partial f}{\partial x}(x(t), y(t)) \right|, \left| \frac{\partial f}{\partial y}(x(t), y(t)) \right| \right\} \rightarrow 0
$$

as $t \rightarrow \infty$.

This example could be extended easily to the case where $f$ is defined as the product of arbitrarily many functions with bounded second derivatives.

4 Application to Neural Networks with Multiple Layers

In order to implement and analyze the DSGD algorithm for minimizing a particular objective function, there are three tasks: 1) Define the family of norms for the space, 2) Identify a duality structure to use, and 3) Verify the generalized gradient smoothness condition of Assumption 5.2. In this section we carry out these steps in the context of a neural network with multiple layers.
We first define the parameter space and the objective function. The network consists of an input layer and $K$ non-input layers. We are going to consider the case that each layer is fully connected to the previous one and uses the same activation function. Networks with heterogeneous layer types (consisting for instance of convolutional layers, softmax layers, etc.) and networks with biases at each layer can also be accommodated in our theory.

Let the input to the network be of dimensionality $n_0$, and let $n_1, \ldots, n_K$ specify the number of nodes in each of $K$ non-input layers. For $k = 1, \ldots, K$ define $W_k = \mathbb{R}^{n_k \times n_{k-1}}$ to be the space of $n_k \times n_{k-1}$ matrices; a matrix in $w_k \in W_k$ specifies weights from nodes in layer $k-1$ to nodes in layer $k$. The overall parameter space is then $W = W_1 \times \ldots \times W_K$. We define the output of the network as follows. For an input $x \in \mathbb{R}^{n_0}$, and weights $w = (w_1, \ldots, w_K) \in W$, the output is $y^K(w; x) \in \mathbb{R}^{n_K}$ where $y^0(w; x) = y$ and for $1 \leq k \leq K$,

$$y^k_i(w; x) = \sigma \left( \sum_{j=1}^{n_{k-1}} w_{k,i,j} y^{k-1}_j(w; x) \right), \quad i = 1, 2, \ldots, n_k.$$  

Given $m$ input/output pairs $(x_1, z_1), (x_2, z_2), \ldots, (x_m, z_m)$, where $(x_n, z_n) \in \mathbb{R}^{n_0} \times \mathbb{R}^{n_K}$, we seek to minimize the empirical error

$$f(w) = \frac{1}{m} \sum_{i=1}^{m} f_i(w),$$  \hspace{1cm} (12)

where the $f_i$ are

$$f_i(w) = \| y^K(w; x_i) - z_i \|_2^2, \quad i = 1, 2, \ldots, m.$$  \hspace{1cm} (13)

and $\| \cdot \|_2$ is the Euclidean norm.

### 4.1 Layer-wise gradient smoothness for Neural Networks

Our assumptions on the activation $\sigma$, the inputs $x_i$, and targets $z_i$, are as follows:

**Assumption 4.1**

i. **(Activation bounds)** The activation function $\sigma$ and its first two derivatives are bounded. Formally, $\| \sigma \|_\infty \leq 1$, $\| \sigma' \|_\infty < \infty$, and $\| \sigma'' \|_\infty < \infty$.

ii. **(Input/Target bounds)** $\| x_i \|_\infty \leq 1$ and $\| z_i \|_\infty \leq 1$ for $i = 1, 2, \ldots, m$.

Note that the first part of the assumption is satisfied by the sigmoid function $\sigma(u) = 1/(1 + e^{-u})$ and also the hyperbolic tangent function $\sigma(u) = -1 + 2/(1 + e^{-2u})$. Note that this assumption is not satisfied by the ReLU function $\sigma(u) = \max\{0, u\}$. The second part of Assumption 4.1 states that the components of the inputs and targets are between $-1$ and $1$.

In Proposition 4.3 we establish that, under Assumption 4.1, the restriction of the objective function to the weights in any particular layer is a function with a bounded second derivative. To confirm the boundedness of the second derivative, any norm on the weight matrices can be used, because on finite
dimensional spaces all norms are strongly equivalent. However, different norms will lead to different specific bounds. For the purposes of gradient descent, each norm and Lipschitz bound implies a different quadratic upper bound on the objective, which in general may lead to a variety of update steps, hence defining different algorithms. Our construction considers the induced matrix norms corresponding to the vector norms \( \| \cdot \|_q \) for \( 1 \leq q \leq \infty \).

**Assumption 4.2** For some \( q \in [1, \infty) \) and all \( 1 \leq i \leq K \), each space \( \mathbb{R}^{n_i} \) has the norm \( \| \cdot \|_q \).

We are going to be working with the matrix norm induced by the given choice of \( q \). Recall that, for an \( r \times c \) matrix \( A \), if \( q = 1 \), then,

\[
\| A \|_1 = \max_{1 \leq j \leq c} \sum_{i=1}^{r} |A_{i,j}|,
\]

while if \( q = 2 \),

\[
\| A \|_2 = \max_{1 \leq i \leq \min\{r,c\}} \sigma_i(A),
\]

where for a matrix \( A \), we define \( \sigma(A) = (\sigma_1(A), \ldots, \sigma_{\min\{r,c\}}(A)) \) to be the vector of singular values of \( A \). Lastly, if \( q = \infty \),

\[
\| A \|_\infty = \max_{1 \leq i \leq r} \sum_{j=1}^{c} |A_{i,j}|.
\]

That is, when \( q = 1 \) the matrix norm is the maximum absolute column sum, when \( q = 2 \) the norm is the largest singular value, also known as the spectral norm, and when \( q = \infty \) the norm is the largest absolute row sum [23].

For ease of notation, throughout this section, we will assume that all the layers have the same number of nodes. Formally, this means \( n_i = n_K \) for \( i = 0, \ldots, K \). Also, at times we use the subvector notation \( z_{1:i} \) to denote the first \( i \) components of a vector \( z \). Next, let us introduce a set of functions that will be used to express our bounds on the second derivatives. Let \( r_0 = 1 \), and for \( 1 \leq n \leq K - 1 \) the function \( r_n \) is

\[
r_n(z_1, \ldots, z_n) = \| \sigma' \|_\infty \prod_{i=1}^{n} z_i.
\]

Then define \( v_n \) recursively, with \( v_0 = 0 \), and for \( 1 \leq n \leq K - 1 \), the function \( v_n \) is

\[
v_n(z_1, \ldots, z_n) = \| \sigma'' \|_\infty \| \sigma' \|_\infty^{2(n-1)} \prod_{i=1}^{n} z_i^2 + \| \sigma' \|_\infty z_n v_{n-1}(z_1, \ldots, z_{n-1}).
\]

Define constants \( d_{q,1}, d_{q,2} \) and \( c_q \) as in Table 2 Then for \( 0 \leq n \leq K - 1 \) the function \( s_n \) is

\[
s_n(z_1, \ldots, z_n) = d_{q,2} c_q^2 \| \sigma' \|_\infty^2 r_1^2(z_1, \ldots) + d_{q,1} c_q^2 \| \sigma' \|_\infty^2 v_1(z_1, \ldots) + d_{q,1} c_q^2 \| \sigma'' \|_\infty r_1(z_1, \ldots). \]
Proposition 4.3 Let Assumptions 4.1 and 4.2 hold, and let \( q \) be the constant from Assumption 4.2. Let the spaces \( W_1, \ldots, W_K \) have the norm induced by \( \| \cdot \|_q \) and define functions \( p_1, \ldots, p_K \) as

\[
p_i(w) = \sqrt{s_{K-i}(\|w_{i+1}\|_q, \ldots, w_K\|_q)} + 1. \tag{14}
\]

Let \( f \) be as in (12). Then for all \( w \in W \) and \( 1 \leq i \leq K \), the bound \( \| \frac{\partial^2 f}{\partial w_i^2}(w) \|_q \leq p_i(w)^2 \) holds.

For example, a network with one hidden layer yields polynomials \( p_1, p_2 \) where

\[
p_1(w) = \sqrt{s_1(\|w_2\|_q)} + 1
= \sqrt{d_2 q c_2^2 \|\sigma''\|_\infty^2 r_1(\|w_2\|_q)^2 + d_2 q c_2^2 \|\sigma''\|_\infty^2 v_1(\|w_2\|_q) + d_2 q c_2^2 r_1(\|w_2\|_q) + 1}
= \sqrt{(d_2 q c_2^2 \|\sigma''\|_\infty^2 + d_2 q c_2^2 \|\sigma''\|_\infty^2 \|\sigma''\|_\infty) \|w_2\|_q^2 + d_2 q c_2^2 \|\sigma''\|_\infty \|\sigma''\|_\infty \|w_2\|_q + 1}, \tag{15a}
\]

\[
p_2(w) = \sqrt{s_0 + 1}
= \sqrt{d_2 q c_2^2 \|\sigma''\|_\infty^2 r_0^2 + d_2 q c_2^2 \|\sigma''\|_\infty^2 v_0 + d_2 q c_2^2 \|\sigma''\|_\infty r_0 + 1}
= \sqrt{c_2^2(d_2 q c_2^2 \|\sigma''\|_\infty^2 + d_2 q c_2^2 \|\sigma''\|_\infty) + 1}. \tag{15b}
\]

Note that in Proposition 4.3, the norm of the Hessian matrix is bounded by a polynomial in the norms of the weights, and terms of a similar form appear in norm-based complexity measures for deep networks [35, 32, 31].

Proposition 4.4 Let \( f : \mathbb{R}^n \to \mathbb{R} \) be a function with continuous derivatives up to 2nd order. Let \( \| \cdot \| \) be an arbitrary norm on \( \mathbb{R}^n \) and let \( \rho \) be a corresponding duality map. Suppose that \( \sup_w \sup_{\|u_1\| = \|u_2\| = 1} \left\| \frac{\partial^2 f}{\partial w^2}(w) \cdot (u_1, u_2) \right\| \leq L \). Then for any \( \epsilon > 0 \) and any \( \Delta \in \mathbb{R}^n \), \( f(w - \epsilon \Delta) \leq f(w) - \epsilon \frac{\partial f}{\partial w}(w) \cdot \Delta + \epsilon^2 \frac{L}{2} \|\Delta\|^2 \). In particular, \( f \left( w - \epsilon \rho \left( \frac{\partial f}{\partial w}(w) \right) \right) \leq f(w) - \epsilon \left( 1 - \frac{1}{2} \epsilon \right) \| \frac{\partial f}{\partial w}(w) \|^2 \).
This proposition motivates the following greedy algorithm: Identify a layer $i^*$ such that $i^* = \arg\max_{1 \leq i \leq K} \frac{1}{p_i(w)} \| \frac{\partial f}{\partial w_i}(w) \|$ and update parameter $w_{i^*}$, using a step-size $\frac{1}{p_{i^*}(w)}$ in the direction $\rho \left( \frac{\partial f}{\partial w_{i^*}}(w) \right)$. As a consequence of Proposition 4.3 and Proposition 4.4, this update will lead to a decrease in the objective of at least $\frac{1}{2} \left( p_{i^*}(w) \right)^2 \| \frac{\partial f}{\partial w_{i^*}}(w) \|^2$. This greedy algorithm is depicted (in a slightly generalized form) in Algorithm 4.1. In the remainder of this section, we will show how this sequence of operations can be explained with a particular duality structure on $\mathbb{R}^n$, in order to apply the convergence theorems of Section 3.

4.2 Family of norms and duality structure

In this section we define a family of norms and associated duality structure that encodes the layer-wise update criteria. The family of norms is constructed using the functions $p_i$ from (14) as follows. For any $w = (w_1, \ldots, w_K) \in W$ and any $(u_1, \ldots, u_K) \in W$, define $\|(u_1, \ldots, u_K)\|_w$ as

$$\|(u_1, \ldots, u_K)\|_w = p_1(w)\|u_1\|_q + \ldots + p_K(w)\|u_K\|_q.$$  

(16)

Note that the family of norms and the polynomials $p$ also depend on the user-supplied parameter $q$ from Assumption 4.2, although we omit this from the notation for clarity.

To obtain the duality structure, we derive duality maps for matrices with the norm $\| \cdot \|_q$, and then use a general construction for product spaces. The first part is summarized in the following Proposition. Note that when we use the $\arg\max$ to find the index of the largest entry of a vector, any tie-breaking rule can be used in case there are multiple maxima. For instance, the $\arg\max$ may be defined to return the smallest such index.

**Proposition 4.5** Let $\ell \in \mathcal{L}(\mathbb{R}^{r \times c}, \mathbb{R})$ be a linear functional defined on a space of matrices with the norm $\| \cdot \|_q$ for $q \in \{1, 2, \infty\}$. Then the dual norm is

$$\|\ell\|_q = \begin{cases} \sum_{j=1}^{c} \max_{1 \leq r \leq r} |\ell_{i,j}| & \text{if } q = 1, \\ \min_{(r,c)} \sum_{i=1}^{r} \sigma_i(\ell) & \text{if } q = 2, \\ \max_{1 \leq i \leq c} \sum_{j=1}^{c} |\ell_{i,j}| & \text{if } q = \infty. \end{cases}$$  

(17)

**Possible choices for duality maps are as follows:**

For $q = 1$, the duality map $\rho_1$ sends $\ell$ to a matrix that picks out a maximum in each column: $\rho_1(\ell) = \|\ell\|_1 m$ where $m$ is the $r \times c$ matrix

$$m_{i,j} = \begin{cases} \text{sgn}(\ell_{i,j}) & \text{if } i = \arg\max_{1 \leq k \leq r} |\ell_{k,j}|, \\ 0 & \text{otherwise}. \end{cases}$$  

(18)
For $q = 2$ the duality map $\rho_2$ normalizes the singular values of $\ell$: If $\ell = U\Sigma V^T$ is the singular value decomposition of $\ell$, written in terms of column vectors as $U = [u_1, \ldots, u_c], V = [v_1, \ldots, v_c]$, and denoting the rank of the matrix $\ell$ by $\text{rank}\ell$, then

$$\rho(\ell)_2 = \|\ell\|_2 \sum_{i=1}^{\text{rank}\ell} u_i v_i^T. \tag{19}$$

For $q = \infty$, the duality map $\rho_\infty$ sends $\ell$ to a matrix that picks out a maximum in each row: $\rho_\infty(\ell) = \|\ell\|_\infty m$ where $m$ is the $r \times c$ matrix

$$m_{i,j} = \begin{cases} \text{sgn}(\ell_{i,j}) & \text{if } j = \arg \max_{1 \leq k \leq c} |\ell_{i,k}|, \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

The proof of this proposition is in the appendix.

Next, we construct a duality map for a product space from duality maps on the components. Recall that in a product vector space $Z = X_1 \times \ldots \times X_K$, each linear functional $\ell \in \mathcal{L}(Z, \mathbb{R})$ uniquely decomposes as $\ell = (\ell_1, \ldots, \ell_K) \in \mathcal{L}(X_1, \mathbb{R}) \times \ldots \times \mathcal{L}(X_K, \mathbb{R})$.

**Proposition 4.6** If $X_1, \ldots, X_K$ are normed spaces, carrying duality maps $\rho_{X_1}, \ldots, \rho_{X_K}$ respectively, and the product $Z = X_1 \times \ldots \times X_K$ has norm $\| (x_1, \ldots, x_K) \|_Z = p_1 \|x_1\|_{X_1} + \ldots + p_K \|x_K\|_{X_K}$, for some positive coefficients $p_1, \ldots, p_K$, then the dual norm for $Z$ is

$$\| (\ell_1, \ldots, \ell_K) \|_Z = \max \left\{ \frac{1}{p_1} \|\ell_1\|_{X_1}, \ldots, \frac{1}{p_K} \|\ell_K\|_{X_K} \right\} \tag{21}$$

and a duality map is given by

$$\rho_Z(\ell_1, \ldots, \ell_K) = \left( 0, \ldots, \frac{1}{p_{i^*}} \rho_{X_{i^*}}(\ell_{i^*}), \ldots, 0 \right)$$

where $i^* = \arg \max_{1 \leq i \leq K} \left\{ \frac{1}{p_i} \|\ell_i\|_{X_i} \right\}$.

See the appendix for a proof of Proposition 4.6. Based on Proposition 4.6 and the definition of the family of norms from (16), the dual norm at a point $w \in W = W_1 \times \ldots \times W_K$ is

$$\| (\ell_1, \ldots, \ell_K) \|_w = \max_{1 \leq i \leq K} \frac{1}{p_i(w)} \|\ell_i\|_q. \tag{22}$$

We define the duality structure on the neural net parameter space as follows:

1. Each space $W_1, \ldots, W_K$ has duality map $\rho_q(\cdot)$, defined by Proposition 4.5.
2. The duality map at each point $w$ is defined according to Proposition 4.6:

$$\rho_w(\ell_1, \ldots, \ell_K) = \left( 0, \ldots, \frac{1}{p_{i^*(w)}} \rho_q(\ell_{i^*}), \ldots, 0 \right) \tag{23}$$

where $i^* = \arg \max_{1 \leq i \leq K} \left\{ \frac{1}{p_{i}(w)} \|\ell_i\|_q \right\}$. 
4.3 Convergence Analysis

Throughout this section, we associate with $W$ the family of norms $\| \cdot \|_w$ from (16) and duality structure $\rho_w$ from (23), and the function $f$ is defined as in (12). The convergence analysis of Algorithm 3.1 is based on the idea that the update performed in the algorithm is exactly equivalent to taking a step in the direction of the duality map (23) as applied to the derivative of $f$, so the algorithm is simply a special case of Algorithm 3.1. Recall that the convergence property of Algorithm 3.1 depends on verifying the generalized smoothness condition set forth in Assumption 3.2. This smoothness condition is confirmed in the following proposition.

**Lemma 4.7** Let Assumptions 4.1 and 4.2 hold, and let $q$ be the constant chosen in Assumption 4.2. Let $f$ defined as in (12). Then Assumption 3.2 is satisfied with $L = 1$.

Now that Assumption 3.2 has been established, we can proceed to the analysis of batch and stochastic DSGD.

4.4 Batch analysis

First we consider analysis of Algorithm 4.1 running in Batch mode. Each iteration starts on Line 4 by computing the derivatives of the objective function. This is a standard back-propagation step. Next, on Line 8, for each layer $i$ the polynomials $p_i$ and the $q$-norms of the derivatives $g_i$ are computed. Note that for any $i < K$, computing $p_i$ will require the matrix norms $\| w_{i+1} \|_q, \ldots, \| w_K \|_q$. In Line 9 we identify which layer $i$ has the largest value of $\| g_i(t) \|_q/p_i(w(t))$. Note that this is equivalent to maximizing $\| g_i(t) \|_q^2/2p_i(w(t))^2$, which is exactly the lower bound guaranteed by Proposition 4.4. Having chosen the layer, in Lines 10 through 13 we perform the update of layer $i^*$, keeping parameters in other layers fixed.

**Theorem 4.8** Let the function $f$ be defined as in (12), let Assumptions 4.1 and 4.2 hold, and let $q$ be the constant chosen in Assumption 4.2. Associate with $W$ the family of norms $\| \cdot \|_w$ from (16) and duality structure $\rho_w$ from (23). Consider running Algorithm 4.1 in batch mode, using step-size $\epsilon = 1$. Then $\min_{1 \leq t \leq T} \| g_{i^*}(w(t)) \|_{w(t)}^2 \leq \delta$ when $T \geq 2f(w(1))/\delta$.

**Proof** It is evident that the update performed in Algorithm 4.1 running in batch mode is of the form $w(t + 1) = w(t) - \epsilon \Delta(t)$, where $\epsilon = 1$ and $\Delta(t) = \rho_w(t)(\frac{\partial f}{\partial w}(w(t)))$. Hence the algorithm is a particular case of Algorithm 3.1. We have established Assumption 3.2 in Lemma 4.7 and the result follows by Corollary 4.4, using $L = 1$ and $f^* = 0$. 

Algorithm 4.1: Duality structure gradient descent for a multi-layer neural network

1. **input:** Parameter $q \in \{1, 2, \infty\}$, training data $(y_i, z_i)$ for $1 \leq i \leq m$, initial point $w(1) \in W$, step-size $\epsilon$, selection of mode Batch or Stochastic, and batch-size $b$ (only required for Stochastic mode.)

2. for $t = 1, 2, \ldots$ do
   3. if Mode = Batch then
      4. Compute full derivative $g(t) = \frac{\partial f}{\partial w}(w(t))$.
   5. else if Mode = Stochastic then
      6. Compute mini-batch derivative $g(t) = \frac{1}{b} \sum_{j \in B(t)} \frac{\partial f}{\partial w}(w(t))$.
   7. end
   8. Compute $\frac{1}{p_1(w(t))} \|p_1(w(t))\|_q, \ldots, \frac{1}{p_K(w(t))} \|p_K(w(t))\|_q$. (Using (14) and Prop. 4.5)
   9. Select layer to update: $i^* = \arg \max_{1 \leq i \leq K} \frac{1}{p_i(w(t))} \|p_i(w(t))\|_q$.
   10. Update $w(t+1)_{i^*} = w(t)_{i^*} - \epsilon \frac{1}{p_{i^*}(w(t))^2} \rho_q(g_{i^*}(t))$. (Using Prop. 4.5)
   11. for $i \in \{1, 2, \ldots, K\} \setminus \{i^*\}$ do
      12. Copy previous parameter: $w(t+1)_{i} = w(t)_{i}$.
   13. end
   14. end

To get some intuition for this convergence bound, note that the local derivative norm may be lower bounded as

$$\left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)} \geq \max_{1 \leq i \leq K} \frac{\partial f}{\partial w_i}(w(t)) \sum_{i=1}^{K} \frac{\|p_i(w(t))\|_q}{K \sum_{j=1}^{K} p_j(w(t))}.$$

Therefore, using a step-size $\epsilon = 1$, a consequence of the convergence bound is

$$\min_{1 \leq t \leq T} \frac{\sum_{i=1}^{K} \left\| \frac{\partial f}{\partial w_i}(w(t)) \right\|_q}{K \sum_{j=1}^{K} p_j(w(t))} \leq \delta$$

when $T \geq 2f(w(1))/\delta$. In this inequality, the term on the left-hand side is the magnitude of the gradient relevant to a fixed norm independent of the weights $w$, divided by a term that is an increasing function of the weight norms $\|w(t)\|$.

Remark 4.1 Note that in our analysis of DSGD for neural networks, it is important that the abstract theory is not constrained to update schemes based on inner-product norms. In our case, the family of norms on the parameter space $W$ is defined so that the corresponding duality structure $(\mathcal{P}, \langle \cdot \rangle)$ generates

...
updates that are confined to a single layer. This feature will not be present in the duality map for any inner product norm, since the duality map for an inner product norm is always linear. More explicitly, suppose that \( \ell_1 \) and \( \ell_2 \) are linear functionals and \( \rho \) is a duality map for an inner product norm. If \( \rho(\ell_1) \) has non-zero components in only the first layer, and \( \rho(\ell_2) \) only has non-zero components in the second layer, then, due to linearity, \( \rho(\ell_1 + \ell_2) = \rho(\ell_1) + \rho(\ell_2) \) has non-zero components in both layers.

Next, let us consider the setting of mini-batch duality structure stochastic gradient descent. This corresponds to executing the steps of Algorithm 4.1 in with “stochastic” mode, where instead of computing the full derivative at each iteration, approximate derivatives are calculated by averaging the gradient of our loss function over some number of randomly selected instances in our training set. Formally, this is expressed in Line 6 of Algorithm 4.1. We represent \( b \) randomly chosen instances as a random subset \( B(t) \subseteq \{1, \ldots, m\}^b \) and the gradient estimate \( g(t) \) is

\[
g(t) = \frac{1}{b} \sum_{j \in B(t)} \frac{\partial f_j}{\partial w}(w(t)).
\]

(24)

We first show that this gradient estimate has a uniformly bounded variance relative to the family of norms (16).

**Lemma 4.9** Let Assumptions 4.1 and 4.2 hold and let \( q \) be the constant chosen in Assumption 4.2. Let \( g(t) \) be as in (24) and define \( \delta(t) = \frac{\partial f}{\partial w}(w(t)) - g(t) \). Then the variance of \( g(t) \) is bounded as

\[
\mathbb{E} \left[ ||\delta(t)||^2_{w(t)} \middle| F(t - 1) \right] \leq \frac{1}{b} \times 32Kn_{\max}^{1+2/q}4^{-4/q}.
\]

(25)

**Remark 4.2** Note that the right-hand side of (25) is bounded independently of \( w(1), \ldots, w(t - 1) \). This is notable as such a guarantee cannot be made in standard (Euclidean) SGD, a fact we formally prove in Proposition A.3.

Now that we have established a bound on the variance of the gradient estimates \( g(t) \), we can move to the performance guarantee for stochastic gradient descent.

**Theorem 4.10** Let the function \( f \) be defined as in (12), let Assumptions 4.1 and 4.2 hold let \( q \) be the constant chosen in Assumption 4.2. Associate with \( W \) the family of norms (16) and duality structure (23). Set \( \sigma^2 = \frac{32}{b}Kn_{\max}^{1+2/q}4^{-4/q} \). Consider running Algorithm 3.1 in stochastic mode, with a batch size \( b \) and step-size \( \epsilon = \frac{1}{4} \frac{\gamma - \sigma^2}{\gamma + \sigma^2} \). Then for any \( \gamma > \sigma^2 \) if \( \tau \), is the stopping time (5) it holds that

\[
\mathbb{E}[\tau] \leq \frac{16G\sigma^2}{(\gamma + \sigma^2)^2} + \frac{16(G + \sigma^2)}{\gamma + \sigma^2} + 16.
\]
Proof The reasoning follows the proof of Theorem 4.8: Assumption 3.2 was established in Lemma 4.7, and Assumption 3.3 follows from Lemma 4.9, and hence the result follows from Corollary 3.6 using $L = 1, c = 0, \text{ and } f^* = 0$.

Note that our result requires that $\gamma$ be at least $\sigma^2$. This is in contrast to the deterministic case (Theorem 4.8) which does not restrict $\gamma$. An interesting avenue of future work would be to see whether this bound can be improved.

5 Numerical Experiment

The previous section established convergence guarantees for DSGD, in both batch (Theorem 4.8) and minibatch (Theorem 4.10) settings. In this section we investigate the practical efficiency of DSGD with numerical experiments on several machine learning benchmark problems. These benchmarks included the MNIST [31], Fashion-MNIST [52], SVHN [41], and CIFAR-10 [28] image classification tasks. In our experiments, the networks all had one hidden layer ($K = 2$). The hidden layer had $n_1 = 300$ units, and the output layer had $n_2 = 10$ units (one for each class). For the MNIST and Fashion-MNIST datasets, the input size was $n_0 = 784$ and, for the SVHN and CIFAR-10 datasets the input size is $n_0 = 3072$. The nonlinearity used in all the experiments was the logistic function $\sigma(x) = 1/(1 + e^{-x})$. For all datasets, the objective function is defined as in Equation (12). The number of training instances was $m = 60,000$ for MNIST and Fashion-MNIST, $m = 50,000$ for CIFAR-10, and $m = 73,257$ in the SVHN experiment. In all cases, a training pair $(y_n, t_n)$ consists of an image and a 10 dimensional indicator vector representing the label for the image.

The details of the DSGD procedure are shown in Algorithm 4.1. Note that the algorithm calculates different matrix norms and duality maps depending on the choice of $q$. For instance, when $q = 2$, computing the polynomials $p_1$ involves computing the spectral norm of the weight-matrix $w_2$, while computing the norms of $g_1$ and $g_2$ uses the norm dual to the spectral norm, as defined in the second case of Equation (17).

For experiments where DSGD is used in batch mode, the theoretically specified step-size $\epsilon = 1$ was used. In all other cases, the choice of step-size was determined experimentally using a validation set (details of the validation procedure, as well as weight initialization, are deferred to an appendix.) In the batch experiments, the algorithm ran for 20,000 weight updates. In the stochastic algorithms, each mini-batch had 128 training examples, and training ran for 500 epochs.

5.1 Batch DSGD using theoretically specified step-sizes

We performed several experiments involving DSGD in batch mode using the theoretically prescribed step-size $\epsilon = 1$ from Theorem 4.8 in order to understand the practicality of the algorithm. This was achieved by comparing the performance of DSGD with two other layer-wise training algorithms termed
Fig. 2 A comparison of batch DSGD with layer-wise algorithms. For each dataset and choice of $q \in \{1, 2, \infty\}$ we plot the training error for of DSGD as well as the best layer-wise algorithm among RANDOM and SEQUENTIAL. Best viewed in color.

RANDOM and SEQUENTIAL. In the RANDOM algorithm, the layer to update is chosen uniformly at random at each iteration. In the SEQUENTIAL algorithm, the layer to update alternates deterministically at each iteration. For both RANDOM and SEQUENTIAL, the step-sizes are chosen based on performance on a validation set. For each of the three algorithms (DSGD, RANDOM, and SEQUENTIAL), we repeated optimization using three different underlying norms $q = 1, 2, \text{ or } \infty$. Some of the results are shown in Figure 2 which indicates the trajectory of the training error over the course of optimization. Note that although DSGD does not have the best performance when measured in terms of final training error, it does carry the benefit of having theoretically justified step-sizes, while the other layer-wise algorithms use step-sizes defined through heuristics. An additional plot featuring the trajectory of testing accuracy for these experiments may be found in the appendix (Figure 6).

As the DSGD algorithm selects the layer to update at runtime, based on the trajectory of weights, it may be of interest to consider how these updates are distributed. This information is presented in Figure 3 for the MNIST and CIFAR-10 datasets. Interestingly, when using the norm $\| \cdot \|_1$, all updates occur in the second layer. For the norm $\| \cdot \|_2$, the rates of updates in each layer remained relatively constant throughout optimization. For $\| \cdot \|_{\infty}$, there was a greater range in the rate of updates in each layer as training progressed.

Let us remark on the runtime performance of DSGD compared with the other layer-wise algorithms. Compared to standard DSGD has the additional step of
computing the duality map and norms of the gradients, and the norm of the weights. However, for the batch algorithms the time per epoch is dominated by forward and backward passes over the network. The other layer-wise algorithms that were compared against also compute duality maps, but not norms of the weights. Due to this, epochs of DSGD are only about 2% - 3% slower than their random and sequential counterparts. Data sets and code generated during the current study are available from the author on reasonable request.

5.2 Practical variants of DSGD

In this section we compared a variant of DSGD with SGD. The variant of DSGD that we consider is termed DSGD ALL. In this algorithm, the step-sizes are computed as in Line 10 of Algorithm 4.1, but the update is performed in both layers, instead of only one as is done in DSGD. This is to enable a more accurate comparison with algorithms that update both layers. The variants of SGD we considered were standard SGD using Euclidean updates (SGD_STANDARD), and SGD using updates corresponding to the $\| \cdot \|_1$, $\| \cdot \|_2$, and $\| \cdot \|_\infty$ norms. For all the algorithms, the step-size was determined using performance on a validation
Fig. 4 A comparison of dsgd with gradient descent and variants of gradient descent using several different norms. Each figure plots the value of the testing accuracy for the dataset. Best viewed in color.

set, following the protocol set forth in the Appendix. The trajectories of testing accuracy for the algorithms is shown in Figure 4. We observe that for all the datasets, the variant of dsgd_all using the norm $\| \cdot \|_2$ performs the best among the dsgd algorithms. However, we also observed that sgd_standard outperformed dsgd. Corresponding plots for the training error may be found in Figure 5 in the appendix.

In terms of performance, dsgd requires more work at each update due to the requirement of computing the matrix norms. In the minibatch scenario, a higher percentage of time is spent on these calculations compared to the batch scenario, where the time-per-epoch was dominated by forward and backward passes over the entire dataset. Because of this, the dsgd algorithm corresponding to $\| \cdot \|_2$ is the slowest among the algorithms, taking about 4 times longer than standard sgd. For the dsgd variants using $\| \cdot \|_1$ or $\| \cdot \|_\infty$, calculations of the relevant matrix norms and duality maps can be done very efficiently, and hence these algorithms operate essentially at the same speed as standard sgd. This motivates future work into efficient variations of dsgd, perhaps using approximate and/or delayed duality map and norm computations.

6 Discussion

This work was motivated by the fact that gradient smoothness assumptions used in certain optimization analyses may be too strict to be applicable in problems involving neural networks. To address this, we sought an algorithm
for training neural networks that is both practical and admits a non-asymptotic convergence analysis. Our starting point was the observation that the empirical error function for a multilayer network has a Layer-wise gradient smoothness property. We showed how a greedy algorithm that updates one layer at a time can be explained with a geometric interpretation involving a family of norms. That is, the steps of the algorithm (choosing one layer at a time in a greedy fashion) flow naturally from the gradient descent procedure, by using a certain family of norms (a geometric construct.) Different variants of the algorithm can be generated by varying the underlying norm on the state-space, and the choice of norm can have a significant impact on the practical efficiency.

Our abstract algorithmic framework can in some cases provide non-asymptotic performance guarantees while making less restrictive assumptions compared to vanilla gradient decent. In particular, the analysis does not assume that the objective function has a Lipschitz gradient in the usual Euclidean sense. The class of functions that the method applies to includes neural networks with arbitrarily many layers, subject to some mild conditions on the data set (the components of the input and output data should be bounded) and the activation function (boundedness of the derivatives of the activation function.)

Although it was expected that the method would yield step sizes that were too conservative to be competitive with standard gradient descent, this turned out not to be the case. This may be due to that that DSGD integrates more problem structure into the algorithm compared to standard gradient descent. Various problem data was used to construct the family of norms, such as the hierarchical structure of the network, bounds on various derivatives, and bounds on the input.

Acknowledgments

This material is based upon work supported by the U.S. Department of Energy, Office of Science, under contract number DE-0012704.

References

1. Ralph Abraham, Jerrold E Marsden, and Tudor Ratiu. Manifolds, tensor analysis, and applications, volume 75. Springer Science & Business Media, 2012.
2. P-A Absil, Robert Mahony, and Rodolphe Sepulchre. Optimization algorithms on matrix manifolds. Princeton University Press, 2009.
3. Zeyuan Allen-Zhu and Elad Hazan. Variance reduction for faster non-convex optimization. In Proceedings of the 33rd International Conference on Machine Learning, pages 699–707, 2016.
4. Shun-Ichi Amari. Natural gradient works efficiently in learning. Neural computation, 10(2):251–276, 1998.
5. Peter L Bartlett, Dylan J Foster, and Matus J Telgarsky. Spectrally-normalized margin bounds for neural networks. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 6240–6249. 2017.

6. Heinz H. Bauschke, Jérôme Bolte, and Marc Teboulle. A descent lemma beyond lipschitz gradient continuity: First-order methods revisited and applications. *Mathematics of Operations Research*, 42(2):330–348, 2017.

7. Heinz H. Bauschke, Jérôme Bolte, Jiawei Chen, Marc Teboulle, and Xianfu Wang. On linear convergence of non-euclidean gradient methods without strong convexity and lipschitz gradient continuity. *Journal of Optimization Theory and Applications*, 182(3):1068–1087, April 2019. doi: 10.1007/s10957-019-01516-9. URL: https://doi.org/10.1007/s10957-019-01516-9.

8. E. G. Birgin, J. L. Gardenghi, J. M. Martínez, S. A. Santos, and Ph. L. Toint. Worst-case evaluation complexity for unconstrained nonlinear optimization using high-order regularized models. *Mathematical Programming*, 163(1):359–368, May 2017. ISSN 1436-4646.

9. Jérôme Bolte, Shoham Sabach, Marc Teboulle, and Yakov Vaisbourd. First order methods beyond convexity and lipschitz gradient continuity with applications to quadratic inverse problems. *SIAM Journal on Optimization*, 28(3):2131–2151, 2018.

10. N. Boumal, P.-A. Absil, and C. Cartis. Global rates of convergence for nonconvex optimization on manifolds. *IMA Journal of Numerical Analysis*, To appear, 2018.

11. Coralia Cartis, Nicholas IM Gould, and Philippe L Toint. Adaptive cubic regularisation methods for unconstrained optimization. part i: motivation, convergence and numerical results. *Mathematical Programming*, 127(2):245–295, 2011.

12. Charles Chidume. *Geometric properties of Banach spaces and nonlinear iterations*, volume 1965. Springer, 2009.

13. Frank E Curtis, Daniel P Robinson, and Mohammadreza Samadi. A trust region algorithm with a worst-case iteration complexity of $o(\epsilon^{-3/2})$ for nonconvex optimization. *Mathematical Programming*, 162(1-2):1–32, 2017.

14. W. C. Davidon. Variable metric method for minimization. *AEC Research and Development Report ANL-5990 (Rev. TID-4500, 14th Ed.)*, 11 1959. doi: 10.2172/422000.

15. William C Davidon. Variable metric method for minimization. *SIAM Journal on Optimization*, 1(1):1–17, 1991.

16. Damek Davis, Dmitriy Drusvyatskiy, and Kellie J MacPhee. Stochastic model-based minimization under high-order growth. *arXiv preprint arXiv:1807.00255*, 2018.

17. K. Deimling. *Nonlinear functional analysis*. Springer-Verlag, 1985.
18. John Duchi, Elad Hazan, and Yoram Singer. Adaptive subgradient methods for online learning and stochastic optimization. *Journal of Machine Learning Research*, 12(Jul):2121–2159, 2011.

19. Clement Farabet, Camille Couprie, Laurent Najman, and Yann LeCun. Learning hierarchical features for scene labeling. *IEEE transactions on pattern analysis and machine intelligence*, 35(8):1915–1929, 2013.

20. Benjamin Fehrman, Benjamin Gess, and Arnulf Jentzen. Convergence rates for the stochastic gradient descent method for non-convex objective functions. *Journal of Machine Learning Research*, 21(136):1–48, 2020. URL http://jmlr.org/papers/v21/19-636.html.

21. Saeed Ghadimi and Guanghui Lan. Stochastic first- and zeroth-order methods for nonconvex stochastic programming. *SIAM Journal on Optimization*, 23(4):2341–2368, 2013.

22. G. E. Hinton and R. R. Salakhutdinov. Reducing the dimensionality of data with neural networks. *Science*, 313(5786):504–507, 2006. ISSN 0036-8075.

23. Roger A. Horn and Charles R. Johnson, editors. *Matrix Analysis*. Cambridge University Press, New York, NY, USA, 1986.

24. Ruinan Jin, Yu Xing, and Xingkang He. On the convergence of mSGD and adagrad for stochastic optimization. In *International Conference on Learning Representations*, 2022. URL https://openreview.net/forum?id=g5tANwND04i.

25. Rie Johnson and Tong Zhang. Accelerating stochastic gradient descent using predictive variance reduction. In *Advances in Neural Information Processing Systems* 26, pages 315–323, 2013.

26. Ali Kavis, Kfir Yehuda Levy, and Volkan Cevher. High probability bounds for a class of nonconvex algorithms with adagrad stepsize. In *International Conference on Learning Representations*, 2022. URL https://openreview.net/forum?id=dSw0QtRMJKO.

27. Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *Proceedings of the 3rd International Conference on Learning Representations (ICLR)*, 2014.

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

29. Alex Krizhevsky, Ilya Sutskever, and Geoff Hinton. Imagenet classification with deep convolutional neural networks. In *Advances in Neural Information Processing Systems* 25, pages 1106–1114, 2012.

30. Takio Kurita. Iterative weighted least squares algorithms for neural networks classifiers. In Shuji Doshiba, Koichi Furukawa, Klaus P. Jantke, and Toyaki Nishida, editors, *Algorithmic Learning Theory: Third Workshop, ALT ’92 Tokyo, Japan, October 20–22, 1992 Proceedings*, pages 75–86, Berlin, Heidelberg, 1993. Springer Berlin Heidelberg.

31. Yann LeCun. The mnist database of handwritten digits. http://yann.lecun.com/exdb/mnist/, 1998.

32. Honglak Lee, Roger Grosse, Rajesh Ranganath, and Andrew Y Ng. Convolutional deep belief networks for scalable unsupervised learning of hierarchical representations. In *Proceedings of the 26th annual international conference*
33. Xiaoyu Li and Francesco Orabona. On the convergence of stochastic gradient descent with adaptive stepsizes. *arXiv preprint arXiv:1805.08114*, 2018.

34. Xiangru Lian, Ce Zhang, Huan Zhang, Cho-Jui Hsieh, Wei Zhang, and Ji Liu. Can decentralized algorithms outperform centralized algorithms? a case study for decentralized parallel stochastic gradient descent. In *Advances in Neural Information Processing Systems 30*, pages 5330–5340. 2017.

35. Tengyuan Liang, Tomaso Poggio, Alexander Rakhlin, and James Stokes. Fisher-rao metric, geometry, and complexity of neural networks. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 888–896, 2019.

36. E.H. Lieb, Keith Ball, and E.A. Carlen. Sharp uniform convexity and smoothness inequalities for trace norms. *Inventiones mathematicae*, 115(3):463–482, 1994.

37. H. Lu, R. Freund, and Y. Nesterov. Relatively smooth convex optimization by first-order methods, and applications. *SIAM Journal on Optimization*, 28(1):333–354, 2018.

38. Vien V. Mai and Mikael Johansson. Stability and convergence of stochastic gradient clipping: Beyond lipschitz continuity and smoothness. In Marina Meila and Tong Zhang, editors, *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pages 7325–7335. PMLR, 18–24 Jul 2021. URL https://proceedings.mlr.press/v139/mai21a.html.

39. Eric Moulines and Francis R. Bach. Non-asymptotic analysis of stochastic approximation algorithms for machine learning. In J. Shawe-Taylor, R. S. Zemel, P. L. Bartlett, F. Pereira, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems 24*, pages 451–459. Curran Associates, Inc., 2011.

40. Yurii Nesterov. *Introductory lectures on convex optimization: A basic course*, volume 87. Springer Science & Business Media, 2013.

41. Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bissacco, Bo Wu, and Andrew Y Ng. Reading digits in natural images with unsupervised feature learning. In *NIPS Workshop on Deep Learning and Unsupervised Feature Learning*, 2011.

42. Behnam Neyshabur, Ryota Tomioka, and Nathan Srebro. Norm-based capacity control in neural networks. In Peter Grünwald, Elad Hazan, and Satyen Kale, editors, *Proceedings of The 28th Conference on Learning Theory*, volume 40 of *Proceedings of Machine Learning Research*, pages 1376–1401, Paris, France, 03–06 Jul 2015. PMLR.

43. Lam et. al Nguyen. Sgd and hogwild: Convergence without the bounded gradients assumption. In *ICML*, 2018.

44. Yann Ollivier. Riemannian metrics for neural networks i: feedforward networks. *Information and Inference: A Journal of the IMA*, 4(2):108, 2015.
45. S. Reddi, A. Hefny, S. Sra, B. Poczos, and A. Smola. Stochastic variance reduction for nonconvex optimization. In *International conference on machine learning*, 2016.

46. Ruslan Salakhutdinov and Geoffrey E. Hinton. Learning a nonlinear embedding by preserving class neighbourhood structure. In *International Conference on Artificial Intelligence and Statistics*, pages 412–419, 2007.

47. Tom Schaul, Sixin Zhang, and Yann LeCun. No more pesky learning rates. In *Proceedings of the 30th International Conference on International Conference on Machine Learning - Volume 28*, pages III–343–III–351, 2013.

48. Nitish Srivastava and Ruslan Salakhutdinov. Multimodal learning with deep boltzmann machines. *The Journal of Machine Learning Research*, 15(1):2949–2980, 2014.

49. T. Tieleman and G. Hinton. Lecture 6.5—RmsProp: Divide the gradient by a running average of its recent magnitude. COURSERA: Neural Networks for Machine Learning, 2012.

50. Rachel Ward, Xiaoxia Wu, and Leon Bottou. AdaGrad stepsizes: Sharp convergence over nonconvex landscapes. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 6677–6686, Long Beach, California, USA, 09–15 Jun 2019. PMLR.

51. D. Williams. *Probability with Martingales*. Cambridge University Press, 1991.

52. Han Xiao, Kashif Rasul, and Roland Vollgraf. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms, 2017.

53. Hongyi Zhang, Sashank J. Reddi, and Suvrit Sra. Riemannian svrg: Fast stochastic optimization on riemannian manifolds. In Advances in Neural Information Processing Systems 29, pages 4592–4600, 2016.

54. Jingzhao Zhang, Tianxing He, Suvrit Sra, and Ali Jadbabaie. Why gradient clipping accelerates training: A theoretical justification for adaptivity. In *International Conference on Learning Representations*, 2020.

55. Siqi Zhang and Niao He. On the convergence rate of stochastic mirror descent for nonsmooth nonconvex optimization. *arXiv preprint arXiv:1806.04781*, 2018.
Appendix

Further experimental details

For algorithms other than batch DSGD, we withheld 1/6 of the training data as validation data for tuning step-sizes. We ran gradient descent on the remaining 5/6 of the dataset, for each choice of \( \epsilon \in \{0.001, 0.01, 0.1, 1, 10\} \), and evaluated the validation error after optimization. The step-size that gave the smallest validation error was used for the full experiments. In all cases, network weights were initially uniformly distributed in the interval \([-1, 1]\).

![Fig. 5](image_url) A comparison of DSGD with gradient descent (GD) and variants of GD using several different norms. The plots show the training error for the dataset. Best viewed in color.

![Fig. 6](image_url) A comparison of batch DSGD with layer-wise algorithms. For each dataset and choice of \( q \in \{1, 2, \infty\} \) we plot the testing accuracy of DSGD as well as the best layer-wise algorithm among random and sequential. Best viewed in color.
Proofs of main results

A.1 Proof of Lemma 3.4

Let \( w = (w_1, w_2, w_3, w_4) \) denote a particular choice of parameters. The chain-rule gives

\[
\frac{\partial^2 f}{\partial w_1 \partial w_3} (w) = 2g(w; 1) \frac{\partial^2 y}{\partial w_1 \partial w_3} (w; 1) + 2 \frac{\partial y}{\partial w_3} (w; 1) \frac{\partial y}{\partial w_1} (w; 1).
\]

The derivatives of \( y \) appearing in this equation are as follows:

\[
\begin{align*}
\frac{\partial y}{\partial w_1} (w; 1) &= \sigma'(w_3\sigma(w_1) + w_4\sigma(w_2))\sigma(w_1), \\
\frac{\partial^2 y}{\partial w_1 \partial w_3} (w; 1) &= \sigma'(w_3\sigma(w_1) + w_4\sigma(w_2))w_3\sigma'(w_1), \\
\frac{\partial^2 y}{\partial w_1 \partial w_3} (w; 1) &= \sigma''(w_3\sigma(w_1) + w_4\sigma(w_2))\sigma(w_1)w_3\sigma'(w_1) + \sigma'(w_3\sigma(w_1) + w_4\sigma(w_2))\sigma'(w_1).
\end{align*}
\]

Let \( z \) be any non-positive number, and define the curve \( w : [0, \infty) \to \mathbb{R} \) as

\[ w(\epsilon) = \left( 1, 1, \epsilon, \frac{1}{\sigma(1)}(z - \epsilon \sigma(1)) \right). \]

Then

\[
\frac{\partial^2 f}{\partial w_1 \partial w_3} (w(\epsilon)) = \left( 2\sigma(z)\sigma''(z)\sigma'(1) + 2\sigma'(z)\sigma(1)\sigma'(1) \right)\epsilon + \sigma'(z)\sigma'(1).
\]

Note that since \( z \) is non-positive, we guarantee \( \sigma''(z) \geq 0 \), and therefore the coefficient of \( \epsilon \) in this equation is positive. We conclude that \( \lim_{\epsilon \to \infty} \frac{\partial^2 f}{\partial w_1 \partial w_3} (w(\epsilon)) = +\infty. \]

A.2 Proof of Lemma 3.4

Set \( \ell_1 = \ell + \delta \) and \( \ell_2 = -\ell \). Plugging these values into (87) of Lemma A.4 yields

\[
||\delta||^2 \geq ||\ell + \delta||^2 - 2\ell \cdot \rho(\ell + \delta) + c||\ell||^2
\]

(27)

Apply (87) again, this time with \( \ell_1 = \ell \) and \( \ell_2 = \delta \), obtaining

\[
||\ell + \delta||^2 \geq ||\ell||^2 + 2\delta \cdot \rho(\ell) + c||\delta||^2
\]

(28)

Combining (27) and (28), then,

\[
||\delta||^2 \geq \left(||\ell||^2 + 2\delta \cdot \rho(\ell) + c||\delta||^2\right) - 2\ell \cdot \rho(\ell + \delta) + c||\ell||^2
\]

\[
= (1 + c)||\ell||^2 + 2\delta \cdot \rho(\ell) + c||\delta||^2 - 2\ell \cdot \rho(\ell + \delta)
\]

Rearranging terms and dividing both sides of the equation by two,

\[
\frac{\ell \rho(\ell + \delta)}{2} \geq \left( \frac{1 + c}{2} \right) ||\ell||^2 + \delta \cdot \rho(\ell) - \left( \frac{1 - c}{2} \right) ||\delta||^2
\]

Taking expectations, we obtain (8a).

Next, applying (77) with \( x = 2\ell \) and \( y = 2\delta \) yields

\[
||\ell + \delta||^2 \leq 2 \left(||\ell||^2 + ||\delta||^2\right) - c||\ell - \delta||^2
\]

(29)
Setting $\ell_1 = \ell$ and $\ell_2 = -\delta$ in (87), we get
\[
||\ell - \delta||^2 \geq ||\ell||^2 - \delta \cdot \rho(\ell) + c||\delta||^2
\] (30)

Combining (29) and (30),
\[
||\ell + \delta||^2 \leq 2 (||\ell||^2 + ||\delta||^2) - c \left( (||\ell||^2 + \delta \cdot \rho(\ell)) - c||\delta||^2 \right)
\] (31)

Taking expectations gives (8b).

A.3 Proof of Theorem 3.5

By Assumption 3.2 we know that
\[
f(w(t + 1)) \leq f(w(t)) - \epsilon \frac{\partial f}{\partial w}(w(t)) \cdot \rho_w(t) (g(t)) + c^2 L^2 ||g(t)||^2_{w(t)}.
\]

Using the definition of $\delta(t)$ given in Assumption 3.3 this is equivalent to
\[
f(w(t + 1)) \leq f(w(t)) - \epsilon \frac{\partial f}{\partial w}(w(t)) \cdot \rho_w(t) \left( \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right) + c^2 L^2 \left( \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right) \left\| \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right\|_{w(t)}^2.
\] (32)

Summing (32) over $t = 1, 2, \ldots, N$ yields
\[
f(w(N + 1)) \leq f(w(1)) - \epsilon \sum_{t=1}^{N} \frac{\partial f}{\partial w}(w(t)) \cdot \rho_w(t) \left( \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right) + c^2 L^2 \sum_{t=1}^{N} \left\| \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right\|_{w(t)}^2.
\] (33)

Rearranging terms, and noting that $f(w(N + 1)) \geq f^*$,
\[
\epsilon \sum_{t=1}^{N} \frac{\partial f}{\partial w}(w(t)) \cdot \rho_w(t) \left( \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right) \leq G + c^2 L^2 \sum_{t=1}^{N} \left\| \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right\|_{w(t)}^2.
\] (34)

According to Equation (8a), for all $t$ it holds that
\[
E \left[ \left\| \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right\|_{w(t)}^2 | F(t - 1) \right] \geq \left( \frac{1 + \epsilon}{2} \right) \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 - \left( \frac{1 - \epsilon}{2} \right) \sigma^2,
\] (35)

while Equation (8b) implies
\[
E \left[ \left\| \frac{\partial f}{\partial w}(w(t)) + \delta(t) \right\|_{w(t)}^2 | F(t - 1) \right] \leq (2 - \epsilon) \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 + (2 - \epsilon^2) \sigma^2.
\] (36)

For $n \geq 1$ we define the stopping time $\tau \wedge n$ to be the minimum of $\tau$ and the constant value $n$. Applying Proposition A.3, inequality (35), and using the law of total expectation, it holds that for any $n$,
\[
E \left[ \sum_{t=1}^{\tau \wedge n} \left( \frac{1 + \epsilon}{2} \right) \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 - \left( \frac{1 - \epsilon}{2} \right) \sigma^2 \right] \geq E \sum_{t=1}^{\tau \wedge n} \left( \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 - \left( \frac{1 - \epsilon}{2} \right) \sigma^2 \right).
\] (37)
Applying Proposition A.5 a second time, in this case to inequality (36), we see that

\[
E \left[ \sum_{t=1}^{\tau_n} \left\| \frac{\partial f}{\partial w}(w(t)) + \epsilon(t) \right\|_{w(t)}^2 \right] \leq E \left[ \sum_{t=1}^{\tau_n} \left( (2 - c) \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 + (2 - c^2) \sigma^2 \right) \right].
\]  

(38)

Combining (34) with (37) and (38) and rearranging terms,

\[
\epsilon \left( \frac{1 + c}{2} - \frac{L}{2} \epsilon(2 - c) \right) E \left[ \sum_{t=1}^{\tau_n} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 \right] \leq G + \epsilon \left( \frac{L}{2} \epsilon(2 - c^2) + \frac{1 - c}{2} \right) \sigma^2 E[\tau \wedge n].
\]  

(39)

Next, note that

\[
\sum_{t=1}^{\tau_n} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 \geq \sum_{t=1}^{\tau_n-1} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 \geq \gamma(n - 1).
\]  

(40)

Combining (39) with (40) yields

\[
\epsilon \left( \frac{1 + c}{2} - \frac{L}{2} \epsilon(2 - c) \right) \gamma E[\tau \wedge n] - 1 \leq G + \epsilon \left( \frac{L}{2} \epsilon(2 - c^2) + \frac{1 - c}{2} \right) \sigma^2 E[\tau \wedge n].
\]

By (9), this can be rearranged into

\[
E[\tau \wedge n] \leq \frac{2G + \epsilon(1 + c - Le(2 - c)) \gamma}{\epsilon(1 + c - Le(2 - c)) \gamma - \epsilon(Le(2 - c^2) + 1 - c) \sigma^2}.
\]

Since the right-hand side of this equation is independent of \(n\), the claimed inequality follows by the monotone convergence theorem. \(\Box\)

### A.4 Proof of Corollary 3.6

We first consider case 2 of the corollary. Using the given value of \(\epsilon\) in conjunction with (10),

\[
E[\tau] \leq \frac{2G + (1 + c - Le(2 - c)) \gamma}{\epsilon(1 + c - Le(2 - c)) \gamma - \epsilon(Le(2 - c^2) + 1 - c) \sigma^2}.
\]  

(41)

Note that \(1 + c - Le(2 - c) \leq 1 + c \leq 2\). Therefore

\[
(8LG + 4L\gamma(1 + c - Le(2 - c)))((2 - c)\gamma + (2 - c^2)\sigma^2) \leq 8LG(2 - c^2)\sigma^2 + 8LG(2 - c)\gamma + 8L\gamma(2 - c)\gamma + 8L\gamma(2 - c^2)\sigma^2 = 8LG(2 - c^2)\sigma^2 + 8LG(2 - c)(G + \sigma^2)\gamma + 8LG(2 - c)\gamma^2 \leq 8LG(2 - c^2)\sigma^2 + 8LG(2 - c)(G + \sigma^2)\gamma + 8LG(2 - c)\gamma^2.
\]  

(42)

Combining (41) with (42),

\[
E[\tau] \leq \frac{8LG(2 - c^2)\sigma^2}{((1 + c)\gamma + (1 - c)\sigma^2)^2} + \frac{8LG(2 - c)(G + \sigma^2)\gamma}{((1 + c)\gamma + (1 - c)\sigma^2)^2} + \frac{8LG(2 - c)\gamma^2}{((1 + c)\gamma + (1 - c)\sigma^2)^2}.
\]

Note that \(\gamma \leq (1 + c)\gamma + (1 - c)\sigma^2\) implies

\[
E[\tau] \leq \frac{8LG(2 - c^2)\sigma^2}{(1 + c)\gamma + (1 - c)\sigma^2} + \frac{8LG(2 - c)(G + \sigma^2)}{(1 + c)\gamma + (1 - c)\sigma^2} + 8LG(2 - c).
\]

The result for case 1 (standard sgd) follows by setting \(c = 1\) in the above equation. \(\Box\)
A.5 Proof of Corollary 3.7

For \( t \geq 0 \), set \( \eta(t) = \frac{\partial f}{\partial w}(w(t)) \). Then Assumption 3.2 implies

\[
 f(w(t + 1)) \leq f(w(t)) - \epsilon \frac{\partial f}{\partial w}(w(t)) \cdot \rho_w \left( \frac{\partial f}{\partial w}(w(t)) \right) + \epsilon^2 \frac{L}{2} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2.
\]

Invoking the duality map properties (44) and (46),

\[
 \leq f(w(t)) - \epsilon \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 + \frac{L}{2} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2
 = f(w(t)) + \epsilon \left( \frac{L}{2} \epsilon - 1 \right) \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2.
\]

From the last inequality it is clear that the function decreases at iteration \( t \) unless \( \frac{\partial f}{\partial w}(w(t)) = 0 \). Summing our inequality over \( t = 1, 2, \ldots, T \) yields

\[
 f(w(T)) \leq f(w(1)) + \epsilon \left( \frac{L}{2} T - 1 \right) \sum_{t=1}^{T} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2.
\]

(43)

Upon rearranging terms and using that \( f(w(T)) > f^* \), we find that

\[
 \sum_{t=1}^{T} \left\| \frac{\partial f}{\partial w}(w(t)) \right\|_{w(t)}^2 \leq \frac{2(f(1)) - f^*)}{\epsilon(2 - L\epsilon)}.
\]

(44)

Let \( w^* \) be an accumulation point of the algorithm; this is defined as a point such that for any \( \gamma > 0 \) the ball \( \{ w \in \mathbb{R}^n | \left\| w - w^* \right\| < \gamma \} \) is entered infinitely often by the sequence \( w(t) \) (any norm \( \| \cdot \| \) can be used to define the ball.) Then there is a subsequence of iterates \( w(m(1)), w(m(2)), \ldots \) with \( m(k) < m(k + 1) \) such that \( w(m(k)) \rightarrow w^* \). We know from (44) that \( \| \frac{\partial f}{\partial w}(w(m(k))) \|_{w(m(k))} \rightarrow 0 \), and the same must hold for any subsequence. Hence \( \| \frac{\partial f}{\partial w}(w(m(k))) \|_{w(m(k))} \rightarrow 0 \). As the map \( (w, \ell) \rightarrow \left\| \ell \right\|_w \) is continuous on \( \mathbb{R}^n \times L(\mathbb{R}^n, \mathbb{R}) \), (see for instance [17], Proposition 27.7) it must be that \( \| \frac{\partial f}{\partial w}(w^*) \|_{w^*} = 0 \) Since \( \| \cdot \|_{w^*} \) is a norm, then \( \frac{\partial f}{\partial w}(w^*) = 0 \).

□

A.6 Proof of Proposition 1.3

Let us first recall some notation for the composition of a bilinear map with a pair of linear maps: if \( B : U \times U \rightarrow V \) is a bilinear map then \( B(A_1 \circ A_2) \) is the bilinear map which sends \( (u_1, u_2) \) to \( B(A_1 u_1, A_2 u_2) \). In addition, if \( B : U \times U \rightarrow V \) is a bilinear map, then for any \( (u_1, u_2) \in U \times U \) the inequality \( \| B(u_1, u_2) \|_V \leq \| B \| \| u_1 \|_U \| u_2 \|_U \) holds. It follows that if \( A_1 : Z \rightarrow U \) and \( A_2 : Z \rightarrow U \) are any linear maps, then

\[
\| B(A_1 \circ A_2) \| \leq \| B \| \| A_1 \|_A \| A_2 \|_A.
\]

(45)

To prove the proposition, it suffices to consider the case of a single input/output pair \((x, z) \in \mathbb{R}^m \times \mathbb{R}^n \). In this case, we can express the function \( f \) as

\[
 f(w) = J(y^K(x, w))
\]

(46)

where \( J(y) = \| y - z \|_2^2 \) is the squared distance of a state \( y \) to the target \( z \) and \( y^K(x, w) \) is the output of a \( K \)-layer neural network with input \( x \). The output \( y^K \) is defined recursively as

\[
y^i(x, w) = \begin{cases} 
 h(y^{i-1}(x, w_{i-1}), w_i) & \text{if } 2 \leq i \leq K, \\
 h(x, w_1) & \text{if } i = 1,
\end{cases}
\]

(47)
where the function \( h(y, w) \) represents the computation performed by a single layer in the network:

\[
h_k(y, w) = \sigma \left( \sum_{j=1}^{n} w_{kj} y_j \right), \quad k = 1, 2, \ldots, n. \tag{48}\]

Taking the second derivative of \( (48) \) with respect to the input parameter, we have, for any

\[
\frac{\partial^2 f}{\partial w_i^2}(w) = \frac{\partial^2 f}{\partial x^2}(y^K(x, w)) \left( \frac{\partial y^K}{\partial w_i}(x, w) \right)^2 + \frac{\partial^2 J}{\partial y}(y^K(x, w)) \frac{\partial^2 y^K}{\partial w_i^2}(x, w). \tag{49}\]

To find bounds on these terms we will use the following identity: for \( 0 \leq k \leq i \),

\[
y^i(x, w_{1:k}) = y^{i-k}(y^k(x, w_{1:k}), w_{k+1:i}) \tag{50}\]

with the convention that \( y^0(x) = x \). Differentiating Equation \( (50) \), with respect to \( w_i \) for \( 1 \leq i \leq K \) gives

\[
\frac{\partial y^i}{\partial w_i}(x, w_{1:K}) = \frac{\partial y^{i-1}}{\partial x}(y^i(x, w_{1:i}), w_{i+1:K}) \frac{\partial h}{\partial w}(y^{i-1}(x, w_{1:i-1}), w_i) \tag{51}\]

and differentiating a second time yields

\[
\frac{\partial^2 y^i}{\partial w_i^2}(x, w_{1:K}) = \frac{\partial^2 y^{i-1}}{\partial x^2}(y^i(x, w_{1:i}), w_{i+1:K}) \left( \frac{\partial h}{\partial w}(y^{i-1}(x, w_{1:i-1}), w_i) \right)^2 + \frac{\partial^2 h}{\partial y}(y^{i-1}(x, w_{1:i-1}), w_i) \frac{\partial^2 y^{i-1}}{\partial x^2}(y^i(x, w_{1:i}), w_{i+1:K}). \tag{52}\]

Next, we consider the terms \( \frac{\partial y^n}{\partial x} \) and \( \frac{\partial^2 y^n}{\partial x^2} \) appearing in the two preceding equations \( \eqref{51} \) and \( \eqref{52} \). By differentiating equation \( (47) \) with respect to the input parameter, we have, for any input \( u \) and parameters \( a_1, a_2, \ldots, a_n \),

\[
\frac{\partial y^n}{\partial x}(u, a_1:n) = \frac{\partial h}{\partial y}(y^{n-1}(u, a_1:n-1), a_n) \frac{\partial y^{n-1}}{\partial x}(u, a_1:n-1), \tag{53}\]

and upon differentiating a second time,

\[
\frac{\partial^2 y^n}{\partial x^2}(u, a_1:n) = \frac{\partial^2 h}{\partial y^2}(y^{n-1}(u, a_1:n), a_n) \left( \frac{\partial y^{n-1}}{\partial x}(u, a_1:n-1) \right)^2 + \frac{\partial^2 h}{\partial y}(y^{n-1}(u, a_1:n-1), a_n) \frac{\partial^2 y^{n-1}}{\partial x^2}(u, a_1:n-1). \tag{54}\]

We will use some bounds on \( h \) in terms of the norm \( \| \cdot \|_q \). It follows from Lemma \( \ref{56} \) that the following bounds hold for any \( 1 \leq q \leq \infty \):

\[
\left\| \frac{\partial h}{\partial y}(y, w) \right\|_q \leq \|\sigma\|_\infty \|w\|_q, \quad \left\| \frac{\partial h}{\partial w}(y, w) \right\|_q \leq \|\sigma\|_\infty \|y\|_q. \tag{55}\]

\[
\left\| \frac{\partial^2 h}{\partial y^2}(y, w) \right\|_q \leq \|\sigma\|_\infty \|w\|_q^2, \quad \left\| \frac{\partial^2 h}{\partial w^2}(y, w) \right\|_q \leq \|\sigma\|_\infty \|y\|_q^2. \tag{56}\]

Combining \( \eqref{53} \) with \( \eqref{55} \) we obtain the following inequalities: For \( n > 1 \),

\[
\left\| \frac{\partial y^n}{\partial x}(u, a_1:n) \right\|_q \leq \left\| \sigma\|_\infty \|a_n\|_q \left\| \frac{\partial y^{n-1}}{\partial x}(u, a_1:n-1) \right\|_q \quad \text{if } n > 1, \]

\[
\left\| \frac{\partial y^n}{\partial x}(u, a_1:n) \right\|_q \leq \left\| \sigma\|_\infty \|a_1\|_q \left\| \frac{\partial y^{n-1}}{\partial x}(u, a_1:n-1) \right\|_q \quad \text{if } n = 1. \tag{56}\]
Combining the two cases in inequality (60), and using the definition of $r_n$ we find that, for $n \geq 1$,
\[
\left\| \frac{\partial^2 y^n}{\partial x^n} (u, a_{1:n}) \right\|_q \leq r_n (\|a_1\|_q, \ldots, \|a_n\|_q). \tag{57}
\]

Now we turn to the second derivative $\frac{\partial^2 u^n}{\partial x^n}$. Taking norms in Equation (54), and applying (59), (57), and (45), we obtain the following inequalities. If $n \geq 1$,
\[
\left\| \frac{\partial^2 y^n}{\partial x^2} (u, a_{1:n}) \right\|_q \leq \|\sigma''\|_\infty \|a_1\|_q^2 \|\sigma'\|^2 (n-1) \prod_{i=1}^{n-1} \|a_i\|_q + \|\sigma''\|_\infty \|a_n\|_q \left\| \frac{\partial^2 x^n}{\partial y^2} (u, a_{1:n-1}) \right\|_q
\]

While for $n = 1$,
\[
\left\| \frac{\partial^2 y^n}{\partial x^2} (u, a_{1:n}) \right\|_q \leq \|\sigma''\|_\infty \|a_1\|_q^2. \tag{58}
\]

Combining (51), (59), and (57),
\[
\left\| \frac{\partial y^K}{\partial x} (x, w_{1:K}) \right\|_q \leq \left\| \frac{\partial y^{K-1}}{\partial y} (y'(x, w_{1:K}), w_{1:K}) \right\|_q \|\sigma'\|_\infty \|y^{K-1}(x, w_{1:K})\|_q \leq r_{K-1} (\|w_{1:K}\|_q, \ldots, \|w_{1:K}\|_q) \|\sigma''\|_\infty c_q
\]

where the number $c_q$, defined in Table 2 is the $q$-norm of the vector $(1, 1, \ldots, 1) \in \mathbb{R}^n$.

Combining (52), (59), (57), and (58),
\[
\left\| \frac{\partial^2 y^K}{\partial x^2} (x, w_{1:K}) \right\|_q \leq \left\| \frac{\partial^2 y^{K-1}}{\partial x^2} (y'(x, w_{1:K}), w_{1:K}) \right\|_q \|\sigma'\|^2 c_q^2 + \left\| \frac{\partial y^{K-1}}{\partial x} (y'(x, w_{1:K}), w_{1:K}) \right\|_q \|\sigma''\|_\infty c_q^2 \leq r_{K-1} (\|w_{1:K}\|_q, \ldots, \|w_{1:K}\|_q) \|\sigma''\|_\infty c_q^2. \tag{60}
\]

Now we arrive at bounding the derivatives of the function $f$. As shown in Lemma A.7 in the appendix, the following inequalities hold:
\[
\sup_{w,x} \left\| \frac{\partial f}{\partial y} (y^K(x, w)) \right\|_q \leq d_{q,1}. \tag{61a}
\]
\[
\sup_{w,x} \left\| \frac{\partial^2 f}{\partial y^2} (y^K(x, w)) \right\|_q = d_{q,2}. \tag{61b}
\]
where $d_{q,1}$ and $d_{q,2}$ are as in Table 2. Combining (19), (59), (60), (61a) and (61b), it holds that for $i = 1, \ldots, K$,
\[
\left\| \frac{\partial^2 f}{\partial y_i^2} (x, w_{1:K}) \right\|_q \leq d_{q,2} \left\| \frac{\partial y^K}{\partial w_i} (x, w) \right\|_q + d_{q,1} \left\| \frac{\partial^2 y^K}{\partial x^2} (x, w) \right\|_q \leq d_{q,2} c_q^2 \|\sigma'\|^2 r_{K-1} (\|w_{1:K}\|_q, \ldots, \|w_{1:K}\|_q) + d_{q,1} c_q^2 \|\sigma''\|_\infty r_{K-1} (\|w_{1:K}\|_q, \ldots, \|w_{1:K}\|_q) = s_{K-1} (\|w_{1:K}\|_q, \ldots, \|w_{1:K}\|_q) < p_i (w)^2.
\]
\]
A.7 Proof of Proposition 4.4

Let for any \( w \in \mathbb{R}^n, \Delta \in \mathbb{R}^n \) and let \( \epsilon > 0 \). Applying the fundamental theorem of calculus, first on the function \( f \) and then on its derivative, we have

\[
\begin{align*}
f(w - \epsilon \Delta) &= f(w) - \epsilon \int_0^1 \frac{\partial f}{\partial w}(w - \lambda \epsilon \Delta) \cdot \Delta d\lambda \\
&= f(w) - \epsilon \int_0^1 \left[ \frac{\partial f}{\partial w}(w) \cdot \Delta + \epsilon \int_0^1 \frac{\partial^2 f}{\partial w^2}(w + \tau \epsilon \Delta) \cdot (\Delta, \Delta) d\tau \right] d\lambda \\
&= f(w) - \epsilon \frac{\partial f}{\partial w}(w) \cdot \Delta + \epsilon^2 \int_0^1 \int_0^1 \frac{\partial^2 f}{\partial w^2}(w + \tau \epsilon \Delta) \cdot (\Delta, \Delta) d\tau d\lambda.
\end{align*}
\]

Using our assumption on the second derivative,

\[
\begin{align*}
\leq f(w) - \epsilon \frac{\partial f}{\partial w}(w) \cdot \Delta + \epsilon^2 L^2 \|\Delta\|^2.
\end{align*}
\]

Letting \( \Delta = \rho(\frac{\partial f}{\partial w}(w)) \), and using the two defining equations of duality maps (4a and 4b), we see that

\[
\begin{align*}
\leq f(w) - \epsilon \frac{\partial f}{\partial w}(w) \cdot \Delta + \epsilon^2 L^2 \left\| \frac{\partial f}{\partial w}(w) \right\|^2.
\end{align*}
\]

Combining the terms yields the result. \( \square \)

A.8 Proof of Proposition 4.5

Let \( \ell \) be given and consider \( q = \infty \). For any matrix \( A \) with \( \|A\|_\infty = 1 \),

\[
\ell(A) = \sum_{i=1}^r \sum_{j=1}^c \ell_{i,j} A_{i,j} \leq \sum_{i=1}^r \max_{1 \leq j \leq c} |\ell_{i,j}| \tag{62}
\]

since each row sum \( \sum_{j=1}^c |A_{i,j}| \) is at most 1. Let \( m \) be the matrix defined in equation (20).

Clearly this matrix has maximum-absolute-row-sum 1. Furthermore,

\[
\ell(m) = \sum_{i=1}^r \max_{1 \leq j \leq c} |\ell_{i,j}|. \tag{63}
\]

Combining equation (63) with the inequality (62) confirms that the dual norm is \( \|\ell\|_\infty = \sum_{i=1}^r \max_{1 \leq k \leq c} |\ell_{i,k}| \).

For \( q = 2 \), that the duality between the spectral norm is the sum of singular values, or trace norm, is well-known, and can be proved for instance as in the proof of Theorem 7.4.24 of [23].

For the duality maps, let the matrix \( \rho_\infty(\ell) \) be defined as in (20). Then

\[
\|\rho_\infty(\ell)\|_\infty = \|\ell\|_\infty \|m\|_\infty = \|\ell\|_\infty
\]

and \( \ell \cdot \rho_\infty(\ell) = \|\ell\|_\infty \ell(m) = \|\ell\|_2^2 \).

For \( q = 2 \), let the \( \ell = U \Sigma V^T \) be the singular value decomposition of \( \ell \), and let the matrix \( \rho_2(\ell) \) be defined as in (19). Then \( \ell \cdot \rho_2(\ell) = \|\ell\|_2 \ell(A) \) where \( A \) is the matrix \( A = \sum_{i=1}^{\text{rank} \ell} u_i v_i^T \).
It remains to show that $\ell(A) = \sum_{i=1}^{\text{rank } \ell} \sigma_i(\ell)$:

$$
\ell(A) = \text{tr} \left( (U \Sigma V^T)^T A \right) \\
= \text{tr} \left( V \Sigma^T U^T U V^T \right) \\
= \text{tr} \left( \sum_{j=1}^{\text{rank } \ell} \sum_{i=1}^{\text{rank } \ell} \sigma_i(\ell) u_i u_i^T \right) \\
= \text{tr} \left( \sum_{i=1}^{\text{rank } \ell} \sigma_i(\ell) v_i v_i^T \right) \\
= \sum_{i=1}^{\text{rank } \ell} \sigma_i(\ell).
$$

In the second to last inequality we used the fact that the columns of $U$ are orthogonal. In the last inequality we used the linearity of trace together with the fact that the columns of $V$ are unit vectors (that is, $\text{tr}(v_i v_i^T) = 1$).

\[ \square \]

### A.9 Proof of Proposition 4.6

First we compute the dual norm on $Z$. For any $u = (u_1, \ldots, u_K) \in X_1 \times \ldots X_K$ with $\|u\|_Z = 1$, we have

$$
\ell \cdot u = (\ell_1 \cdot u_1) + \ldots + (\ell_K \cdot u_K) \leq \frac{p_1}{p_1} \|\ell_1\|_{X_1} \|u_1\|_{X_1} + \ldots + \frac{p_K}{p_K} \|\ell_K\|_{X_K} \|u_K\|_{X_K} \\
\leq (p_1 \|u_1\|_{X_1} + \ldots + p_K \|u_K\|_{X_K}) \max_{1 \leq i \leq K} \left\{ \frac{1}{p_i} \|\ell_i\|_{X_i} \right\} \\
= \max_{1 \leq i \leq K} \left\{ \frac{1}{p_i} \|\ell_i\|_{X_i} \right\}.
$$

Then, for any $u = (u_1, \ldots, u_K) \in X_1 \times \ldots X_K$, we have

$$
\|\ell\|_Z \leq \max_{1 \leq i \leq K} \left\{ \frac{1}{p_i} \|\ell_i\|_{X_i} \right\}.
$$

Define $i^\ast$ as

$$
i^\ast = \arg \max_{1 \leq i \leq K} \left\{ \frac{1}{p_i} \|\ell_i\|_{X_i} \right\}.
$$

To show (64) is in fact an equality, consider the vector $u$ defined as

$$
u = (u_1, \ldots, u_K) = \left(0, \ldots, \frac{1}{\|\ell_i^\ast\|_{X_i^\ast} \rho_{X_i^\ast} (\ell_i^\ast)}, \ldots, 0\right).
$$

The norm of this vector is

$$
\|u\|_Z = p_i^\ast \frac{1}{\|\ell_i^\ast\|_{X_i^\ast}} \|\rho_{X_i^\ast} (\ell_i^\ast)\| = \frac{1}{\|\ell_i^\ast\|} \|\ell_i^\ast\| = 1,
$$

and

$$
\ell \cdot u = \frac{1}{\|\ell_i^\ast\|} \ell_i^\ast \cdot \rho_{X_i^\ast} (\ell_i^\ast) = \frac{1}{\|\ell_i^\ast\|} \|\ell_i^\ast\|^2 = \frac{\|\ell_i^\ast\|_{X_i^\ast}}{p_i^\ast}.
$$

Therefore the dual norm is given by (21).
Next, we show that the function \( \rho_Z \) defined in Proposition 4.6 is a duality map, by verifying the conditions (4b) and (4d). Firstly,

\[
\ell \cdot \rho_Z(\ell) = \ell \cdot \left( 0, \ldots, \frac{1}{(p_1^*)} \rho_{X_{i^*}}( \ell_{i^*}), \ldots, 0 \right) = \frac{1}{(p_1^*)} \ell_{i^*} \cdot \rho_{X_{i^*}}( \ell_{i^*})
\]

\[
= \frac{1}{(p_1^*)} \| \ell_{i^*} \|_{X_{i^*}}^2
\]

This shows that (4b) holds. It remains to show \( \| \rho_Z(\ell) \|_Z = \| \ell \|_Z \). By definition of \( i^* \), we have

\[
\rho_Z(\ell) = \left( 0, \ldots, \frac{1}{(p_1^*)} \rho_{X_{i^*}}( \ell_{i^*}), \ldots, 0 \right)
\]

so

\[
\| \rho_Z(\ell) \|_Z = p_1^* \frac{1}{(p_1^*)^2} \| \rho_{X_{i^*}}( \ell_{i^*}) \|_{X_{i^*}} = \frac{1}{p_1^*} \| \ell_{i^*} \|_{X_{i^*}} = \| \ell \|_Z.
\]

\[\square\]

A.10 Proof of Lemma 4.7

Let \( w \in W \) and \( \eta \in \mathcal{L}(W, \mathbb{R}) \) be arbitrary. Let \( i^* = \arg \max_{1 \leq i \leq K} \left\{ \frac{1}{(p_i^*)} \| \eta_i \|_q \right\} \). Then \( \rho_w(\eta) \) is of the form \( \rho_w(\eta) = (0, \ldots, \Delta_{i^*}, \ldots, 0) \), where \( \Delta_{i^*} \in W_{i^*} \) is \( \Delta_{i^*} = \frac{1}{(p_1^*) \rho_\eta(\eta_{i^*})} \). Applying Taylor’s theorem, it holds that

\[
f(w + \epsilon \rho_w(\eta)) = f(w) + \epsilon \frac{\partial f}{\partial w}(w) \cdot \rho_w(\eta) + \epsilon^2 \int_0^1 \int_0^1 \frac{\partial^2 f}{\partial w^2}(w + u \epsilon \rho_w(\eta)) \cdot (\rho_w(\eta), \rho_w(\eta)) \, du \, d\lambda.
\]  

(65)

The only components of \( \rho_w(\eta) \) that are potentially non-zero are those corresponding to layer \( i^* \). Then

\[
\frac{\partial^2 f}{\partial w^2}(w + u \epsilon \rho_w(\eta)) \cdot (\rho_w(\eta), \rho_w(\eta)) = \frac{\partial^2 f}{\partial w^2_{i^*}}(w + u \epsilon \rho_w(\eta)) \cdot (\Delta_{i^*}, \Delta_{i^*}).
\]  

(66)

According to Proposition 4.3

\[
\left| \frac{\partial^2 f}{\partial w^2_{i^*}}(w + u \epsilon \rho_w(\eta)) \cdot (\Delta_{i^*}, \Delta_{i^*}) \right| \leq p_1^*(w + u \epsilon \rho_w(\eta))^2 \| \Delta_{i^*} \|_q^2.
\]  

(67)

Since the function \( p_1^* \) only depends on the weights in layers \( (i^* + 1), (i^* + 2), \ldots, K \), it holds that

\[
p_1^*(w + u \epsilon \rho_w(\eta)) = p_1^*(w).
\]  

(68)

By the definition of the dual norm (23)

\[
p_1^*(w^*) \| \Delta_{i^*} \|_q = \| \eta \|_w.
\]  

(69)

By combining Equations (65) - (69) then,

\[
\left| f(w + \epsilon \rho_w(\eta)) - f(w) + \epsilon \frac{\partial f}{\partial w}(w) \cdot \rho_w(\eta) \right| \leq \epsilon^2 \frac{1}{2} \| \eta \|_w^2.
\]

\[\square\]
A.11 Proof of Lemma 4.9

Define the norm \( \| \cdot \|_{1,q} \) on \( \mathcal{L}(W, \mathbb{R}) = \mathcal{L}(W_1 \times \ldots \times W_K, \mathbb{R}) \) as
\[
\| (\ell_1, \ldots, \ell_K) \|_{1,q} = \max_{1 \leq t \leq K} \| \ell_t \|_{q}.
\]
(70)

For each \( w \in W \) there is a linear map \( A(w(t)) \) on \( W \) such that the norm \( \| \cdot \|_{w(t)} \) on the dual space \( \mathcal{L}(W, \mathbb{R}) \) can be represented as
\[
\| \ell \|_{w(t)} = \| A(w(t)) \ell \|_{1,q}.
\]
(71)

This can be deduced from inspecting the formula \( \mathbb{2} \). Although not material for our further arguments, \( A(w(t)) \) is a block-structured matrix, with coefficients \( A(w(t))_{i,j} = 0 \) whenever \( i, j \) correspond to parameters in separate layers, and \( A(w(t))_{i,j} = \frac{1}{p_n(w)} \) when \( i, j \) are both weights in layer \( k \).

In general, if \( q \in [1, \infty] \) and \( A \) is an \( n_K \times n_K \) matrix, then, with the convention that \( 1/\infty = 0 \),
\[
n^{-1/2 - 1/q} \| A \|_2 \leq \| A \|_q \leq n^{1/2 - 1/q} \| A \|_2.
\]
(72)

This is well known; see for instance \( \mathbb{23} \) Section 5.6. Also, the Frobenius norm on \( n_K \times n_K \) matrices satisfies
\[
\| A \|_2 \leq \| A \|_F \leq n^{1/2} \| A \|_2.
\]
(73)

Combining (72) and (73), then,
\[
n^{-1/2 - 1/2 - 1/q} \| A \|_F \leq \| A \|_q \leq n^{1/2 - 1/2 - 1/q} \| A \|_F.
\]
(74)

It follows from (74) and Proposition A.1 that for any linear functional \( \ell \in \mathcal{L}(\mathbb{R}^{n_K \times n_K}, \mathbb{R}) \),
\[
n^{-1/2 - 1/2 - 1/q} \| \ell \|_F \leq \| \ell \|_q \leq n^{1/2 + 1/2 - 1/q} \| \ell \|_F.
\]
(75)

Inequality (75), together with the definition (70), means that for any \( \ell \in \mathcal{L}(W, \mathbb{R}) \),
\[
n^{-1/2 - 1/2 - 1/q} \max_{1 \leq t \leq K} \| \ell_t \|_F \leq \| \ell \|_{1,q} \leq n^{1/2 + 1/2 - 1/2 - 1/q} \max_{1 \leq t \leq K} \| \ell_t \|_F.
\]
(76)

For any vector \( u \) in \( \mathbb{R}^K \) we have,
\[
K^{-1/2} \| u \|_2 \leq \| u \|_{\infty} \leq \| u \|_2.
\]
(77)

Combining (76) and (77) implies that for all \( \ell \in \mathcal{L}(W, \mathbb{R}) \),
\[
K^{-1/2} n^{-1/2 - 1/2 - 1/q} \| \ell \|_2 \leq \| \ell \|_{1,q} \leq n^{1/2 + 1/2 - 1/2 - 1/q} \| \ell \|_2.
\]
(78)

Let \( k_3 = K n^{1 + 2(1/2 - 1/2 - 1/q)} \). Then
\[
\mathbb{E} \left[ \| \delta(t) \|_{w(t)}^2 \mid \mathcal{F}(t-1) \right] = \mathbb{E} \left[ \| A(w(t)) \delta(t) \|_{1,q}^2 \mid \mathcal{F}(t-1) \right] \quad \text{(by (71))}
\leq n^{1 + 1/2 - 1/q} \mathbb{E} \left[ \left\| A(w(t)) \delta(t) \right\|_2^2 \mid \mathcal{F}(t-1) \right] \quad \text{(by (78))}
\leq \frac{1}{b} n^{1 + 1/2 - 1/2 - 1/q} \mathbb{E} \left[ \left\| A(w(t)) \left( \frac{\partial f}{\partial w}(w(t)) - \frac{\partial f_i}{\partial w}(w(t)) \right) \right\|_2^2 \mid \mathcal{F}(t-1) \right]
\leq \frac{1}{b} k_3 \mathbb{E} \left[ \left\| A(w(t)) \left( \frac{\partial f}{\partial w}(w(t)) - \frac{\partial f_i}{\partial w}(w(t)) \right) \right\|_{1,q}^2 \mid \mathcal{F}(t-1) \right] \quad \text{(by (78)).}
\]

In the third step, we used the fact that \( b \) items in a mini-batch reduces the (Euclidean) variance by a factor of \( b \) compared to using a single instance, which we have represented with the random index \( i \in \{1, 2, \ldots, m\} \).
Applying the Equation (71) once more, this yields
\[
E \left[ \| \delta(t) \|_{w(t)}^2 | F(t - 1) \right] \leq \frac{1}{b} k_b E \left[ \left\| \frac{\partial f_i}{\partial w}(w(t)) - \frac{\partial f_i}{\partial w}(w(t)) \right\|_{w(t)}^2 | F(t - 1) \right].
\] (79)

Next, observe that for any pair \( i, j \) in \( \{1, 2, \ldots, m\} \),
\[
\left\| \frac{\partial f_i}{\partial w}(w(t)) - \frac{\partial f_i}{\partial w}(w(t)) \right\|_{w(t)}^2 \leq 2 \left( \left\| \frac{\partial f_i}{\partial w}(w(t)) \right\|_{w(t)}^2 + \left\| \frac{\partial f_j}{\partial w}(w(t)) \right\|_{w(t)}^2 \right).
\] (80)

Applying the chain rule to the function \( f_i \) as defined in Equation (13), and using Inequalities (79), (79), we see that for all \( w, i, \) and \( k, \)
\[
\left\| \frac{\partial f_i}{\partial w_k}(w) \right\|_q \leq d_{q,1} \left\| \frac{\partial y}{\partial w_k}(x; w) \right\|_q \leq d_{q,1} r_{K-K}(\|w_k\|_q, \ldots, \|w_r\|_q) |z|_q |z|_q \leq d_{q,1} r_{K-K}(\|w_k\|_q, \ldots, \|w_r\|_q). \] (81)

Using the definition of \( p_k \) from (14), then for any \( w, i, \) and \( k, \)
\[
\left\| \frac{\partial f_i}{\partial w_k}(w) \right\|_q \leq d_{q,1} p_k(w). \] (82)

By examining the ratio \( d_{q,1}/\sqrt{d_{q,2}} \) in the four cases presented in Table 2, we see that
\[
\frac{d_{q,1}}{\sqrt{d_{q,2}}} = \sqrt{5} \times n_{\min(1/2,1/4)}. \] (83)

Combining (82), (83) with the definition of the dual norm at \( w \) presented at Equation (72),
\[
\left\| \frac{\partial f_i}{\partial w}(w(t)) \right\|_{w(t)} \leq \sqrt{5} \times n_{\min(1/2,1/4)}. \] (84)

Using (79) and (80) together with (84),
\[
E \left[ \| \delta(t) \|_{w(t)}^2 | F(t - 1) \right] \leq \frac{32}{b} k_b n_{\min(1,2/4)} \leq \frac{32}{b} K n_{\max(1/2,1/4)}. \]

This confirms (25).

\[ \square \]

Auxiliary results

**Proposition A.1.** Let \( \| \cdot \|_A, \| \cdot \|_B \) be norms on \( \mathbb{R}^n \), such that for all \( w \in \mathbb{R}^n \) the inequality \( \|w\|_A \leq K \|w\|_B \) holds. Then for any \( \ell \in L(\mathbb{R}^n, \mathbb{R}) \), it holds that \( \|\ell\|_B \leq K \|\ell\|_A \).

**Proof.** Given a norm \( \| \cdot \| \) on \( \mathbb{R}^n \), the corresponding dual norm on \( L(\mathbb{R}^n, \mathbb{R}) \) can be expressed as \( \|\ell\| = \sup_{u \neq 0} \frac{|\ell(u)|}{\|u\|} \). Using this formula, and the assumption on \( \| \cdot \|_A, \| \cdot \|_B \), then,
\[
\|\ell\|_B = \sup_{u \neq 0} \frac{|\ell(u)|}{\|u\|_B} \leq \sup_{u \neq 0} \frac{|\ell(u)|}{\|u\|_A} K = K \sup_{u \neq 0} \frac{|\ell(u)|}{\|u\|_A} = K \|\ell\|_A.
\]
Proposition A.2 In the context of the neural network model defined by (1) and the objective function $f$ of (2), consider the following family of norms on $\mathbb{R}^4$:

$$\| (w_1, w_2, w_3, w_4) \|_w = p_1(w) |w_1| + p_2(w) |w_2| + p_3(w) |w_3| + p_4(w) |w_4|,$$

where $p_1, ..., p_4$ are defined as follows:

$$p_1(w) = \sqrt{\frac{1}{8} |w_3| + \frac{5}{128} |w_3|^2 + 1},$$

$$p_2(w) = \sqrt{\frac{1}{8} |w_4| + \frac{5}{128} |w_4|^2 + 1},$$

$$p_3(w) = p_4(w) = \sqrt{\frac{5}{8}}.$$

Then a duality structure for the family of norms $\| \cdot \|_w$ is given by

$$\rho_w(\ell_1, ..., \ell_4) = \begin{cases} 0, & \text{if } \ell_1 = 0, \\ \frac{1}{p_1(w)^2} \ell_1, & \text{otherwise} \end{cases}$$

where $i^* = \arg \max_{1 \leq i \leq 4} \left\{ \frac{1}{p_i(w)} |\ell_i| \right\}$.

Additionally, with this family of norms and duality structure, Assumption 3.2 holds with $L = 1$.

Proof We provide an abbreviated proof, and for more details see the detailed proof for Proposition 3.3. Next, we must verify the Lipschitz-like condition of (3.2). The following inequalities, which follow from basic calculus, will be essential:

$$\left| \frac{\partial^2 f}{\partial w_1^2} (w) \right| \leq \frac{1}{8} |w_3| + \frac{5}{128} |w_3|^2$$

(85)

(86)

Above, we have used the bounds $\| \sigma \|_\infty = 1, \| \sigma' \|_\infty = \frac{1}{4},$ and $\| \sigma'' \|_\infty \leq \frac{1}{4}$. Let $\eta = (\eta_1, \eta_2, \eta_3, \eta_4)$ be an arbitrary vector in $\mathbb{R}^4$. Let us investigate the four possible cases for $\rho_w(\eta)$. First, consider the case of $\rho_w(\eta) = (\frac{1}{p_1(w)} \eta_1, 0, 0, 0)$. Observe that, by (85), the function $\epsilon \mapsto f(w + \epsilon \rho_w(\eta))$ has a $K$-Lipschitz continuous gradient, where $K = \frac{|\eta_1|^2}{p_1(w)^2} \left( \frac{1}{8} |w_3| + \frac{5}{128} |w_3|^2 \right) \leq \frac{|\eta_1|^2}{p_1(w)^2}$. Hence

$$\left| f(w + \epsilon \rho_w(\eta)) - f(w) - \frac{\partial f}{\partial w}(w) \cdot \rho_w(\eta) \right| \leq \frac{1}{2} \epsilon^2 \frac{|\eta_1|^2}{p_1(w)^2} \leq \frac{1}{2} \epsilon^2 \|\eta\|_w^2$$

(86)

The case of $\rho_w(\eta) = (0, \frac{1}{p_2(w)} \eta_2, 0, 0)$ is handled similarly, due to the symmetry between $w_1$ and $w_2$.

If $\rho_w(\eta) = (0, 0, \frac{1}{p_3(w)} \eta_3, 0)$ then, similarly, the function $\epsilon \mapsto f(w + \epsilon \rho_w(\eta))$ has a $K$-Lipschitz gradient where $K = \frac{|\eta_3|^2}{p_3(w)^2} \frac{5}{8} = \frac{|\eta_3|^2}{p_3(w)^2}$, leading to the inequality

$$\left| f(w + \epsilon \rho_w(\eta)) - f(w) - \epsilon \frac{\partial f}{\partial w}(w) \cdot \rho_w(\eta) \right| \leq \frac{1}{2} \epsilon^2 \|\eta\|_w^2$$

Again, by symmetry the case $\rho_w(\eta) = (0, 0, 0, \frac{1}{p_4(w)} \eta_4)$ is handled similarly.
Proposition A.3 In the context of the neural network model defined by $f$, consider the objective function
\[ f(w_1, w_2, w_3, w_4) = \frac{1}{2} |y(w_1, w_2, w_3, w_4; 1)|^2 + \frac{1}{2} |y(w_1, w_2, w_3, w_4; 0) - 1|^2 , \]
which corresponds to training the network to map input $x = 1$ to output 0, and input $x = 0$ to output 1. Define $\delta_1(w) = 2y(w; 1)\frac{\partial y}{\partial w}(w; 1)$ and $\delta_2(w) = 2(y(w; 0) - 1)\frac{\partial y}{\partial w}(w; 0)$, so that
\[ \frac{\partial f}{\partial w}(w) = \frac{1}{2} [\delta_1(w) + \delta_2(w)] . \]
Consider the gradient estimator that computes $\delta_1(w)$ or $\delta_2(w)$ with equal probability. Then
\[ \lim_{w \to \infty} \frac{1}{2} \sum_{i=1}^2 \| \delta_i(w) - \frac{\partial f}{\partial w}(w) \|^2 = +\infty \]
Proof It suffices to show that $\| \delta_1(w) - \delta_2(w) \|^2$ is an increasing function of $\| w \|$. Focusing on the component of $\delta_1(w) - \delta_2(w)$ corresponding to $w_1$, we have
\[ \delta_{1,1}(w) = 2y(w; 1)\frac{\partial y}{\partial w}(w; 1) = 2y(w; 1)\sigma'(w_3\sigma(w_1) + w_4\sigma(w_2))w_3\sigma'(w_1) \]
and
\[ \delta_{2,1}(w) = 2(y(w; 0) - 1)\frac{\partial y}{\partial w}(w; 0) = 2(y(w; 0) - 1)\sigma'(w_3\sigma(0) + w_4\sigma(0))w_3 \times 0 = 0 . \]
Hence
\[ \| \delta_{1,1}(w) - \delta_{2,1}(w) \|^2 = \| 2y(w; 1)\sigma'(w_3\sigma(w_1) + w_4\sigma(w_2))w_3\sigma'(w_1) \|^2 . \]
Let $z$ be any number, and define the curve $w : [0, \infty) \to \mathbb{R}$ as
\[ w(\epsilon) = \left(1, 1, \epsilon, \frac{1}{\sigma(1)}(z - \epsilon\sigma(1)) \right) . \]
Note that
\[ w_3\sigma(w_1) + w_4\sigma(w_2) = \epsilon\sigma(1) + \frac{1}{\sigma(1)}(z - \epsilon\sigma(1))\sigma(1) = y \]
and therefore
\[ \| \delta_{1,1}(w(\epsilon)) - \delta_{2,1}(w(\epsilon)) \|^2 = 2\sigma(z)\sigma'(z)\sigma'(1)^2z^2 . \]
Clearly, the right hand side of this equation tends to $\infty$ as $\epsilon \to \infty$.

Lemma A.4 (Corollary 4.17 of [12]) Let $\| \cdot \|$ be a norm on $\mathbb{R}^n$ that is 2-uniformly convex with parameter $c$, and let $\rho$ be a duality map for $\| \cdot \|$. Then for any $\ell_1, \ell_2$ in $L(\mathbb{R}^n, \mathbb{R})$, \[ \| \ell_1 + \ell_2 \|^2 \geq \| \ell_1 \|^2 + 2\ell_2 \cdot \rho(\ell_1) + c\| \ell_2 \|. \] (87)
Proof This is follows from Corollary 4.17 of [12], using $p = 2$.

Proposition A.5 Let $\tau$ be a stopping time with respect to a filtration $\{ F_t \}_{t=0,1,\ldots}$. Suppose there is a number $c < \infty$ such that $\tau \leq c$ with probability one. Let $x_1, x_2, \ldots$ be any sequence of random variables such that each $x_t$ is $F_t$-measurable and $\mathbb{E}[\| x_t \|] < \infty$. Then
\[ \mathbb{E} \left[ \sum_{t=1}^\tau x_t \right] = \mathbb{E} \left[ \sum_{t=1}^\tau \mathbb{E}[x_t | F_{t-1}] \right] . \] (88)
Proof We argue that (88) is a consequence of the optional stopping theorem (Theorem 10.10 in [51]). Define \( S_0 = 0 \) and for \( t \geq 1 \), let \( S_t = \sum_{i=1}^{t} (x_i - \mathbb{E}[x_i | F_{i-1}]) \). Then \( S_0, S_1, \ldots \) is a martingale with respect to the filtration \( \{F_t\}_{t=0,1,\ldots} \), and the optional stopping theorem implies \( \mathbb{E}[S_\tau] = \mathbb{E}[S_0] \). But \( \mathbb{E}[S_0] = 0 \), and therefore \( \mathbb{E}[S_\tau] = 0 \), which is equivalent to (88).

Lemma A.6 Let \( h : \mathbb{R}^n \times \mathbb{R}^{n \times n} \to \mathbb{R}^n \) be the function defined by Equation (48). Let \( \mathbb{R}^n \) have the norm \( \| \cdot \|_q \) for \( 1 \leq q \leq \infty \) and equip the matrices \( \mathbb{R}^{n \times n} \) with the corresponding induced norm. Then the following inequalities hold:

\[
\left\| \frac{\partial h}{\partial y} (y, w) \right\|_q \leq \|\sigma\|_\infty \|w\|_q, \quad \left\| \frac{\partial h}{\partial w} (y, w) \right\|_q \leq \|\sigma\|_\infty \|y\|_q, \\
\left\| \frac{\partial^2 h}{\partial y^2} (y, w) \right\|_q \leq \|\sigma''\|_\infty \|w\|_q^2, \quad \left\| \frac{\partial^2 h}{\partial w^2} (y, w) \right\|_q \leq \|\sigma''\|_\infty \|y\|_q^2.
\]

Proof Define the pointwise product of two vectors in \( \mathbb{R}^n \) as \( u \odot v = (u_1 v_1, \ldots, u_n v_n) \). We will rely on the following two properties that are shared by the norms \( \| \cdot \|_q \) for \( 1 \leq q \leq \infty \).

Firstly, for all vectors \( u, v \),

\[\|u \odot v\|_q \leq \|u\|_q \|v\|_q. \tag{89}\]

Secondly, for any \( n \times n \) diagonal matrix \( D \), \( \|D\|_q = \max_{1 \leq i \leq n} |D_{i,i}| \). Recall that the component functions of \( h \) are \( h_i(y, w) = \sigma \left( \sum_{k=1}^{n} w_{i,k} y_k \right) \). Then for \( 1 \leq i, j \leq n \),

\[
\frac{\partial h_i}{\partial y_j} (y, w) = \sigma' \left( \sum_{k=1}^{n} w_{i,k} y_k \right) w_{i,j}.
\]

Set \( D(x, w) \) to be the \( n \times n \) diagonal matrix

\[D(y, w)_{i,i} = \sigma' \left( \sum_{k=1}^{n} w_{i,k} y_k \right), \tag{90}\]

Then \( \frac{\partial h}{\partial y} (y, w) = D(y, w)w \). Hence

\[
\left\| \frac{\partial h}{\partial y} (y, w) \right\|_q = \|D(y, w)w\|_q \\
\leq \|D(y, w)\|_q \|w\|_q \\
= \sup_{1 \leq i \leq n} \|D(y, w)_{i,i}\| \|w\|_q \\
\leq \|\sigma\|_\infty \|w\|_q.
\]

Observe that for \( 1 \leq i, j, l \leq n \),

\[
\frac{\partial h_i}{\partial w_{j,l}} (y, w) = \begin{cases} 
\sigma' \left( \sum_{k=1}^{n} w_{i,k} y_k \right) y_l & \text{if } j = i, \\
0 & \text{else}.
\end{cases}
\]
Let $\Delta$ be an $n \times n$ matrix such that $\|\Delta\|_q = 1$. Then $\frac{\partial}{\partial w}(y, w) \cdot \Delta$ is a vector in $\mathbb{R}^n$ with $i$th component

$$\left(\frac{\partial}{\partial w}(y, w) \cdot \Delta\right)_i = \sum_{j=1}^{n} \sum_{l=1}^{n} \frac{\partial h}{\partial w_j}(y, w) \Delta_{j,l}$$

$$= \sum_{l=1}^{n} \frac{\partial h}{\partial w_i}(y, w) \Delta_{i,l}$$

$$= \sum_{l=1}^{n} \sigma' \left(\sum_{k=1}^{n} w_{i,k} y_k\right) y_l \Delta_{i,l}$$

$$= \sigma' \left(\sum_{k=1}^{n} w_{i,k} y_k\right) \sum_{l=1}^{n} \Delta_{i,l} y_l$$

$$= (D(x, w)\Delta y)_i$$

where $D$ is as in (90). Hence

$$\left\|\frac{\partial}{\partial w}(y, w) \cdot \Delta\right\|_q = \|D(y, w)\Delta y\|_q$$

$$\leq \|D(y, w)\|_q \|\Delta\|_q \|y\|_q$$

and therefore $\left\|\frac{\partial}{\partial w}(y, w)\right\|_q \leq \|\sigma'\|_\infty \|y\|_q$. Observe that

$$\frac{\partial^2}{\partial y \partial y}(y, w) = \sigma'' \left(\sum_{k=1}^{n} w_{i,k} y_k\right) w_{i,j} w_{i,l}$$

That means $\frac{\partial^2}{\partial y \partial y}(y, w) \cdot (u, v)$ is a vector with components

$$\left(\frac{\partial^2}{\partial y \partial y}(x, w) \cdot (u, v)\right)_i = \sum_{j=1}^{n} \sum_{l=1}^{n} \sigma'' \left(\sum_{k=1}^{n} w_{i,k} y_k\right) w_{i,j} w_{i,l} u_j v_l$$

$$= \sigma'' \left(\sum_{k=1}^{n} w_{i,k} y_k\right) \left(\sum_{j=1}^{n} w_{i,j} u_j\right) \left(\sum_{l=1}^{n} w_{i,l} v_l\right)$$

$$= E(y, w)_{i,i} (Wu)_i (Wv)_i$$

where $E$ is the diagonal matrix

$$E(y, w)_{i,i} = \sigma'' \left(\sum_{k=1}^{n} w_{i,k} y_k\right). \quad (91)$$

Using the notation $\odot$ for the entry-wise product of vectors, then

$$\frac{\partial^2}{\partial y \partial y}(x, w) \cdot (u, v) = E(x, w) \cdot ((wu) \odot (wv)).$$

Then

$$\left\|\frac{\partial^2}{\partial y \partial y}(y, w) \cdot (u, v)\right\|_q = \|E(y, w) \cdot (wu) \odot (wv)\|_q$$

$$\leq \|E(y, w)\|_q \|(wu) \odot (wv)\|_q$$

$$\leq \|E(y, w)\|_q \|wu\|_q \|wv\|_q$$

$$\leq \|E(y, w)\|_q \|w\|_q^2 \|v\|_q.$$
Duality Structure Gradient Descent

Hence \( \left\| \frac{\partial^2 h}{\partial y^2} (y, w) \right\|_q \leq \|\sigma''\|_\infty \|w\|_q^2 \). Observe that

\[
\frac{\partial^2 h}{\partial w^2}(x, w) = \begin{cases} \sigma'' \left( \sum_{k=1}^n w_{i,k} y_k \right) y_i y_m & \text{if } j = i \text{ and } k = i, \\ 0 & \text{else.} \end{cases}
\]

Hence for matrices \( u, v \), \( \frac{\partial^2 h}{\partial w^2}(y, w) \cdot (u, v) \) is a vector with entries

\[
\frac{\partial^2 h}{\partial y^2}(y, w) \cdot (u, v) = \begin{cases} \sigma'' \left( \sum_{k=1}^n w_{i,k} x_k \right) y_i y_m u_{i,l} v_{i,m} & \text{if } j = i \text{ and } k = i, \\ 0 & \text{else.} \end{cases}
\]

where \( E \) is as in (91). Hence

\[
\frac{\partial^2 h}{\partial w^2}(y, w) \cdot (u, v) = E(y, w) \cdot ((uy)_i \odot (vy)_i)
\]

which means

\[
\left\| \frac{\partial^2 h}{\partial y^2}(y, w) \cdot (u, v) \right\|_q \leq \|E(y, w)\|_q \|uy\|_q \|vy\|_q
\]

\[
\leq \|E(y, w)\|_q \|u\|_q \|v\|_q \|y\|_q^2.
\]

Therefore \( \left\| \frac{\partial^2 h}{\partial y^2}(y, w) \cdot (u, v) \right\|_q \leq \|\sigma''\|_\infty \|y\|_q^2 \).

**Lemma A.7** Let \( z \in \mathbb{R}^n \) and define the function \( J : \mathbb{R}^n \to \mathbb{R} \) as

\[
J(y) = \sum_{i=1}^n (y_i - z_i)^2
\]

Then for all \( y, z \in \mathbb{R}^n \) such that \( \|y - z\|_\infty \leq 2 \), and \( 1 \leq q \leq \infty \),

\[
\left\| \frac{\partial J}{\partial y}(y) \right\|_q \leq \begin{cases} 4 & \text{if } q = 1, \\ 4n(q-1)/q & \text{if } 1 < q < \infty, \\ 4n & \text{if } q = \infty, \end{cases}
\]

and

\[
\left\| \frac{\partial^2 J}{\partial y^2}(y) \right\|_q \leq \begin{cases} 2 & \text{if } 1 \leq q \leq 2, \\ 2n(q-2)/q & \text{if } 2 < q < \infty, \\ 2n & \text{if } q = \infty. \end{cases}
\]

**Proof** By direct calculation, the components of the derivative of \( J \) are \( \frac{\partial J}{\partial y_i}(y) = 2(y_i - z_i) \), and therefore

\[
\left\| \frac{\partial J}{\partial y_i}(y) \right\|_q = 2\|y_i - z_i\|_q^2.
\]
where \( \| \cdot \|_q^* \) represents the norm dual to \( \| \cdot \|_q \). When \( q = 1 \), the dual norm is \( \| \cdot \|_\infty \), for \( 1 \leq q < \infty \), the dual of norm \( \| \cdot \|_q \) is \( \| \cdot \|_q^{q/(q-1)} \) and finally the dual of the norm \( \| \cdot \|_\infty \) is \( \| \cdot \|_1 \).

This yields
\[
\frac{\partial J}{\partial x}(y) = \begin{cases} 
2\|y - z\|_\infty & \text{if } q = 1 \\
2\|y - z\|_{q/(q-1)} & \text{if } 1 < q < \infty, \\
2\|y - z\|_1 & \text{if } q = \infty
\end{cases}
\] (93)

Equation (92) follows by combining (93) with our assumption that \( \|y - z\|_\infty \leq 2 \).

For the second derivative, the components are
\[
\frac{\partial^2 J}{\partial y_i \partial y_j} = \begin{cases} 
0 & \text{if } i \neq j, \\
2 & \text{if } i = j.
\end{cases}
\]

Then for any vectors \( u, v \),
\[
\frac{\partial J^2}{\partial y^2}(y) \cdot (u, v) = 2 \sum_{i=1}^n u_i v_i.
\]

Therefore
\[
\left\| \frac{\partial J^2}{\partial y^2}(y) \right\|_q = 2 \sup_{\|u\|_q = \|v\|_q = 1} \sum_{i=1}^n u_i v_i
\]
\[
= 2 \sup_{\|u\|_q = 1} \|u\|_{q^*}
\]

To bound the final term in the above equation, we consider four cases. The first case is that \( q = 1 \). In this situation, \( \|u\|_{q^*} = \|u\|_\infty \leq 1 \). The second case is that \( 1 < q < 2 \). Then \( q/(q-1) > q \), and hence \( \|u\|_{q^*} \leq \|u\|_q = 1 \). The third case is when \( 2 \leq q < \infty \). Here, \( q/(q-1) \leq q \), and we appeal to the following inequality: If \( 1 \leq r < q \), then \( \|\cdot\|_r \leq n^{\frac{1}{r}-\frac{1}{q}} \|\cdot\|_q \).

Applying this inequality with \( r = q/(q-1) \), we obtain \( \|u\|_{q^*} \leq n^{(q-2)/q} \|u\|_q = n^{(q-2)/q} \).

Finally, if \( q = \infty \) we have \( \|u\|_{q^*} = \|u\|_1 \leq n \).