Tune smarter not harder: A principled approach to tuning learning rates for shallow nets

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Abstract—Effective hyper-parameter tuning is essential to guarantee the performance that neural networks have come to be known for. In this work, a principled approach to choosing the learning rate is proposed for shallow feedforward neural networks. We associate the learning rate with the gradient Lipschitz constant of the objective to be minimized while training. An upper bound on the mentioned constant is derived and a search algorithm, which always results in non-divergent traces, is proposed to exploit the derived bound. It is shown through simulations that the proposed search method significantly out-performs the existing tuning methods such as Tree Parzen Estimators (TPE). The proposed method is applied to two different existing applications, namely, channel estimation in a wireless communication system and prediction of the exchange currency rates, and it is shown to pick better learning rates than the existing methods using the same or lesser compute power.

I. INTRODUCTION

Deep neural networks have made significant improvements to fields like speech and image processing [1], communications [2], [3], computer vision, etc. [4]. These networks are typically trained using an iterative optimization algorithm such as Gradient Descent (GD) or its multiple variants [5], [6]. To successfully deploy these networks for various applications, the hyper-parameters of the network, namely the width and the depth of the network and the learning rate used for training should be carefully tuned [7].

Initially, manual search and grid search were the most popular approaches [8]. The authors of [9] then showed that randomly chosen trials were more efficient in terms of search time for hyper-parameter optimization than a grid-based search. However, in both the methods, the observations from the previous samples are not utilized to choose values for the subsequent trials. To remedy this, Sequential Model-Based Optimization (SMBO) was introduced to perform hyper-parameter tuning where the next set of hyper-parameters to be evaluated are chosen based on the previous trials [10]. Some of the well-known models for Bayesian optimization are Gaussian Processes [11], random forests [12] and TPE [13].

In the methods listed here so far, the tuning of hyper-parameters is typically performed as a black-box module, i.e., without utilizing any information about the objective function to be minimized. There exist many applications in which the architecture of the network is fixed, for which the number of layers and the width of the network are already specified and are not treated as hyper-parameters. Given such an architecture, the learning rate is an important hyper-parameter as it determines the speed of convergence of the optimization algorithm [14]. In such cases, it would be beneficial if the learning rate is derived as a function of the objective as it can be simply recomputed for a new set of inputs instead of tuning the learning rate from scratch. This would require a theoretical analysis of the objective function. Although neural networks are applied to varied applications, little is known about its theoretical properties when the network consists of multiple hidden layers. Most theoretical works such as [15], [16] are available for networks with one or two hidden layers, which we call shallow networks.

Although deep neural networks are popular in computer vision and image processing where the function to be learnt is complex due to its multi-dimensional nature, applications in areas like wireless communication and finance predictions still employ shallow feedforward neural networks as evidenced by works in [17]–[21]. In [18], channel estimation for OFDM systems was done using a single hidden layer neural network. Shallow networks were also used in applications like user equipment (UE) Localization [21], symbol detection in high-speed OFDM underwater acoustic communication [22] and Direction of Arrival (DoA) estimation [20]. In all the above applications, the architecture for a given application was fixed and the learning rate was chosen by either manual tuning or grid search.

For such applications which employ a fixed shallow architecture, a theory-based approach for choosing the learning rate will save the computation which would otherwise be spent on tuning the hyper-parameters. The learning rate of the optimization algorithm has been associated with the Lipschitz properties of the objective function, namely the Lipschitz constant of the gradient of the objective function [23]. Although, there has been significant interest in analyzing the Lipschitz properties of neural networks in recent literature [24], [25], these works focus on the Lipschitz constant of the output of the network which plays an important role in analysing the stability of the network, and not on the gradient Lipschitz constant of the objective which is required for quantifying the learning rate.
A. Motivation

In the existing works on hyper-parameter optimization, the choice of learning rate is often treated as a separate module that is to be performed before the training; they do not employ any information about the function that should be optimized. As an alternative, we wish to associate the learning rate with the parameters of the problem, thereby providing a theoretical justification to the choice of learning rate and also use this to tune in a smarter fashion.

In typical tuning methods, there is a clear trade-off between the number of trials of the search algorithm that is allowed and the performance of the chosen learning rate. If one decides to adopt a higher number of trials then, one is more likely to achieve a better learning rate. However, there is no guarantee that the chosen learning rate will lead to convergent behaviour of GD given any fixed number of trials. In the proposed method, we wish to provide the user with the same trade-off between the number of trials and the performance, whilst ensuring that chosen learning rate always results in convergence irrespective of the number of trials allowed.

B. Contributions

A theory-based approach to determine the learning rate for shallow networks is proposed. The contributions of this work are four-fold. Firstly, using classic literature \[23\], the learning rate is associated with the gradient Lipschitz constant of the objective function. Secondly, the upper bound on gradient Lipschitz constants for feedforward neural networks consisting of one and two layers are derived for popular activation functions, namely, ReLU and sigmoid. The bounds, initially in terms of eigenvalues of large Hessian matrices, are simplified to yield easy-to-implement expressions that can be adapted to a given architecture. Thirdly, the derived bound on the gradient Lipschitz constant is utilized for determining the learning rate; an algorithm, ‘BinarySearch’, is introduced for this search. The proposed algorithm is shown to outperform the popular hyper-parameter tuning estimator, TPE, in terms of the loss achieved, while ensuring convergence. Finally, the utility of the proposed method is also demonstrated using two applications: channel estimation in the case of Orthogonal Frequency Division Multiplexing (OFDM) systems and the prediction of exchange rates for currencies.

C. Notation

We use bold upper-case letters, say \(A\) to denote matrices and \(A_{ij}, A^i\) to denote their \((i,j)\)th element and the \(i\)th column respectively. The maximum eigenvalue of \(A\) is denoted as \(\lambda_{\text{max}}(A)\); the maximum diagonal entry is denoted as \(D_{\text{max}}(A)\). The bold lower-case letters \(x, y\) denote vectors. All vectors are column vectors unless stated otherwise. The \(\ell_2\) norm of a vector is denoted as \(\|\cdot\|\). The \(\ell_1\) and \(\ell_\infty\) norms of a vector \(x\) are denoted as \(|x|_1 = \sum_i x_i\) and \(|x|_\infty = \max_i x_i\) respectively. The indicator function denoted as \(\mathbb{1}_E\) takes the value 1 when \(E\) is true and value 0 otherwise. The symbols \(\nabla\) and \(\nabla^2\) denote the first and second derivatives respectively.

II. Definitions and Background

**Definition 1.** A differentiable function \(f : \mathbb{R}^d \to \mathbb{R}\) is said to be an \(\alpha\)-gradient Lipschitz if for any \(x_1, x_2\) in the domain of \(f\), and for \(\alpha > 0\),

\[
\|\nabla f(x_1) - \nabla f(x_2)\| \leq \alpha \|x_1 - x_2\|, \tag{1}
\]

where \(\alpha\) is known as the gradient Lipschitz constant. The smallest such constant is known as the optimal constant, denoted by \(\alpha^*\).

Nesterov’s seminal work \[23\] discusses the following theorem which guarantees the convergence of the GD algorithm.

**Lemma 1.** \[23\] For an \(\alpha\)-gradient Lipschitz function \(f : \mathbb{R}^d \to \mathbb{R}\), gradient descent with a step size \(\eta \leq 1/\alpha\) produces a decreasing sequence of objective values and the optimal step size is given by \(\eta^* = 1/\alpha\).

For a doubly differentiable function \(f\) with gradient Lipschitz constant as \(\alpha\), we have \[23\]

\[
\nabla^2 f(x) \leq \alpha I \quad \forall x. \tag{2}
\]

This implies that all eigenvalues of the matrix \(\nabla^2 f(x) - \alpha I\) should be less than or equal to zero for all values of \(x\). This is achieved when the maximum eigenvalue satisfies this condition. Therefore, the gradient Lipschitz constant of a double differentiable function is given by

\[
\alpha^* = \max_{x} \lambda_{\text{max}}(\nabla^2 f(x)). \tag{3}
\]

We use \[3\] in the following sections to derive the required constant. Note that any \(\alpha > \alpha^*\) also satisfies \[2\]. Therefore, if the exact value for \(\alpha^*\) cannot be determined, an upper bound on \(\alpha^*\) can be derived. The learning rate derived from the upper bound also results in a decreasing sequence of iterates according to Lemma \[1\]. This signifies that the learning rate derived as the inverse of the gradient Lipschitz constant or any upper bound will always result in convergence of the gradient descent algorithm. This implication is used by us to guarantee the convergence of GD while training neural networks.

III. Deriving the Gradient Lipschitz Constant for a Single Hidden Layer Neural Network

In this section, a neural network with a single hidden layer consisting of \(k\) neurons with activation function \(act(.)\) is considered, as given in Fig. 1. We derive the gradient Lipschitz constant for two different popular activation functions: sigmoid and ReLU. The weight vector from the input to the \(j\)th hidden layer neuron is denoted as \(w^j\) where \(w^j \in \mathbb{R}^d\) for \(j = 1, \ldots k\). The column vector \(w\) refers to the stack of vectors \(w^1, \ldots, w^k\); \(w \in \mathbb{R}^{kd}\). The output of the network is taken as the sum of outputs from each of the hidden layer neurons and is given by \(f(x, w) = \sum_{j=1}^{k} act(x^T w^j)\) for input \(x\). The training data is denoted as a set of points \((x(i), y(i))\) for \(i = 1, \ldots N\). The aim of the network is to learn the function \(f\) given the training data. Throughout, we consider the quadratic loss function namely,

\[
l(w) = \frac{1}{2N} \sum_{i=1}^{N} \left( \sum_{j=1}^{k} act(x(i)^T w^j) - y(i) \right)^2. \tag{4}
\]
A. Sigmoid activation

The sigmoid activation is defined as \( \sigma(x) = \frac{1}{1 + \exp(-x)} \). The gradient Lipschitz constant for a single hidden layer network with sigmoid activation function is derived in this section. Initially, we consider a single data point, \((x, y)\), and then extend it to a database.

**Theorem 1.** The gradient Lipschitz constant for a single-hidden layer feedforward network with sigmoid activation when considering quadratic loss function in (4) with \( \text{act}(.) = \sigma(.) \) and \( N = 1 \) is given by,

\[
\alpha^* = \min \left( \frac{|k-y|}{10} + \frac{k}{16} \cdot 0.1176(k-1) + \frac{|y|}{10} + 0.077 \right) \|x\|^2.
\]

**(5)**

**Proof:** As the loss function is doubly differentiable, the required constant is \( \alpha^* = \max_w \lambda_{\text{max}}(\nabla^2 l(w)) \). Note,

\[
\nabla l(w) = \left( \sum_{j=1}^{k} \sigma(x^Tw^j) - y \right) \begin{bmatrix} \sigma(x^Tw^1) \sigma(x^Tw^2) \cdots \sigma(x^Tw^k) \end{bmatrix} x
\]

Define,

\[
\hat{b}(x, w) = \begin{bmatrix} \sigma(x^Tw^1) \sigma(x^Tw^2) \cdots \sigma(x^Tw^k) \end{bmatrix},
\]

where the vector \( \hat{b}(x, w) \in \mathbb{R}^k \). Let \( \text{Diag}_m(k_m) \) denote a diagonal matrix whose non-zero entry in the \( m_{th} \) row is \( k_m \). The Hessian matrix computed using the product rule of differentiation is given by,

\[
\nabla^2 l(w) = \left( \text{Diag}_m \left( \sum_{j=1}^{k} \sigma(x^Tw^j) - y \right) \sigma(x^Tw^m) \right)\left(1 - \sigma(x^Tw^m)\right)\left(1 - 2\sigma(x^Tw^m)\right)
\]

\[
+ \hat{b}(x, w)\hat{b}(x, w)^T \otimes xx^T.
\]

**(8)**

The gradient Lipschitz constant is given by

\[
\alpha^* = \max_{w} \lambda_{\text{max}} \left[ \left( \text{Diag}_m \left( \sum_{j=1}^{k} \sigma(x^Tw^j) - y \right) \sigma(x^Tw^m) \right)\left(1 - \sigma(x^Tw^m)\right)\left(1 - 2\sigma(x^Tw^m)\right) 
\]

\[
+ \hat{b}(x, w)\hat{b}(x, w)^T \otimes xx^T \right].
\]

**(9)**

Note (9) involves a maximization over all possible values of \( w \) and an eigenvalue computation for every value. We use the structure of the matrix to provide a simplified solution. We use the following property of Kronecker products [26].

**Lemma 2.** Let \( A \in \mathbb{R}^{n \times n} \) have eigenvalues \( \lambda_i, i \in n \), and let \( B \in \mathbb{R}^{m \times m} \) have eigenvalues \( \mu_j, j \in m \), then the mn eigenvalues of \( A \otimes B \) are given by

\[
\lambda_1\mu_1, \cdots, \lambda_1\mu_m, \lambda_2\mu_1, \cdots, \lambda_2\mu_m, \cdots, \lambda_n\mu_m.
\]

Therefore, the maximum eigenvalue of the Kronecker product will be the product of the maximum eigenvalues, if the maximum eigenvalue of the diagonal matrix is positive; else, it will be zero. As we are maximizing over all possible values of \( w \), we can always ensure that the maximum eigenvalue is positive. Since \( xx^T \) is rank one with a single non-zero eigenvalue, \( x^T x \), using Lemma 2 we have,

\[
\alpha^* = \max_{w} \lambda_{\text{max}}(P)x^T x,
\]

**(10)**

where \( P \) is defined as

\[
P = \text{Diag}_m \left( \sum_{j=1}^{k} \sigma(x^Tw^j) - y \right) \sigma(x^Tw^m) \left(1 - \sigma(x^Tw^m)\right)\left(1 - 2\sigma(x^Tw^m)\right) + \hat{b}(x, w)\hat{b}(x, w)^T.
\]

**(11)**

A bound can be obtained to find the maximum eigenvalue of \( P \) using the Weyl’s inequality which states that for Hermitian matrices \( A \) and \( B \),

\[
\lambda_{\text{max}}(A + B) \leq \lambda_{\text{max}}(A) + \lambda_{\text{max}}(B).
\]

**(12)**

Using the above inequality, the observation that \( \hat{b}(x, w)\hat{b}(x, w)^T \) is rank-1 and that the eigenvalues of
We now use the following bounds on the sigmoid derivatives, one obtains,
\[
\lambda_{\text{max}}(P) \leq \max_m \left( \sum_{j=1}^{k} \sigma(x^T w^j) - y \right) \sigma(x^T w^m) \\
(1 - \sigma(x^T w^m))(1 - 2\sigma(x^T w^m)) + \hat{b}(x, w) + b(x, w).
\]
(13)

Combining (10) and (13),
\[
\alpha^* \leq \max \left( \max_m \left( \sum_{j=1}^{k} \sigma(x^T w^j) - y \right) \left( \nabla^2 \sigma(x^T w^m) + \sum_{j=1}^{k} (\nabla \sigma(x^T w^j))^2 \right) \|x\|^2 \right).
\]
(14)
The expression in (14) can be written in terms of the derivatives of sigmoid function as given below:
\[
\alpha^* \leq \max \left( \max_m \left( \sum_{j=1}^{k} \sigma(x^T w^j) - y \right) \nabla^2 \sigma(x^T w^m) + \sum_{j=1}^{k} (\nabla \sigma(x^T w^j))^2 \right) \|x\|^2.
\]
(15)

We now use the following bounds on the sigmoid derivatives to bound (15):
\[
0 \leq \sigma(x) \leq 1 \quad \forall x
\]
(16)
\[
\nabla_x \sigma(x) = \sigma(x)(1 - \sigma(x)) \leq \frac{1}{4} \quad \forall x
\]
(17)
\[
\nabla_x^2 \sigma(x) = \sigma(x)(1 - \sigma(x))(1 - 2\sigma(x)) \leq \frac{1}{10} \quad \forall x.
\]
(18)

Using the above conditions to individually maximize each of the terms in (15),
\[
\alpha^* \leq \left[ \frac{|k - y|}{10} + \frac{k}{16} \right] \|x\|^2.
\]
(19)

We note that tighter bounds may be achieved by maximizing the expression in (15) as a whole instead of each individual term. As the maximization in (15) is over the weights \(w\), considering the terms consisting of \(w\),
\[
\max_m \left( \sum_{j=1}^{k} \sigma(x^T w^j) - y \right) \nabla^2 \sigma(x^T w^m) + \sum_{j=1}^{k} (\nabla \sigma(x^T w^j))^2 \right) \|x\|^2.
\]
(20)

Note that maximizing (20) with respect to \(w\) maximizes (15). Let us assume that the index that maximizes the inner maximization with respect to \(m\) is \(\bar{m}\). Therefore, the expression in (20) is now rewritten as
\[
\left( \sum_{j=1}^{k} \sigma(x^T w^j) - y \right) \nabla^2 \sigma(x^T w^{\bar{m}}) + \sum_{j=1}^{k} (\nabla \sigma(x^T w^j))^2.
\]
(21)

We use the following inequality that \(a - b \leq |a| + |b|\) on the first term. Combining the terms corresponding to \(\bar{m}\) and using (18) to bound the second derivative,
\[
\max_w \left[ \frac{1}{10} \left( \sum_{j=1}^{k} \sigma(x^T w^j) + |y| \right) + \sum_{j=1}^{k} (\nabla \sigma(x^T w^j))^2 \right.
\]
\[
+ \sigma(x^T w^{\bar{m}}) \nabla^2 \sigma(x^T w^{\bar{m}}) + (\nabla \sigma(x^T w^{\bar{m}}))^2 \right].
\]
(22)

We then maximize each of these terms individually leading to the following bounds:

- \(\sigma(x) + (\nabla \sigma(x))^2 \leq 0.1176 \quad \forall x\)
- \(\sigma(x) \nabla^2 \sigma(x) + (\nabla \sigma(x))^2 \leq 0.0770 \quad \forall x\)

Incorporating the above, we get the following bound on the gradient Lipschitz constant
\[
\alpha^* \leq \left[ (k - 1)0.1176 + \frac{|y|}{10} + 0.0770 \right] \|x\|^2.
\]
(23)

Depending on the value of \(k\) and \(y\), we find that either of the bounds in (19) and (23) can prove tighter. As both of them are upper bounds, we pick the least one of them. The final expression for the upper bound on the gradient Lipschitz constant when a single data point \((x, y)\) is taken is given by,
\[
\alpha^* \leq \min \left( \frac{|k - y|}{10} + \frac{k}{16}, \frac{|y|}{10} + 0.1776(k - 1) \right.
\]
\[
+ \left. \frac{|y|}{10} + 0.0770 \right) \|x\|^2.
\]
(24)

Extending this to multiple data points \((x(i), y(i))\) for \(i = 1, \ldots, N\), the bound on \(\alpha^*\) is given by
\[
\alpha^* \leq \frac{1}{N} \sum_{i=1}^{N} \min \left[ \frac{|k - y(i)|}{10} + \frac{k}{16}, \frac{|y(i)|}{10} + 0.1776(k - 1) \right.
\]
\[
+ \left. \frac{|y(i)|}{10} + 0.0770 \right) \|x(i)\|^2.
\]
(25)

Given the number of neurons in the hidden layer, \(k\), and the data set, the upper bound can be found by simply evaluating the expression derived in (25); the inverse of this bound gives a learning rate which always guarantees that GD will converge. The bound increases with increase in width of the network as well as the norm of the input. It is noted that the bound depends on data only through its norm. Therefore, if different data sets with similar Euclidean norms are encountered, the derived bound can simply be reused.

**B. ReLU activation**

The ReLU activation function is given by \(s(x) = \max(0, x)\). Initially, consider a single data point \((x, y)\) for deriving the gradient Lipschitz constant.
Theorem 2. The gradient Lipschitz constant for a single-hidden layer feedforward network with ReLU activation when considering quadratic loss function in (4) when \( act(.) = s(.) \) and \( N = 1 \) is given by
\[ \alpha^* = k \| x \|^2. \]  
(26)

Proof: Please see Appendix A.

We now extend the derivation of the gradient Lipschitz constant for a multiple input database. The result in Theorem 2 can be extended to \( N \) inputs as
\[ \alpha^* = \frac{1}{N} \max_{w} \lambda_{\max} \left( \sum_{i=1}^{N} a(x(i), w)a(x(i), w)^T \right). \]  
(27)
where
\[ a(x, w) \triangleq \left[ \mathbb{I}_{\{x^Tw^1 \geq 0\}} x \ldots \mathbb{I}_{\{x^Tw^k \geq 0\}} x \right]^T. \]  
(28)
This involves a maximization over all possible weights and we would like to derive a closed form expression. It is observed that the Hessian matrix in this specific problem is structured; it is the sum of outer products of the vector \( a(x(i), w) \) where the vector consists of \( x(i) \) multiplied by appropriate indicators. We wish to exploit the structure of the Hessian matrix to arrive at an elegant solution which can be easily evaluated. Towards that end, we state and prove the following lemma.

Lemma 3. For a vector \( a(x(i), w) \) as defined in (28), the following relation holds
\[ \lambda_{\max} \left( \sum_{i=1}^{N} \bar{a}(x(i))\bar{a}(x(i))^T \right) \geq \lambda_{\max} \left( \sum_{i=1}^{N} a(x(i), w)a(x(i), w)^T \right) \quad \forall w, \]  
(29)
where
\[ \bar{a}(x) \triangleq [x \ldots x]^T \quad (k \text{ terms}). \]  
(30)
Proof: Please see Appendix B.

Lemma 3 holds for all values of \( w \); therefore, it also holds for that \( w \) which maximizes the maximum eigenvalue in (27). In essence, Lemma 3 provides an upper bound on the constant \( \alpha^* \). It is also noted that as \( \bar{a}(x(i)) \) is an instance of \( a(x(i), w) \) for a specific \( w \),
\[ \max_{w} \lambda_{\max} \left( \sum_{i=1}^{N} a(x(i), w)a(x(i), w)^T \right) \geq \lambda_{\max} \left( \sum_{i=1}^{N} \bar{a}(x(i))\bar{a}(x(i))^T \right). \]  
(31)
Hence, (31) gives a lower bound on the constant \( \alpha^* \). From (29) and (31), it is evident that the upper and the lower bounds coincide and must be equal to the exact value of \( \alpha^* \), i.e.,
\[ \alpha^* = \lambda_{\max} \left( \frac{1}{N} \sum_{i=1}^{N} \bar{a}(x(i))\bar{a}(x(i))^T \right). \]  
(32)

The exact gradient Lipschitz constant for a single hidden layer network with ReLU activation has been derived in (32). We no longer need the perform the brute force maximization over all weight values as was required in (22). Instead evaluating \( \alpha^* \) is now reduced to finding the maximum eigenvalue of a \( kd \times kd \) matrix. We note that the value of \( \alpha^* \) only depends on the data vectors \( x(i) \) and the number of neurons \( k \). As the dimension of the problem increases, the eigenvalue computation will get intensive; in such cases, we can employ well-established bounds like Gershgorin and Brauer’s ovals of Cassini to provide easily computable upper bounds on \( \alpha^* \). For convenience, these theorems are stated here.

Theorem 3 (Gershgorin’s Circles theorem [28]). For a square matrix \( A \), the upper bound on the maximum eigenvalue is,
\[ \lambda_{\max}(A) \leq \max_{i} (a_{ii} + R_i(A)), \]  
(33)
where \( R_i(A) = \sum_{i \neq j} |a_{ij}| \).

Theorem 4 (Brauer’s Ovals of Cassini). For a square matrix \( A \), the upper bound on the maximum eigenvalue is given by
\[ \lambda_{\max}(A) \leq \max_{i \neq j} \left( a_{ii} + a_{jj} \right) \]  
(34)
\[ + \sqrt{(a_{ii} - a_{jj})^2 + R_i(A)R_j(A)}, \]  
where \( R_i(A) = \sum_{i \neq j} |a_{ij}| \).

The bound in Theorem 4 is guaranteed to be provide a bound which is not worse than the Gershgorin bound [29]. The bounds stated above can be used to provide an upper bound on the gradient Lipschitz constant if eigenvalue computation is a constraint. The inverse of the derived constant \( \alpha^* \) or its upper bound can be used as the learning rate while training the network, and this will guarantee convergence of GD.

IV. DERIVING THE GRADIENT LIPSCHITZ CONSTANT FOR A TWO HIDDEN LAYER NEURAL NETWORK

Here, we focus on a shallow architecture with two hidden layers between the input and output layers as illustrated in Fig. 2. The weight matrix between the input and the first hidden layer is denoted as \( V \in \mathbb{R}^{d \times k_1} \) where \( k_1 \) is the number of neurons in the first hidden layer. The weight matrix between the two hidden layers is denoted as \( W \in \mathbb{R}^{k_1 \times k_2} \) where \( k_2 \) is the number of neurons in the second hidden layer. The output of the network is the sum of the outputs of the neurons in the second hidden layer. Let us denote the parameters of the network \( V, W \) as a single vector \( \theta \). Note that the dimension of \( \theta \) is \( k_1(d + k_2) \).

\[ \theta = [V^{1T} \ldots V^{k_1T} W^{1T} \ldots W^{k_2T}]^T \]  
(35)

This derivation is challenging as it is not a straight-forward extension of the single layer case; the Hessian involves two weight matrices \( V, W \) to be optimized over. The squared loss function is considered whose expression is given by,
\[ l(\theta) = \frac{1}{2N} \sum_{i=1}^{N} \left( \sum_{l_1=1}^{k_2} \sum_{l_2=1}^{k_1} act(x(i))^T V^{l_1} W_{l_1l_2} \right) - y(i))^2. \]  
(36)
A. Sigmoid activation

Here, we derive the gradient Lipschitz constant of a 2-hidden layer network with sigmoid activation function. As done previously, we initially consider a single data tuple \((x, y)\) where \(x \in \mathbb{R}^d\) and \(y \in \mathbb{R}\).

**Theorem 5.** The gradient Lipschitz constant for a two hidden layer feedforward network with sigmoid activation when considering quadratic loss function in (36) with \(\text{act}(.) = \sigma(.)\) and \(N = 1\) is given by,

\[
\alpha^* \leq k_1 \left( \frac{k_2 \beta \|x\|}{16} \right)^2 + \frac{k_1 k_2}{16} + \max \left( \frac{1}{10} + \left[ \frac{1}{4} + \frac{\beta}{1000} \right] k_1 |x| + \left[ \frac{1}{4} + \frac{\beta}{10} \right] k_2 \|x\|_\infty + \left[ \frac{\beta}{100} + \frac{1}{4} \right] k_1 k_2 \|x\|_1 \|x\|_\infty |k_2 - y| \right)
\]  

\[(37)\]

when \(|\theta_i| < \beta\) \forall i for \(\theta\) as defined in (35).

**Proof:** Please see Appendix [C].

This is further extended to the case of \(N\) inputs and the obtained constant is given by

\[
\alpha^* \leq \frac{1}{N} \sum_{i=1}^{N} \left[ k_1 \left( \frac{k_2 \beta \|x(i)\|}{16} \right)^2 + \frac{k_1 k_2}{16} + \max \left( \frac{1}{10} + \left[ \frac{1}{4} + \frac{\beta}{1000} \right] k_1 |x(i)| + \left[ \frac{1}{4} + \frac{\beta}{10} \right] k_2 \|x(i)\|_\infty + \left[ \frac{\beta}{100} + \frac{1}{4} \right] k_1 k_2 \|x(i)\|_1 \|x(i)\|_\infty |k_2 - y(i)| \right) \right].
\]  

\[(38)\]

We note that increase in dimension of the architecture will lead to an increase in the bound. The derived bound also depends on the maximum value in the weight matrix. Therefore, the bound is tighter when there are no spurious values with large magnitude in the weight matrix.

B. ReLU Activation

Initially, consider a single data tuple \((x, y)\) where \(x \in \mathbb{R}^d\) and \(y \in \mathbb{R}\).

**Theorem 6.** The gradient Lipschitz constant for a two hidden layer feedforward network with ReLU activation when considering quadratic loss function in (36) with \(\text{act}(.) = s(.)\) and \(N = 1\) is given by

\[
\alpha^* \leq k_1 (d + k_2) \beta^2 \|x\|^2 + \max((A_{max} k_2 |x|_{\infty}, A_{max} |x|_1)),
\]  

\[(39)\]

where \(A_{max} = k_1 k_2 \beta^2 \|x\| - y\) when \(|\theta| < \beta\) \forall i.

**Proof:** Please see the supplementary material.

Extending to a database of \(N\) inputs, i.e., \((x(i), y(i))\) for \(i = 1,...,N\), the following bound is obtained on the gradient Lipschitz constant,

\[
\alpha^* \leq \frac{1}{N} \sum_{i=1}^{N} \left( k_1(d + k_2) \beta^2 \|x(i)\|^2 + \max((A_{max}(i) k_2 |x(i)|_{\infty}, A_{max}(i) |x(i)|_1)) \right),
\]  

\[(40)\]

where \(A_{max}(i) = k_1 k_2 \beta^2 \|x(i)\| - y(i)\). The derived bound depends on the dimension of the problem and on the factor \(\beta\) which is the maximum magnitude in the weight matrix. The bound increases linearly with increase in any of the following parameters: \(k_1, k_2, d\) and quadratically on \(\beta\).

V. PROPOSED SEARCH ALGORITHM

We propose an algorithm that uses the derived bounds from previous sections to arrive at a learning rate which exhibits faster convergence than using the inverse of the derived bound.

A. Why is a search algorithm required?

For a derived upper bound \(\alpha\), the corresponding learning rate is found as \(\eta = 1/\alpha\). Note that \(\eta < \eta^*\) (where \(\eta^* = 1/\alpha^*\)) and therefore, any learning rate derived from an upper bound is guaranteed to result in non-increasing traces for GD. However, there may exist learning rates that are greater than \(\eta\) which lead to faster convergence.

Even when the exact value of gradient Lipschitz constant is available, optimality over all possible initializations is considered. However, in practical scenarios, the range of values with which the neural networks are initialized are restricted and hence, we do not require a universally optimal learning rate. In other words, we can afford to have learning rates even higher than \(\eta^*\) as long as it guarantees monotonically decreasing iterates in the region where the weights are initialized.

Summarizing, the motivations for proposing a search are two-fold: the derived bounds may be loose which gives room for finding better learning rates, and we wish to exploit the weight initialization to find a learning rate customized to the initialization.

B. Proposed algorithm

The search is for a learning rate which leads to faster convergence than the inverse of the derived bound, while ensuring that it produces decreasing iterates. This search can be conducted by employing a search interval customized for a given data set and weight initialization. The start-of-the-art
hyper-parameter tuning libraries such as HyperOpt[13] allow the user to set the search space. In our work, we adopt the HyperOpt implementation of TPE[13]. As they do not utilize the information regarding the objective, the search for learning rate is typically conducted in the interval $[0, 1]$.

The algorithm is inspired by binary search [30]. The algorithm is initialized with a learning rate that is guaranteed to converge (i.e., $1/\alpha$ where $\alpha$ is the derived bound) and is allowed a certain number of trials. If the learning rate chosen in a trial results in a converging trace of GD, a higher learning rate is chosen for the next trial; else, a lower learning rate is chosen. The learning rate leading to the lowest loss is reported at the end of the search algorithm. We note that as the algorithm is initialized with a convergent learning rate, it never yields a divergent learning rate, unlike other search algorithms like grid search, random search and HyperOpt. The proposed algorithm is described in Algorithm 1. Note that in the algorithm, $Loss(\eta, T)$ refers to the value of the loss function at the end of $T$ epochs using the learning rate $\eta$.

C. Advantages and remarks

The inverse of the derived gradient Lipschitz constant always acts as a valid learning rate. Therefore, in applications where a slower convergence is acceptable, this method is highly useful since it allows one to actually skip hyperparameter tuning altogether.

In other search methods, the search space is often considered as $[0, 1]$. However, there may be applications where the inverse of the gradient Lipschitz constant is greater than one. This in turn implies that the proposed method will choose learning rates greater than one whilst guaranteeing convergence whereas the traditional methods with restricted search space, say $[0, 1]$ will choose a learning rate less than one.

In the case that the optimal learning rate is of a very low order, search algorithms like random search or HyperOpt may always encounter diverging behaviour even after the allotted number of evaluations are utilized. However, in the case of the proposed BinarySearch algorithm, we are guaranteed to find a learning rate which would result in a successful GD epoch. These advantages are demonstrated with the help of simulations in the forthcoming section.

D. Simulation Results

The effectiveness of the proposed algorithm is compared against HyperOpt. As HyperOpt is already shown to outperform random search [13], we only compare with the HyperOpt tool that uses the TPE. To do so, we run 100 experiments with the same number of evaluations allotted for both HyperOpt and BinarySearch. To compare optimization strategies, we can opt for any of the following metrics:

- Best-found value: The loss achieved during the best-performing evaluation in an experiment is compared and the fraction of times BinarySearch outperforms HyperOpt is tabulated.
- Best trace: The best trace for both the competing algorithms are compared. The learning rate leading to the least area under the convergence curve is said to yield the best trace.

The synthetic simulation is inspired from the setting in works like [15], [16] that deal with the theoretical properties of shallow networks. We consider a data base with points $(x(i), y(i))$ for $i = 1, \ldots, N$ where $x(i) \sim N(0, I)$ similar to [15]. It is assumed that there is an underlying network known as the teacher network with weights $w^*$. The weights of the teacher network are also sampled from a zero mean unit variance Gaussian distribution. The corresponding labels $y(i)$ are generated by passing the data through the teacher network. For our simulations, we consider $N = 100$ with $T$ epochs.

The network to be trained is referred to as the student network. The weights of the student network are initialized using Xavier initialization [31] and the quadratic loss function is employed. The optimization algorithm used for training is GD and it is run for $T$ epochs. The algorithms, both BinarySearch and HyperOpt, are allowed a fixed number of evaluations. This is repeated for 100 experiments (each with a different data base and weight initialization). All results reported are over 100 experiments.

1) One hidden layer networks: For a single hidden layer, we run GD for $T = 100$ epochs. We note that the best learning rate chosen by HyperOpt after the stipulated number of evaluations sometimes still lead to unsuccessful GD epochs in case of ReLU activation, i.e., the iterates diverge while our method never leads to divergent behaviour. The fraction of times that divergent behaviour is observed for HyperOpt is tabulated in Table I. In the remaining successful experiments, we compare the final loss obtained using the learning rate chosen by both BinarySearch and HyperOpt. The fraction of experiments in which BinarySearch outperforms (results in a lower 'best-found value’ than) HyperOpt is tabulated in Table II.

---

1 In this manuscript, we refer to the TPE implementation in the HyperOpt library as simply HyperOpt.

https://sigopt.com/blog/evaluating-hyperparameter-optimization-strategies/
We notice that for higher number of evaluations, BinarySearch always outperforms HyperOpt. It should be noted that these comparisons are performed after eliminating the experiments for which HyperOpt diverges. For instance, for the configuration $d = k = 20$ with 5 evaluations using ReLU activation, BinarySearch outperforms HyperOpt 73% out of the $100 - 37 = 63$ successful experiments. If we also consider the divergent experiments, BinarySearch outperforms HyperOpt 83% of the times. In the case of sigmoid activation, the divergent behaviour is not observed. As the gradient of the loss function is of a small order of magnitude (in the order of $10^{-5}$), GD does not diverge for higher learning rates. Also, the learning rate derived as the inverse of gradient Lipschitz constant for $d = 2, k = 3, N = 100$ is 1.78 which itself is greater than 1. This implies that any learning rate less than 1.78 will never lead to divergent behaviour and learning rates greater than 1.78 can be explored. One can argue that the derived bound can be used to modify the search interval of existing algorithms; this is discussed at the end of this section.

The metric, ‘best-found value’ grades an algorithm based on the final loss value that the algorithm converges to. We also need a metric to quantify the performance in terms of the convergence rate. Hence, we also provide the best-trace graphs for a two-hidden layer network. We note that these comparisons are performed after eliminating the experiments even after allowing 20 evaluations for HyperOpt. In case of sigmoid activation, it is again noted that there is no divergent behaviour. The fraction of the remaining experiments in which BinarySearch outperforms HyperOpt is tabulated in Table IV. It is noticed that the proposed method overtakes the existing method at higher dimensions. Best-trace graphs for a two-hidden layer network resembles the graphs for a single hidden layer and are not produced due to lack of space.

The number of experiments which return unusable (divergent) learning rates increases. For example, in the case of ReLU activation with $k_1 = 10, k_2 = 10$, we obtain divergent learning rates for 44% of the experiments even after allowing 20 evaluations for HyperOpt. In case of sigmoid activation, we note that for a neural network with sigmoid activation function, GD converges for learning rates greater than 1. Hence, the learning rate corresponding to the derived bound ($> 1$) may be set as the lower limit of the search

2) Two hidden layer networks: For a two hidden layer network, we run GD for $T = 200$ epochs as it takes greater number of epochs to converge than the single hidden layer. Similar to the case of a single hidden layer, the fraction of experiments for which HyperOpt chooses divergent values for a network with ReLU activation is tabulated in Table III. We note that as the dimensions of the problem gets bigger,
We now derive an upper bound on the gradient Lipschitz constant of the said loss function. To find the gradient Lipschitz constant of the said loss function, we bound the maximum eigenvalue of the Hessian of \( l(\theta) \). Note that, in this application, the architecture consists of multiple outputs nodes. Therefore, the result in Theorem \( \text{I} \) cannot be used as it is. The bound on the gradient Lipschitz constant hence is derived for this specific case, and the final constant is given by

\[
\alpha^* \leq \frac{1}{N} \sum_{i=1}^{N} \left[ k_1 k_2 \frac{\beta^2}{16} \|x(i)\|_\infty \|x(i)\|_1 + \sum_{l_2=1}^{k_2} \left[ (k_1 \beta - \alpha_{l_2}) \frac{\beta}{10} \|x(i)\|_\infty \|x(i)\|_1 \right] + \frac{k_1 k_2}{4} \beta \|x(i)\|_\infty + \frac{k_1}{4} (k_1 \beta - \min_m o_m) \|x(i)\|_1 \right].
\]

**Sketch of Proof:** The elements of the Hessian matrix \( \nabla^2 l(\theta) \) are computed and the Gerschgorin theorem (Theorem \( \text{III} \)) is then applied to obtain the above result.

1) **Finding the gradient Lipschitz constant:** We follow the notation introduced in Section \( \text{IV} \) where the weight matrix between the input and hidden layer is denoted by \( V \) and the weight matrix between the hidden and output layer is denoted as \( W \). Let the data points be denoted as \((x(i), \alpha(i))\) for \( i = 1, \ldots, N \). Each element of the output vector is denoted as \( o(i)_{l_2} \) where \( l_2 = 1, \ldots, M \). The loss function is given by

\[
l(\theta) = \frac{1}{2N} \sum_{i=1}^{N} \sum_{l_2=1}^{2M} \left[ \left( \sum_{l_1=1}^{k} \sigma(x(i)^T V^T W_{l_1, l_2}) - o(i)_{l_2} \right)^2 \right].
\]

We now consider a OFDM system with \( M = 64 \) sub-carriers where all the sub-carriers consist of the pilot symbol. The pilots are transmitted through the channel and received. All the simulations are performed in the frequency domain. It is assumed that the channel impulse responses are available for training. As done in [18], the number of inputs and outputs to the neural network are \( 2M \) and the number of neurons in the hidden layer are \( k = 10 \).

For our simulations, we have considered a QPSK constellation and an SNR of 10dB.

The learning rate chosen in the paper is a fixed learning rate 0.05. The loss corresponding to the fixed learning rate after \( T = 100 \) time steps is 0.068. The learning rate chosen by Algorithm \( \text{I} \) and the corresponding loss in tabulated in Table \( \text{VI} \). We can see that the proposed method finds a learning rate that is comparable to the one suggested by manual tuning with as low as 5 evaluations. We can also see that the loss that the algorithm converges to is lower than the loss arrived at by using 0.05 as the learning rate.

**VI. APPLICATIONS**

Feedforward shallow networks are widely used in the context of resource allocation [32], wireless communication [18, 20], financial predictions [19] and weather forecasting [33]. In this section, we illustrate the utility of the proposed algorithm in two specific applications.

A. **Channel Estimation in OFDM systems**

The use of neural network for channel estimation is advocated in as traditional estimation methods such as Least Squares and MMSE suffer from lack of accuracy and high computational complexity respectively [17, 18]. We now describe the architecture employed in [18]. A pilot-based channel estimation is considered. A single hidden layer with \( k \) neurons with sigmoid activation function is employed. The real and the imaginary parts of the received pilots are fed separately into the network and the corresponding channel impulses are estimated at the output. The output layer (with linear activation function) has the same number of neurons as the input layer, say \( 2M \) for estimating the channel response the real and imaginary parts of \( M \) sub-carriers. The component-wise sum of the squared difference between the estimated and actual channel response is the objective function to be minimized. The learning rate employed in the paper is 0.05 and is chosen through manual tuning, which usually involves searching through trial and error which is a laborious process. We now derive an upper bound on the gradient Lipschitz constant of the objective and apply Algorithm \( \text{I} \) to find the learning rate.

1) **Finding the gradient Lipschitz constant:** We follow the notation introduced in Section \( \text{IV} \) where the weight matrix between the input and hidden layer is denoted by \( V \) and the weight matrix between the hidden and output layer is denoted as \( W \). Let the data points be denoted as \((x(i), \alpha(i))\) for \( i = 1, \ldots, N \). Each element of the output vector is denoted as \( o(i)_{l_2} \) where \( l_2 = 1, \ldots, M \). The loss function is given by

\[
l(\theta) = \frac{1}{2N} \sum_{i=1}^{N} \sum_{l_2=1}^{2M} \left[ \left( \sum_{l_1=1}^{k} \sigma(x(i)^T V^T W_{l_1, l_2}) - o(i)_{l_2} \right)^2 \right].
\]

We now consider a OFDM system with \( M = 64 \) sub-carriers where all the sub-carriers consist of the pilot symbol. The pilots are transmitted through the channel and received. All the simulations are performed in the frequency domain. It is assumed that the channel impulse responses are available for training. As done in [18], the number of inputs and outputs to the neural network are \( 2M \) and the number of neurons in the hidden layer are \( k = 10 \).

For our simulations, we have considered a QPSK constellation and an SNR of 10dB.

The learning rate chosen in the paper is a fixed learning rate 0.05. The loss corresponding to the fixed learning rate after \( T = 100 \) time steps is 0.068. The learning rate chosen by Algorithm \( \text{I} \) and the corresponding loss in tabulated in Table \( \text{VI} \). We can see that the proposed method finds a learning rate that is comparable to the one suggested by manual tuning with as low as 5 evaluations. We can also see that the loss that the algorithm converges to is lower than the loss arrived at by using 0.05 as the learning rate.

B. **Exchange rate prediction**

Neural networks are used in various aspects of finance such as debt risk assessment, currency prediction, business risk failure, etc. [34]. Applications such as exchange rate prediction hold great importance in the economy. In [19], a single hidden

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**TABLE III:** Fraction of times HyperOpt diverges for 2 hidden layer ReLU

| ReLU activation | Sigmoid activation |
|-----------------|--------------------|
| No. of evaluations | No. of evaluations |
| \( d \) | \( k_1 \) | \( k_2 \) | 5 | 10 | 20 | 5 | 10 | 20 |
| 5 | 3 | 2 | 0.45 | 0.65 | 0.39 | 1 | 0.98 | 0.95 |
| 10 | 5 | 3 | 0.58 | 0.67 | 0.61 | 1 | 0.99 | 0.96 |
| 5 | 10 | 5 | 0.52 | 0.62 | 0.73 | 0.4 | 0.93 | 0.96 |
| 10 | 10 | 10 | 0.56 | 0.66 | 0.86 | 0 | 1 | 1 |

**TABLE IV:** Fraction of times the best value for BinarySearch outperforms HyperOpt for 2 hidden layer out of successful experiments

| No. of evaluations | 5 | 10 | 20 |
|--------------------|---|----|----|
| Learning rate     | 0.033 | 0.062 | 0.084 |
| Loss              | 0.0004 | 3.53e-6 | 3.27 e-23 |
layer neural network is considered where the neurons employ the sigmoid activation function. In the mentioned work, prediction is done using daily, monthly or quarterly steps. For the sake of our demonstration, we consider the daily step prediction. The exchange rates for the previous $d = 5$ days are fed as the input to the network and the prediction for the next day is made. The architecture of the network is the same as the one demonstrated in Fig. I with $d = 5$ input neurons, $k = 10$ neurons at the hidden layer and one output neuron. The data for the experiment is obtained from the website 
http://www.global-view.com/forex-trading-tools/forex-history/index.html as in [19].

The data is organized as $(x(i), y(i))$ for $i = 1, \ldots, N$ training samples; note that $x(i) \in \mathbb{R}^d$ represents the daily step (change in the exchange rate from the previous day) for the past five days and $y(i)$ is the rate for the day (which is the quantity to be estimated). We implement [19] with a slight modification: the network proposed in the paper uses a threshold within every neuron which is also a parameter to be tuned; instead, in this implementation, we add a column of ones to the data to compensate for threshold. Hence, we have $x(i) \in \mathbb{R}^{d+1}$.

We are justified in doing so as we would tune the weight vector corresponding to the $d + 1$th input to the hidden layer instead of tuning the threshold. The loss function used in [19] is given by

$$l(w) = \frac{1}{2N} \sum_{i=1}^{N} \left( \sum_{j=1}^{k} \sigma(x(i)^T w^j) - y(i) \right)^2 , \quad (42)$$

where $w$ denotes the weights of the network to be optimized and $\sigma(.)$ denotes the sigmoid activation function. We note that the loss function is the similar to (3) and hence the bound derived in (25) in Section III can be used.

The paper recommends GD as the optimization algorithm to be used; however, it does not recommend any tuning method for the learning rate for this application. We employ the BinarySearch method proposed in Algorithm I and tabulate the losses encountered after tuning the learning rate for $T = 500$ time steps in Table VI.

|      | No. of evaluations |
|------|-------------------|
|      | 5                 | 10                | 20                |
| BinarySearch | 0.254             | 0.2532            | 0.253             |
| HyperOpt   | 0.255             | 0.255             | 0.254             |

TABLE VI: Loss encountered for exchange rate prediction by Algorithm I and HyperOpt

performs well as compared to HyperOpt using TPE and is able to achieve the optimal loss within a small number of iterations. As it is noted that both the algorithms converge to similar losses, we wish to demonstrate the convergence graphs by plotting the best-trace graphs. From Fig. 5 we note that the proposed BinarySearch algorithm converges faster.

In this section, we demonstrated that the proposed method can be used effectively to tune the learning rate for applications that involve a shallow feedforward network. We considered two popular and very different applications in the communication and finance sector where neural networks are used and

![Fig. 5: Best trace comparison for exchange rate prediction network with 10 evaluations](image)

we demonstrated that the proposed method is competitive with state-of-the-art tuning algorithms.

VII. CONCLUDING REMARKS

In this work, we proposed a theory-based approach for determining the learning rate for a shallow feedforward neural network. We derived the gradient Lipschitz constant for fixed architectures and developed a search algorithm that employs the derived bound to find a better learning rate while ensuring convergence. While the existing algorithms tune harder, i.e., employ higher number of evaluations in order to find a suitable learning rate, we can tune smarter by searching over an interval which is customized to the objective. When allowed the same number of evaluations, we demonstrated that the proposed method outperforms state-of-the-art methods such as HyperOpt in terms of convergence in both synthetic and real data.

APPENDIX A

PROOF OF THEOREM 2

As the function is doubly differentiable, the required constant is $\alpha^* = \max_w \lambda_{\text{max}}(\nabla^2 l(w))$.

$$\nabla l(w) = \left( \sum_{j=1}^{k} s(x^T w^j) - y \right) \begin{bmatrix} \mathbb{I}_{\{x^T w^j \geq 0\}} \mathbf{x} \\ \vdots \\ \mathbb{I}_{\{x^T w^k \geq 0\}} \mathbf{x} \end{bmatrix}$$ (43)

$$\nabla^2 l(w) = \begin{bmatrix} \mathbb{I}_{\{x^T w^1 \geq 0\}} \mathbf{x} & \cdots & \mathbb{I}_{\{x^T w^k \geq 0\}} \mathbf{x} \\ \vdots & \ddots & \vdots \\ \mathbb{I}_{\{x^T w^k \geq 0\}} \mathbf{x} & \cdots & \mathbb{I}_{\{x^T w^k \geq 0\}} \mathbf{x} \end{bmatrix}^T$$

$$= \mathbf{a}(x, w) \mathbf{a}(x, w)^T$$ (44)

where

$$\mathbf{a}(x, w) \triangleq \begin{bmatrix} \mathbb{I}_{\{x^T w^1 \geq 0\}} \mathbf{x} \\ \vdots \\ \mathbb{I}_{\{x^T w^k \geq 0\}} \mathbf{x} \end{bmatrix}.$$ (45)

Although the ReLU function given by $\max(0, x)$ is non-differentiable at $x = 0$, the work in [16] states that if the input is assumed to be from the Gaussian distribution, the
loss function becomes smooth, and the gradient is well defined everywhere. The gradient is given by \( \mathbb{I}_{[x \geq 0]} \) where \( \mathbb{I} \) is the indicator function. By a similar argument, we consider the second derivative to be zero over the entire real line. Note that the Gaussian assumption is only to ensure that the derivative of the ReLU function is defined at \( x = 0 \) due to the smoothness for theoretical tractability. The gradient Lipschitz constant is given by

\[
\alpha^* = \max_w \lambda_{\text{max}}(\nabla^2 l(w)) = \max_w \lambda_{\text{max}}(a(x, w)^T a(x, w)^T). \tag{46}
\]

We note that \( a(x, w)^T a(x, w)^T \) is a rank-1 matrix and therefore, its only non-zero eigenvalue is given by \( a(x, w)^T a(x, w) = \|a(x, w)\|^2 \), which is also the maximum eigenvalue. Substituting in \( \alpha^* \),

\[
\alpha^* = \max_w \|a(x, w)\|^2. \tag{47}
\]

The norm is maximized when all the entries of the vector are non-zero, i.e., when all the indicators correspond to 1. Let us define

\[
\bar{a}(x) \triangleq [x \ldots x]^T, \tag{48}
\]

which is a stack of the input vector repeated \( k \) times. Therefore, the required constant is given by

\[
\alpha^* = \|\bar{a}(x)\|^2 = k \|x\|^2. \tag{49}
\]

In this case, we note that the derived constant for a single data point is not a bound, but the exact gradient Lipschitz constant and it is a function of the number of neurons, \( k \), and the norm of the input vector.

**APPENDIX B**

**PROOF OF LEMMA**

The Rayleigh quotient of a Hermitian matrix \( A \) and a non-zero vector \( g \) is given by \( g^T A g \) and reaches the maximum eigenvalue when the vector \( g \) is the eigen vector corresponding to the maximum eigenvalue \( \lambda_{\text{max}} \).

\[
\lambda_{\text{max}}(A) = \max_{\|g\|=1} g^T A g. \tag{50}
\]

Also, observe that for any other vector of unit norm \( h \neq g \),

\[
g^T A g > h^T A h. \tag{51}
\]

In the following proof, denoting \( x(i) \) as \( x_i \) and the principal eigen vectors of \( \sum_{i=1}^{N} \bar{a}(x_i)\bar{a}(x_i)^T \) and \( \sum_{i=1}^{N} a(x_i, w)^T a(x_i, w)^T \) as \( \bar{g}, g_i \) and \( \tilde{g} \) respectively,

\[
\lambda_{\text{max}} \left( \sum_{i=1}^{N} \bar{a}(x_i)\bar{a}(x_i)^T \right) = \tilde{g}^T \left( \sum_{i=1}^{N} \bar{a}(x_i)\bar{a}(x_i)^T \right) \tilde{g} \\
= \sum_{i=1}^{N} \tilde{g}^T (\bar{a}(x_i)\bar{a}(x_i)^T) \tilde{g} \\
\geq \sum_{i=1}^{N} g_i^T (\bar{a}(x_i)\bar{a}(x_i)^T) g_i^T.
\]

Note that as \( (a(x_i, w)\bar{a}(x_i)\bar{a}(x_i)^T) \) is a rank-1 matrix, the principal eigen vector is given by \( g_i = a(x_i, w) \). Hence,

\[
\sum_{i=1}^{N} g_i^T \bar{a}(x_i)\bar{a}(x_i)^T g_i^T \\
= \sum_{i=1}^{N} a(x_i, w)^T (\bar{a}(x_i)\bar{a}(x_i)) a(x_i, w). \tag{52}
\]

Considering each term in the summation,

\[
a(x_i, w)^T (\bar{a}(x_i)\bar{a}(x_i)) a(x_i, w) \\
= (a(x_i, w)\bar{a}(x_i)\bar{a}(x_i)^T) a(x_i, w) \\
= \left( \sum_{j=1}^{k} \mathbb{I}_{[x_j^T w^j \geq 0]} x_j^T x_i \right) \left( \sum_{j=1}^{k} \mathbb{I}_{[x_j^T w^j \geq 0]} x_j^T x_i \right) \\
= \left( \sum_{j=1}^{k} \mathbb{I}_{[x_j^T w^j \geq 0]} x_j^T x_i \right) \left( \sum_{j=1}^{k} \mathbb{I}_{[x_j^T w^j \geq 0]} x_j^T x_i \right) \\
= \sum_{j=1}^{k} \mathbb{I}_{[x_j^T w^j \geq 0]} x_j^T x_i \sum_{j=1}^{k} \mathbb{I}_{[x_j^T w^j \geq 0]} x_j^T x_i \\
= a(x_i, w)^T (a(x_i, w)\bar{a}(x_i)\bar{a}(x_i)^T) a(x_i, w).
\]

Using this result in \( \alpha^* \),

\[
\sum_{i=1}^{N} a(x_i, w)^T (\bar{a}(x_i)\bar{a}(x_i)) a(x_i, w) \\
= \sum_{i=1}^{N} a(x_i, w)^T (a(x_i, w)\bar{a}(x_i)\bar{a}(x_i)^T) a(x_i, w) \\
\geq \sum_{i=1}^{N} \tilde{g}^T (a(x_i, w)\bar{a}(x_i)\bar{a}(x_i)^T) \tilde{g} \\
= \tilde{g}^T \left( \sum_{i=1}^{N} a(x_i, w)^T a(x_i, w)^T \right) \tilde{g} \\
= \lambda_{\text{max}} \left( \sum_{i=1}^{N} a(x_i, w)^T a(x_i, w)^T \right).
\]

Hence proved.

**APPENDIX C**

**PROOF OF THEOREM**

The loss function is doubly differentiable, and hence,

\[
\alpha^* = \max_{\theta} \lambda_{\text{max}}(\nabla^2 l(\theta)). \tag{53}
\]
The first-order partial derivatives are initially computed as follows,

\[
\frac{\partial l(\theta)}{\partial \theta} = A \frac{\partial A}{\partial \theta} = \left[ \begin{align*}
\left( \sum_{l_2=1}^{k_2} [q_{l_2} \sigma(x^T V^{l_2}) (1 - \sigma(x^T V^{l_2})) W_{l_1 l_2} x] \right) \\
\vdots \\
\left( \sum_{l_2=1}^{k_2} [q_{l_2} \sigma(x^T V^{k_2_1}) (1 - \sigma(x^T V^{k_2_1})) W_{k_1 l_2} x] \right)
\end{align*} \right] \frac{\partial A}{\partial \theta}
\]

where we define the following terms,

\[
A \triangleq \left( \sum_{l_2=1}^{k_2} \sigma \left( \sum_{l_1=1}^{k_1} \sigma(x^T V^{l_1}) W_{l_1 l_2} x \right) - y \right),
\]

\[
q_l \triangleq \sigma \left( \sum_{l_1=1}^{k_1} \sigma(x^T V^{l_1}) W_{l_1 a} \right) \left( 1 - \sigma \left( \sum_{l_1=1}^{k_1} \sigma(x^T V^{l_1}) W_{l_1 a} \right) \right),
\]

\[
q'_l \triangleq \sigma \left( \sum_{l_1=1}^{k_1} \sigma(x^T V^{l_1}) W_{l_1 a} \right) \left( 1 - \sigma \left( \sum_{l_1=1}^{k_1} \sigma(x^T V^{l_1}) W_{l_1 a} \right) \right) \left( 1 - 2 \sigma \left( \sum_{l_1=1}^{k_1} \sigma(x^T V^{l_1}) W_{l_1 a} \right) \right).
\]

The term \( q_l \) is the first derivative and \( q'_l \) is the second derivative of \( \sigma \left( \sum_{l_1=1}^{k_1} \sigma(x^T V^{l_1}) W_{l_1 a} \right) \). We now compute the elements of the required Hessian matrix.

\[
\frac{\partial^2 l(\theta)}{\partial V^i \partial V^j} = \left( \sum_{l_2=1}^{k_2} [q_{l_2} \sigma(x^T V^{l_2}) (1 - \sigma(x^T V^{l_2})) W_{l_1 l_2} x] \right) \frac{\partial^2 A}{\partial \theta^i \partial \theta^j}
\]

It is observed that the elements of the Hessian matrix depend on the values of the parameters in \( \theta \) (through \( A \)) unlike the case with a single hidden layer in which the parameters only appeared as indicators. As the maximization is over \( \theta \), the elements of the matrix \( V \) and \( W \) can be scaled up arbitrarily and the obtained upper bound will be infinity, which is a trivial upper bound. To avoid this, it is assumed that the magnitude of the weights are restricted; i.e., \( |a_i| < \beta \; \forall i \). The Hessian matrix can be written in the following form:

\[
\nabla^2 l(\theta) = \left( \frac{dA}{d\theta} \right) \left( \frac{dA}{d\theta} \right)^T + M,
\]

where the first terms in all the second order partial derivative elements (given in (59) - (62)) are accounted for in \( \left( \frac{dA}{d\theta} \right) \left( \frac{dA}{d\theta} \right)^T \). The rest of the additive terms are represented by the matrix \( M \). Applying Weyl’s inequality (i.e., (12)),

\[
\lambda_{\text{max}}(\nabla^2 l(\theta)) \leq \lambda_{\text{max}} \left( \left( \frac{dA}{d\theta} \right) \left( \frac{dA}{d\theta} \right)^T \right) + \lambda_{\text{max}}(M).
\]

We note that the first term in the above equation is a rank one matrix and has a maximum eigenvalue of \( \| \frac{dA}{d\theta} \|^2 \). The required gradient Lipschitz constant is obtained by maximizing (64).
over all values of $\theta$ and is given by

$$\max_{\theta} \lambda_{\text{max}}(\nabla^2 l(\theta)) \leq \max_{\theta} \left\| \frac{dA}{d\theta} \right\|^2 + \max_{\theta} \lambda_{\text{max}}(M)$$

(65)

Focusing on the first term in (65), the vector $\frac{dA}{d\theta}$ consists of $k_1 k_2$ terms of the form $q_j \sigma(\cdot)$ and $k_1$ terms of the form $\sum_{i=1}^{k_2} q_i \nabla (x(T^IV^k)W_{il}\mathbf{x})$ where $a = 1, \ldots, k_1$. Recall from (16) that $\sigma(\cdot) \leq 1$ and from (17) that $q(\cdot) \leq \frac{1}{2}$. Therefore,

$$\max_{\theta} \left\| \frac{dA}{d\theta} \right\|^2 = k_1 \left( \frac{k_2 \beta \|x\|}{16} \right)^2 + k_1 k_2 \frac{16}{16}$$

(66)

where $\beta = \max \theta_i$. We now focus on the second additive term in (65). To bound the maximum eigenvalue of $M$, the Gershgorin’s theorem (stated in Theorem 3) is employed. Considering the terms in (59) - (62) that are not included in $(\frac{dA}{d\theta})(\frac{dA}{d\theta})^T$, we bound the maximum row sum over all possible values of $\theta$. The row sum can be computed in one of two possible ways considering elements from (a) $\frac{\partial^2 l(\theta)}{$$\partial V_i \partial V_j$}$ or (b) $\frac{\partial^2 l(\theta)}{$$\partial W_{ij} \partial V_{ij}$}$ and $\frac{\partial^2 l(\theta)}{$$\partial W_{ij} \partial V_{ij}$}$.

The maximum value taken by $A$ is $|k_2 - y|$ as the sigmoid function has a maximum value of one. Recall that $q_k$ is a first derivative and $q_k'$ is a second derivative of the sigmoid function. Using the bounds on derivatives stated in (16) - (18),

$$\max_{\theta} \lambda_{\text{max}}(M) \leq |k_2 - y| \max \left\{ \frac{1}{10} \frac{\beta}{10} + \frac{1}{4} + \frac{1}{4}, \frac{k_1 \|x\|}{4}, \frac{k_1 k_2 \|x\|}{4}, \frac{k_1 k_2 \|x\|}{4}, k_1 \frac{k_1 k_2 \|x\|}{4}, \right\}$$

(67)

where the first argument in the maximization corresponds to case (a) and the second argument corresponds to case (b) of computing the row sum. Combining (66) and (67).

$$\alpha^* \leq \max \left\{ \frac{1}{10} + \left[ \frac{1}{4} + \frac{1}{10} \right] \frac{k_1 \|x\|}{4}, \frac{1}{4} + \frac{1}{4}, \frac{1}{4} + \frac{1}{10} \right\}$$

(68)

\[ \frac{k_1 k_2 \|x\|}{4}, \frac{k_1 k_2 \|x\|}{4}, k_1 k_2 \frac{k_1 k_2 \|x\|}{4}, \frac{k_1 k_2 \|x\|}{4}, k_1 \frac{k_1 k_2 \|x\|}{4}, \right\}

**APPENDIX D**

**Proof of Theorem 6**

The aim is to find the gradient Lipschitz constant of $l(\theta)$. For a doubly differentiable function, the required constant is given by

$$\alpha^* = \max_{\theta} \lambda_{\text{max}}(\nabla^2 l(\theta)).$$

(69)

In order to find the Hessian, we initially find the first-order partial derivatives:

$$\frac{\partial l(\theta)}{\partial \theta} = A \frac{\partial A}{\partial \theta}$$

(70)

\[ \begin{bmatrix} \sum_{i=1}^{T_2} \left[ q_i \mathbf{1}_{\{x^T \mathbf{V}^i \geq 0\}} W_{il} \mathbf{x} \right] \\ \vdots \\ \sum_{i=1}^{k_2} \left[ q_i \mathbf{1}_{\{x^T \mathbf{V}^k \geq 0\}} W_{il} \mathbf{x} \right] \\ q_1 s(x^T \mathbf{V}^k) \\ \vdots \\ q_k s(x^T \mathbf{V}^k) \end{bmatrix} \]

(71)

where

$$A \triangleq \left( \sum_{i=1}^{k_2} s \left( \sum_{i=1}^{k_1} s(x^T \mathbf{V}^k) W_{il} \mathbf{x} \right) \right) - y$$

(72)

$$q_a \triangleq I_{x^T \mathbf{V}^k \geq 0}.$$ 

(73)

Similar to one-hidden layer ReLU case, we assume that the gradients of $q_a$ with respect to $W_{i,j}$ and $\mathbf{V}^i$ are 0 and 0 respectively. Now, the second-order partial derivatives are derived.

$$\frac{\partial^2 l(\theta)}{\partial W_{ij} \partial V_{i'j'}} = q_{i'} s(x^T \mathbf{V}^i') \left( q_{i'} s(x^T \mathbf{V}^i') \right)^T$$

(74)

$$\frac{\partial^2 l(\theta)}{\partial V_{i''} \partial V_{i''}} = \left( \sum_{i=1}^{k_2} q_i \mathbf{1}_{\{x^T \mathbf{V}^k \geq 0\}} W_{il} \mathbf{x} \right) \left( \sum_{i=1}^{k_2} q_i \mathbf{1}_{\{x^T \mathbf{V}^k \geq 0\}} W_{il} \mathbf{x} \right)^T$$

(75)

$$\frac{\partial^2 l(\theta)}{\partial W_{ij} \partial V_{i'}} = A q'_{i'} I_{\{x^T \mathbf{V}^k \geq 0\}} \mathbf{1}_{\{i'=i'\}} x^T + \left( \sum_{i=1}^{k_2} q_i \mathbf{1}_{\{x^T \mathbf{V}^k \geq 0\}} W_{il} \mathbf{x} \right) \left( q_{i'} s(x^T \mathbf{V}^i') \right)$$

(76)

$$\frac{\partial^2 l(\theta)}{\partial W_{ij} \partial V_{i'}} = A q_{i'} \mathbf{1}_{\{x^T \mathbf{V}^k \geq 0\}} \mathbf{1}_{\{i'=i\}} x + \left( \sum_{i=1}^{k_2} q_i \mathbf{1}_{\{x^T \mathbf{V}^k \geq 0\}} W_{il} \mathbf{x} \right) \left( q_{i'} s(x^T \mathbf{V}^i') \right).$$

(77)

Note that the Hessian is a square matrix of dimension $k_1 (d + k_2) \times k_1 (d + k_2)$. On putting the Hessian matrix together, it is observed that the Hessian can be written as a sum of two matrices as given below

$$\nabla^2 l(\theta) = \left( \frac{dA}{d\theta} \right) \left( \frac{dA}{d\theta} \right)^T + M,$$

(78)

where $M$ is a matrix with all the elements as zero except for the additional elements corresponding to $\frac{\partial^2 l(\theta)}{\partial W_{ij} \partial V_{i'}}$ and $\frac{\partial^2 l(\theta)}{\partial W_{ij} \partial V_{i'}}$ where $i = i'$. The main diagonal elements of the matrix are always zero and it is also symmetric; there are 2$d k_1 k_2$ non-zero elements in the matrix.
Using Weyl's inequality stated in (12),
\[
\lambda_{\max}(\nabla^2 l(\theta)) \leq \lambda_{\max} \left( \left( \frac{dA}{d\theta} \right)^T \frac{dA}{d\theta} \right) + \lambda_{\max}(M) \]
\[
= \left\| \frac{dA}{d\theta} \right\|^2 + \lambda_{\max}(M). \tag{79}
\]

The maximum eigenvalue of the matrix \(M\) can be bounded using the Brauer’s Ovals of Cassini bound (stated in Theorem 4).
\[
\lambda_{\max}(M) \leq \max_{i \neq j} \left( \frac{m_{ii} + m_{jj}}{2} + \sqrt{(m_{ii} - m_{jj})^2 + R_i(M) R_j(M)} \right) \tag{80}
\]
where \(R_i(M) = \sum_{j \neq i} |m_{ij}|\). It is noted that all diagonal elements are always zero and multiple rows have similar row sums. Therefore, the bound reduces to
\[
\lambda_{\max}(M) \leq \max_i R_i(M) \tag{82}
\]
This is the same as the Gersgorin’s bound obtained for the matrix \(M\). Note that the elements of the matrix \(M\) are the first terms in (76) and (77) corresponding to the case when \(i = i’\). The structure of the matrix \(M\) is such that the maximum row sum can be computed in one of two ways: \(Ak\) times the maximum element of vector \(x\), or \(A\) times the sum of elements of \(x\). Therefore, while maximizing over \(\theta\), the maximum row sum of \(M\) is given by
\[
\max_i R_i(M) = \max(Ak_2 \theta |x|_\infty, A |x|_1), \tag{83}
\]
where \(|x|_\infty = \max_i x_i\) and \(|x|_1 = \sum_i x_i\).
We can write (80) as
\[
\lambda_{\max}(\nabla^2 l(\theta)) \leq \left\| \frac{dA}{d\theta} \right\|^2 + \max\{A(k_2 \theta |x|_\infty, A |x|_1). \tag{84}
\]
To obtain the desired bound on the gradient Lipschitz constant, we maximize over all possible values of \(\theta\) to obtain,
\[
\max_{\theta} \lambda_{\max}(\nabla^2 l(\theta)) \leq \max_{\theta} \left\| \frac{dA}{d\theta} \right\|^2 + \max \lambda_{\max}(M). \tag{85}
\]
The first term is an outer product of vectors (matrix of rank 1) and hence, the eigenvalue is given by their inner product. The vector \(\frac{dA}{d\theta}\) consists of \(k_1(d + k_2)\) terms each with an indicator, an element from \(\theta\) and the input vector. Recall that to avoid arbitrary scaling of the derived bound, we impose the following restriction that \(|\theta_i| \leq \beta\) \(\forall i\). Therefore,
\[
\max_{\theta} \left\| \frac{dA}{d\theta} \right\|^2 = k_1(d + k_2) \beta^2 \|x\|^2. \tag{86}
\]
To maximize the second term in (85), we note that the scalar term \(A\) is a sum of \(k_1k_2\) combinations of product of two weight parameters with the data vector \(x\). The maximum value that the scalar \(A\) can take is denoted by \(A_{\max} = k_1k_2\beta^2 \|x\|^2 - y\). Therefore, the second term is maximized as
\[
\max_{\theta} \lambda_{\max}(M) = \max(A_{\max}k_2 \theta |x|_\infty, A_{\max} |x|_1), \tag{87}
\]
where \(A_{\max} = k_1k_2\beta^2 \|x\|^2 - y\). Combining (85), (86) and (87), we obtain
\[
\alpha^* \leq k_1(d + k_2) \beta^2 \|x\|^2 + \max(A_{\max}k_2 \theta |x|_\infty, A_{\max} |x|_1). \tag{88}
\]
An upper bound on the gradient Lipschitz constant for a two hidden layer ReLU network is derived.

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