Abstract

The Lipschitz constant of a network plays an important role in many applications of deep learning, such as robustness certification and Wasserstein Generative Adversarial Network. We introduce a semidefinite programming hierarchy to estimate the global and local Lipschitz constant of a multiple layer deep neural network. The novelty is to combine a polynomial lifting for ReLU functions derivatives with a weak generalization of Putinar’s positivity certificate. This idea could also apply to other, nearly sparse, polynomial optimization problems in machine learning. We empirically demonstrate that our method not only runs faster than state-of-the-art linear programming based method, but also provides sharper bounds.

Keywords: Polynomial Optimization, Lipschitz Constant, Neural Network.

1 Introduction

Throughout this paper, we focus on the multiple layer neural networks $F$ whose activation function is ReLU, which is simply defined as $\text{ReLU}(x) = \max\{0, x\}$ for $x \in \mathbb{R}$. The main purpose is to propose a computationally efficient method to give a valid upper bound of the Lipschitz constant of the network. Recall that a function $f$, defined on $\mathcal{X} \subseteq \mathbb{R}^n$, is $L$-Lipschitz with respect to the norm $\| \cdot \|$ means that for all $x, y \in \mathcal{X}$, we have $|f(x) - f(y)| \leq L\|x - y\|$. The Lipschitz constant of $f$ with respect to norm $\| \cdot \|$, denoted by $L_f$, is the infimum of all
those valid $L$s:

$$L_f^{\|\cdot\|} := \inf \{ L : \forall x, y \in \mathcal{X}, |f(x) - f(y)| \leq L\|x - y\| \}.$$  \hspace{1cm} (1)

The Lipschitz constant of a neural network plays an important role in many applications of deep learning and robustness certification of deep neural networks has emerged as a hot topic. See, e.g., recent contributions by [29, 7] based on semidefinite programming (SDP), by [6, 39] based on linear programming (LP), by [32] based on mixed integer programming (MIP), and by [5, 40, 38, 37] based on the outer polytope of the feasible domain. Instead of certifying robustness directly, another possible route is to compute upper bounds of the Lipschitz constant of the neural network [33].

Another example is the Wasserstein Generative Adversarial Network (WGAN) [3]. Instead of estimating the Wasserstein distance of two distinct measures using its dual on the space of functions whose Lipschitz constants are at most 1, one uses the space encoded by neural networks whose Lipschitz constants are at most 1. But this requires a precise estimation of the Lipschitz constant of a neural network. See recent contributions by [9] based on heuristic penalties, by [23] based on upper bounds, and by [2] based on choices of activation functions.

Recently there has been a growing interest in polynomial optimization for such deep learning applications. For instance, in [29], robustness certification is modeled as a quadratically constrained quadratic problem (QCQP) for ReLU network. Similarly, in [19], an upper bound on the Lipschitz constant of an ELU network is obtained by solving a polynomial optimization problem (POP).

One important reason why polynomial optimization flows into the trend is because, in contrast to optimization problems with more general functions, powerful (global) positivity certificates are available for POP. Such certificates are needed if the goal is to approximate the global optimum as closely as desired [15].

Such positivity certificates have been already applied with success in various areas of science and engineering. The first attempt to compute lower bounds of a QCQP by solving an SDP can be traced back to [30]. Recently this Shor’s relaxation has been applied to certify robustness of neural networks in [29]. Krivine-Stengle’s certificates [13, 31, 17] are implemented via an LP-based hierarchy and provide approximations from below that converge to the global minimum of a POP. In [19], Krivine-Stengle’s certificates are used to bound the Lipschitz constant of neural networks. Putinar’s certificate [27, 15] is implemented via an SDP-based hierarchy (a.k.a., “Lasserre’s hierarchy”) and provides approximations from below (resp. above) that converge to the global minimum (resp. maximum) of a POP. Various applications in and outside optimization are described in, e.g., [14]; in particular, see also its application to large scale optimal power flow (OPF) problems in [24, 25] and for roundoff error certification in [22].

In terms of computational complexity, the LP-based hierarchy is cheaper than the SDP-based hierarchy, but has been proven to be less efficient for combinatorial 0/1 optimization [20], and cannot converge in finitely many steps for continuous POPs. Lasserre’s hierarchy has also become a basic tool to prove/disprove
Khot’s celebrated Unique Games Conjecture (UGC) [12]. Finally, other weaker positivity certificates can be used, e.g., the DSOS/SDSOS [1] framework which is based on LP/second-order cone programming, or the hybrid BSOS hierarchy [17], which combines features of the LP and SDP hierarchies, with semidefiniteness constraints of constant size, fixed in advance and chosen by the user.

1.1 Related Works

For multiple layer deep neural networks, we can obtain an upper bound of its Lipschitz constant by a simple product of the layer-wise Lipschitz constants [11]. However this kind of upper bound is extremely loose and has many limitations for further applications, as shown in [11]. Still using products of the layer-wise Lipschitz constants, [34] propose an improvement via a finer reformulation for calculating the Lipschitz constant of each layer.

Instead of approaching the goal successively by estimating the Lipschitz constant of neural networks in each layer, [19] propose a QCQP formulation to estimate the Lipschitz constant of neural networks. Then by solving its Shor’s relaxation they obtain an upper bound of the Lipschitz constant. Alternatively, by using Krivine-Stengle positivity certificates of higher degree (but LP-based), [19] obtain tighter upper bounds. By another SDP-based method, [8] provide an upper bound of the Lipschitz constant for a multiple layer neural network. However this method is restricted to the $L_2$-norm whereas most deep learning applications are rather concerned with the $L_\infty$-norm.

1.2 Preliminaries and Notations

Denote by $F$ the multiple layer neural network, $m$ the number of hidden layers, $p_0, p_1, \ldots, p_m$ the number of nodes in the input layer and each hidden layer. For simplicity, $(p_0, p_1, \ldots, p_m)$ will denote the layer structure of network $F$. Let $x_0$ be the initial input, and $x_1, \ldots, x_m$ be the activation vectors in each hidden layer. Each $x_i$, $i = 1, \ldots, m$, is obtained by a weight $A_i$, a bias $b_i$, and an activation function $\sigma$, i.e., $x_i = \sigma(A_i x_{i-1} + b_i)$. In this paper, we consider coordinatewise application of the Rectified Linear Units (ReLU) activation function, which is defined as $\text{ReLU}(x) = \max\{0, x\}$ for $x \in \mathbb{R}$, and whose derivative is the Heaviside function $\text{ReLU}'(x) = 1_{\{x>0\}}$ for $x \in \mathbb{R}$.

We assume that the last layer in our neural network is a softmax layer with $K$ entries, that is, the network is a classifier for $K$ labels. For each label $k \in \{1, \ldots, K\}$, the score of label $k$ is obtained by an affine product with the last activation vector, i.e., $c_k^T x_m$ for some $c_k \in \mathbb{R}^{p_m}$. The final output is the label with the highest score, i.e., $y = \arg \max_k c_k^T x_m$.

1.3 Contribution

• We first express both graphs of ReLU and ReLU’ functions via basic closed semialgebraic sets, i.e., sets defined with finite conjunctions of polynomial
Indeed, if \( y = \text{ReLU}(x) \) and \( z = \text{ReLU}'(x) \), then equivalently:

\[
y(y - x) = 0; \quad y \geq x, \ y \geq 0. \tag{2}
\]
\[
z(z - 1) = 0; \quad (z - 1/2) x \geq 0. \tag{3}
\]

Being exact, this semi-algebraic reformulation is a noticeable improvement compared to the model proposed in [19] where the derivative of ReLU is simply replaced with a decision variable lying between 0 and 1 (and so is only approximated).

Next we provide a heuristic approach based on an SDP-hierarchy for nearly sparse polynomial optimization problems. In such problems one assumes that only a few affine constraints destroy a sparsity pattern satisfied by the other constraints. This new approach is mainly based on the sparse version of the Lasserre’s hierarchy, popularized in [35, 16]. It provides upper bounds tighter than those obtained by the LP-based hierarchy in [19].

### 1.4 Main Results

In the recent work [19] the authors exploit a certain sparsity structure arising from a neural network. Consider a neural network \( F \) with one single hidden layer, and 4 nodes in each layer. The network \( F \) is said to have a sparsity of 2 if its weight matrix \( A \) is symmetric, of the form:

\[
\begin{pmatrix}
* & * & 0 & 0 \\
* & * & * & 0 \\
0 & * & * & * \\
0 & 0 & * & *
\end{pmatrix}
\]  

(4)

Larger sparsity values refer to symmetric matrices with band structure of a given size. This sparsity structure (4) of the networks greatly influences the number of variables involved in the LP program to solve in [19]. This is in deep contrast with our method which does not require the weight matrix to be as in (4). Hence when the network is fully-connected, our method is more efficient and provides tighter upper bounds.

Table 1 and 2 give a brief comparison outlook of the results obtained by our method and the method in [19]. The abbreviation “HR-2” stands for the second-order SDP-based method we propose, and “LipOpt-3/4” stands for the LP-based method from [19] (which uses Krivine-Stengle’s positivity certificate of degree 3 or 4). The numerical result is the global Lipschitz upper bound for neural networks of different sizes. We vary the size of the sparsity pattern (4) of \( F \), and compare the upper bound and running time obtained by each method. All execution times have been computed by averaging over ten runs.

### 2 Problem Setting

In this section, we recall basic facts about optimization and build the polynomial optimization model for estimating Lipschitz constant of neural networks.
Table 1: Global Lipschitz constant of networks of size (80, 80) obtained by (HR-2) and (LipOpt-3) on various sparsities $s$. Results relate to 10 random networks and the table displays averages. Apart from $s = 10$, which is not significative, HR-2 obtains much better bounds and is also much more efficient than LipOpt-3.

|       | $s = 10$ | $s = 20$ | $s = 30$ | $s = 40$ |
|-------|----------|----------|----------|----------|
| HR-2  | OBJ. 1.45 | 2.05     | 2.41     | 2.68     |
|       | TIME 3.14 | 7.78     | 8.61     | 9.82     |
| LipOpt-3 | OBJ. 1.42 | 2.55     | 3.47     | 4.23     |
|       | TIME 22.4 | 69.6     | 224      | 415      |

Table 2: Global Lipschitz constant of networks of size (20, 20, 10) obtained by (HR-2) and (LipOpt-3, LipOpt-4) on various sparsities $s$. For HR-2, we use the approximation technique introduced at the end of Section 4.2 in order to reduce the objective to degree 2. The table displays averages over 10 random networks. The upper bounds obtained by HR-2 are tighter than LipOpt-3. LipOpt-4 improves slightly over HR-2 only for $s = 6$ at the price of a much higher computation time. For $s = 8$, LipOpt-4 reports numerical issues.

|       | $s = 2$  | $s = 4$  | $s = 6$  | $s = 8$  |
|-------|----------|----------|----------|----------|
| HR-2  | OBJ. 0.08 | 0.25     | 0.42     | 0.55     |
|       | TIME 0.67 | 0.62     | 0.65     | 1.30     |
| LipOpt-3 | OBJ. 0.10 | 0.23     | 0.44     | 0.76     |
|       | TIME 0.12 | 0.54     | 0.63     | 0.80     |
| LipOpt-4 | OBJ. 0.10 | 0.23     | 0.41     | -        |
|       | TIME 0.87 | 100.98   | 1261.25  | -        |

2.1 Polynomial Optimization

In a polynomial optimization problem (POP), one computes the global minimum (or maximum) of a multivariate polynomial function on a basic closed semialgebraic set. If the semialgebraic set is the whole space, the problem is unconstrained, and constrained otherwise. Given a positive integer $n \in \mathbb{N}$, let $x = (x_1, \ldots, x_n)^T$ be a vector of decision variables, and denote by $[n]$ the set $\{1, \ldots, n\}$. A POP has the canonical form:

$$
\inf_{x \in \mathbb{R}^n} \{ f(x) : f_i(x) \geq 0, i \in [p]; g_j(x) = 0, j \in [q] \},
$$

(POP)

where $f, f_i, g_j$ are all polynomials in $n$ variables. With $I \subset \{1, \ldots, n\}$, let $x_I := (x_i)_{i \in I}$ and let $\mathbb{R}[x]$ be the space of real polynomials in the variables $x$ while $\mathbb{R}[x_I]$ is the space of real polynomials in the variables $x_I$. 


In particular, if the objective $f$ and constraints $f_i, g_j$ in POP are all of degree at most 2, we say that the problem is a quadratically constrained quadratic problem (QCQP). The Shor’s relaxation of a QCQP is a semidefinite program which can be solved efficiently numerically. If all polynomials involved in (POP) are affine then the problem is a linear program (LP).

2.2 Semidefinite Programming

Semidefinite programming (SDP) is a subfield of convex conic optimization concerned with the optimization of a linear objective function over the intersection of the cone of positive semidefinite matrices with an affine subspace. A real symmetric $n \times n$ matrix $M$ is said to be positive semidefinite (PSD) if $z^T M z \geq 0$ for all $z \in \mathbb{R}^n$. An SDP can be written in the canonical form:

$$\min_{X \in S^n} \{(C, X)_{S^n} : (A_k, X)_{S^n} = b_k, k \in [m] ; X \succeq 0\},$$

(SDP)

where $S^n$ denotes the space of all real symmetric $n \times n$ matrices, and $(\cdot, \cdot)_{S^n}$ denotes the Frobenius scalar product in $S^n$, i.e., $(A, B)_{S^n} = \sum_{i,j} a_{ij}b_{ij}$ for all $A = \{a_{ij}\}_{ij}, B = \{b_{ij}\}_{ij} \in S^n$.

2.3 Lipschitz Constant Estimation Problem (LCEP)

Suppose we train a neural network $F$ for $K$-classifications and denote by $A_i, b_i, c_k$ its parameters already defined in section 1.2. Thus for an input $x_0 \in \mathbb{R}^{p_0}$, the targeted score of label $\sigma(k)$ at point $x_0$ is $\nabla F_k(x_0) = (\prod_{i=1}^m A_i^T \text{diag}(\sigma'(z_i)))c_k$. We fix a targeted label (label 1 for example) and omit the symbol $k$ for simplicity. According to [19] (Theorem 1), the Lipschitz constant $L_F^{||\cdot||}$ of $F$ with respect to norm $|| \cdot ||$, is the supremum of the gradient’s dual norm, i.e.:

$$L_F^{||\cdot||} = \sup_{x_0 \in \Omega} \| (\prod_{i=1}^m A_i^T \text{diag}(\sigma'(z_i)))c \|_*,$$  \hspace{1cm} (5)

where $\Omega$ is the input space, and $|| \cdot ||_*$ is the dual norm of $|| \cdot ||$, which is defined by $||x||_* := \sup_{x \in \Omega} ||(t, x)||$ for all $x \in \mathbb{R}^n$. When $\Omega = \mathbb{R}^n$, $L_F^{||\cdot||}$ is the global Lipschitz constant of $F$ with respect to norm $|| \cdot ||$. In many cases we are also interested in the local Lipschitz constant of a neural network constrained in a small neighborhood of a fixed input $x_0$. In this situation the input space $\Omega$ is often the ball around $x_0 \in \mathbb{R}$ with radius $\varepsilon$: $\Omega = \{x : ||x - x_0|| \leq \varepsilon\}$. In particular, with the $L_\infty$-norm (and using $l \leq x \leq u \Leftrightarrow (x - l)(x - u) \leq 0$), the input space $\Omega$ is the basic semialgebraic set:

$$\Omega = \{x : (x - x_0 + \varepsilon)(x - x_0 - \varepsilon) \leq 0\}.$$  \hspace{1cm} (6)
Combining (2), (3) and (5), LCEP for neural networks with respect to the norm $||\cdot||$, is the following POP:

\[
\max_{x, y, t} \quad t^T \left( \prod_{i=1}^{m} A_i^T \text{diag}(y_i) \right) c
\]

\begin{align*}
\text{s.t.} & \quad y_i (y_i - 1) = 0, (y_i - 1/2)(A_i x_{i-1} + b_i) \geq 0, i \in [m]; \\
& \quad x_{i-1} (x_{i-1} - A_{i-1} x_{i-2} - b_{i-1}) = 0, 2 \leq i \leq m; \\
& \quad x_{i-1} \geq 0, x_{i-1} \geq A_{i-1} x_{i-2} + b_{i-1}, 2 \leq i \leq m; \\
& \quad t^2 \leq 1, (x_0 - \bar{x}_0 + \varepsilon)(x_0 - \bar{x}_0 - \varepsilon) \leq 0.
\end{align*}

In [19] the authors only use the constraint $0 \leq y_i \leq 1$ on the variables $y_i$, only capturing the Lipschitz character of the considered activation function. We could use the same constraints, this would allow to use activations which do not have semi-algebraic representations such as the Exponential Linear Unit (ELU). However, such a relaxation, despite very generally is a lot coarser than the one we propose. Indeed, LCEP treats an exact formulation of the derivative of the ReLU function by exploiting its semi-algebraic character.

3 Lasserre’s Hierarchy

In this section we briefly introduce the Lasserre’s hierarchy [15] which has already many successful applications in and outside optimization [18]. In the Lasserre’s hierarchy for optimization one approximates the global optimum of the POP

\[
\inf_{x \in \mathbb{R}^n} \{ f(x) : g_i(x) \geq 0, i \in [p] \}, \quad \text{(Opt)}
\]

(where $f, g_i$ are all polynomials in $\mathbb{R}[x]$), by solving a hierarchy of SDPs of increasing size. Equality constraints can also be taken into account easily. Each SDP is a semidefinite relaxation of (Opt) in the form:

\[
\rho_d = \inf_{y} \{ L_Y(f) : L_Y(1) = 1, M_d(y) \succeq 0, M_{d-\omega_i}(g_i y) \succeq 0, i \in [p] \}, \quad \text{(MomOpt-d)}
\]

where $\omega_i = \lceil \deg(g_i)/2 \rceil$, $y = (y_\alpha)_{\alpha \in \mathbb{N}_d^2}$, $L_Y : \mathbb{R}[x] \rightarrow \mathbb{R}$ is the so-called Riesz linear functional:

\[
f (\sum_{\alpha} f_\alpha x^\alpha) \mapsto L_Y(f) := \sum_{\alpha} f_\alpha y_\alpha, \quad f \in \mathbb{R}[x],
\]

and $M_d(y)$, $M_{d-\omega_i}(g_i y)$ are moment matrix and localizing matrix respectively; see [18] for precise definitions and more details. The semidefinite program (MomOpt-d) is the $d$-th order moment relaxation of problem (Opt). As a result, when $K := \{ x : g_i(x) \geq 0, i \in [p] \}$ is compact, one obtains a monotone sequence of lower bounds $(\rho_d)_{d \in \mathbb{N}}$ with the property $\rho_d \uparrow f^*$ as $d \rightarrow \infty$ under a certain technical Archimedean condition; the latter is easily satisfied by including
a quadratic redundant constraint $M - \|x\|^2 \geq 0$ in the definition of $K$ (redundant as $K$ is compact and $M$ is large enough). At last but not least and interestingly, generically the latter convergence is finite [26]. Ideally, one expects an optimal solution $\mathbf{y}^*$ of $\text{MomOpt-d}$ to be the vector of moments up to order $2d$ of the Dirac measure $\delta_{\mathbf{x}^*}$ at a global minimizer $\mathbf{x}^*$ of $\text{Opt}$.

For illustration purpose and without going into details, consider the following simple example where we want to minimize $x_1 x_2$ over the unit disk on $\mathbb{R}^2$. That is:

$$\inf_{\mathbf{x} \in \mathbb{R}^2} \{ f(\mathbf{x}) = x_1 x_2 : g(\mathbf{x}) = 1 - x_1^2 - x_2^2 \geq 0 \}. \quad (7)$$

For $d = 1$, $\mathbf{y} = \{y_{00}, y_{01}, y_{10}, y_{11}, y_{20}\} \in \mathbb{R}^6$, $L_y(f) = y_{11}$, and

$$M_1(\mathbf{y}) = \begin{pmatrix} y_{00} & y_{10} & y_{01} \\ y_{10} & y_{20} & y_{11} \\ y_{01} & y_{11} & y_{02} \end{pmatrix}.$$ 

As $\omega = \lceil \deg(g)/2 \rceil = 1$, $M_0(g \mathbf{y}) \succeq 0$ simply translates to the linear constraint $L_y(g) = 1 - y_{20} - y_{02} \geq 0$. Therefore $\text{MomOpt-d}$ with $d = 1$ reads:

$$\inf_{\mathbf{y} \in \mathbb{R}^6} \{ y_{11} : y_{00} = 1, M_1(\mathbf{y}) \succeq 0, 1 - y_{20} - y_{02} \geq 0 \}, \quad (8)$$

with optimal value $\rho_1 = -1/2 = f^*$. It turns out that $\text{[8]}$ is exactly Shor’s relaxation applied to $\text{[7]}$. In fact, for QCQP the first-order moment relaxation (i.e., $\text{MomOpt-d}$ with $d = 1$) is exactly Shor’s relaxation.

### 3.1 Convergent SDP Relaxations exploiting Sparsity [35]

The hierarchy $\text{MomOpt-d}$ is often referred to as dense Lasserre’s hierarchy since we do not exploit any possible sparsity pattern of the POP. Therefore, if one solves $\text{MomOpt-d}$ with interior point methods (as all current SDP solvers do), then the dense hierarchy is limited to POPs of modest size. Indeed the $d$-th order dense moment relaxation $\text{MomOpt-d}$ involves $(n + 2d^2)$ variables and a moment matrix $M_d(\mathbf{y})$ of size $(n + d^2) = O(n^2)$ at fixed $d$. Fortunately, large-scale POPs often exhibit some structured sparsity patterns which can be exploited to yield a sparse version of $\text{MomOpt-d}$, as initially demonstrated in [35]. As a result, wider applications of Lasserre’s hierarchy have been possible.

Assume that the set of variables in $\text{Opt}$ can be divided into several subsets indexed by $I_k$, for $k \in [l]$, i.e., $[n] = \bigcup_{k=1}^l I_k$, and suppose that the following assumptions hold:

A1: The function $f$ is a sum of polynomials, each involving variables of only one subset, i.e., $f(\mathbf{x}) = \sum_{k=1}^l f_k(\mathbf{x}_{I_k})$;

A2: Each constraint also involves variables of only one subset, i.e., $g_i \in \mathbb{R}[\mathbf{x}_{I_k(i)}]$ for some $k(i) \in \{1, \cdots, l\}$;
A3: The subsets $I_k$ satisfy the Running Intersection Property (RIP): for every $k \in [l-1]$, $I_{k+1} \cap \bigcup_{j=1}^{k} I_j \subseteq I_{s}$, for some $s \leq k$.

A POP with such a sparsity pattern is of the form:
\[
\inf_{x \in \mathbb{R}^n} \{ f(x) : g_l(x_{I_{k(l)}}) \geq 0, i \in [p] \}, \quad \text{(SpOpt)}
\]
and its associated sparse Lasserre’s hierarchy reads:
\[
\theta_d = \inf_y \{ L_y(f) : L_y(1) = 1, M_d(y, I_k) \succeq 0, k \in [l] \};
\]
\[
M_{d-\omega_i}(g_i, y, I_{k(i)}) \succeq 0, i \in [p], \quad \text{(MomSpOpt-d)}
\]
where $d$, $\omega_i$, $y$, $L_y$ are defined as in (MomOpt-d) but with a crucial difference. The matrix $M_d(y, I_k)$ (resp. $M_{d-\omega_i}(g_i, y, I_k)$) is a submatrix of the moment matrix $M_d(y)$ (resp. localizing matrix $M_{d-\omega_i}(g_i y)$) with respect to the subset $I_k$, and hence of much smaller size $O(\tau_k^d)$ if $|I_k| =: \tau_k \ll n$.

For illustration, consider the following POP:
\[
\inf_{x \in \mathbb{R}^2} \{ x_1 x_2 + x_2 x_3 : x_1^2 + x_2^2 \leq 1, x_2^2 + x_3^2 \leq 1 \}.
\]
Define the subsets $I_1 = \{1,2\}$, $I_2 = \{2,3\}$. It is easy to check that assumptions A1, A2 and A3 hold. Define $y = \{y_{000}, y_{100}, y_{010}, y_{001}, y_{200}, y_{110}, y_{101}, y_{020}, y_{011}, y_{002} \} \in \mathbb{R}^{10}$. For $d = 1$, the first-order dense moment matrix reads:
\[
M_1(y) = \begin{pmatrix}
  y_{000} & y_{100} & y_{010} & y_{001} \\
  y_{100} & y_{200} & y_{110} & y_{101} \\
  y_{010} & y_{110} & y_{020} & y_{011} \\
  y_{001} & y_{101} & y_{011} & y_{002}
\end{pmatrix},
\]
whereas the sparse moment matrix $M_1(y, I_1)$ (resp. $M_1(y, I_2)$) is the submatrix of $M_1(y)$ taking red and pink (resp. blue and pink) entries. That is, $M_1(y, I_1)$ and $M_1(y, I_2)$ are submatrices of $M_1(y)$, obtained by restricting to rows and columns concerned with subsets $I_1$ and $I_2$ only.

Therefore, if the maximum size $\tau$ of the subsets is such that $\tau \ll n$, then solving (MomSpOpt-d) rather than (MomOpt-d) results in drastic computational savings. In fact, even with not so large $n$, (MomOpt-d) with $d = 2$ is out of reach for currently available SDP solvers.

Finally, $\theta_d \leq f^*$ for all $d$ and moreover, if the subsets $I_k$ satisfy RIP, then we still obtain the convergence $\theta_d \uparrow f^*$ as $d \to \infty$, like for the dense relaxation (MomOpt-d).

3.2 Link between SDP and Sum-of-Square (SOS)

The primal and dual of Lasserre’s hierarchy (MomOpt-d) nicely illustrate the duality between moments and positive polynomials. Indeed for each fixed $d$, the dual of (MomOpt-d) reads:
\[
\sup_{t \in \mathbb{R}} \{ t : f - t = \sigma_0 + \sum_{i=1}^{p} \sigma_i g_i \}, \quad \text{(SOS-d)}
\]
where $\sigma_0$ is a sum-of-squares (SOS) polynomial of degree at most $2d$, and $\sigma_j$ are SOS polynomials of degree at most $2(d - \omega_i), \omega_i = \lceil \deg(g_j)/2 \rceil$. The right-hand-side of the identity in \((\text{SOS-d})\) is nothing less than Putinar’s positivity certificate \([27]\) for the polynomial $x \mapsto f(x) - t$ on the compact semialgebraic set ${\{x : g_i(x) \geq 0, i \in [p]\}}$.

Similarly, the dual problem of \((\text{MomSpOpt-d})\) implements the sparse Putinar’s positivity certificate \([16, 35]\).

The specific MATLAB toolboxes Gloptipoly \([10]\) and YALMIP \([21]\) can solve the hierarchy \((\text{MomOpt-d})\) and its sparse variant \((\text{MomSpOpt-d})\).

4 Heuristic Approaches

For illustration purpose, consider 1-hidden layer networks. Then in \((\text{LCEP})\) we can define natural subsets $I_i = \{y_1^{(i)}, x_0\}, i \in [p_1]$ (w.r.t. constraints $y_1(y_1 - 1) = 0, (y_1 - 1/2)(A_i x_0 + b_i) \geq 0$, and $(x_0 - x_0 + \varepsilon)(x_0 - x_0 - \varepsilon) \leq 0$); and $J_j = \{t^{(j)}\}$, $j \in [p_0]$ (w.r.t. constraints $t^2 \leq 1$). Clearly, $I_i, J_j$ satisfy the RIP condition and are subsets with smallest possible size. Recall that $x_0 \in \mathbb{R}^{p_0}$. Hence $|I_i| = 1 + p_0$ and the maximum size of the PSD matrices is $\lceil 1 + p_0 + d \rceil$. Therefore, as in real deep neural networks $p_0$ can be as large as 1000, the second-order sparse Lasserre’s hierarchy \((\text{MomOpt-d})\) cannot be implemented in practice.

4.1 Nearly Sparse POP

In fact \((\text{LCEP})\) can be considered as a “nearly sparse” POP, i.e., a sparse POP with some additional “bad” constraints that violate the sparsity assumptions. More precisely, suppose that $f, g_i$ and subsets $I_k$ satisfy assumptions \(A1, A2\) and \(A3\). Let $g$ be a polynomial that violates \(A2\). Then we call the POP

\[
\inf_{x \in \mathbb{R}^n} \{f(x) : g(x) \geq 0, g_i(x) \geq 0, i \in [p]\},
\]

a nearly sparse POP because only one constraint, namely $g \geq 0$, does not satisfy the sparsity pattern \(A2\). This single “bad” constraint $g \geq 0$ precludes us from applying the sparse Lasserre hierarchy \((\text{MomOpt-d})\).

\([30]\) have adapted \((\text{MomSpOpt-d})\) to solve nearly sparse POPs. But the method is limited to nearly sparse POPs with very few “bad” constraints. In the procedure one includes a set of artificial variables for each bad constraint, and the initial subsets are then augmented by two such variables times the number of bad constraints. In \((\text{LCEP})\), we have $p_1$ “bad” constraints $(y_1 - 1/2)(A_i x_{i-1} + b_i) \geq 0$. Thus the maximal size of the subsets (initially $\tau$) would be no less than $\tau + 2p_1$, which does not yield any improvement.
4.2 Heuristic Relaxation

In this situation, we propose a heuristic method which can be applied to problems with arbitrary many constraints that possibly destroy the sparsity. The key idea of our algorithm is:

(i) Keep the “nice” sparsity pattern defined without the bad constraints;

(ii) Associate only low-order localizing matrix constraints to the “bad” constraints.

For illustration, consider problem (NlySpOpt). We already have a sparsity pattern with subsets $I_k$ and an additional “bad” constraint $g \geq 0$ (assumed to be quadratic). Then we consider the sparse moment relaxations $\text{MomSpOpt-d}$ applied to (NlySpOpt) without the bad constraint $g \geq 0$ and simply add two constraints: (i) the moment constraint $M(y) \geq 0$ (with full dense first-order moment matrix $M_1(y)$), and (ii) the linear moment inequality constraint $L_y(g) \geq 0$ (which is the lowest-order localizing matrix constraint $M_0(g(y)) \geq 0$).

To see why the full moment constraint $M_1(y) \geq 0$ is needed, consider the toy problem (9). Recall that the subsets we defined are $I_1 = \{1, 2\}$, $I_2 = \{2, 3\}$. Now suppose that we need to consider an additional “bad” constraint $(1 - x_1 - x_2 - x_3)^2 = 0$. After developing $L_y(g)$, one needs to consider the moment variable $y_{103}$ corresponding to the monomial $x_1 x_3$ in the expansion of $g = (1 - x_1 - x_2 - x_3)^2$, and $y_{103}$ does not appear in the moment matrices $M_d(y, I_1)$ and $M_d(y, I_2)$ because $x_1$ and $x_3$ are not in the same subset. However $y_{103}$ appears in $M_1(y)$ (which is a $n \times n$ matrix).

The $d$-th order heuristic hierarchy (HR-$d$) reads:

$$\inf_y \{ L_y(f) : M_1(y) \geq 0, M_d(y, I_k) \geq 0, k \in [l] ;$$

$$M_{d-\omega_i}(g_i, y, I_{k(i)}) \geq 0, i \in [p] ;$$

$$L_y(g) \geq 0, L_y(1) = 1 \} , \quad \text{(MomNlySpOpt-d)}$$

where $y$, $L_y$, $M_d(y, I_k)$, $M_{d-\omega_i}(g_i, y, I_{k(i)})$ have been defined in section 3.1.

Now let us see how this works for problem (LCEP). First introduce new variables $z_i$ with associated constraints $z_i - A_i x_{i-1} - b_i = 0$, so that all “bad” constraints are affine. Equivalently, we may and will consider the single “bad” constraint $g \geq 0$ with

$$g(z_1, \ldots, x_0, x_1, \ldots) = - \sum_i ||z_i - Ax_{i-1} - b_i||^2,$$

and solve $\text{MomNlySpOpt-d}$. We briefly sketch the rationale behind this reformulation. Let $(y^d)_{d \in \mathbb{N}}$ be a sequence of optimal solutions of $\text{MomNlySpOpt-d}$. If $d \to \infty$, then $y^d \to y$ (possibly for a subsequence $(d_k)_{k \in \mathbb{N}}$), and $y$ corresponds to the moment sequence of a measure $\mu$ supported on $\{ (x, z) : g_i(x, z) \geq 0, i \in [p] ; \int g d\mu \geq 0 \}$. But as $-g$ is a square, $\int g d\mu \geq 0$ implies $g = 0, \mu$-a.e., and therefore $z_i = Ax_{i-1} + b_i, \mu$-a.e. This is why we do not need to consider the higher-order constraints $M_d(g(y)) \geq 0$ for $d > 0$; only $M_0(g(y)) \geq 0$ is sufficient. In fact, we impose the stronger linear constraints $L_y(g) = 0$ and $L_y(z_i - Ax_{i-1} - b_i) = 0$ for all $i \in [p]$. 

For simplicity, assume that the neural networks have only one single hidden layer, i.e., $m = 1$. Denote by $A, b$ the weight and bias respectively. As in $[6]$, we use the fact that $l \leq x \leq u$ is equivalent to $(x - l)(x - u) \leq 0$. Then the local Lipschitz constant estimation problem with respect to $L_\infty$-norm can be written as:

$$\max_{x,y,z,t} \{ t^T A^T \text{diag}(y) c : (z - Ax - b)^2 = 0, \quad t^2 \leq 1, (x - x_0 + \varepsilon)(x - x_0 - \varepsilon) \leq 0, \quad y(y - 1) = 0, (y - 1/2)z \geq 0 \}.$$ (LCEP-MLP)

Define the subsets of \{LCEP-MLP\} to be $I^i = \{x^i, t^i\}$, $J^j = \{y^j, z^j\}$ for $i \in [p_0], j \in [p_1]$, where $p_0, p_1$ are the number of nodes in the input layer and hidden layer respectively. Then the second-order ($d = 2$) heuristic relaxation of (LCEP-MLP) is the following SDP:

$$\inf_y \{ L_y(t^T A^T \text{diag}(y) c) : L_y(1) = 1, M_1(y) \succeq 0, \quad M_2(y, I^i) \succeq 0, i \in [p_0]; M_2(y, J^j) \succeq 0, j \in [p_1]; \quad L_y(z - Ax - b) = 0, L_y((z - Ax - b)^2) = 0, \quad M_1((y_j - 1)y, J^j) \succeq 0, j \in [p_1]; \quad M_1((y_j - 1/2)z, J^j) \succeq 0, j \in [p_1]; \quad M_1((x^{(i)} - \bar{x}_0^{(i)} + \varepsilon)(x^{(i)} - \bar{x}_0^{(i)} - \varepsilon)y, I^i) \succeq 0, \in [p_0]; \quad M_1(t^2_y, I^i) \succeq 0, i \in [p_0] \}. \quad \text{(MomLCEP-2)}$$

The $d$-th order heuristic relaxation \{MomNlySpOpt-$d$\} also applies to multiple layer neural networks. However, if the neural network has $m$ hidden layers, then the criterion in \{LCEP\} is of degree $m + 1$. If $m \geq 2$, then the first-order moment matrix $M_1(y)$ is no longer sufficient, as moments of degree $> 2$ are not encoded in $M_1(y)$ and some may not be encoded in the moment matrices $M_2(y, I^i)$, if they include variables of different subsets.

As a remedy, one possibility is to lift the problem and include artificial variables to obtain an equivalent quadratic objective function. For example, if $xyz$ appear in the criterion, introduce a new variable $s$ and the quadratic constraint $s = yz$, so that $xyz$ is now $xs$ which is bilinear. The price to pay is the addition of variables and constraints.

Another possibility is to approximate the cubic term $xyz$ on the domain $B$ (a box) of $x, y, z$, by a quadratic polynomial: for instance, $xyz \leq p(x, y, z) := \frac{1}{2}xy + \frac{1}{2}yz + \frac{1}{2}xz - \frac{3}{4}x - \frac{1}{4}y - \frac{1}{4}z + \frac{1}{4}$ on $B$ and $p$ minimizes $\max_{(x,y,z) \in B} |q - xyz|$ over all polynomials upper bounds $q$ of degree 2. Of course this would be done off-line as a pre-treatment of the problem (see Section A.2) to replace the initial objective function $f$ by a quadratic polynomial that overestimates $f$. In both cases (lifting or approximation) we may loose some accuracy.
5 Experiments

In this section, we provide results for the global and local Lipschitz constants of random networks of fixed size (80, 80) and with various sparsities. We also compute bounds of a real trained 1-hidden layer network. The complete results can be found in Appendix B and C. For all experiments we focus on the $L_\infty$-norm, the most interesting case for real applications. Let us first provide an overview of the methods with which we compare our results.

**SHOR**: Shor’s relaxation applied to (LCEP). Note that this is different from Shor’s relaxation described in [19] since we apply it to a different QCQP.

**HR-2**: second-order heuristic relaxation applied to (LCEP).

**LipOpt-3**: LP-based method by [19] with degree 3.

**LBS**: lower bound obtained by sampling 50000 random points and evaluating the dual norm of the gradient.

The reason why we list LBS here is because LBS is a valid lower bound on the Lipschitz constant. Therefore all methods should provide a result not lower than LBS, a basic necessary condition of consistency.

As discussed in section 2.3, if we want to estimate the global Lipschitz constant, we need the input space $\Omega$ to be the whole space. In consideration of numerical issues, we set $\Omega$ to be the ball of radius 10 around the origin. For the local Lipschitz constant, we set by default the radius of the input ball as $\varepsilon = 0.1$. In both cases, we compute the Lipschitz constant with respect to the first label. All experiments are run on a personal laptop with a 4-core i5-6300HQ 2.3GHz CPU and 8GB of RAM. We use the (Python) code provided by [19] to execute the experiments for LipOpt. For HR-2 and SHOR, we use the YALMIP toolbox (MATLAB) [21] with MOSEK as a backend to calculate the Lipschitz constants for random networks. For trained network, we implement our algorithm on Julia [4] with MOSEK optimizer to accelerate the computation.

*Remark*: For local Lipschitz constant bound, [19] do not provide codes for LipOpt and thus we are not able to compare with their method.

5.1 Random Network

We first compare the upper bounds for (80, 80) networks, whose weights and biases are randomly generated. We use the codes provided by [19] to generate networks with various sparsities. For each fixed sparsity, we generate 10 different random networks, and apply all the methods to them repeatedly. Then we compute the average upper bound and average running time of those 10 experiments.

[1] https://openreview.net/forum?id=rJe4_xSFDE
Figure 1: Lipschitz constant upper bounds with respect to $L_\infty$ norm obtained by HR-2, SHOR, LipOpt-3 and LBS. We generate random networks of size (80, 80) with sparsity 5, 10, 15, 20, 25, 30, 35, 40. In the meantime, we display median and quartiles over 10 random networks draws.

Figure 2: Running time of HR-2, SHOR, LipOpt-3 and LBS. We generate random networks of size (80, 80) with sparsity 5, 10, 15, 20, 25, 30, 35, 40. In the meantime, we display median and quartiles over 10 random networks draws.

Figure 1 displays a comparison of average upper bounds of global and local Lipschitz constants. For global bounds, we can see from Figure 1 that when the sparsity of the network is small (5, 10, etc.), the LP-based method LipOpt-3 is slightly better than the SDP-based method HR-2. As the sparsity increases, HR-2 provides tighter bounds. Figure 2 shows that LipOpt-3 is more efficient than HR-2 only for sparsity 5. When the networks are dense or nearly dense, our method not only takes much less time, but also gives tighter upper bounds. For global Lipschitz constant estimation, SHOR and HR-2 give nearly the same
Table 3: Comparison of upper bounds of global Lipschitz constant and running time on trained network SDP-NN obtained by HR-2, SHOR, LipOpt-3 and LBS. The network is a fully connected neural network with one hidden layer, with 784 nodes in the input layer and 500 nodes in the hidden layer. The network is for 10-classification, we calculate the upper bound with respect to label 2.

|       | HR-2 | SHOR | LipOpt-3 | LBS |
|-------|------|------|----------|-----|
|       | Glob. Bound | 14.56 | 17.85 | OfM | 9.69 |
|       | Time | 12246 | 2869 | OfM | -   |
|       | Loc. Bound | 12.70 | 16.07 | - | 8.20 |
|       | Time | 20596 | 4217 | - | -   |

upper bounds. However, in the local case, HR-2 provides strictly tighter bounds than SHOR. In both global and local cases, SHOR has smaller computational time than HR-2.

5.2 Trained Network

We use the MNIST classifier (SDP-NN) described in [28]. The network is of size (784, 500). In Table 3, we see that the LipOpt-3 algorithm runs out of memory when applied to the real network SDP-NN to compute the global Lipschitz bound. In contrast, SHOR and HR-2 still work and moreover, HR-2 provides tighter upper bounds than SHOR in both global and local cases. As a trade-off, the running time of HR-2 is around 5 times longer than that of SHOR.

6 Conclusion and Future Work

Optimization Aspect: In this work, we propose a new heuristic moment relaxation based on the dense and sparse Lasserre’s hierarchy. In terms of performance, our method provides bounds no worse than Shor’s relaxation and better bounds in many cases. In terms of computational efficiency, our algorithm also applies to nearly sparse polynomial optimization problems without running into computational issue.

Machine Learning Aspect: The ReLU function and its derivative ReLU’ are semialgebraic. This semialgebraic character is easy to handle exactly in polynomial optimization (via some lifting) so that one is able to apply moment relaxation techniques to the resulting POP. Moreover, our heuristic moment relaxation provides tighter bounds than Shor’s relaxation and the state-of-the-art LP-based algorithm in [19].

https://worksheets.codalab.org/worksheets/0xa21e794020bb474d8804ec7bc0543f52/
Future research: The heuristic relaxation is designed for QCQP (e.g. problem (LCEP) for 1-hidden layer networks). As the number of hidden layer increases, the degree of the objective function also increases and the approach must be combined with lifting or approximation techniques described in [1,2] in order to replace the initial criterion by a quadratic polynomial. Efficient derivation of approximate sparse certificates for high degree polynomials should allow to enlarge the spectrum of applicability of such techniques to larger size networks and broader classes of activation functions. This is an exciting topic of future research.

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A Lifting and Approximation Techniques for Cubic Terms

As discussed at the end of Section 4.2, for 2-hidden layer networks, one needs to reduce the objective function to degree 2 so that the HR-2 algorithm can be adapted to problem (LCEP). Precisely, problem (LCEP) for 2-hidden layer networks is the following POP:

\[
\begin{align*}
\max_{x, y, t} & \quad t^T A_1^T \text{diag}(y_1) A_2^T \text{diag}(y_2) c \\
\text{s.t.} & \quad y_1(y_1 - 1) = 0, (y_1 - 1/2)(A_1 x_0 + b_1) \geq 0, \\
& \quad y_2(y_2 - 1) = 0, (y_2 - 1/2)(A_2 x_1 + b_2) \geq 0, \\
& \quad x_1(x_1 - A_1 x_0 - b_1) = 0, x_1 \geq 0, x_1 \geq A_1 x_0 + b_1; \\
& \quad t^2 \leq 1, (x_0 - \bar{x}_0 + \varepsilon)(x_0 - \bar{x}_0 - \varepsilon) \leq 0.
\end{align*}
\]

A.1 Lifting Technique

Define new decision variable \( s := y_1 y_2^T \), so that the degree of objective is reduced to 2. Problem (LCEP-MLP_2) can now be reformulated as:

\[
\begin{align*}
\max_{x, y, t} & \quad \sum_i t_i (\text{diag}(A_1^{(i)}) A_2^T \text{diag}(c), s) \\
\text{s.t.} & \quad y_1(y_1 - 1) = 0, (y_1 - 1/2)(A_1 x_0 + b_1) \geq 0, \\
& \quad y_2(y_2 - 1) = 0, (y_2 - 1/2)(A_2 x_1 + b_2) \geq 0, \\
& \quad x_1(x_1 - A_1 x_0 - b_1) = 0, x_1 \geq 0, x_1 \geq A_1 x_0 + b_1; \\
& \quad t^2 \leq 1, (x_0 - \bar{x}_0 + \varepsilon)(x_0 - \bar{x}_0 - \varepsilon) \leq 0, s = y_1 y_2^T.
\end{align*}
\]

For problem (ReducedLCEP-MLP_2), we have \( p_1 p_2 \) more variables (\( s \)) and constraints (\( s = y_1 y_2^T \)), where \( y_1 \in \mathbb{R}^{p_1} \) and \( y_2 \in \mathbb{R}^{p_2} \). Even when \( p_1 = p_2 = 100 \), we add 10000 variables and constraints, which will cause a memory issue. This is why we use the following approximation technique as a remedy.

A.2 Approximation Technique

The idea of this approximation technique is to replace every cubic term in the objective of (LCEP-MLP_2) by a quadratic function. For illustration purpose, take \( xyz \) defined on \([0, 1]^3\) as an example. We want to find a quadratic function \( p(x, y, z) \) defined on \([0, 1]^3\) such that for all quadratic function \( \tilde{p}(x, y, z) \geq xyz \) on \([0, 1]^3\),

\[
\max_{x, y, z \in [0, 1]} |p(x, y, z) - xyz| \leq \max_{x, y, z \in [0, 1]} |\tilde{p}(x, y, z) - xyz|.
\]
This can be reformulated as the following SOS hierarchy (based on the Putinar’s certificate [27, 15]): for $d \geq 1$,

$$\inf_{\lambda, p, \sigma, \tau_i} \lambda$$ \quad (10)

subject to

\[
\begin{align*}
\lambda - p(x, y, z) + xyz &= \sigma_0(x, y, z) - \sigma_1(x, y, z)x(x - 1) \\
-\sigma_2(x, y, z)y(y - 1) - \sigma_3(x, y, z)z(z - 1), \\
p(x, y, z) - xyz &= \tau_0(x, y, z) - \tau_1(x, y, z)x(x - 1) \\
-\tau_2(x, y, z)y(y - 1) - \tau_3(x, y, z)z(z - 1).
\end{align*}
\]

where $p$ is a quadratic function, $\sigma_0$ and $\tau_0$ are SOS of degree at most $2d$, $\sigma_i$ and $\tau_i$ are SOS of degree at most $2(d - 1)$. By solving (10) with SOS of degrees up to 4 ($d = 2$), we get

$$xyz \leq \frac{1}{2} xy + \frac{1}{2} yz + \frac{1}{2} zx - \frac{1}{4} x - \frac{1}{4} y - \frac{1}{4} z + \frac{1}{4} =: q_1(x, y, z).$$

Similarly, we have

$$xyz \geq \frac{1}{2} xy + \frac{1}{2} yz + \frac{1}{2} zx - \frac{1}{4} x - \frac{1}{4} y - \frac{1}{4} z =: q_2(x, y, z).$$

Finally, the $L_\infty$-distance between $xyz$ and $q_1$ (or $q_2$) is

$$\max_{x, y, z \in [0, 1]} |q_1(x, y, z) - xyz| = \max_{x, y, z \in [0, 1]} |q_2(x, y, z) - xyz| = \frac{1}{4}.$$

\section*{B Global Lipshitz Constant Estimation for Random Networks}

We use the experimental settings described in Section 5.

\subsection*{B.1 1-Hidden Layer Networks}

Figure 3 displays the average upper bounds of global Lipschitz constant and the running time of different algorithms for 1-hidden layer random networks of different sizes and sparsities. We can see from Figure 3a that when the size of the network is small (10, 20, etc.), the LP-based method LipOpt-3 is slightly better than the SDP-based method HR-2. However, when the size and sparsity of the network increase, HR-2 provides tighter bounds. From Figure 3b, we can see that LipOpt-3 is more efficient than HR-2 only when the size or the sparsity of the network is small (for (10, 10) networks, or for (40, 40) networks of sparsity 5, etc.). When the networks are dense or nearly dense, our method not only takes much less time, but also gives much tighter upper bounds. For global Lipschitz constant estimation, SHOR and HR-2 give nearly the same upper bounds. This is because the sizes of the toy networks are quite small. For big real network, as shown in Table 3, HR-2 provides strictly tighter bound than SHOR. Finally, SHOR is more efficient than HR-2 and LipOpt-3 in terms of computational complexity.
Figure 3: Global Lipschitz constant upper bounds (left) and running time (right) for 1-hidden layer networks with respect to $L_\infty$-norm obtained by Shor, HR-2, LipOpt-3 and LBS. We generate random networks of size 10, 20, 40, 80. For size 10, we consider sparsity 2, 4, 6, 8, 10; for size 20, we consider sparsity 4, 8, 12, 16, 20; for size 40 and 80, we consider sparsity 5, 10, 15, 20, 25, 30, 35, 40. In the meantime, we display median and quartiles over 10 random networks draws.

B.2 2-Hidden Layer Networks

For 2-hidden layer networks, we use the approximation technique described in Section A.2 in order to reduce the objective to degree 2. Figure 4 displays the average upper bounds of global Lipschitz constant and the running time of different algorithms for 2-hidden layer random networks of different sizes and sparsities. We can see from Figure 4a that the SDP-based method HR-2 performs consistently better than the LP-based method LipOpt-3 in all cases. When we increase the degree of LipOpt-3 to 4, we observe a significant improvement. However, according to Figure 4b, the running time of LipOpt-4 increases extremely rapidly. This happens in particular for networks of sparsity 6. For size (5, 5, 10), the running time of LipOpt-4 is 10 times longer than HR-2; for size (10, 10, 10), it is 100 times longer; and for size (15, 15, 10), it is even 1000 times longer. Due to some timing issues or numerical issues, the LipOpt-4 algorithm doesn’t provide valid upper bounds for (15, 15, 10) networks of sparsity 10, (20, 20, 10) networks of size 8 and 10.

C Local Lipschitz Constant Estimation for Random Networks

We use the experimental settings described in Section 5.
Figure 4: Global Lipschitz constant upper bounds (left) and running time (right) for 2-hidden layer networks with respect to $L_\infty$-norm obtained by HR-2, SHOR, LipOpt-3, LipOpt-4 and LBS. We generate random networks of size 5, 10, 15, 20. For each size, we consider sparsity 2, 4, 6, 8, 10. In the meantime, we display median and quartiles over 10 random networks draws.

C.1 1-Hidden Layer Networks

Figure 5 displays the average upper bounds of local Lipschitz constant and the running time of different algorithms for 1-hidden layer random networks of different sizes and sparsities. By contrast with the global case, we can see from Figure 5a that HR-2 gives strictly tighter upper bounds than SHOR. As a trade-off, HR-2 takes more computational time than SHOR. According to Figure 5b, the running time of HR-2 is around 5 times longer than SHOR.

C.2 2-Hidden Layer Networks

For 2-hidden layer networks, we use the approximation technique described in Section A.2 in order to reduce the objective to degree 2. Figure 6a and 6b displays the average upper bounds of local Lipschitz constant and the running time of different algorithms for 2-hidden layer random networks of different sizes and sparsities. By contrast with the global case, we can see from Figure 6a that HR-2 gives strictly tighter upper bounds than SHOR. As a trade-off, HR-2 takes more computational time than SHOR. According to Figure 6b, the running time of HR-2 is just around 5 times longer than SHOR.
Figure 5: Local Lipschitz constant upper bounds (left) and running time (right) for 1-hidden layer networks with respect to $L_\infty$-norm obtained by HR-2, SHOR and LBS. By default, $\varepsilon = 0.1$. We generate random networks of size 10, 20, 40, 80. For size 10, we consider sparsity 2, 4, 6, 8, 10; for size 20, we consider sparsity 4, 8, 12, 16, 20; for size 40 and 80, we consider sparsity 5, 10, 15, 20, 25, 30, 35, 40. In the meantime, we display median and quartiles over 10 random networks draws.

Figure 6: Local Lipschitz constant upper bounds (left) and running time (right) for 2-hidden layer networks with respect to $L_\infty$-norm obtained by HR-2, SHOR and LBS. By default, $\varepsilon = 0.1$. We generate random networks of size 20, 30, 40, 50. For each size, we consider sparsity 10, 20, 30, 40, 50. In the meantime, we display median and quartiles over 10 random networks draws.