On the Tightness of Semidefinite Relaxations for Certifying Robustness to Adversarial Examples

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Abstract

The robustness of a neural network to adversarial examples can be provably certified by solving a convex relaxation. If the relaxation is loose, however, then the resulting certificate can be too conservative to be practically useful. Recently, a less conservative robustness certificate was proposed, based on a semidefinite programming (SDP) relaxation of the ReLU activation function. In this paper, we describe a geometric technique that determines whether this SDP certificate is *exact*, meaning whether it provides both a lower-bound on the size of the smallest adversarial perturbation, as well as a globally optimal perturbation that attains the lower-bound. Concretely, we show, for a least-squares restriction of the usual adversarial attack problem, that the SDP relaxation amounts to the nonconvex projection of a point onto a hyperbola. The resulting SDP certificate is exact if and only if the projection of the point lies on the major axis of the hyperbola. Using this geometric technique, we prove that the certificate is exact over a single hidden layer under mild assumptions, and explain why it is usually conservative for several hidden layers. We experimentally confirm our theoretical insights using a general-purpose interior-point method and a custom rank-2 Burer-Monteiro algorithm.

1 Introduction

It is now well-known that neural networks are vulnerable to *adversarial examples*: imperceptibly small changes to the input that result in large, possibly targeted change to the output [1–3]. Adversarial examples are particularly concerning for safety-critical applications like self-driving cars and smart grids, because they present a mechanism for erratic behavior and a vector for malicious attacks.

Methods for analyzing robustness to adversarial examples work by formulating the problem of finding the *smallest* perturbation needed to result in an adversarial outcome. For example, this could be the smallest change to an image of the digit “3” for a given model to misclassify it as an “8”. The *size* of this smallest change serves as a *robustness margin*: the model is robust if even the smallest adversarial change is still easily detectable.

Computing the robustness margin is a nonconvex optimization problem. In fact, methods that *attack* a model work by locally solving this optimization, usually using a variant of gradient descent [3–6]. A successful attack demonstrates vulnerability by explicitly stating a small—but not necessarily the smallest—adversarial perturbation. Of course, failed attacks do not prove robustness, as there is always the risk of being defeated by stronger attacks in the future. Instead, robustness can be *certified* by proving lower-bounds on the robustness margin [7–18]. Training against a robustness certificate (as an adversary) in turn produces models that are certifiably robust to adversarial examples [10, 19, 20].

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The most useful robustness certificates are *exact*, meaning that they also explicitly state an adversarial perturbation whose size matches their lower-bound on the robustness margin, thereby proving global optimality [7–9]. Unfortunately, the robustness certification problem is NP-hard in general, so most existing methods for exact certification require worst-case time that scales exponentially with respect to the number of neurons. In contrast, *conservative* certificates are more scalable because the have polynomial worst-case time complexity [10–18]. Their usefulness is derived from their level of conservatism. The issue is that a pessimistic assessement for a model that is ostensibly robust can be attributed to either undue conservatism in the certificate, or an undiscovered vulnerability in the model. Also, training against an overly conservative certificate will result in an overly cautious model that is too willing to sacrifice performance for perceived safety.

Recently, Raghunathan et al. [21] proposed a less conservative certificate based on a *semidefinite programming* (SDP) relaxation of the rectified linear unit (ReLU) activation function. Their empirical results found it to be significantly less conservative than competing approaches, based on linear programming or propagating Lipschitz constants. In other domains, ranging from integer programming [22, 23], polynomial optimization [24, 25], matrix completion [26, 27], to matrix sensing [28], the SDP relaxation is often *tight*, in the sense that it is formally equivalent to the original combinatorially hard problem. Within our context, tightness corresponds to exactness in the robustness certificate. Hence, the SDP relaxation is a good candidate for exact certification in polynomial time, possibly over some restricted class of models or datasets.

This paper aims to understand when the SDP relaxation of the ReLU becomes tight, with the goal of characterizing conditions for exact robustness certification. Our main contribution is a geometric technique for analyzing tightness, based on splitting a least-squares restriction of the adversarial attack problem into a sequence of projection problems. The final problem projects a point onto a nonconvex hyperboloid (i.e. a high-dimensional hyperbola), and the SDP relaxation is tight if and only if this projection lies on the major axis of the hyperboloid. Using this geometric technique, we prove that the SDP certificate is generally exact for a single hidden layer. The certificate is usually conservative for several hidden layers; we use the same geometric technique to offer an explanation for why this is the case.

Notations. Denote *vectors* in boldface lower-case $\mathbf{x}$, *matrices* in boldface upper-case $\mathbf{X}$, and *scalars* in non-boldface x, X. The bracket denotes *indexing* $\mathbf{x}[i]$ starting from 1, and also *concatenation*, which is row-wise via the comma $[a, b]$ and column-wise via the semicolon $[a; b]$. The i-th canonical basis vector $\mathbf{e}_i$ satisfies $\mathbf{e}_i[i] = 1$ and $\mathbf{e}_i[j] = 0$ for all $j \neq i$. The usual *inner product* is $\langle \mathbf{a}, \mathbf{b} \rangle = \sum_i \mathbf{a}[i]\mathbf{b}[i]$, and the usual rectified linear unit activation function is $\mathrm{ReLU}(\mathbf{x}) \equiv \max\{\mathbf{x}, 0\}$.

2 Main results

Let $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ be a feedforward ReLU neural network classifier with ℓ hidden layers

$$\mathbf{f}(\mathbf{x}_0) = \mathbf{x}_\ell \text{ where } \quad \mathbf{x}_{k+1} = \mathrm{ReLU}(\mathbf{W}_k \mathbf{x}_k + \mathbf{b}_k) \quad \text{for all } k \in \{0, 1, \ldots, \ell - 1\}, \tag{2.1}$$

that takes an input $\hat{\mathbf{x}} \in \mathbb{R}^n$ (say, an image of a hand-written single digit) labeled as belonging to the i-th of m classes (say, the 5-th of 10 possible classes of single digits), and outputs a prediction vector $\mathbf{s} = \mathbf{W}_\ell \mathbf{f}(\hat{\mathbf{x}}) + \mathbf{b}_\ell \in \mathbb{R}^m$ whose i-th element is the largest, as in $\mathbf{s}[i] > \mathbf{s}[j]$ for all $j \neq i$. Then, the problem of finding an adversarial example $\mathbf{x}$ that is similar to $\hat{\mathbf{x}}$ but causes an incorrect j-th class to be ranked over the i-th class can be posed

$$d_j^\star \quad = \quad \min_{\mathbf{x} \in \mathbb{R}^n} \quad \|\mathbf{x} - \hat{\mathbf{x}}\| \quad \text{subject to} \quad (2.1), \quad \langle \mathbf{w}, \mathbf{f}(\mathbf{x}) \rangle + b \leq 0, \tag{A}$$

where $\mathbf{w} = \mathbf{W}_\ell^T(\mathbf{e}_i - \mathbf{e}_j)$ and $b = \mathbf{b}_\ell^T(\mathbf{e}_i - \mathbf{e}_j)$. In turn, the adversarial example $\mathbf{x}^\star$ most similar to $\hat{\mathbf{x}}$ over *all* incorrect classes gives a *robustness margin* $d^\star = \min_{j \neq i} d_j$ for the neural network.

In practice, the SDP relaxation for problem (A) is often loose. To understand the underlying mechanism, we study a slight modification that we call its *least-squares restriction*

$$L^\star \quad = \quad \min_{\mathbf{x} \in \mathbb{R}^n} \quad \|\mathbf{x} - \hat{\mathbf{x}}\| \quad \text{subject to} \quad (2.1), \qquad \|\mathbf{f}(\mathbf{x}) - \hat{\mathbf{z}}\| \leq \rho, \tag{B}$$

where $\hat{\mathbf{z}} \in \mathbb{R}^m$ is the targeted output, and $\rho > 0$ is a radius parameter. Problem (A) is equivalent to problem (B) taken at the limit $\rho \to \infty$, because a half-space is just an infinite-sized ball

$$\|\mathbf{z} + \mathbf{w}\left(b/\|\mathbf{w}\|^2 + \rho/\|\mathbf{w}\|\right)\|^2 \leq \rho^2 \quad \Longleftrightarrow \quad \tfrac{\|\mathbf{w}\|}{2\rho}\|\mathbf{z} + \mathbf{w}\left(b/\|\mathbf{w}\|^2\right)\|^2 + [\langle \mathbf{w}, \mathbf{z} \rangle + b] \leq 0 \tag{2.2}$$

with a center $\hat{\mathbf{z}} = -\mathbf{w}\left(b/\|\mathbf{w}\|^2 + \rho/\|\mathbf{w}\|\right)$ that tends to infinity alongside the ball radius ρ. The SDP relaxation for problem (B) is often tight for finite values of the radius ρ. The resulting solution $\mathbf{x}$ is a *strictly* feasible (but suboptimal) attack for problem (A) that causes misclassification $\langle \mathbf{w}, \mathbf{f}(\mathbf{x})\rangle + b < 0$. The corresponding optimal value $L^\star$ gives an upper-bound $d_{\text{ub}} \equiv L^\star \geq d^\star$ that converges to an equality as $\rho \to \infty$. (See Appendix E for details.)

In Section 5, we completely characterize the SDP relaxation for problem (B) over a single hidden neuron, by appealing to the underlying geometry of the relaxation. In Section 6, we extend these insights to partially characterize the case of a single hidden layer.

Theorem 2.1 (One hidden neuron)**.** *Consider the one-neuron version of problem (B), explicitly written*

$$L^\star \quad = \quad \min_{x} \quad |x - \hat{x}| \quad \textit{subject to} \quad |\mathrm{ReLU}(x) - \hat{z}| \leq \rho. \tag{2.3}$$

The SDP relaxation of (2.3) yields a tight lower-bound $L_{\text{lb}} = L^\star$ and a globally optimal $x^\star$ satisfying $|x^\star - \hat{x}| = L_{\text{lb}}$ if and only if one of the two conditions hold: (i) $\rho \geq |\hat{z}|$; or (ii) $\rho < \hat{z}/(1 - \min\{0, \hat{x}/\hat{z}\})$.

Theorem 2.2 (One hidden layer)**.** *Consider the one-layer version of problem (B), explicitly written*

$$L^\star \quad = \quad \min_{\mathbf{x}\in\mathbb{R}^n} \quad \|\mathbf{x} - \hat{\mathbf{x}}\| \quad \textit{s.t.} \quad \|\mathrm{ReLU}(\mathbf{W}\mathbf{x}) - \hat{\mathbf{z}}\| \leq \rho \tag{2.4}$$

The SDP relaxation of (2.3) yields a tight lower-bound $L_{\text{lb}} = L^\star$ and a globally optimal $\mathbf{x}^\star$ satisfying $\|\mathbf{x}^\star - \hat{\mathbf{x}}\| = L_{\text{lb}}$ if one of the two conditions hold: (i) $\rho \geq \|\mathrm{ReLU}(\mathbf{W}\hat{\mathbf{x}}) - \hat{\mathbf{z}}\|$; or (ii) $\rho < \hat{z}_{\min}/2(1+\kappa)$ and $\|\mathbf{W}\hat{\mathbf{x}} - \hat{\mathbf{z}}\|_\infty < \hat{z}_{\min}^2/(2\rho\kappa)$ where $\hat{z}_{\min} = \min_i \hat{z}_i$ and $\kappa = \|\mathbf{W}\|^2\|(\mathbf{W}\mathbf{W}^T)^{-1}\|_\infty$.

The lack of a weight term in (2.3) and a bias term in (2.3) and (2.4) is without loss of generality, as these can always be accommodated by shifting and scaling $\mathbf{x}$ and $\hat{\mathbf{x}}$. Intuitively, Theorem 2.1 and Theorem 2.2 say that the SDP relaxation tends to be tight if the output target $\hat{\mathbf{z}}$ is *feasible*, meaning that there exists some choice of $\mathbf{u}$ such that $\hat{\mathbf{z}} = \mathbf{f}(\mathbf{u})$. (The condition $\rho < \hat{z}_{\min}/2(1+\kappa)$ is sufficient for feasibility.) Conversely, the SDP relaxation tends to be loose if the radius $\rho > 0$ lies within an intermediate band of "bad" values. For example, over a single neuron with a feasible $\hat{z} = 1$, the relaxation is loose if and only if $\hat{x} \leq 0$ and $1/(1 + |\hat{x}|) \leq \rho < 1$. These two general trends are experimentally verified in Section 8.

In the case of multiple layers, the SDP relaxation is usually loose, with a notable exception being the trivial case with $L^\star = 0$.

Corollary 2.3 (Multiple layers)**.** *If $\rho \geq \|\mathbf{f}(\hat{\mathbf{x}}) - \hat{\mathbf{z}}\|$, then the SDP relaxation of problem (B) yields the tight lower-bound $L_{\text{lb}} = L^\star = 0$ and the globally optimal $\mathbf{x}^\star = \hat{\mathbf{x}}$ satisfying $\|\mathbf{x}^\star - \hat{\mathbf{x}}\| = 0$.*

The proof is given in Appendix E. In Section 7, we explain the looseness of the relaxation for multiple layers using the geometric insight developed for the single layer. As mentioned above, the general looseness of the SDP relaxation for problem (B) then immediately implies the general looseness for problem (A).

3 Related work

Adversarial attacks, robustness certificates, and certifiably robust models. Adversarial examples are usually found by using projected gradient descent to solve problem (A) with its objective and constraint swapped [3–6]. Training a model against these empirical attacks generally yield very resilient models [4–6]. It is possible to certify robustness exactly despite the NP-hardness of the problem [7–9, 29]. Nevertheless, conservative certificates show greater promise for scalability because they are polynomial-time algorithms. From the perspective of tightness, the next most promising techniques after the SDP relaxation are relaxations based on linear programming (LP) [10–13], though techniques based on propagating bounds and/or Lipschitz constants tend to be much faster in practice [14–18]. Aside from training a model against a robustness certificate [10, 19, 20], certifiably robust models can also be constructed by randomized smoothing [30–32].

Tightness of SDP relaxations. The geometric techniques used in our analysis are grounded in the classic paper of Goemans and Williamson [33] (see also [34–36]), but our focuses are different: they prove general bounds valid over entire classes of SDP relaxations, whereas we identify specific SDP relaxations that are exactly tight. In the sense of tight relaxations, our results are reminescent of the guarantees by Candès and Recht [26], Candès and Tao [27] (see also [37, 38]) on the matrix completion problem, but our approaches are very different: their arguments are based on using the dual to imply tightness in the primal, whereas our proof analyzes the primal directly.

After this paper was submitted, we became aware of two parallel work [39, 40] that also study the tightness of SDP relaxations for robustness to adversarial examples. The first, due to Fazlyab et al. [39], uses similar techniques like the S-procedure to study a different SDP relaxation constructed from robust control techniques. The second, due to Dvijotham et al. [40], studies the same SDP relaxation within the context of a different attack problem, namely the version of Problem (A) with the objective replaced by the infinity norm distance $\|\mathbf{x} - \hat{\mathbf{x}}\|_\infty$.

Efficient algorithms for SDPs. While SDPs are computationally expensive to solve using off-the-shelf algorithms, efficient formulation-specific solvers were eventually developed once their use case became sufficiently justified. In fact, most state-of-the-art algorithms for phase retrieval [41–44] and collaborative filtering [45–49] can be viewed as highly optimized algorithms to solve an underlying SDP relaxation. Our rank-2 Burer-Monteiro algorithm in Section 8 is inspired by Burer et al. [50]. It takes strides towards an efficient algorithm, but the primary focus of this paper is to understand the use case for robustness certification.

4 Preliminary: Geometry of the SDP relaxation

The SDP relaxation of Raghunathan et al. [21] is based on the observation that the rectified linear unit (ReLU) activation function $z = \mathrm{ReLU}(x) \equiv \max\{0, x\}$ is equivalent to the inequalities $z \geq 0$, $z \geq x$, and $z(z - x) \leq 0$. Viewing these as quadratics, we apply a standard technique (see Shor [51] and also [24, 25, 33]) to rewrite them as linear inequalities over a positive semidefinite matrix variable,

$$z \geq 0, \quad z \geq x, \quad Z \leq Y, \quad \mathbf{G} = \begin{bmatrix} 1 & x & z \\ x & X & Y \\ z & Y & Z \end{bmatrix} \succeq 0, \quad \mathrm{rank}(\mathbf{G}) = 1. \tag{4.1}$$

In essence, the reformulation collects the inherent nonconvexity of $\mathrm{ReLU}(\cdot)$ into the constraint $\mathrm{rank}(\mathbf{G}) = 1$, which can then be deleted to yield a convex relaxation. If the relaxation has a unique solution $\mathbf{G}^\star$ satisfying $\mathrm{rank}(\mathbf{G}^\star) = 1$, then we say that it is *tight*.[1] In this case, the globally optimal solution $x^\star, z^\star$ to the original nonconvex problem can be found by solving the SDP relaxation in polynomial time and factorizing the solution $\mathbf{G}^\star = \mathbf{g}\mathbf{g}^T$ where $\mathbf{g} = [1; x^\star; z^\star]^T$.

It is helpful to view $\mathbf{G}$ as the *Gram matrix* associated with the vectors $\mathbf{e}, \mathbf{x}, \mathbf{z} \in \mathbb{R}^p$ in an ambient p-dimensional space, where p is the order of $\mathbf{G}$ (here $p = 3$). The individual elements of $\mathbf{G}$ correspond to the inner products terms associated with $\mathbf{e}, \mathbf{x}, \mathbf{z}$, as in

$$\langle \mathbf{e}, \mathbf{z} \rangle \geq \max\{0, \langle \mathbf{e}, \mathbf{x} \rangle\}, \quad \|\mathbf{z}\|^2 \leq \langle \mathbf{z}, \mathbf{x} \rangle, \quad \|\mathbf{e}\|^2 = 1, \quad \mathbf{G} = \begin{bmatrix} \langle \mathbf{e}, \mathbf{e} \rangle & \langle \mathbf{e}, \mathbf{x} \rangle & \langle \mathbf{e}, \mathbf{z} \rangle \\ \langle \mathbf{e}, \mathbf{x} \rangle & \langle \mathbf{x}, \mathbf{x} \rangle & \langle \mathbf{x}, \mathbf{z} \rangle \\ \langle \mathbf{e}, \mathbf{z} \rangle & \langle \mathbf{x}, \mathbf{z} \rangle & \langle \mathbf{z}, \mathbf{z} \rangle \end{bmatrix}, \tag{4.2}$$

and $\mathrm{rank}(\mathbf{G}) = 1$ corresponds to *collinearity* between $\mathbf{x}$, $\mathbf{z}$, and $\mathbf{e}$, as in $\|\mathbf{e}\|\|\mathbf{x}\| = |\langle \mathbf{e}, \mathbf{x} \rangle|$ and $\|\mathbf{e}\|\|\mathbf{z}\| = |\langle \mathbf{e}, \mathbf{z} \rangle|$. From the Gram matrix perspective, the SDP relaxation works by allowing the underlying vectors $\mathbf{x}$, $\mathbf{z}$, and $\mathbf{e}$ to take on arbitrary directions; the relaxation is tight if and only if *all* possible solutions $\mathbf{e}^\star, \mathbf{x}^\star, \mathbf{z}^\star$ are collinear.

Figure 1 shows the underlying geometry the ReLU constraints (4.2) as noted by Raghunathan et al. [21]. Take $\mathbf{z}$ as the variable and fix $\mathbf{e}, \mathbf{x}$. Since $\mathbf{e}$ is a unit vector, we may view $\langle \mathbf{e}, \mathbf{x} \rangle$ and $\langle \mathbf{e}, \mathbf{z} \rangle$ as the "$\mathbf{e}$-axis coordinates" for the vectors $\mathbf{x}$ and $\mathbf{z}$. The constraint $\langle \mathbf{e}, \mathbf{z} \rangle \geq \max\{0, \langle \mathbf{e}, \mathbf{x} \rangle\}$ is then a *half-space* that restricts the "$\mathbf{e}$-coordinate" of $\mathbf{z}$ to be nonnegative and greater than that of $\mathbf{x}$. The constraint $\langle \mathbf{z}, \mathbf{z} - \mathbf{x} \rangle \leq 0$ is rewritten as $\|\mathbf{z} - \mathbf{x}/2\|^2 \leq \|\mathbf{x}/2\|^2$ by completing the square; this is a *sphere* that restricts $\mathbf{z}$ to lie within a distance of $\|\mathbf{x}/2\|$ from the center $\mathbf{x}/2$. Combined, the ReLU constraints (4.2) constrain $\mathbf{z}$ to lie within a *spherical cap*—a portion of a sphere cut off by a plane.

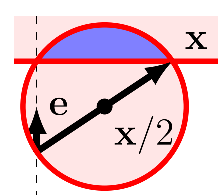

Fig. 1 – The ReLU constraints (4.2) describe a spherical cap.

[1] If a rank-1 solution exists but is nonunique, then we do not consider the SDP relaxation tight because the rank-1 solution cannot usually be found in polynomial time. Indeed, an interior-point method converges onto a maximum rank solution, but this can be rank-1 only if it is unique.

5 Tightness for one hidden neuron

Now, consider the SDP relaxation of the one-neuron problem (2.3), explicitly written as

$$L_{\text{lb}}^2 = \min_{\mathbf{G}} \quad X - 2x\hat{x} + \hat{x}^2 \quad \text{s.t.} \quad \begin{matrix} z \geq \max\{0, x\},\ Z \leq Y, \\ Z - 2z\hat{z} + \hat{z}^2 \leq \rho^2, \end{matrix} \quad \mathbf{G} = \begin{bmatrix} 1 & x & z \\ x & X & Y \\ z & Y & Z \end{bmatrix} \succeq 0. \quad (5.1)$$

Viewing the matrix variable $\mathbf{G} \succeq 0$ as the Gram matrix associated with the vectors $\mathbf{e}, \mathbf{x}, \mathbf{z} \in \mathbb{R}^p$ where $p = 3$ rewrites (5.1) as the following

$$L_{\text{lb}} = \min_{\mathbf{x},\mathbf{z},\mathbf{e} \in \mathbb{R}^p} \|\mathbf{x} - \hat{x}\,\mathbf{e}\| \quad \text{s.t.}\ \langle \mathbf{z}, \mathbf{e} \rangle \geq \max\{\langle \mathbf{x}, \mathbf{e} \rangle, 0\},\ \|\mathbf{z}\|^2 \leq \langle \mathbf{z}, \mathbf{x} \rangle,\ \|\mathbf{z} - \hat{z}\,\mathbf{e}\| \leq \rho. \quad (5.2)$$

The SDP relaxation (5.1) has a unique rank-1 solution if and only if its nonconvex vector interpretation (5.2) has a unique solution that aligns with $\mathbf{e}$. The proof for the following is given in Appendix A.

Lemma 5.1 (Collinearity and rank-1)**.** *Fix $\mathbf{e} \in \mathbb{R}^p$. Then, problem (5.2) has a unique solution $\mathbf{x}^\star$ satisfying $\|\mathbf{x}^\star\| = |\langle \mathbf{x}^\star, \mathbf{e} \rangle|$ if and only if problem (5.1) has a unique solution $\mathbf{G}^\star$ satisfying* $\operatorname{rank}(\mathbf{G}^\star) = 1$.

We proceed to solve problem (5.2) by rewriting it as the composition of a convex projection over $\mathbf{z}$ with a nonconvex projection over $\mathbf{x}$, as in:

$$\phi(\mathbf{x}, \hat{z}) \quad = \quad \min_{\mathbf{z} \in \mathbb{R}^p} \quad \|\mathbf{z} - \hat{z}\mathbf{e}\| \quad \text{subject to} \quad \langle \mathbf{e}, \mathbf{z} \rangle \geq \max\{\langle \mathbf{e}, \mathbf{x} \rangle, 0\}, \quad \|\mathbf{z}\|^2 \leq \langle \mathbf{z}, \mathbf{x} \rangle, \quad (5.3)$$

$$L_{\text{lb}} \quad = \quad \min_{\mathbf{x} \in \mathbb{R}^p} \quad \|\mathbf{x} - \hat{x}\mathbf{e}\| \quad \text{subject to} \quad \phi(\mathbf{x}, \hat{z}) \leq \rho. \quad (5.4)$$

Problem (5.3) is clearly the projection of the point $\hat{z}\mathbf{e}$ onto the spherical cap shown in Figure 1. In a remarkable symmetry, it turns out that problem (5.4) is the projection of the point $\hat{x}\mathbf{e}$ onto a *hyperboloidal cap*—a portion of a high-dimensional hyperbola cut off by a plane—with the optimal $\mathbf{x}^\star$ in problem (5.2) being the resulting projection. In turn, our goal of verifying collinearity between $\mathbf{x}^\star$ and $\mathbf{e}$ amounts to checking whether $\hat{x}\mathbf{e}$ projects onto the major axis of the hyperboloid.

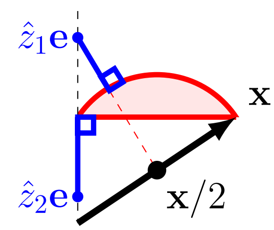

Fig. 2 – Problem (5.3) is the projection of a point onto a spherical cap.

To turn this intuitive sketch into a rigorous proof, we begin by solving the convex projection (5.3) onto the spherical cap. Figure 2 shows the corresponding geometry. There are two distinct scenarios: **i)** For $\hat{z}_1\mathbf{e}$ that is *above* the spherical cap, the projection must intersect the upper, round portion of the spherical cap along the line from $\hat{z}_1\mathbf{e}$ to $\mathbf{x}/2$. This yields a distance of $\phi(\mathbf{x}, \hat{z}_1) = \|\hat{z}_1\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\|$. **ii)** For $\hat{z}_2\mathbf{e}$ that is *below* the spherical cap, the projection is simply the closest point directly above, at a distance of $\phi(\mathbf{x}, \hat{z}_2) = \max\{0, \langle \mathbf{e}, \mathbf{x} \rangle\} - \hat{z}_2$.

It turns out that the conditional statements are unnecessary; the distance $\phi(\mathbf{x}, \hat{z})$ simply takes on the larger of the two values derived above. In Appendix B, we prove this claim algebraically, thereby establishing the following.

Lemma 5.2 (Projection onto spherical cap)**.** *The function $\phi : \mathbb{R}^p \times \mathbb{R} \to \mathbb{R}$ defined in (5.3) satisfies*

$$\phi(\mathbf{x}, \hat{z}) = \max\{\max\{0, \langle \mathbf{e}, \mathbf{x} \rangle\} - \hat{z}, \quad \|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\|\}. \quad (5.5)$$

Taking $\mathbf{x}$ as the variable, we see from Lemma 5.2 that each level set $\phi(\mathbf{x}, \hat{z}) = \rho$ is either: 1) a *hyperplane* normal to $\mathbf{e}$ at the intercept $\hat{z} + \rho$; or 2) a two-sheet *hyperboloid* centered at $\hat{z}\mathbf{e}$, with semi-major axis ρ and focal distance $|\hat{z}|$ in the direction of $\mathbf{e}$. Hence, the sublevel set $\phi(\mathbf{x}, \hat{z}) \leq \rho$ is a hyperboloidal cap as claimed.

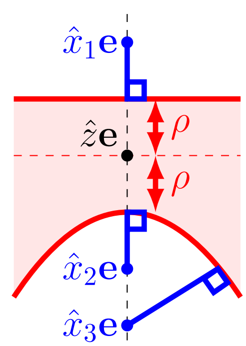

Fig. 3 – Problem (5.4) is the projection of a point onto a hyperbolidal cap.

We proceed to solve the nonconvex projection (5.4) onto the hyperboloidal cap. This shape degenerates into a half-space if the semi-major axis ρ is longer than the focal distance, as in $\rho \geq |\hat{z}|$, and becomes empty altogether with a negative center, as in $\hat{z} < -\rho$. Figure 3 shows the geometry of projecting onto a *nondegenerate* hyperboloidal cap with $\hat{z} > \rho$. There are three distinct scenarios: **i)** For $\hat{x}_1\mathbf{e}$ that is either *above* or *interior* to the hyperboloidal cap, the projection is either the closest point directly below or the point itself, as in $\mathbf{x}^\star = \min\{\hat{z}+\rho, \hat{x}_1\}\mathbf{e}$; **ii)** For $\hat{x}_2\mathbf{e}$ that is *below* and *sufficiently close* to the hyperboloidal cap, the projection lies at the top of the hyperbolid sheet at $\mathbf{x}^\star = (\hat{z}-\rho)\mathbf{e}$; **iii)** For $\hat{x}_3\mathbf{e}$ that is *below* and *far away* from the hyperboloidal cap, the projection lies somewhere along the side of the hyperboloid.

Evidently, the first two scenarios correspond to choices of $\mathbf{x}^\star$ that are collinear to $\mathbf{e}$, while the third scenario does not. To resolve the boundary between the second and third scenarios, we solve the projection onto a hyperbolidal cap in closed-form.

Lemma 5.3 (Projection onto nondegenerate hyperboloidal cap)**.** *Given* $\mathbf{e} \in \mathbb{R}^p$, $\hat{x} \in \mathbb{R}$, *and* $\hat{z} > \rho > 0$, *define* $\mathbf{x}^\star$ *as the solution to the following projection*

$$\min_{\mathbf{x}\in\mathbb{R}^p} \quad \|\mathbf{x}-\hat{x}\mathbf{e}\|^2 \quad \textit{s.t.} \quad \langle \mathbf{e},\mathbf{x}\rangle - \hat{z} \le \rho, \quad \|\hat{z}\mathbf{e}-\mathbf{x}/2\| - \|\mathbf{x}/2\| \le \rho.$$

Then, $\mathbf{x}^\star$ *is unique and satisfies* $\|\mathbf{x}^\star\| = |\langle \mathbf{e},\mathbf{x}^\star\rangle|$ *if and only if* $(\hat{z}-\hat{x}) < \hat{z}^2/\rho$.

We defer the proof of Lemma 5.3 to Appendix C, but note that the main idea is to use the S-lemma (see e.g. [52, p. 655] or [53]) to solve the minimization of a quadratic (the distance) subject to a quadratic constraint (the nondegenerate hyperboloid). Resolving the degenerate cases and applying Lemma 5.3 to the nondegenerate case yields a proof of our main result.

Proof of Theorem 2.1. If $\hat{z} < -\rho$, then the hyperbolidal cap $\phi(\mathbf{x},\hat{z}) \le \rho$ is empty as $\rho < -\hat{z} \le \phi(\mathbf{x},\hat{z})$. In this case, problem (5.4) is infeasible. If $|\hat{z}| \le \rho$, then the hyperbolidal cap $\phi(\mathbf{x},\hat{z}) \le \rho$ degenerates into a half-space $\langle \mathbf{e},\mathbf{x}\rangle \le \hat{z}+\rho$, because $\|\hat{z}\mathbf{e}-\mathbf{x}/2\|-\|\mathbf{x}/2\| \le \|\hat{z}\mathbf{e}\|+\|\mathbf{x}/2\|-\|\mathbf{x}/2\| = |\hat{z}| \le \rho$. In this case, the projection $\mathbf{x}^\star = \min\{\hat{z}+\rho,\hat{x}\}\mathbf{e}$ is clearly collinear to $\mathbf{e}$, so $|\hat{z}| \le \rho$ is the first condition of Theorem 2.1. Finally, if $\hat{z} > \rho$, Lemma 5.3 says that $\mathbf{x}^\star$ is collinear with $\mathbf{e}$ whenever $(\hat{z}-\hat{x}) < \hat{z}^2/\rho$, which is rewritten $\hat{x} > \hat{z}(1-\hat{z}/\rho)$. Under $\hat{z} > \rho$, this is equivalent to $\rho < \hat{z}/(1-\hat{x}/\hat{z})$. Finally, taking the intersection of these two constraints yields $\rho < \hat{z}/(1-\min\{0,\hat{x}/\hat{z}\})$, which is the second condition of Theorem 2.1. □

6 Tightness for one layer

Our analysis of the one-hidden-neuron case extends to the one-hidden-layer case without significant modification. Here, the semidefinite relaxation reads

$$L_{\text{lb}}^2 = \min_{\mathbf{G}} \quad \operatorname{tr}(\mathbf{X}) - 2\langle \mathbf{x},\hat{\mathbf{x}}\rangle + \|\hat{\mathbf{x}}\|^2 \tag{6.1}$$
$$\text{s.t.} \quad \begin{matrix} \mathbf{z} \ge \max\{0,\mathbf{W}\mathbf{x}\},\ \operatorname{diag}(\mathbf{W}\mathbf{Z}) \le \operatorname{diag}(\mathbf{W}\mathbf{Y}), \\ \operatorname{tr}(\mathbf{Z}) - 2\langle \mathbf{z},\hat{\mathbf{z}}\rangle + \|\hat{\mathbf{z}}\|^2 \le \rho^2, \end{matrix} \quad \mathbf{G} = \begin{bmatrix} 1 & \mathbf{x} & \mathbf{z} \\ \mathbf{x} & \mathbf{X} & \mathbf{Y} \\ \mathbf{z} & \mathbf{Y}^T & \mathbf{Z} \end{bmatrix} \succeq 0.$$

Viewing the matrix variable $\mathbf{G} \succeq 0$ in the corresponding SDP relaxation (6.1) as the Gram matrix associated a set of length-p vectors (where $p = m+n+1$ is the order of the matrix $\mathbf{G}$) yields the following[2]

$$L_{\text{lb}}^2 = \min_{\mathbf{x}_j,\mathbf{z}_i\in\mathbb{R}^p} \quad \textstyle\sum_j \|\mathbf{x}_j - \hat{x}_j\,\mathbf{e}\|^2 \tag{6.2}$$
$$\text{s.t.} \quad \begin{matrix} \langle \mathbf{e},\mathbf{z}_i\rangle \ge \max\left\{0, \langle \mathbf{e}, \sum_j W_{i,j}\mathbf{x}_j\rangle\right\}, \\ \|\mathbf{z}_i\|^2 \le \langle \mathbf{z}_i, \sum_j W_{i,j}\mathbf{x}_j\rangle, \end{matrix} \quad \textstyle\sum_i \|\mathbf{z}_i - \hat{z}_i\,\mathbf{e}\|^2 \le \rho^2 \text{ for all } i,$$

with indices $i \in \{1,2,\ldots,m\}$ and $j \in \{1,2,\ldots,n\}$. We will derive conditions for the SDP relaxation (6.1) to have a unique, rank-1 solution by fixing $\mathbf{e}$ in problem (6.2) and verifying that every optimal $\mathbf{x}_j^\star$ is collinear with $\mathbf{e}$ for all j. The proof for the following is given in Appendix A.

Lemma 6.1 (Collinearity and rank-1)**.** *Fix* $\mathbf{e} \in \mathbb{R}^p$. *Then, problem (6.2) has a unique solution* $\mathbf{x}_1^\star, \mathbf{x}_2^\star, \ldots, \mathbf{x}_n^\star$ *satisfying* $\|\mathbf{x}_j^\star\| = |\langle \mathbf{x}_j^\star, \mathbf{e}\rangle|$ *if and only if problem (6.1) has a unique solution* $\mathbf{G}^\star$ *satisfying* $\operatorname{rank}(\mathbf{G}^\star) = 1$.

[2] To avoid visual clutter we will abbreviate $\sum_{j=1}^n x_j$ and "for all $i \in \{1,2,\ldots,n\}$" as $\sum_j x_j$ and "for all i" whenever the ranges of indices are clear from context.

Problem (6.2) can be rewritten as the composition of a series of projections over $\mathbf{z}_i$, followed by a sequence of nonconvex projections over $\mathbf{x}_j$, as in

$$L_{\text{lb}}^2 = \min_{\mathbf{x}_j \in \mathbb{R}^p, a_i \geq 0} \quad \textstyle\sum_j \|\mathbf{x}_j - \hat{x}_j\, \mathbf{e}\|^2 \quad \text{s.t.} \quad \phi(\textstyle\sum_j W_{i,j}\mathbf{x}_j, \hat{z}_i) \leq \rho_i \text{ for all } i, \quad \textstyle\sum_i \rho_i^2 \leq \rho^2, \tag{6.3}$$

where ϕ was previously defined in the one-neuron convex projection (5.3). Whereas in the one-neuron case we are projecting a single point onto a single hyperboloidal cap, the one-layer case requires us to project n points onto the intersection of n hyperboloidal caps. This has a closed-form solution only when all the hyperboloids are nondegenerate.

Lemma 6.2 (Projection onto several hyperboloidal caps)**.** *Given $\mathbf{W} = [W_{i,j}] \in \mathbb{R}^{m\times n}$, $\hat{\mathbf{x}} = [\hat{x}_j] \in \mathbb{R}^n$, $\hat{\mathbf{z}} = [\hat{z}_i] \in \mathbb{R}^m$, $\mathbf{e} \in \mathbb{R}^p$, and ρ_i satisfying $\hat{z}_i > \rho > 0$, define $\mathbf{x}_j^\star$ as the solution to the following projection*

$$\min_{\mathbf{x}_j \in \mathbb{R}^p} \quad \textstyle\sum_j \|\mathbf{x}_j - \hat{x}_j \mathbf{e}\|^2 \quad \textit{s.t.} \quad \begin{array}{r} \langle \mathbf{e}, \sum_j W_{i,j}\mathbf{x}_j\rangle - \hat{z}_i \leq \rho_i \textit{ for all } i, \\ \|\hat{z}_i \mathbf{e} - \sum_j W_{i,j}\mathbf{x}_j/2\| - \|\sum_j W_{i,j}\mathbf{x}_j/2\| \leq \rho_i \textit{ for all } i. \end{array}$$

If $\rho_{\max}\|\mathbf{W}\|^2\|(\mathbf{W}\mathbf{W}^T)^{-1}(\mathbf{W}\hat{\mathbf{x}} - \hat{\mathbf{z}})\|_\infty + \rho_{\max}^2(1 + \|\mathbf{W}\|^2\|(\mathbf{W}\mathbf{W}^T)^{-1}\|_\infty) < \hat{z}_{\min}^2$ holds with $\rho_{\max} = \max_i \rho_i$ and $\hat{z}_{\min} = \min_i \hat{z}_i$, then $\mathbf{x}_j^\star$ is unique and satisfies $\|\mathbf{x}_j^\star\| = |\langle \mathbf{e}, \mathbf{x}_j^\star\rangle|$ for all j.

We defer the proof of Lemma 6.2 to Appendix D, but note that the main idea is to use the *lossy* S-lemma to solve the minimization of one quadratic (the distance) over several quadratic constraints (the hyperboloids). Theorem 2.2 then follows immediately from Lemma 6.2 and Corollary 2.3.

7 Looseness for multiple layers

Unfortunately, the SDP relaxation is not usually tight for more than a single layer. Let $\mathbf{f}(x) = \mathrm{ReLU}(\mathrm{ReLU}(x))$ denote a two-layer neural network with a single neuron per layer. The corresponding instance of problem (B) is essentially the same as problem (2.3) from Section 5 for the one-layer one-neuron network, because $\mathrm{ReLU}(\mathrm{ReLU}(x)) = \mathrm{ReLU}(x)$ holds for all x. However, constructing the SDP relaxation and taking the Gram matrix interpretation reveals the following (with $p = 4$)

$$L_{\text{lb}} = \min_{\mathbf{x},\mathbf{z},\mathbf{e} \in \mathbb{R}^p} \|\mathbf{x} - \hat{x}\, \mathbf{e}\| \quad \text{s.t.} \quad \begin{array}{c} \langle \mathbf{z}, \mathbf{e}\rangle \geq \max\{\langle \mathbf{x}, \mathbf{e}\rangle, 0\}, \ \|\mathbf{z}\|^2 \leq \langle \mathbf{z}, \mathbf{x}\rangle, \\ \langle \mathbf{z}, \mathbf{e}\rangle - \hat{z} \leq \rho, \ \|\hat{z}\mathbf{e} - \mathbf{z}/2\| - \|\mathbf{z}/2\| \leq \rho, \end{array} \tag{7.1}$$

which is *almost* the same as problem (5.2) from Section 5, except that the convex ball constraint $\|\hat{z}\mathbf{e} - \mathbf{z}\| \leq \rho$ has been replaced by a nonconvex hyperboloid. As we will see, it is this hyperbolic geometry that makes it harder for the SDP relaxation to be tight.

Denote $x^\star$ as the solution to both instances of problem (B). The point $\mathbf{u} = x^\star \mathbf{e}$ must be the unique solution to (7.1) and (5.2) in order for their respective SDP relaxations to be tight. Now, suppose that $\hat{x} < 0$ and $\hat{z} > \rho > 0$, so that both instances of problem (B) have $x^\star = \hat{z} - \rho > 0$. Both (5.2) and (7.1) are convex over $\mathbf{x}$; fixing $\mathbf{z}$ and optimizing over $\mathbf{x}$ in each case yields $\|\mathbf{x}^\star - \hat{x}\mathbf{e}\| = \|\mathbf{z}\| - \hat{x}\cos\theta$ where $\cos\theta = \langle \mathbf{e}, \mathbf{z}\rangle/\|\mathbf{z}\|$. In order for $\mathbf{u}$ to be the unique solution, we need $\|\mathbf{z}\| - \hat{x}\cos\theta$ to be globally minimized at $\mathbf{z} = \mathbf{u}$. As shown in Figure 4, $\|\mathbf{z}\|$ is clearly minimized at $\mathbf{z}^\star = \mathbf{u}$ over the ball constraint $\|\hat{z}\mathbf{e} - \mathbf{z}\| \leq \rho$, but the same is not obviously true for the hyperbolid $\|\hat{z}\mathbf{e} - \mathbf{z}/2\| - \|\mathbf{z}/2\| \leq \rho$. Some detailed computation readily confirm the geometric intuition that $\mathbf{u}$ is generally a local minimum over the circle, but not over the hyperbola.

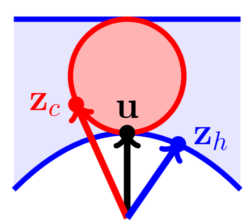

Fig. 4 – Any point $\mathbf{z}_c$ on the circle clearly satisfies $\|\mathbf{z}_c\| > \|\mathbf{u}\|$, but a point $\mathbf{z}_h$ on the hyperbola may have $\|\mathbf{z}_h\| \approx \|\mathbf{u}\|$.

8 Numerical experiments

Dataset and setup. We use the MNIST dataset of 28×28 images of handwritten digits, consisting of 60,000 training images and 10,000 testing images. We remove and set aside the final 1,000 images from the training set as the verification set. All our experiments are performed on an Intel Xeon E3-1230 CPU (4-core, 8-thread, 3.2-3.6 GHz) with 32 GB of RAM.

Architecture. We train two small fully-connected neural network ("dense-1" and "dense-3") whose SDP relaxations can be quickly solved using MOSEK [54], and a larger convolutional network

("CNN") whose SDP relaxation must be solved using a custom algorithm described below. The "dense-1" and "dense-3" models respectively have one and three fully-connected layer(s) of 50 neurons, and are trained on a 4×4 maxpooled version of the training set (each image is downsampled to 7×7). The "CNN" model has two convolutional layers (stride 2) with 16 and 32 filters (size 4×4) respectively, followed by a fully-connected layer with 100 neurons, and is trained on the original dataset of 28×28 images. All models are implemented in tensorflow and trained over 50 epochs using the SGD optimizer (learning rate 0.01, momentum 0.9, "Nesterov" true).

Rank-2 Burer-Monteiro algorithm ("BM2"). We use a rank-2 Burer–Monteiro algorithm to solve instances of the SDP relaxation on the "CNN" model, by applying a local optimization algorithm to the following (see Appendix F for a detailed derivation and implementation details)

$$\begin{aligned} \min_{\mathbf{u}_k,\mathbf{v}_k\in\mathbb{R}^n} \quad & \|\mathbf{u}_0-\hat{\mathbf{x}}\|^2+\|\mathbf{v}_0\|^2 \\ \text{s.t.} \quad & \operatorname{diag}(\mathbf{u}_{k+1}\mathbf{u}_{k+1}^T+\mathbf{v}_{k+1}\mathbf{v}_{k+1}^T) \le \operatorname{diag}((\mathbf{W}_k\mathbf{u}_k+\mathbf{b}_k)\mathbf{u}_{k+1}^T+\mathbf{W}_k\mathbf{v}_{k+1}\mathbf{v}_{k+1}^T) \\ & \mathbf{u}_{k+1} \ge \max\{0, \mathbf{W}_k\mathbf{u}_k+\mathbf{b}_k\}, \qquad \|\mathbf{u}_\ell-\hat{\mathbf{z}}\|^2+\|\mathbf{v}_\ell\|^2 \le \rho^2 \qquad \text{for all } k. \end{aligned} \tag{BM2}$$

Let $\{\mathbf{u}_k^\star, \mathbf{v}_k^\star\}$ be a locally optimal solution satisfying the first- and second-order optimality conditions (see e.g. [55, Chapter 12]). If $\mathbf{v}_0^\star = 0$, then by induction $\mathbf{u}_{k+1}^\star = \mathrm{ReLU}(\mathbf{W}_k\mathbf{u}_k^\star + \mathbf{b}_k)$ and $\mathbf{v}_k^\star = 0$ for all k. It then follows from a well-known result of Burer and Monteiro [56] (see also [57, 58] and in particular [59, Lemma 1]) that $\{\mathbf{u}_k^\star, \mathbf{v}_k^\star\}$ corresponds to a rank-1 solution of the SDP relaxation, and is therefore *globally optimal*. Of course, such a solution must not exist if the relaxation is loose; even when it does exist, the algorithm might still fail to find it if it gets stuck in a *spurious* local minimum with $\mathbf{v}_0^\star \neq 0$. Our experience is that the algorithm consistently succeeds whenever the relaxation is tight, but admittedly this is not guaranteed.

Tightness for problem (B). Our theoretical results suggest that the SDP relaxation for problem (B) should be tight for one layer and loose for multiple layers. To verify, we consider the first k layers of the "dense-3" and "CNN" models over a range of radii ρ. In each case, we solve 1000 instances of the SDP relaxation, setting $\hat{\mathbf{x}}$ to be a new image from the verification set, and $\hat{\mathbf{z}} = \mathbf{f}(\mathbf{u})$ where $\mathbf{u}$ is the *previous* image used as $\hat{\mathbf{x}}$. MOSEK solved each instance of "dense-3" in 5-20 minutes and BM2 solved each instance of "CNN" in 15-60 minutes. We mark $\mathbf{G}^\star$ as numerically rank-1 if $\lambda_1(\mathbf{G}^\star)/\lambda_2(\mathbf{G}^\star) > 10^3$, and plot the success rates in Figure 5a. Consistent with Theorem 2.2, the relaxation over one layer is most likely to be loose for intermediate values of ρ. Consistent with Corollary 2.3, the relaxation eventually becomes tight once ρ is large enough to yield a trivial solution. The results for CNN are dramatic, with an 100% success rate over a single layer, and a 0% success rate for two (and more) layers. BM2 is less successful for very large and very small ρ in part due to numerical issues associated with the factor-of-two exponent in $\|\mathbf{z}-\hat{\mathbf{z}}\|^2 \le \rho^2$.

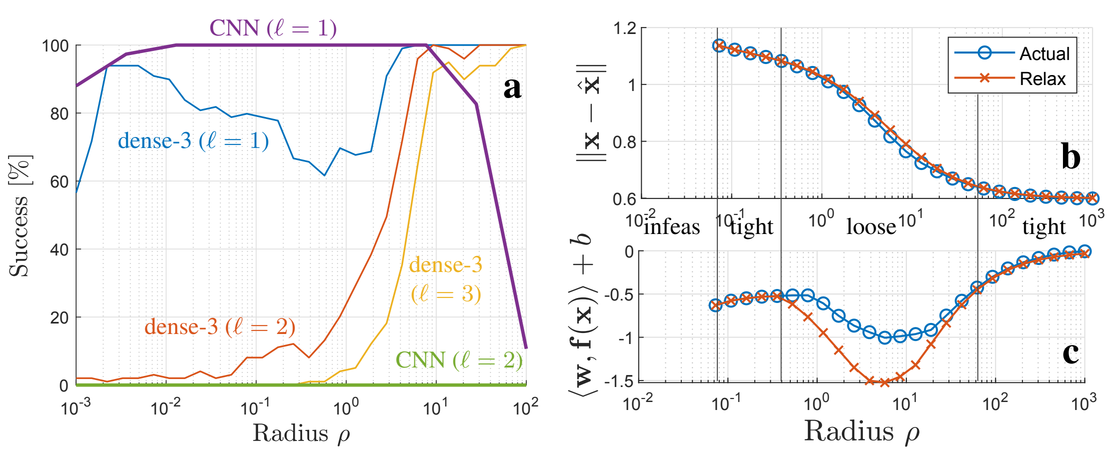

Fig. 5 – a. The SDP relaxation for problem (B) is generally tight over a single layer, and loose over multiple layers. **b.** Viewing problem (A) as (B) taken at the limit $\rho \to \infty$, the resulting SDP relaxation can be close to, but not exactly, tight, for finite values of ρ. **c.** The SDP relaxation of (B) can produce a near-optimal attack $\mathbf{x}$ satisfying $\langle \mathbf{w}, \mathbf{f}(\mathbf{x})\rangle + b < 0$ for problem (A), even when relaxation itself is not actually tight.

Application to problem (A). Viewing problem (A) as problem (B) in the limit $\rho \to \infty$, we consider a finite range of values for ρ, and solve the corresponding SDP relaxation with $\hat{\mathbf{z}} = -\mathbf{w}(b/\|\mathbf{w}\|^2 + \rho/\|\mathbf{w}\|)$. Here, the SDP relaxation is generally loose, so BM2 does not usually succeed, and we must resort to using MOSEK to solve it on the small "dense-1" model. Figure 5b compares the relaxation objective $\sqrt{\mathrm{tr}(\mathbf{X}) - 2\langle \hat{\mathbf{x}}, \mathbf{x}\rangle + \|\hat{\mathbf{x}}\|^2}$ with the actual distance $\|\mathbf{x} - \hat{\mathbf{x}}\|$, while Figure 5c compares the feasibility predicted by the relaxation $\langle \mathbf{w}, \mathbf{z}\rangle + b$ with the actual feasibility $\langle \mathbf{w}, \mathbf{f}(\mathbf{x})\rangle + b$. The relaxation is tight for $0.07 \le \rho \le 0.4$ and $\rho \ge 60$ so the plots coincide. The relaxation is loose for $0.4 \le \rho \le 60$, and the relaxation objective is strictly greater than the actual distance because $\mathbf{X} \succ \mathbf{x}\mathbf{x}^T$. The resulting attack $\mathbf{x}$ must fail to satisfy $\|\mathbf{f}(\mathbf{x}) - \hat{\mathbf{z}}\| \le \rho$, but in this case it is still *always* feasible for problem (A). For $\rho < 0.07$, the SDP relaxation is infeasible, so we deduce that the output target $\hat{\mathbf{z}}$ is not actually feasible.

9 Conclusions

This paper presented a geometric study of the SDP relaxation of the ReLU. We split the a modification of the robustness certification problem into the composition of a convex projection onto a spherical cap, and a nonconvex projection onto a hyperboloidal cap, so that the relaxation is tight if and only if the latter projection lies on the major axis of the hyperboloid. This insight allowed us to completely characterize the tightness of the SDP relaxation over a single neuron, and partially characterize the case for the single layer. The multilayer case is usually loose due to the underlying hyperbolic geometry, and this implies looseness in the SDP relaxation of the original certification problem. Our rank-2 Burer-Monteiro algorithm was able to solve the SDP relaxation on a convolution neural network, but better algorithms are still needed before models of realistic scales can be certified.

Broader Impact

This work contributes towards making neural networks more robust to adversarial examples. This is a crucial roadblock before neural networks can be widely adopted in safety-critical applications like self-driving cars and smart grids. The ultimate, overarching goal is to take the high performance of neural networks—already enjoyed by applications in computer vision and natural language processing—and extend towards applications in societal infrastructure.

Towards this direction, SDP relaxations allow us to make mathematical guarantees on the robustness of a given neural network model. However, a blind reliance on mathematical guarantees leads to a false sense of security. While this work contributes towards robustness of neural networks, much more work is needed to understand the appropriateness of neural networks for societal applications in the first place.

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A Uniqueness of a Rank-1 Solution

Consider the rank-constrained semidefinite program

$$\begin{aligned} \underset{\mathbf{x}\in\mathbb{R}^n,\ \mathbf{X}\in\mathbb{R}^{n\times n}}{\text{minimize}} \quad & \langle \mathbf{D}, \mathbf{X}\rangle + \langle \mathbf{f}, \mathbf{x}\rangle \\ \text{subject to} \quad & \langle \mathbf{A}_i, \mathbf{X}\rangle + \langle \mathbf{b}_i, \mathbf{x}\rangle \le c_i \quad \text{for all } i \in \{1, 2, \dots, m\}, \\ & \begin{bmatrix} 1 & \mathbf{x}^T \\ \mathbf{x} & \mathbf{X} \end{bmatrix} \succeq 0, \quad \operatorname{rank}(\mathbf{X}) \le p, \end{aligned} \tag{A.1}$$

and its corresponding nonconvex optimization interpretation

$$\begin{aligned} \underset{\mathbf{v}_1,\mathbf{v}_2,\dots,\mathbf{v}_n\in\mathbb{R}^p}{\text{minimize}} \quad & \sum_{k=1}^{n}\sum_{j=1}^{n} \langle \mathbf{v}_j, \mathbf{v}_k\rangle \langle \mathbf{D}, \mathbf{e}_k\mathbf{e}_j^T\rangle + \sum_{j=1}^{n} \langle \mathbf{e}, \mathbf{v}_j\rangle\langle \mathbf{f}, \mathbf{e}_j\rangle \\ \text{subject to} \quad & \sum_{k=1}^{n}\sum_{j=1}^{n} \langle \mathbf{v}_j, \mathbf{v}_k\rangle \langle \mathbf{A}_i, \mathbf{e}_k\mathbf{e}_j^T\rangle + \sum_{j=1}^{n} \langle \mathbf{e}, \mathbf{v}_j\rangle\langle \mathbf{b}_i, \mathbf{e}_j\rangle \le c_i \quad \text{for all } i \in \{1, 2, \dots, m\}, \end{aligned} \tag{A.2}$$

where $\mathbf{e}$ is an arbitrary, fixed unit vector satisfying $\|\mathbf{e}\| = 1$. Our main result in this section is that we can guarantee a rank-1 solution to (A.1) to be *unique*, and hence computable via an interior-point method, by verifying that every solution to (A.2) is collinear with the unit vector $\mathbf{e}$.

Definition A.1. Fix $\mathbf{e} \in \mathbb{R}^p$ with $\|\mathbf{e}\| = 1$. We say that $\mathbf{v} \in \mathbb{R}^p$ is *collinear* or that it satisfies *collinearity* if $|\langle \mathbf{e}, \mathbf{v}\rangle| = \|\mathbf{v}\|$.

Theorem A.2 (Unique rank-1)**.** *Fix $\mathbf{e} \in \mathbb{R}^p$ with $\|\mathbf{e}\| = 1$, and write $\mathcal{V}^\star$ as the resulting solution set associated with (A.2). Then, problem (A.1) has a unique solution satisfying $\mathbf{X}^\star = \mathbf{x}^\star(\mathbf{x}^\star)^T$ if and only if $\mathbf{v}_1^\star, \mathbf{v}_2^\star, \dots, \mathbf{v}_n^\star$ are collinear for all $(\mathbf{v}_1^\star, \mathbf{v}_2^\star, \dots, \mathbf{v}_n^\star) \in \mathcal{V}^\star$.*

We briefly defer the proof of Theorem A.2 to discuss its consequences. In the case of ReLU constraints, if the input vectors $\mathbf{x}_j$ are collinear, then the output vectors $\mathbf{z}_i$ are also collinear.

Lemma A.3 (Propagation of collinearity)**.** *Fix $\mathbf{e} \in \mathbb{R}^p$ with $\|\mathbf{e}\| = 1$. Under the ReLU constraints $\langle \mathbf{e}, \mathbf{z}\rangle \ge \max\{0, \langle \mathbf{e}, \sum_j w_j \mathbf{x}_j\rangle\}$ and $\langle \mathbf{z}, \mathbf{z}\rangle \le \left\langle \mathbf{z}, \sum_j w_j \mathbf{x}_j \right\rangle$, if $\mathbf{x}_j$ is collinear for all j, then $\mathbf{z}$ is also collinear.*

Proof. Let $\mathbf{x}_j = x_j \mathbf{e}$ for all j, and write $\alpha = \sum_j w_j x_j$ for clarity. Observe that $\langle \mathbf{z}, \mathbf{z}\rangle \le \left\langle \mathbf{z}, \sum_j w_j \mathbf{x}_j \right\rangle = \sum_j w_j x_j \langle \mathbf{z}, \mathbf{e}\rangle = \alpha \langle \mathbf{z}, \mathbf{e}\rangle$. If $\alpha < 0$, then $\langle \mathbf{z}, \mathbf{e}\rangle = 0$ and $\langle \mathbf{z}, \mathbf{e}\rangle = 0$ as claimed. If $\alpha \ge 0$, then $\langle \mathbf{e}, \mathbf{z}\rangle \ge \left\langle \mathbf{e}, \sum_j w_j \mathbf{x}_j \right\rangle = \sum_j w_j x_j = \alpha$. Combined with the above, this yields $\langle \mathbf{z}, \mathbf{z}\rangle \le \alpha \langle \mathbf{z}, \mathbf{e}\rangle \le \langle \mathbf{z}, \mathbf{e}\rangle^2$. We actually have $\langle \mathbf{z}, \mathbf{z}\rangle = \langle \mathbf{z}, \mathbf{e}\rangle^2$ as claimed, because $\langle \mathbf{z}, \mathbf{z}\rangle \ge \langle \mathbf{z}, \mathbf{e}\rangle^2$ already holds by the Cauchy–Schwarz inequality. □

Hence, the conditions for the uniqess of the rank-1 solution throughout the main body of the paper are simply special cases of Theorem A.2.

Proof of Lemma 5.1. Observe that the semidefinite program (5.1) is a special instance of (A.1), and that its nonconvex interpretation (5.2) is the corresponding instance of (A.2). In the one-neuron case, Lemma A.3 says that if $\mathbf{x}^\star$ satisfies collinearity, then $\mathbf{z}^\star$ also satisfies collinearity. Or put in another way, $\mathbf{x}^\star$ and $\mathbf{z}^\star$ satisfy collinearity if and only if $\mathbf{x}^\star$ satisfies collinearity. Using the latter as an equivalent condition for the former and substituting into Theorem A.2 yields Lemma 5.1 as desired. □

Proof of Lemma 6.1. We repeat the proof of Lemma 5.1, but note that $\mathbf{x}_j^\star$ and $\mathbf{z}_i^\star$ satisfy collinearity for all i and j if and only if $\mathbf{x}_j^\star$ satisfies collinearity for all j. Using the latter as an equivalent condition for the former and substituting into Theorem A.2 yields Lemma 6.1 as desired. □

The main intuition behind the proof of Theorem A.2 is that a non-collinear solution to (A.2) corresponds to a high rank solution to (A.1) with $\operatorname{rank}(\mathbf{X}^\star) > 1$. In turn, a rank-1 solution is unique if and only if there exists no high-rank solutions; see [60, Theorem 2.4]. To make these ideas rigorous, we begin by reviewing some preliminaries. First, without loss of generality, we can fix $\mathbf{e} = \mathbf{e}_1$, that is, the first canonical basis vector. If we wish to solve (A.2) with a different $\mathbf{e} = \mathbf{e}'$, then we simply need to find an orthonormal matrix $\mathbf{U}$ for which $\mathbf{e}' = \mathbf{U}\mathbf{e}$, for example, using the Gram-Schmidt process. Given a solution $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ (A.2) with $\mathbf{e} = \mathbf{e}_1$, setting $\mathbf{v}'_j = \mathbf{U}\mathbf{v}_j$ yields a solution $\mathbf{v}'_1, \mathbf{v}'_2, \ldots, \mathbf{v}'_n$ to (A.2) with $\mathbf{e} = \mathbf{e}'$, because $\langle \mathbf{v}_k, \mathbf{v}_j \rangle = \langle \mathbf{U}\mathbf{v}_k, \mathbf{U}\mathbf{v}_j \rangle = \langle \mathbf{v}'_k, \mathbf{v}'_j \rangle$ and $\langle \mathbf{e}_1, \mathbf{v}_j \rangle = \langle \mathbf{U}\mathbf{e}_1, \mathbf{U}\mathbf{v}_j \rangle = \langle \mathbf{e}', \mathbf{v}'_j \rangle$.

The equivalence between (A.1) and (A.2) is established by using the solution to one problem to construct a *corresponding solution* satisfying the following relationship

$$\langle \mathbf{x}, \mathbf{e}_j \rangle = \langle \mathbf{e}, \mathbf{v}_j \rangle, \qquad \langle \mathbf{X}, \mathbf{e}_j \mathbf{e}_k^T \rangle = \langle \mathbf{v}_j, \mathbf{v}_k \rangle,$$

for the other problem. In one direction, given a solution $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n \in \mathbb{R}^p$ to (A.2), the corresponding solution to (A.1) is simply

$$\mathbf{x} = [\langle \mathbf{e}, \mathbf{v}_j \rangle]_{j=1}^n = \mathbf{V}^T \mathbf{e}, \qquad \mathbf{X} = [\langle \mathbf{v}_j, \mathbf{v}_k \rangle]_{j,k=1}^n = \mathbf{V}^T \mathbf{V},$$

where $\mathbf{V} = [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_n] \in \mathbb{R}^{p \times n}$. In the other direction, given a solution $\mathbf{x}$ and $\mathbf{X}$ to (A.1), we factorize $\mathbf{X} - \mathbf{x}\mathbf{x}^T = \tilde{\mathbf{V}}^T \tilde{\mathbf{V}}$ so that

$$\begin{bmatrix} 1 & \mathbf{x}^T \\ \mathbf{x} & \mathbf{X} \end{bmatrix} = [\mathbf{e}_1 \quad \mathbf{V}]^T [\mathbf{e}_1 \quad \mathbf{V}], \quad \mathbf{V} = \begin{bmatrix} \mathbf{x}^T \\ \tilde{\mathbf{V}} \end{bmatrix} = [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_n] \in \mathbb{R}^{p \times n}.$$

Then, $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ is a corresponding solution to (A.2) with $\mathbf{e} = \mathbf{e}_1$.

Proof of Theorem A.2. ($\Rightarrow$) Given a rank-1 solution $\mathbf{X}^\star = \mathbf{x}^\star (\mathbf{x}^\star)^T$ of the relaxation (A.1), we set $x_j^\star = \langle \mathbf{e}_j, \mathbf{x}^\star \rangle$ and $\mathbf{v}_j^\star = \langle \mathbf{e}_j, \mathbf{x}^\star \rangle \mathbf{e}$ to obtain a corresponding solution $\mathbf{v}_1^\star, \mathbf{v}_2^\star, \ldots, \mathbf{v}_n^\star$ to (A.2) that satisfies collinearity. By contradiction, suppose that there exists another solution $\mathbf{v}'_1, \mathbf{v}'_2, \ldots, \mathbf{v}'_n$ to (A.2) that does not satisfy collinearity, meaning that there exists some s such that $|\langle \mathbf{e}, \mathbf{v}'_s \rangle| \neq \|\mathbf{v}'_s\|$. Then, its corresponding solution $\mathbf{x}', \mathbf{X}'$ is distinct from $\mathbf{x}^\star, \mathbf{X}^\star$, because $|\langle \mathbf{e}, \mathbf{v}'_s \rangle| \neq \|\mathbf{v}'_s\|$ but $|\langle \mathbf{e}, \mathbf{v}_s^\star \rangle| = \|\mathbf{v}_s^\star\|$, so we can have either $\langle \mathbf{X}^\star - \mathbf{X}', \mathbf{e}_s \mathbf{e}_s^T \rangle = \|\mathbf{v}_s^\star\|^2 - \|\mathbf{v}'_s\|^2 = 0$ or $\langle \mathbf{x}^\star - \mathbf{x}', \mathbf{e}_s \rangle = \langle \mathbf{e}, \mathbf{v}_s^\star - \mathbf{v}'_s \rangle = 0$ but not both at the same time. This contradicts the hypothesis that $\mathbf{X}^\star$ is a unique solution.

($\Leftarrow$) Without loss of generality, we assume that $\mathbf{e} = \mathbf{e}_1$. Given a solution $\mathbf{v}_1^\star, \mathbf{v}_2^\star, \ldots, \mathbf{v}_n^\star$ to (A.2) satisfying collinearity, we set $x_j^\star = \langle \mathbf{e}, \mathbf{v}_j^\star \rangle$, $\mathbf{x}^\star = [x_j^\star]_{j=1}^n$, and $\mathbf{X}^\star = \mathbf{x}^\star (\mathbf{x}^\star)^T$, in order to obtain a corresponding rank-1 solution to (A.1). By contradiction, suppose that there exists another solution $\mathbf{x}', \mathbf{X}'$ to (A.1) that is distinct from $\mathbf{x}^\star, \mathbf{X}^\star$, with corresponding solution $\mathbf{v}'_1, \mathbf{v}'_2, \ldots, \mathbf{v}'_n$ to (A.2). This solution $\mathbf{v}'_1, \mathbf{v}'_2, \ldots, \mathbf{v}'_n$ must satisfy collinearity, or else our hypothesis is immediately violated. Under collinearity, we again set $x'_j = \langle \mathbf{e}, \mathbf{v}'_j \rangle$ such that $\mathbf{x}' = [x'_j]_{j=1}^n$ and $\mathbf{X}' = \mathbf{x}' (\mathbf{x}')^T$. Then, the following

$$\mathbf{v}_j = \frac{1}{2} \mathbf{e}_1 (x_j^\star + x'_j) + \frac{1}{2} \mathbf{e}_2 (x_j^\star - x'_j)$$

yields another solution, since

$$\begin{aligned}
\langle \mathbf{e}_1, \mathbf{v}_j \rangle &= \frac{1}{2}(x_j^\star + x'_j) = \frac{1}{2}(\langle \mathbf{e}_1, \mathbf{v}_j^\star \rangle + \langle \mathbf{e}_1, \mathbf{v}'_j \rangle) \\
\langle \mathbf{v}_j, \mathbf{v}_k \rangle &= \frac{1}{4}(x_j^\star + x'_j)(x_k^\star + x'_k) + \frac{1}{4}(x_j^\star - x'_j)(x_k^\star - x'_k) = \frac{1}{2}(x_j^\star x_k^\star + x'_j x'_k) \\
&= \frac{1}{2}(\langle \mathbf{v}_j^\star, \mathbf{v}_k^\star \rangle + \langle \mathbf{v}'_j, \mathbf{v}'_k \rangle)
\end{aligned}$$

In order for $\mathbf{x}', \mathbf{X}'$ is distinct from $\mathbf{x}^\star, \mathbf{X}^\star$, there must be some choice of s such that $x_s^\star \neq x'_s$, but this means that $\mathbf{v}_s$ does not satisfy collinearity, since $\langle \mathbf{e}_2, \mathbf{v}_s \rangle = \frac{1}{2}(x_s^\star - x'_s) \neq 0$. This contradicts the hypothesis that all solutions $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ to (A.2) satisfy collinearity. □

B Projection onto ReLU Feasbility Set

Fix $\mathbf{e}, \mathbf{x} \in \mathbb{R}^p$ and $\hat{z} \in \mathbb{R}$. Let $\alpha = \max\{\langle \mathbf{e}, \mathbf{x} \rangle, 0\}$, and define ϕ as the projection distance onto the spherical cap defined by the "ReLU feasible set" (5.4), restated here as

$$\phi = \min_{\mathbf{z} \in \mathbb{R}^p} \|\mathbf{z} - \hat{z}\mathbf{e}\| \quad \text{s.t.} \quad \langle \mathbf{e}, \mathbf{z} \rangle \geq \alpha, \quad \|\mathbf{z}\|^2 \leq \langle \mathbf{z}, \mathbf{x} \rangle. \tag{B.1}$$

In the main text, we used intuitive, geometric arguments to prove that

$$\phi = \begin{cases} \alpha - \hat{z} & \hat{z} \le \alpha, \\ \|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\| & \hat{z} > \alpha. \end{cases} \tag{B.2}$$

In this section, we will rigorously verify (B.2) and then prove that the conditional statements are unnecessary, in that ϕ simply takes on the larger of the two values, as in

$$\phi = \max\{\alpha - \hat{z}, \quad \|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\|\}. \tag{B.3}$$

This was stated in the main text as Lemma 5.2.

We first rigorously verify (B.2) by: 1) relaxing a constraint for a specified case; 2) solving the relaxation in closed-form; 3) verifying that the closed-form solution satisfies the original constraints, and must therefore be optimal for the original problem. In the case of $\hat{z} \le \alpha$, the following relaxation

$$\phi_{\mathrm{lb1}} = \min_{\mathbf{z}\in\mathbb{R}^p}\{\|\mathbf{z} - \hat{z}\mathbf{e}\| \quad : \quad \langle \mathbf{e}, \mathbf{z}\rangle \ge \alpha\}$$

has solution $\mathbf{z}^\star = \alpha\mathbf{e}$ that is clearly feasible for (B.1) since $\|\mathbf{z}^\star\|^2 = \langle \mathbf{z}^\star, \mathbf{x}\rangle = \alpha^2$. Hence, this $\mathbf{z}^\star$ must be optimal; its objective $\|\mathbf{z}^\star - \hat{z}\mathbf{e}\| = \alpha - \hat{z}$ yields the desired value of ϕ.

In the case of $\hat{z} > \alpha$, the following relaxation

$$\phi_{\mathrm{lb2}} = \min_{\mathbf{z}\in\mathbb{R}^p}\{\|\mathbf{z} - \hat{z}\mathbf{e}\|^2 \quad : \quad \|\mathbf{z}\|^2 \le \langle \mathbf{z}, \mathbf{x}\rangle\},$$

must have an active constraint at optimality. Otherwise, the solution would be $\mathbf{z} = \hat{z}\mathbf{e}$, but this cannot be feasible as $\hat{z}^2 = \|\mathbf{z}\| \le \langle \mathbf{z}, \mathbf{x}\rangle = \hat{z}\langle \mathbf{e}, \mathbf{x}\rangle \le \hat{z}\alpha$ would contradict $\hat{z} > \alpha \ge 0$. Applying Lagrange multipliers, the solution reads $\mathbf{z}^\star = t \cdot \hat{z}\mathbf{e} + (1-t)\cdot \mathbf{x}/2$ where $t = \|\mathbf{x}/2\|/\|\hat{z}\mathbf{e} - \mathbf{x}/2\|$ is chosen to make the constraint active. We will need the following lemma to verify that $\langle \mathbf{e}, \mathbf{z}^\star\rangle \ge \alpha$.

Lemma B.1. *Let $|v| \le R$. If $u > \sqrt{R^2 - v^2}$, then $Ru/\sqrt{u^2+v^2} \ge \sqrt{R^2 - v^2}$.*

Proof. We will prove that if $u^2 + v^2 > R^2$ then $R^2u^2/(u^2+v^2) + v^2 \ge R^2$. By contradiction, suppose that $R^2u^2/(u^2+v^2) + v^2 < R$. If $u^2 + v^2 = 0$, then the premise is already false. Otherwise, we multiply by $u^2 + v^2 > 0$ to yield $R^2u^2 + v^2(u^2+v^2) < R^2(u^2+v^2)$, or equivalently $v^2(u^2 + v^2 - R^2) < 0$. This last condition is only possible if $v \ne 0$ and $u^2 + v^2 < R^2$, but this again contradicts the premise. ☐

For $u = 2\hat{z} - \langle \mathbf{e}, \mathbf{x}\rangle$, $v = \sqrt{\|\mathbf{x}\|^2 - \langle \mathbf{e}, \mathbf{x}\rangle^2}$, and $R = \|\mathbf{x}\|$, observe that

$$t = \frac{\|\mathbf{x}/2\|}{\|\hat{z}\mathbf{e} - \mathbf{x}/2\|} = \frac{R}{\sqrt{u^2+v^2}}, \qquad \alpha = \max\{\langle \mathbf{e}, \mathbf{x}\rangle, 0\} = \frac{\langle \mathbf{e}, \mathbf{x}\rangle}{2} + \frac{|\langle \mathbf{e}, \mathbf{x}\rangle|}{2}.$$

Then, $\mathbf{z}^\star = t \cdot \hat{z}\mathbf{e} + (1-t)\cdot \mathbf{x}/2$ is feasible for (B.1), because substituting u, v, R into Lemma B.1 yields

$$\hat{z} > \alpha \quad \iff \quad \hat{z} - \frac{\langle \mathbf{e}, \mathbf{x}\rangle}{2} > \frac{|\langle \mathbf{e}, \mathbf{x}\rangle|}{2} \quad \implies \quad t\cdot\left(\hat{z} - \frac{\langle \mathbf{e}, \mathbf{x}\rangle}{2}\right) \ge \frac{|\langle \mathbf{e}, \mathbf{x}\rangle|}{2},$$

and this in turn implies that

$$\langle \mathbf{e}, \mathbf{z}^\star\rangle = \frac{\langle \mathbf{e}, \mathbf{x}\rangle}{2} + t\cdot\left(\hat{z} - \frac{\langle \mathbf{e}, \mathbf{x}\rangle}{2}\right) \ge \frac{\langle \mathbf{e}, \mathbf{x}\rangle}{2} + \frac{|\langle \mathbf{e}, \mathbf{x}\rangle|}{2} = \alpha.$$

Hence, this $\mathbf{z}^\star$ must be optimal; its objective $\|\mathbf{z}^\star - \hat{z}\mathbf{e}\| = (1-t)\|\hat{z}\mathbf{e} - \mathbf{x}/2\|$ yields the desired value of ϕ.

Finally, we prove (5.5) by showing that the conditional statements in (B.2) are unnecessary.

Proof of Lemma 5.2. If $\hat{z} > \alpha$, then clearly $\phi = \phi_{\mathrm{lb2}} \ge 0$ by construction, but $\alpha - \hat{z} < 0$, so $\phi = \max\{\alpha - \hat{z}, \phi_{\mathrm{lb2}}\}$ as desired. For $\hat{z} \le \alpha$, we will proceed by examining two cases. First, suppose that $\hat{z} \ge 0$ and hence $\alpha = \langle \mathbf{e}, \mathbf{x}\rangle$ and $\hat{z} \le \langle \mathbf{e}, \mathbf{x}\rangle$. Then, $\|\hat{z}\mathbf{e} - \mathbf{x}/2\|^2 - \|\mathbf{x}/2\|^2 = \hat{z}(\hat{z} - \langle \mathbf{e}, \mathbf{x}\rangle) \le 0$, and $\|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\| \le 0$, so $\phi = \max\{\phi_{\mathrm{lb1}}, \|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\|\}$ as desired. In the case of $\hat{z} \le 0$, Lemma C.1 shows that $\langle \mathbf{e}, \mathbf{x}\rangle - \hat{z} \le \rho$ implies $\|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\| \le \rho$, since with $u = \langle \mathbf{e}, \mathbf{x}\rangle$, $v = \sqrt{\|\mathbf{x}\|^2 - \langle \mathbf{e}, \mathbf{x}\rangle^2}$, $c = |\hat{z}|$, and $a = \rho$, we have

$$\|\mathbf{x}/2 + |\hat{z}|\mathbf{e}\| - \|\mathbf{x}/2\| \le \rho \qquad \Longleftrightarrow \qquad \frac{\langle \mathbf{e}, \mathbf{x}\rangle + |\hat{z}|}{\rho} \le \sqrt{1 + \frac{\|\mathbf{x}\|^2 - \langle \mathbf{e}, \mathbf{x}\rangle^2}{\hat{z}^2 - \rho^2}}$$

but $\langle \mathbf{e}, \mathbf{x}\rangle - \hat{z} \le \rho$ already implies $\frac{1}{\rho}[\langle \mathbf{e}, \mathbf{x}\rangle + |\hat{z}|] \le 1$. In particular, the fact that $\langle \mathbf{e}, \mathbf{x}\rangle - \hat{z} \le \phi_{\mathrm{lb1}}$ implies $\|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\| \le \phi_{\mathrm{lb1}}$ shows that we have $\phi = \max\{\phi_{\mathrm{lb1}}, \|\hat{z}\mathbf{e} - \mathbf{x}/2\| - \|\mathbf{x}/2\|\}$. $\square$

C Projection onto a hyperbola

Fix $\mathbf{e}, \mathbf{x} \in \mathbb{R}^p$ and $\hat{x}, \hat{z}, \rho \in \mathbb{R}$ such that $\hat{z} > \rho > 0$. Define ψ as the projection distance onto the hyperboloidal cap (5.4), restated here

$$\psi = \min_{\mathbf{x} \in \mathbb{R}^p} \quad \|\mathbf{x} - \hat{x}\mathbf{e}\| \quad \text{s.t.} \quad \langle \mathbf{e}, \mathbf{x}\rangle - \hat{z} \le \rho, \quad \|2\hat{z}\mathbf{e} - \mathbf{x}\| - \|\mathbf{x}\| \le 2\rho. \tag{C.1}$$

Without loss of generality, we can fix $\mathbf{e} = \mathbf{e}_1$ (see Appendix A), and split the coordinates of $\mathbf{x}$ as in $u = \mathbf{x}[1]$ and $\mathbf{v}[j] = \mathbf{x}[1+j]$ for $j \in \{1, 2, \dots, p-1\}$ to rewrite (C.1) as the following

$$\begin{aligned} \psi^2 = \quad & \min_{(u,\mathbf{v}) \in \mathbb{R}^p} \quad (u - \hat{x})^2 + \|\mathbf{v}\|^2 \\ & \text{s.t.} \quad u - \hat{z} \le \rho, \quad \sqrt{(u - 2\hat{z})^2 + \|\mathbf{v}\|^2} - \sqrt{u^2 + \|\mathbf{v}\|^2} \le 2\rho. \end{aligned} \tag{C.2}$$

Observe that the variable $\mathbf{v} \in \mathbb{R}^{p-1}$ only appears in (C.2) via its norm $\|\mathbf{v}\|$. Hence, (C.2) is equivalent to the following problem

$$\begin{aligned} \psi^2 = \quad & \min_{u,v \in \mathbb{R}} \quad (u - \hat{x})^2 + v^2 \\ & \text{s.t.} \quad u - \hat{z} \le \rho, \quad \sqrt{(u - 2\hat{z})^2 + v^2} - \sqrt{u^2 + v^2} \le 2\rho, \end{aligned} \tag{C.3}$$

and a solution $\mathbf{v}^\star$ to (C.2) can be recovered from a solution $v^\star$ to (C.3) by picking any unit vector $\mathbf{s} \in \mathbb{R}^{p-1}$ with $\|\mathbf{s}\| = 1$ and setting $\mathbf{v}^\star = v^\star \mathbf{s}$. We have reduced the projection over a hyperboloid (C.1) into a projection onto a hyperbola (C.3) by taking a quotient over the minor-axis directions. To proceed, we will need the following technical lemma, which is mechancially derived by completing the square and collecting terms.

Lemma C.1. *Given semi-major axis $a > 0$, semi-minor axis $b > 0$, and focus $c = \sqrt{a^2 + b^2}$, the following hold*

$$\sqrt{(u - 2c)^2 + v^2} - \sqrt{u^2 + v^2} \le 2a \qquad \Longleftrightarrow \qquad \frac{u - c}{a} \ge \sqrt{1 + \frac{v^2}{b^2}}, \tag{C.4a}$$

$$\sqrt{(u + 2c)^2 + v^2} - \sqrt{u^2 + v^2} \le 2a \qquad \Longleftrightarrow \qquad \frac{u + c}{a} \le \sqrt{1 + \frac{v^2}{b^2}}. \tag{C.4b}$$

We use Lemma C.1 to rewrite the hyperbolic constraint in (C.3) in quadratic form, as in

$$\psi^2 = \min_{u,v \in \mathbb{R}} \quad (u - \hat{x})^2 + v^2 \quad \text{s.t.} \quad \frac{u - \hat{z}}{\rho} \le 1, \quad \frac{(u - \hat{z})^2}{\rho^2} - \frac{v^2}{\hat{z}^2 - \rho^2} \le 1. \tag{C.5}$$

We will need the following to solve (C.5). This is the main result of this section.

Theorem C.2 (Axial projection onto a hyperbola)**.** *The problem data $\mathbf{a}, \mathbf{x} \in \mathbb{R}^m$, $\mathbf{c} \in \mathbb{R}^m$ and $b \in \mathbb{R}$ satisfy*

$$\mathbf{a}, \mathbf{c} \ne 0, \quad |\langle \mathbf{a}, \mathbf{x}\rangle - b| - 1 < \|\mathbf{a}\|^2 / \|\mathbf{c}\|^2$$

if and only if the following projection

$$(\mathbf{u}^\star, \mathbf{v}^\star) = \arg\min_{\mathbf{u},\mathbf{v}} \left\{ \|\mathbf{u} - \mathbf{x}\|^2 + \|\mathbf{v}\|^2 : (\langle \mathbf{a}, \mathbf{u}\rangle - b)^2 - \langle \mathbf{c}, \mathbf{v}\rangle^2 \le 1 \right\}$$

has a unique solution

$$\begin{aligned} \mathbf{u}^\star &= \mathbf{x} - \mathbf{a}\frac{(\langle \mathbf{a}, \mathbf{x}\rangle - b)}{\|\mathbf{a}\|^2}\left(1 - \frac{1}{|\langle \mathbf{a}, \mathbf{x}\rangle - b|}\right), \\ \mathbf{v}^\star &= 0. \end{aligned}$$

The proof of Theorem C.2 will span the remainder of this section. Lemma 5.3 is clearly a special instance as applied to (C.5).

Proof of Lemma 5.3. If $\hat{x} \geq \hat{z} - \rho$, then relaxing the hyperbolic constraint in (C.5) yields a unique solution of $u^\star = \min\{\hat{x}, \hat{z} + \rho\}$ and $v^\star = 0$. Indeed, this solution also satisfies the hyperbolic constraint, and is therefore optimal for (C.5). Otherwise, if $\hat{x} < \hat{z} - \rho$, then we will use relax the linear constraint in (C.5) and apply Theorem C.2. Here, $\mathbf{a} = 1/\rho$, $b = \hat{z}/\rho$, $\mathbf{c} = 1/\sqrt{\hat{z}^2 - \rho^2}$, and $\mathbf{x} = \hat{x}$, and the condition for (C.5) to have a unique condition $u^\star$ and $v^\star$ with $v^\star = 0$ is

$$|\hat{x} - \hat{z}|/\rho - 1 < (\hat{z}^2 - \rho^2)/\rho^2 \qquad \Longleftrightarrow \qquad |\hat{x} - \hat{z}| < \hat{z}^2/\rho. \tag{C.6}$$

It is easy to verify that the resulting solution is feasible for (C.5), and hence optimal. Under the premise $\hat{x} - \hat{z} < -\rho < 0$, the condition (C.6) is just $\hat{x} > \hat{z} - \hat{z}^2/\rho$, which also implies $\hat{x} \geq \hat{z} - \rho$ because $\hat{z} > \rho$. Hence, we have covered both cases; the condition $(\hat{z} - \hat{x}) < \hat{z}^2/\rho$ guarantees a unique $u^\star$ and $v^\star = 0$ as claimed. □

We will now prove Theorem C.2. The Euclidean projection onto a hyperbola is the minimization of one quadratic function subject to another quadratic function. This is well-known to be a tractable problem via the S-procedure (see e.g. [52, p. 655] or [53]). In its original form, it states that for two quadratics $f(\mathbf{x})$ and $g(\mathbf{x})$ for which there exists $\mathbf{x}_0$ satisfying $g(\mathbf{x}_0) < 0$, that

$$f(\mathbf{x}) \geq 0 \quad \text{holds for all } \mathbf{x} \text{ satisfying } g(\mathbf{x}) \leq 0$$

if and only if there exists $\lambda \geq 0$ such that

$$f(\mathbf{x}) + \lambda g(\mathbf{x}) \geq 0 \quad \text{holds for all } \mathbf{x}.$$

Clearly, a corollary of the S-procedure is strong duality, as in

$$\min_{\mathbf{x}}\{f(\mathbf{x}) : g(\mathbf{x}) \leq 0) \quad = \quad \max_{\lambda \geq 0} \min_{\mathbf{x}}\{f(\mathbf{x}) + \lambda g(\mathbf{x})\},$$

and so the Karush–Kuhn–Tucker conditions allow us to solve the primal by solving the dual, assuming the existence of a strictly feasible point $\mathbf{x}_0$ with $g(\mathbf{x}_0) < 0$. To proceed, we will need the following technical lemma, which is mechancially derived by applying the Sherman-Morrison identity.

Lemma C.3 (Rank-1 update)**.** *Given $\mathbf{a}, \mathbf{x} \in \mathbb{R}^m$, $b \in \mathbb{R}$, and $\lambda > -1/\|\mathbf{a}\|^2$, the following projection*

$$\mathbf{u}^\star = \arg\min_{u \in \mathbb{R}^n} \{\|\mathbf{u} - \mathbf{x}\|^2 + \lambda(\langle \mathbf{a}, \mathbf{u}\rangle - b)^2\}$$

has a unique solution $\mathbf{u}^\star$ satisfying

$$\mathbf{u}^\star = \mathbf{x} - \lambda \mathbf{a}\left(\frac{\langle \mathbf{a}, \mathbf{x}\rangle - b}{1 + \lambda\|\mathbf{a}\|^2}\right), \qquad \langle \mathbf{a}, \mathbf{u}^\star\rangle - b = \frac{\langle \mathbf{a}, \mathbf{x}\rangle - b}{1 + \lambda\|\mathbf{a}\|^2}.$$

$$\|\mathbf{u}^\star - \mathbf{x}\|^2 + \lambda(\langle \mathbf{a}, \mathbf{u}^\star\rangle - b)^2 = \frac{\lambda(\langle \mathbf{a}, \mathbf{x}\rangle - b)^2}{1 + \lambda\|\mathbf{a}\|^2}$$

We will actually solve the most general form of the projection problem.

Lemma C.4 (General projection onto a single hyperbola)**.** *Let $\mathbf{a}, \mathbf{x} \in \mathbb{R}^m$, $\mathbf{c}, \mathbf{y} \in \mathbb{R}^m$ and $b, d \in \mathbb{R}$ satisfy $\mathbf{a}, \mathbf{c} \neq 0$. Let $\mathbf{u}^\star \in \mathbb{R}^m$, $\mathbf{v}^\star \in \mathbb{R}^m$ be solutions to the projection*

$$\phi = \min_{\mathbf{u}, \mathbf{v}} \left\{\|\mathbf{u} - \mathbf{x}\|^2 + \|\mathbf{v} - \mathbf{y}\|^2 : (\langle \mathbf{a}, \mathbf{u}\rangle - b)^2 - (\langle \mathbf{c}, \mathbf{v}\rangle - d)^2 \leq 1\right\},$$

and let $\lambda^\star$ be the unique solution to the Lagrangian dual

$$\phi_{\mathrm{lb}} = \max_{0 \leq \lambda \leq 1/\|\mathbf{c}\|^2} \left\{\lambda\left[\frac{(\langle \mathbf{a}, \mathbf{x}\rangle - b)^2}{1 + \lambda\|\mathbf{a}\|^2} - \frac{(\langle \mathbf{c}, \mathbf{y}\rangle - d)^2}{1 - \lambda\|\mathbf{c}\|^2} - 1\right]\right\}.$$

Then, $\phi = \phi_{\mathrm{lb}}$. Moreover the primal solutions are unique if and only if $\lambda^\star < 1/\|\mathbf{c}\|^2$, with values

$$\mathbf{u}^\star = \mathbf{x} - \lambda^\star \mathbf{a}\left(\frac{\langle \mathbf{a}, \mathbf{x}\rangle - b}{1 + \lambda^\star\|\mathbf{a}\|^2}\right), \qquad v^\star = y + \lambda^\star \mathbf{c}\left(\frac{\langle \mathbf{c}, \mathbf{y}\rangle - d}{1 - \lambda^\star\|\mathbf{c}\|^2}\right).$$

Proof. We define the following two quadratics and corresponding Lagrangian

$$f(\mathbf{u},\mathbf{v}) = \|\mathbf{u}-\mathbf{x}\|^2 + \|\mathbf{v}-\mathbf{y}\|^2,$$
$$g(\mathbf{u},\mathbf{v}) = (\langle \mathbf{a},\mathbf{u}\rangle - b)^2 - (\langle \mathbf{c},\mathbf{v}\rangle - d)^2 - 1,$$
$$L(\mathbf{u},\mathbf{v},\lambda) = f(\mathbf{u},\mathbf{v}) + \lambda g(\mathbf{u},\mathbf{v}).$$

Note that $\mathbf{u}_0 = b\mathbf{a}/\|\mathbf{a}\|$ and $\mathbf{v}_0 = d\mathbf{c}/\|\mathbf{c}\|$ satisfies $g(\mathbf{u}_0,\mathbf{v}_0) < 0$, so strong duality holds via the S-procedure. Next, we apply Lemma C.3 to yield the Lagrangian dual ϕ_{lb} via

$$\min_{\mathbf{u},\mathbf{v}} L(\mathbf{u},\mathbf{v},\lambda) = \begin{cases} \lambda\left[\frac{(\langle \mathbf{a},\mathbf{x}\rangle - b)^2}{1+\lambda\|\mathbf{a}\|^2} - \frac{(\langle \mathbf{c},\mathbf{y}\rangle - d)^2}{1-\lambda\|\mathbf{c}\|^2} - 1\right] & \lambda \le 1/\|\mathbf{c}\|^2, \\ -\infty & \lambda > 1/\|\mathbf{c}\|^2. \end{cases}$$

It is easy to verify that the dual function above is strongly concave over λ, so the solution $\lambda^\star$ is unique. Finally, if $\lambda^\star < 1/\|\mathbf{c}\|^2$, then the Lagrangian $L(\mathbf{u},\mathbf{v},\lambda^\star)$ is strongly convex, and the primal solutions $\mathbf{u}^\star$ and $\mathbf{v}^\star$ are both uniquely determined by minimizing $L(\mathbf{u},\mathbf{v},\lambda^\star)$. Otherwise, if $\lambda^\star = 1/\|\mathbf{c}\|^2$, then $L(\mathbf{u},\mathbf{v},\lambda^\star)$ is weakly convex over $\mathbf{v}$. Here, $\mathbf{u}^\star$ is uniquely determined by minimizing $L(\mathbf{u},\mathbf{v},\lambda^\star)$, but $\mathbf{v}^\star$ can be any choice that satisfies primal feasibility $(\langle \mathbf{a},\mathbf{u}^\star\rangle - b)^2 - (\langle \mathbf{c},\mathbf{v}^\star\rangle - d)^2 = 1$, and is therefore nonunique. □

Finally, we prove Theorem C.2 using Lemma C.4.

Proof of Theorem C.2. The axial projection problem of Theorem C.2 is an instance of the more general projection problem in Lemma C.4 with $\mathbf{y} = 0$ and $d = 0$. The intended claim holds so long as $\lambda^\star < 1/\|\mathbf{c}\|^2$. Now, first order optimality in the Lagrangian dual reads

$$\frac{(\langle \mathbf{a},\mathbf{x}\rangle - b)^2}{(1+\lambda^\star\|\mathbf{a}\|^2)^2} - \frac{(\langle \mathbf{c},\mathbf{y}\rangle - d)^2}{(1-\lambda^\star\|\mathbf{c}\|^2)^2} - 1 = 0,$$

and this implies $1+\lambda^\star\|\mathbf{a}\|^2 = |\langle \mathbf{a},\mathbf{x}\rangle - b|$ and hence $\lambda^\star = (|\langle \mathbf{a},\mathbf{x}\rangle - b| - 1)/\|\mathbf{a}\|^2$. Finally, imposing the bound $\lambda^\star < 1/\|\mathbf{c}\|^2$ on this value yields our desired claim. □

D Projection onto several hyperbolas

Given $\mathbf{W} = [W_{i,j}] \in \mathbb{R}^{m\times n}$, $\hat{\mathbf{x}} = [\hat{x}_j] \in \mathbb{R}^n$, $\hat{\mathbf{z}} = [\hat{z}_i] \in \mathbb{R}^m$, $\mathbf{e} \in \mathbb{R}^p$, and ρ_i satisfying $\hat{z}_i > \rho > 0$, we will partially solve

$$\min_{\mathbf{x}_j \in \mathbb{R}^p} \quad \textstyle\sum_j \|\mathbf{x}_j - \hat{x}_j \mathbf{e}\|^2 \quad \text{s.t.} \quad \begin{aligned} \langle \mathbf{e}, \textstyle\sum_j W_{i,j}\mathbf{x}_j\rangle - \hat{z}_i \le \rho_i \text{ for all } i, \\ \|\hat{z}_i\mathbf{e} - \textstyle\sum_j W_{i,j}\mathbf{x}_j/2\| - \|\textstyle\sum_j W_{i,j}\mathbf{x}_j/2\| \le \rho_i \text{ for all } i. \end{aligned} \tag{D.1}$$

Without loss of generality, we can fix $\mathbf{e} = \mathbf{e}_1$ and split the coordinates of $\mathbf{x}_j$ as in $\mathbf{u}[j] = \mathbf{x}_j[1]$ for all j and $\mathbf{v}_k[j] = \mathbf{x}_j[1+k]$ for all j,k to rewrite (D.1) as the following

$$\begin{aligned} \min_{\mathbf{u},\mathbf{v}_j \in \mathbb{R}^n} \quad & \|\mathbf{u} - \hat{\mathbf{x}}\|^2 + \textstyle\sum_k \|\mathbf{v}_k\|^2 \\ \text{s.t.} \quad & \langle \mathbf{w}_i, \mathbf{u}\rangle - \hat{z}_i \le \rho_i, \\ & \sqrt{(\langle \mathbf{w}_i,\mathbf{u}\rangle - 2\hat{z}_i)^2 + \textstyle\sum_k \langle \mathbf{w}_i,\mathbf{v}_k\rangle^2} - \sqrt{\langle \mathbf{w}_i,\mathbf{u}\rangle^2 + \textstyle\sum_k \langle \mathbf{w}_i,\mathbf{v}_k\rangle^2} \le 2\rho_i, \end{aligned} \tag{D.2}$$

for all i, where $\mathbf{w}_i[j] = \mathbf{W}[i,j]$ is the i-th row of $\mathbf{W}$. Applying Lemma C.1 then rewrites (D.2) as the following.

$$\min_{\mathbf{u},\mathbf{v}_j \in \mathbb{R}^n} \quad \|\mathbf{u} - \hat{\mathbf{x}}\|^2 + \textstyle\sum_k \|\mathbf{v}_k\|^2 \quad \text{s.t.} \quad \sqrt{1 + \frac{\sum_k \langle \mathbf{w}_i,\mathbf{v}_k\rangle^2}{\hat{z}_i^2 - \rho_i^2}} \le \frac{\langle \mathbf{w}_i,\mathbf{u}\rangle - \hat{z}}{\rho_i} \le 1, \tag{D.3}$$

We will need the following to solve (D.3). This is the main result of this section.

Theorem D.1 (Axial projection onto several hyperbolas)**.** *If the problem data $\mathbf{x} \in \mathbb{R}^m$, $\mathbf{a}_i \in \mathbb{R}^m$, $b_i \in \mathbb{R}$, $\mathbf{c}_i \in \mathbb{R}^n$ for $i \in \{1,2,\dots,\ell\}$ satisfy*

$$\|\mathbf{C}\|^2 \cdot (\|(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x} - \mathbf{b})\|_\infty + \|(\mathbf{A}\mathbf{A}^T)^{-1}\|_\infty) < 1$$

where $\mathbf{A}[i,j] = \mathbf{a}_i[j]$, $\mathbf{b}[i] = b_i$, and $\mathbf{C}[i,j] = \mathbf{c}_i[j]$ for all i,j, then the following projection

$$(\mathbf{u}^\star,\mathbf{v}^\star) = \arg\min_{\mathbf{u},\mathbf{v}} \left\{ \|\mathbf{u}-\mathbf{x}\|^2 + \textstyle\sum_j \|\mathbf{v}_j\|^2 : (\langle \mathbf{a}_i,\mathbf{u}\rangle - b_i)^2 - \textstyle\sum_j \langle \mathbf{c}_i,\mathbf{v}_j\rangle^2 \le 1 \quad \textit{for all } i \right\}$$

has a unique solution $(\mathbf{u}^\star,\mathbf{v}^\star)$ with $\mathbf{v}_j^\star = 0$.

The proof of Theorem D.1 will span the remainder of this section. Lemma 6.2 is clearly a special instance as applied to (D.3).

Proof of Lemma 6.2. Write $\mathbf{D}_1 = \mathrm{diag}(\rho_i)$ and $\mathbf{D}_2 = \mathrm{diag}(\sqrt{\hat{z}_i^2 - \rho_i^2})$. Then, we apply Theorem D.1 with $\mathbf{x} = \hat{\mathbf{x}}$, $\mathbf{A} = \mathbf{D}_1^{-1}\mathbf{W}$, $\mathbf{b} = \mathbf{D}_1^{-1}\hat{\mathbf{z}}$, and $\mathbf{C} = \mathbf{D}_2^{-1}\mathbf{W}$. Clearly

$$\|\mathbf{C}\|^2 = \|\mathbf{D}_2^{-1}\mathbf{W}\|^2 \le \|\mathbf{W}\|^2/(\hat{z}_{\min}^2 - \rho_{\max}^2)$$
$$\|(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x}-\mathbf{b})\|_\infty = \|\mathbf{D}_1(\mathbf{W}\mathbf{W}^T)^{-1}(\mathbf{W}\hat{\mathbf{x}}-\hat{\mathbf{z}})\|_\infty \le \rho_{\max}\|(\mathbf{W}\mathbf{W}^T)^{-1}(\mathbf{W}\hat{\mathbf{x}}-\hat{\mathbf{z}})\|_\infty$$
$$\|\mathbf{D}_1(\mathbf{W}\mathbf{W}^T)^{-1}\mathbf{D}_1\|_\infty \le \rho_{\max}^2\|(\mathbf{W}\mathbf{W}^T)^{-1}\|_\infty$$

and hence the condition in Theorem D.1 is the following

$$\rho_{\max}\|\mathbf{W}\|^2\|(\mathbf{W}\mathbf{W}^T)^{-1}(\mathbf{W}\hat{\mathbf{x}}-\hat{\mathbf{z}})\|_\infty + \rho_{\max}^2\|\mathbf{W}\|^2\|(\mathbf{W}\mathbf{W}^T)^{-1}\|_\infty < \hat{z}_{\min}^2 - \rho_{\max}^2$$

which is the same condition stated in Lemma 6.2. □

Our proof of Theorem D.1 is based on a SDP relaxation.

Proof of Theorem D.1. The problem is nonconvex over $\mathbf{v}$, but a convex relaxation is easily constructed by representing the quadratic outer product $\sum_k \mathbf{v}_k\mathbf{v}_k^T$ by $\mathbf{V} \succeq 0$, as in

$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^m,\mathbf{v}\in\mathbb{R}^n}{\text{minimize}} \quad & \frac{1}{2}\|\mathbf{u}-\mathbf{x}\|^2 + \frac{1}{2}\mathrm{tr}(\mathbf{V}) \\ \text{subject to} \quad & -1 \le \langle \mathbf{a}_i, \mathbf{u}\rangle - b_i \le \sqrt{1 + \langle \mathbf{c}_i\mathbf{c}_i^T, \mathbf{V}\rangle} \qquad \text{for all } i \in \{1,2,\dots,\ell\} \end{aligned}$$

with the relaxation being exact whenever $\mathbf{V}^\star = 0$. The corresponding Lagrangian is

$$L(\mathbf{u},\mathbf{V},\xi,\mu) = \frac{1}{2}\|\mathbf{u}-\mathbf{x}\|^2 + \frac{1}{2}\mathrm{tr}(\mathbf{V}) + (\xi-\mu)^T(\mathbf{A}\mathbf{u}-\mathbf{b}) - \sum_{i=1}^{\ell}\left[\xi_i\sqrt{1+\langle \mathbf{c}_i\mathbf{c}_i^T,\mathbf{V}\rangle} + \mu_i\right],$$

over Lagrange multipliers $\xi,\mu \ge 0$. Assuming that $\mathbf{A}^T\mathbf{A} \ne 0$, this problem has strictly feasible primal point $\mathbf{u} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{b}$ and $\mathbf{V} = \mathbf{I}$, and strictly feasible dual point $\xi = \mu = \epsilon\mathbf{1}$ for $\epsilon > 0$. Hence, strong duality is attained as in

$$\min_{\mathbf{V}\succeq 0,\mathbf{u}} \max_{\lambda,\mu\ge 0} L(\mathbf{u},\mathbf{V},\xi,\mu) = \max_{\lambda,\mu\ge 0} \min_{\mathbf{V}\succeq 0,\mathbf{u}} L(\mathbf{u},\mathbf{V},\xi,\mu).$$

Examining the inner minimization over $\mathbf{V} \succeq 0$, note that the associated optimiality conditions read

$$\nabla_{\mathbf{V}} L(\mathbf{u},\mathbf{V}^\star,\xi,\mu) = \mathbf{S} = \frac{1}{2}\left(I - \sum_{i=1}^{q}\frac{\xi_i\mathbf{c}_i\mathbf{c}_i^T}{\sqrt{1+\langle \mathbf{c}_i\mathbf{c}_i^T,\mathbf{V}^\star\rangle}}\right) \succeq 0, \qquad \mathbf{S}\mathbf{V}^\star = 0.$$

Hence, the minimum is attained at $\mathbf{V}^\star = 0$ if and only if $\sum_i \xi_i\mathbf{c}_i\mathbf{c}_i^T \prec I$. We will proceed to solve the dual for the optimal Lagrange multiplier $\xi^\star$ and verify that $\sum_i \xi_i^\star\mathbf{c}_i\mathbf{c}_i^T \prec I$ is satisfied.

In the case that $\mathbf{V}^\star = 0$, the corresponding $\mathbf{u}^\star$ is unique

$$\mathbf{u}^\star = \arg\min_{\mathbf{u}} L(\mathbf{u},0,\lambda,\mu) = \arg\min_{\mathbf{u}} \frac{1}{2}\|\mathbf{u}-\mathbf{x}\|^2 + \mathbf{y}^T(\mathbf{A}\mathbf{u}-\mathbf{b}) = \mathbf{x} - \mathbf{A}^T\mathbf{y}$$

where $\mathbf{y} = \xi - \mu$, and the dual problem is written

$$\max_{\xi,\mu\ge 0}\min_{\mathbf{u}} L(\mathbf{u},0,\xi,\mu) = -\min_{\mathbf{y}}\left\{\frac{1}{2}\|\mathbf{A}^T\mathbf{y}\|^2 - \mathbf{y}^T(\mathbf{A}\mathbf{x}-\mathbf{b}) + \|\mathbf{y}\|_1\right\}.$$

whose optimal conditions read

$$\mathbf{A}\mathbf{A}^T\mathbf{y}^\star - (\mathbf{A}\mathbf{x}-\mathbf{b}) \in \mathrm{sign}(\mathbf{y}^\star) \qquad \text{where } \mathrm{sign}(\alpha) = \begin{cases} +1 & \alpha > 0, \\ [-1,+1] & \alpha = 0, \\ -1 & \alpha < 0. \end{cases}$$

We wish to impose conditions on the data $\mathbf{A}, \mathbf{b}, \mathbf{x}$ to ensure that $\lambda_{\max}(\max\{0, y_i^\star\}\mathbf{c}_i\mathbf{c}_i^T) < 1$ holds at dual optimality. A conservative condition is to use the enclosure $\mathrm{sign}(\alpha) \subset [-1, +1]$ to solve a relaxation

$$\begin{aligned}
&\max_{\mathbf{y}}\left\{\lambda_{\max}\left(\sum_i \max\{0, \mathbf{e}_i^T\mathbf{y}\}\mathbf{c}_i\mathbf{c}_i^T\right) : \mathbf{y} = (\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x} - \mathbf{b} - \mathbf{s}), \quad \mathbf{s} \in \mathrm{sign}(\mathbf{y})\right\} \\
\le&\lambda_{\max}\left(\sum_i \mathbf{c}_i\mathbf{c}_i^T\right) \cdot \max_{\mathbf{y}}\left\{\max_i\{0, \mathbf{e}_i^T\mathbf{y}\} : \mathbf{y} = (\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x} - \mathbf{b} - \mathbf{s}), \quad \mathbf{s} \in \mathrm{sign}(\mathbf{y})\right\} \\
\le&\lambda_{\max}\left(\sum_i \mathbf{c}_i\mathbf{c}_i^T\right) \cdot \max_{\mathbf{y}}\left\{\max_i\{0, \mathbf{e}_i^T\mathbf{y}\} : \mathbf{y} = (\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x} - \mathbf{b} - \mathbf{s}), \quad \|\mathbf{s}\|_\infty \le 1\right\} \\
=&\lambda_{\max}\left(\sum_i \mathbf{c}_i\mathbf{c}_i^T\right) \cdot \max_i\left\{0, \mathbf{e}_i^T(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x} - \mathbf{b} - \mathbf{s})\right\}.
\end{aligned}$$

Hence, if the following holds

$$\|\mathbf{C}\|^2 \cdot \max_i\left\{\mathbf{e}_i^T(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x} - \mathbf{b}) + \sum_{j=1}^n |\mathbf{e}_i^T(\mathbf{A}\mathbf{A}^T)^{-1}\mathbf{e}_j|\right\} < 1$$

or more conservatively, if the following holds

$$\|\mathbf{C}\|^2 \cdot (\|(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{A}\mathbf{x} - \mathbf{b})\|_\infty + \|(\mathbf{A}\mathbf{A}^T)^{-1}\|_\infty) < 1$$

then $\mathbf{V}^\star = 0$ and $\mathbf{u}^\star$ is unique as desired. □

E Further details for multiple layers

In the general ℓ-layer case, the SDP relaxation for problem (A) reads

$$d_{\mathrm{lb}}^2 = \min_{\mathbf{G}_k \succeq 0} \mathrm{tr}(\mathbf{X}_0) - 2\langle\hat{\mathbf{x}}, \mathbf{x}_0\rangle + \|\hat{\mathbf{x}}\|^2 \tag{A-lb}$$

$$\text{s.t.} \quad \begin{array}{c} \mathbf{x}_{k+1} \ge 0, \quad \mathbf{x}_{k+1} \ge \mathbf{W}_k\mathbf{x}_k + \mathbf{b}_k, \\ \mathrm{diag}(\mathbf{X}_{k+1}) \le \mathrm{diag}(\mathbf{W}_k\mathbf{Y}_k^T), \\ \langle\mathbf{w}, \mathbf{x}_\ell\rangle + b \le 0, \end{array} \qquad \mathbf{G}_k = \begin{bmatrix} 1 & \mathbf{x}_k^T & \mathbf{x}_{k+1}^T \\ \mathbf{x}_k & \mathbf{X}_k & \mathbf{Y}_k \\ \mathbf{x}_{k+1} & \mathbf{Y}_k^T & \mathbf{X}_{k+1} \end{bmatrix} \succeq 0 \text{ for all } k,$$

over layer indices $k \in \{0, 1, \ldots, \ell - 1\}$, while the SDP relaxation for problem (B) is almost identical, except the constraint on $\mathbf{x}_\ell$:

$$L_{\mathrm{lb}}^2 = \min_{\mathbf{G}_k \succeq 0} \mathrm{tr}(\mathbf{X}_0) - 2\langle\hat{\mathbf{x}}, \mathbf{x}_0\rangle + \|\hat{\mathbf{x}}\|^2 \tag{B-lb}$$

$$\text{s.t.} \quad \begin{array}{c} \mathbf{x}_{k+1} \ge 0, \quad \mathbf{x}_{k+1} \ge \mathbf{W}_k\mathbf{x}_k + \mathbf{b}_k, \\ \mathrm{diag}(\mathbf{X}_{k+1}) \le \mathrm{diag}(\mathbf{W}_k\mathbf{Y}_k^T), \\ \mathrm{tr}(\mathbf{X}_\ell) - 2\langle\hat{\mathbf{z}}, \mathbf{x}_\ell\rangle + \|\hat{\mathbf{z}}\|^2 \le \rho^2, \end{array} \qquad \mathbf{G}_k = \begin{bmatrix} 1 & \mathbf{x}_k^T & \mathbf{x}_{k+1}^T \\ \mathbf{x}_k & \mathbf{X}_k & \mathbf{Y}_k \\ \mathbf{x}_{k+1} & \mathbf{Y}_k^T & \mathbf{X}_{k+1} \end{bmatrix} \succeq 0 \text{ for all } k,$$

over layer indices $k \in \{0, 1, \ldots, \ell - 1\}$. Note that both (A-lb) and (B-lb) are SDPs over ℓ smaller semidefinite variables, each of order $1 + n_k + n_{k+1}$, rather than over a single large semidefinite variable of order $1 + \sum_{k=1}^{\ell} n_k$. This reduction is from an application of the chordal graph matrix completion of Fukuda et al. [61]; see also [62, Chapter 10].

Now, for the choice $\hat{\mathbf{z}} = \mathbf{u} - \rho\mathbf{w}/\|\mathbf{w}\|$ where $\mathbf{u} = -b\mathbf{w}/\|\mathbf{w}\|^2$, the optimal value $L^\star$ to problem (B) gives an upper-bound to the optimal value $L^\star \ge d^\star$ of problem (A) that converges to an equality at $\rho \to \infty$. At the same time, $L_{\mathrm{lb}} \ge d_{\mathrm{lb}}$ holds for all $\rho > 0$ because problem (A-lb) is always a relaxation of problem (B-lb). To show this, we observe that for this choice of $\hat{\mathbf{z}}$, we have

$$\begin{aligned}
&\mathrm{tr}(\mathbf{X}_\ell) - 2\langle\hat{\mathbf{z}}, \mathbf{x}_\ell\rangle + \|\hat{\mathbf{z}}\|^2 - \rho^2 \\
=&\mathrm{tr}(\mathbf{X}_\ell) - 2\langle\mathbf{u}, \mathbf{x}_\ell\rangle + (2\rho/\|\mathbf{w}\|)\langle\mathbf{w}, \mathbf{x}_\ell\rangle + \|\mathbf{u}\|^2 - (2\rho/\|\mathbf{w}\|)\langle\mathbf{w}, \mathbf{u}\rangle + \rho^2 - \rho^2 \\
=&\underbrace{\mathrm{tr}(\mathbf{X}_\ell) - 2\langle\mathbf{u}, \mathbf{x}_\ell\rangle + \|\mathbf{u}\|^2}_{\ge 0} + (2\rho/\|\mathbf{w}\|)[\langle\mathbf{w}, \mathbf{z}\rangle + b].
\end{aligned}$$

The nonnegativity of this first term follows because

$$\begin{aligned}\mathrm{tr}(\mathbf{X}_\ell) - 2\langle \mathbf{u}, \mathbf{x}_\ell\rangle + \|\mathbf{u}\|^2 &= \mathrm{tr}(\mathbf{X}_\ell - \mathbf{u}\mathbf{x}_\ell^T - \mathbf{x}_\ell \mathbf{u}^T + \mathbf{u}\mathbf{u}^T) \\ &= \mathrm{tr}(\mathbf{X}_\ell - \mathbf{x}_\ell\mathbf{x}_\ell^T + (\mathbf{x}_\ell - \mathbf{u})(\mathbf{x}_\ell - \mathbf{u})^T) \\ &= \mathrm{tr}(\mathbf{X}_\ell - \mathbf{x}_\ell\mathbf{x}_\ell^T) + \|\mathbf{x}_\ell - \mathbf{u}\|^2\end{aligned}$$

and that $\begin{bmatrix} 1 & \mathbf{x}_\ell^T \\ \mathbf{x}_\ell & \mathbf{X}_\ell \end{bmatrix} \succeq 0$ implies $\mathbf{X}_\ell - \mathbf{x}_\ell\mathbf{x}_\ell^T \succeq 0$ by the Schur complement lemma and therefore $\mathrm{tr}(\mathbf{X}_\ell - \mathbf{x}_\ell\mathbf{x}_\ell^T) \geq 0$. Hence, a feasible point $\mathbf{X}_\ell, \mathbf{x}_\ell$ for the relaxation (B-lb) satisfying $\mathrm{tr}(\mathbf{X}_\ell) - 2\langle \hat{\mathbf{z}}, \mathbf{x}_\ell\rangle + \|\hat{\mathbf{z}}\|^2 \leq \rho^2$ must immediately satisfy $\langle \mathbf{w}, \mathbf{z}\rangle + b \leq 0$ and therefore be feasible for the relaxation (A-lb).

If the relaxation (A-lb) is tight, meaning that $d^\star = d_{\mathrm{lb}}$, then the the relaxation (B-lb) must automatically be tight at $\rho \to \infty$, because $d^\star = L^\star \geq L_{\mathrm{lb}} \geq d_{\mathrm{lb}} = d^\star$. But the converse need not hold: the relaxation (A-lb) can still be loose even though (B-lb) is tight, because even with $L^\star = L_{\mathrm{lb}}$ at $\rho \to \infty$, it is still possible to have $d_{\mathrm{lb}} < d^\star$.

The nonlinear interpretation of (B-lb) reads

$$\min_{\mathbf{x}_i^{(k)} \in \mathbb{R}^p} \quad \textstyle\sum_j \|\mathbf{x}_{0,j} - \hat{x}_j \mathbf{e}\|^2 \quad \text{s.t.} \quad \begin{array}{c} \langle \mathbf{e}, \mathbf{x}_i^{(k+1)}\rangle \geq \max\left\{0, \langle \mathbf{e}, \sum_j W_{i,j}^{(k)} \mathbf{x}_j^{(k)} + b_i^{(k)} \mathbf{e}\rangle\right\}, \\ \|\mathbf{x}_i^{(k+1)}\|^2 \leq \langle \mathbf{x}_i^{(k+1)}, \sum_j W_{i,j}^{(k)} \mathbf{x}_j^{(k)} + b_i^{(k)} \mathbf{e}\rangle, \\ \sum_j \|\mathbf{x}_{\ell,j} - \hat{z}_j \mathbf{e}\|^2 \leq \rho^2, \end{array} \quad \text{for all } i, k \tag{E.1}$$

over layer indices $k \in \{0, 1, \ldots, \ell - 1\}$ and neuron indices $i \in \{1, 2, \ldots, n\}$ at each k-th layer. Suppose that problem (B) has a trivial solution $\mathbf{x}^\star = \hat{\mathbf{x}}$ with objective zero. Then, it follows that every solution to (E.1) must be collinear and satisfy $\mathbf{x}_{0,j}^\star = \hat{x}_j \mathbf{e}$, so the relaxation (B-lb) has a unique rank-1 solution via Theorem A.2.

Proof of Corollary 2.3. If $\|\mathbf{f}(\hat{\mathbf{x}}) - \hat{\mathbf{z}}\| \leq \rho$, then problem (E.1) has a minimum of zero, obtained by setting $\mathbf{x}_{0,j}^\star = \hat{x}_j \mathbf{e}$ for all j at the input layer. This choice of $\mathbf{x}_{0,j}^\star$ is unique, because $\sum_j \|\mathbf{x}_{0,j}^\star - \hat{x}_j \mathbf{e}\|^2 = 0$ holds if and only if $\mathbf{x}_{0,j}^\star = \hat{x}_j \mathbf{e}$, so the input layer must be collinear at optimality, meaning that $\|\mathbf{x}_{0,j}^\star\| = |\langle \mathbf{e}, \mathbf{x}_{0,j}^\star\rangle|$ for all j is guaranteed to hold. Then, applying Lemma A.3 shows that $\|\mathbf{x}_{1,i}^\star - b_i^{(1)} \mathbf{e}\| = |\langle \mathbf{e}, \mathbf{x}_{1,i}^\star - b_i^{(1)} \mathbf{e}\rangle|$ and therefore $\|\mathbf{x}_{1,i}^\star\| = |\langle \mathbf{e}, \mathbf{x}_{1,i}^\star\rangle|$ for all i, so the first hidden layer is also collinear. Inductively repeating this argument, if the k-th layer is collinear, as in $\|\mathbf{x}_{k,j}^\star\| = |\langle \mathbf{e}, \mathbf{x}_{k,j}^\star\rangle|$ for all j, then Lemma A.3 shows that the $(k+1)$-th layer is also collinear, as in $\|\mathbf{x}_{k+1,i}^\star\| = |\langle \mathbf{e}, \mathbf{x}_{k+1,i}^\star\rangle|$ for all i. Hence, all solutions to (E.1) are collinear, as in $\|\mathbf{x}_{k,j}^\star\| = |\langle \mathbf{e}, \mathbf{x}_{k,j}^\star\rangle|$ for all j, k. Evoking Theorem A.2 then yields our desired claim. $\square$

F The Rank-2 Burer–Monteiro Algorithm

The Burer-Monteiro algorithm is obtained by using a local optimization algorithm to solve the nonconvex interpretation of (B-lb) stated in (E.1). In particular, fix $p = 2$, define at the k-th layer $\mathbf{u}_k[j] = \langle \mathbf{e}, \mathbf{x}_j^{(k)}\rangle$ and $\mathbf{v}_k[j] = \sqrt{\|\mathbf{x}_j^{(k)}\|^2 - \langle \mathbf{e}, \mathbf{x}_j^{(k)}\rangle^2}$ yields the rank-2 Burer–Monteiro problem (BM2) as desired. In turn, given a solution $\{\mathbf{u}_k^\star, \mathbf{v}_k^\star\}$ to (BM2) satisfying $\mathbf{v}_k^\star = 0$, we recover a *rank deficient* rank-2 solution to (E.1) with $\mathbf{x}_j^{(k)} = \mathbf{u}_k^\star[j]\mathbf{e}$. This rank-deficient solution is guaranteed to be globally optimal if it satisfies first- and second-order optimality; see Burer and Monteiro [56] and also [57, 58] and in particular [59, Lemma 1].

Our MATLAB implementation solves problem (BM2) using `fmincon` with `algorithm='interior-point'`, starting from an initial point selected i.i.d. from the unit Gaussian, and terminating at relative tolerances of 10^{-8}. If the algorithm gets stuck at a spurious local minimum with $\mathbf{v}_0^\star \neq 0$, or if more than 300 iterations or function calls are made, then we restart with a new random initial point; we give up after 5 failed attempts. Empirically, we observed that whenever the SDP relaxation is tight, `fmincon` would consistently converge to a globally optimal solution satisfying $\mathbf{v}_0^\star \approx 0$ within 80 iterations of the first attempt; this suggests an underlying “no spurious local minima” result like that of Boumal et al. [57].