Exactness of SDP Relaxation for Robustness Verification of Neural Networks

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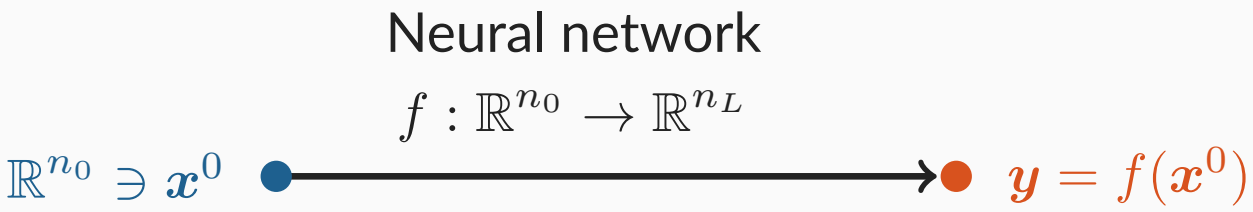
Safety Verification of Neural Networks (NNs)



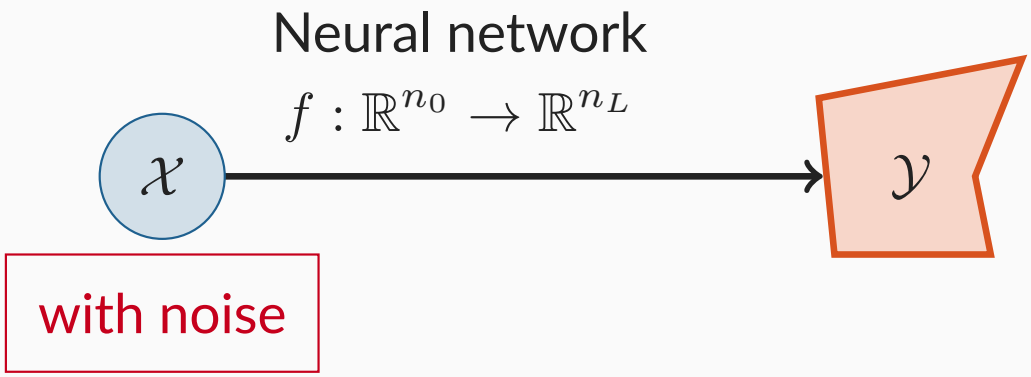
+ noise

- adversarial attacks
- uncertainty

Safety Verification

- Evaluation of the robustness of $\boldsymbol{x}^0$
- By verification of $\mathcal{Y} \subseteq S_y$ from given $\mathcal{X}, f, S_y$

Safety Verification of Neural Networks (NNs)



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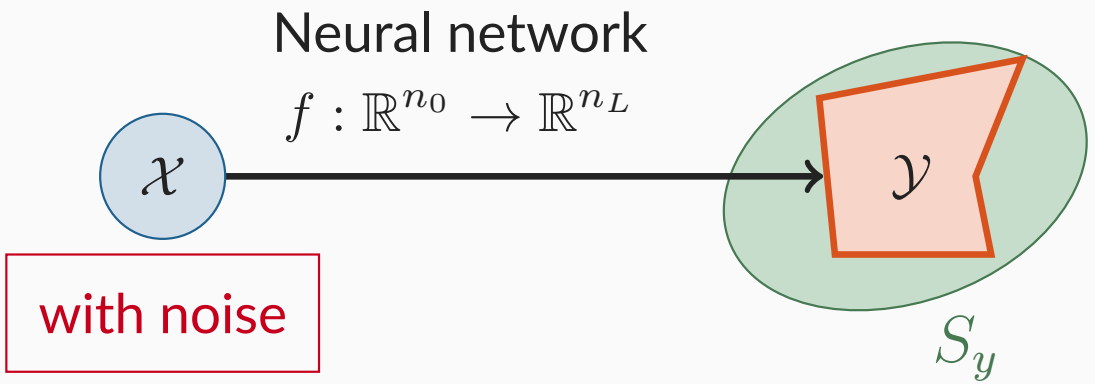


with noise

- adversarial attacks
- uncertainty

same class with y

safety specification set

Safety Verification

- Evaluation of the robustness of x^0
- By verification of $\mathcal{Y} \subseteq S_y$ from given $\mathcal{X}, f, S_y$

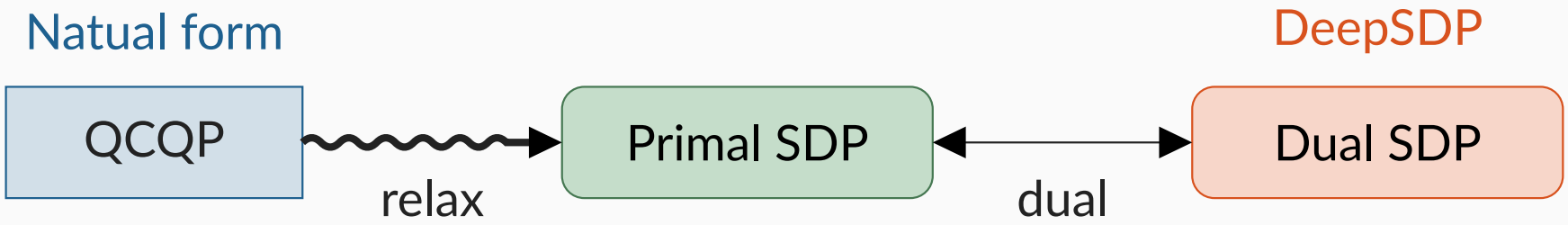
DeepSDP

Semidefinite programming(SDP)-based method can be considered

- Quadratic constraints can formulate NN with ReLU ϕ

$$y = \phi(x) := \max\{0, x\} \quad \Longleftrightarrow \quad \{y \geq 0, \quad y \geq x, \quad y(y - x) = 0\}$$

- DeepSDP is dual of SDP relaxation
  (solvable in polynomial time)



Exactness of Relaxation and Our Motivation

Two gaps exist

- Duality gap (Primal SDP and Dual SDP)
  - $= 0$ under strong duality

- Relaxation gap (QCQP and Primal SDP)
  - $= 0 \iff$ SDP relaxation is *exact*

Motivation of this talk

- Assume strong duality $\Rightarrow$ no duality gap
- Under what conditions is the primal SDP relaxation exact?

Outline

- Introduction

- Quadratically constrained quadratic programming (QCQP)
- Exact semidefinite programming (SDP) relaxation

- Single-layer feed-forward neural network
- QCQP formulation for safety verification
- Exactness conditions for SDP relaxation

- Graphical explanation of exactness

- Summary

QCQP: Quadratically Constrained Quadratic Programming

Quadratic objective function and quadratic constraints

$$
\begin{aligned}
v^* \;:=\; \min_{\boldsymbol{x}\in\mathbb{R}^n} \quad & \boldsymbol{x}^{\mathrm{T}} Q^0 \boldsymbol{x} + 2\big(\boldsymbol{q}^0\big)^{\mathrm{T}} \boldsymbol{x} \\
\text{s.t.} \quad & \boldsymbol{x}^{\mathrm{T}} Q^p \boldsymbol{x} + 2\big(\boldsymbol{q}^p\big)^{\mathrm{T}} \boldsymbol{x} \le b_p, \quad p \in [m] := \{1, \ldots, m\}.
\end{aligned}
\tag{$\mathcal{P}$}
$$

- Generally non-convex & NP-hard
- Approximately solvable via SDP relaxation

SDP Relaxation

QCQP

$$v^* = \min\left\{ \boldsymbol{x}^{\mathrm{T}} Q^0 \boldsymbol{x} + 2\left(\boldsymbol{q}^0\right)^{\mathrm{T}} \boldsymbol{x} \,\middle|\, \boldsymbol{x}^{\mathrm{T}} Q^p \boldsymbol{x} + 2\left(\boldsymbol{q}^p\right)^{\mathrm{T}} \boldsymbol{x} \le b_p,\ p \in [m] \right\} \qquad (\mathcal{P})$$

$$= \min\left\{ Q^0 \bullet X + 2\left(\boldsymbol{q}^0\right)^{\mathrm{T}} \boldsymbol{x} \,\middle|\, \begin{array}{l} X = \boldsymbol{x}\boldsymbol{x}^{\mathrm{T}} \\ Q^p \bullet X + 2\left(\boldsymbol{q}^0\right)^{\mathrm{T}} \boldsymbol{x} \le b_p,\ p \in [m] \end{array} \right\}$$

$$\ge \min\left\{ Q^0 \bullet X + 2\left(\boldsymbol{q}^0\right)^{\mathrm{T}} \boldsymbol{x} \,\middle|\, \begin{array}{l} X \succeq \boldsymbol{x}\boldsymbol{x}^{\mathrm{T}} \\ Q^p \bullet X + 2\left(\boldsymbol{q}^0\right)^{\mathrm{T}} \boldsymbol{x} \le b_p,\ p \in [m] \end{array} \right\} \qquad (\mathcal{P}_{\mathrm{R}})$$

Semidefinite Programming (SDP) Relaxation

$$=: v^*_{\mathrm{SDP}}$$

Notation

- $Q^p \bullet X := \sum_{i,j} Q^p_{ij} X_{ij}$: Frobenius inner product.
- $X \succeq \boldsymbol{x}\boldsymbol{x}^{\mathrm{T}} \iff X - \boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}$ is positive semidefinite.

Exact SDP Relaxation

Def: Exactness

SDP relaxation ($\mathcal{P}_{\mathrm{R}}$) is exact (tight) if $v^* = v^*_{\mathrm{SDP}}$

- Exact $\iff$ ($\mathcal{P}_{\mathrm{R}}$) has a rank-1 solution X^*

$$X^* \succeq \boldsymbol{x}^*(\boldsymbol{x}^*)^{\mathrm{T}} \quad \iff \quad \begin{bmatrix} 1 & (\boldsymbol{x}^*)^{\mathrm{T}} \\ \boldsymbol{x}^* & X^* \end{bmatrix} \succeq O.$$

- Sufficient conditions for general QCQPs have been studied
  - Sparsity and graphs
  - Projection of epigraphs
  - Collinearity of Gram matrix representation

Gram Matrix Transformation

Replace (x, X) in SDP relaxation:

- Fix $e \in \mathbb{R}^s$ with $\|e\| = 1$
- Introduce $u^1, \ldots, u^n \in \mathbb{R}^s$ so that

$$\left[\begin{array}{c|c} 1 & x^{\mathrm{T}} \\ \hline x & X \end{array}\right] = \left[\begin{array}{c|ccc} e^{\mathrm{T}}e & e^{\mathrm{T}}u^1 & \cdots & e^{\mathrm{T}}u^n \\ \hline e^{\mathrm{T}}u^1 & (u^1)^{\mathrm{T}}u^1 & \cdots & (u^1)^{\mathrm{T}}u^n \\ \vdots & \vdots & \ddots & \vdots \\ e^{\mathrm{T}}u^n & (u^n)^{\mathrm{T}}u^1 & \cdots & (u^n)^{\mathrm{T}}u^n \end{array}\right]$$

$$\begin{aligned} Q^p \bullet X + 2(q^p)^{\mathrm{T}}x &= \sum_i \sum_j Q^p_{ij} X_{ij} + 2\sum_i q^p_i x_i \\ &= \sum_i \sum_j Q^p_{ij} (u^i)^{\mathrm{T}} u^j + 2\sum_i q^p_i e^{\mathrm{T}} u^i \end{aligned}$$

Exactness Condition for Gram Matrix Representation

Finally, we obtain

$$
\begin{aligned}
v^*_{\mathrm{SDP}} = \min \quad & \sum_i \sum_j Q^0_{ij} \left(\boldsymbol{u}^i\right)^{\mathrm{T}} \boldsymbol{u}^j + 2 \sum_i q^0_i \boldsymbol{e}^{\mathrm{T}} \boldsymbol{u}^i \\
\text{s.t.} \quad & \sum_i \sum_j Q^p_{ij} \left(\boldsymbol{u}^i\right)^{\mathrm{T}} \boldsymbol{u}^j + 2 \sum_i q^p_i \boldsymbol{e}^{\mathrm{T}} \boldsymbol{u}^i \leq b_p, \quad p \in [m], \\
& \boldsymbol{u}^1, \ldots, \boldsymbol{u}^n \in \mathbb{R}^n.
\end{aligned}
$$

Proposition [Z20]

SDP relaxation is exact if there exist an optimal solution $\left(\boldsymbol{u}^1\right)^*, \ldots, \left(\boldsymbol{u}^n\right)^*$ which are collinear to $\boldsymbol{e}$, i.e.,

$$
\left|\boldsymbol{e}^{\mathrm{T}} \boldsymbol{u}^i\right| = \left\|\boldsymbol{u}^i\right\| \quad \text{for all } i \in [n].
$$

[Z20] Zhang, On the tightness of semidefinite relaxations for certifying robustness to adversarial examples, NeurIPS, 2020.

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Single-layer Neural Networks

W^0, W^1: weight matrices, $\boldsymbol{b}^0, \boldsymbol{b}^1$: bias vectors

Neural network

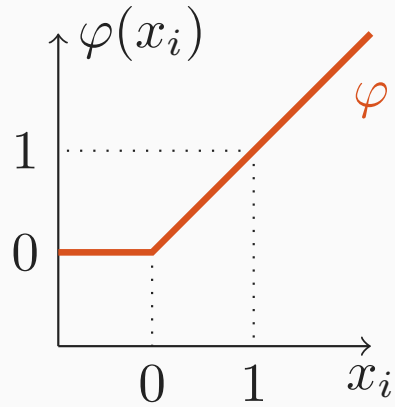
$$\boldsymbol{x}^1 := \phi(W^0 \boldsymbol{x}^0 + \boldsymbol{b}^0),$$
$$f(\boldsymbol{x}^0) := W^1 \boldsymbol{x}^1 + \boldsymbol{b}^1.$$

Note we consider the case that

- $W^1 = I$, and $\boldsymbol{b}^1 = \boldsymbol{0}$.
- ϕ is an element-wise ReLU function, i.e.,

$$\phi(\boldsymbol{x}) := \begin{bmatrix} \varphi(x_1) & \cdots & \varphi(x_n) \end{bmatrix}^{\mathrm{T}},$$

where $\varphi(x_i) := \max\{0, x_i\}$.



Input Set $\mathcal{X} \subseteq \boldsymbol{R}^{n_0}$

Set $\mathcal{X}$ contains the uncertainty and attacks.

- Each input $\boldsymbol{x}^0$ is chosen from $\mathcal{X}$.
- The safety of $\boldsymbol{x}^0$ is evaluated by $\boldsymbol{S}_y$.

Note

$\mathcal{X}$ is not the domain of NN f.

Various shapes are possible.

- hyper-ellipsoid $\quad \mathcal{X} = \{\boldsymbol{x} \mid \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_2 \leq \rho\}$.
- hyper-rectangle $\quad \mathcal{X} = \{\boldsymbol{x} \mid \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_\infty \leq \rho\}$.

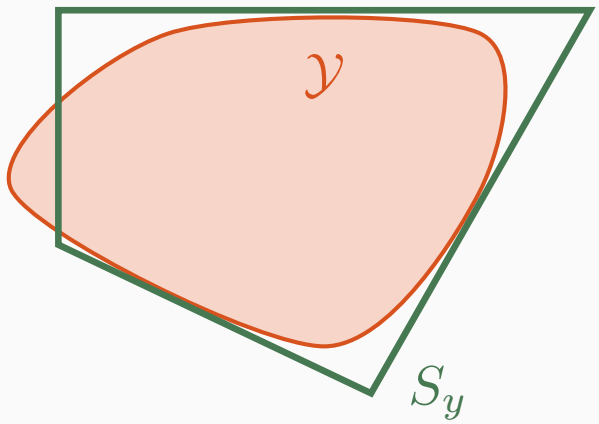
Setting II

This talk covers the case where $\mathcal{X}$ is a hyper-ellipsoid.

Polytope Safety Specification Set

Consider polytope safety specification set S_y

- Let S_y be a quadrilateral below.
- $\mathcal{Y} \subseteq S_y$ can be verified via four half-spaces.



Setting I

Assume that safety specification set S_y is a half-space

$$H \coloneqq \left\{ \boldsymbol{y} \in \mathbb{R}^{n_2} \,\middle|\, \boldsymbol{c}^{\mathrm{T}} \boldsymbol{y} - d \geq 0 \right\}.$$

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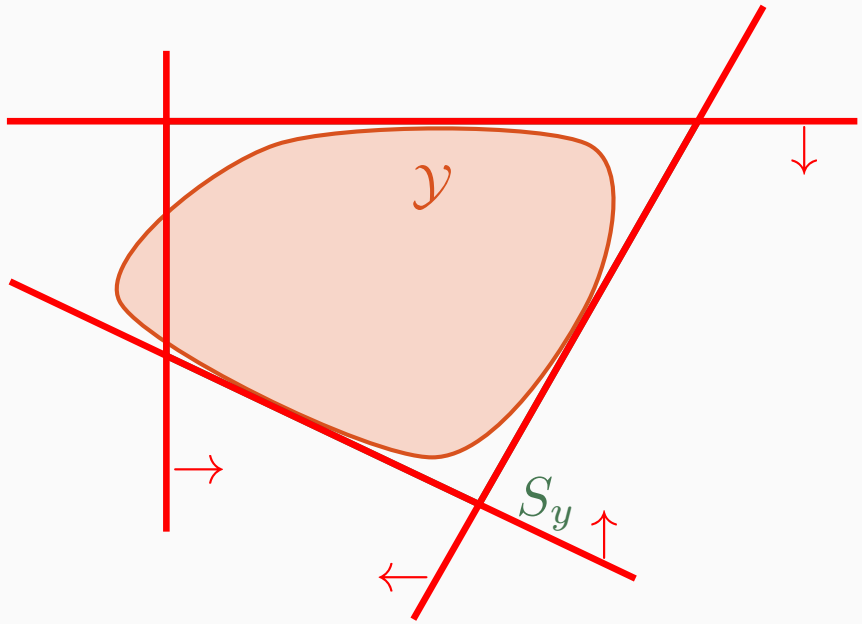

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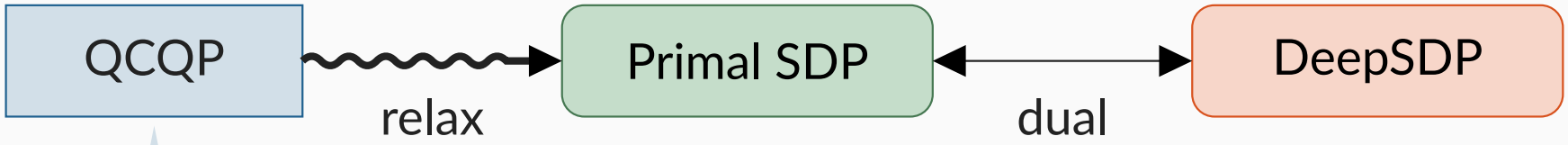
QCQP Formulation

Natual form



$$
\begin{aligned}
\min \quad & 2\boldsymbol{c}^{\mathrm{T}}\boldsymbol{x}^1 \\
\text{s.t.} \quad & \boldsymbol{x}^1 \geq \boldsymbol{0}, \quad \boldsymbol{x}^1 \geq W^0\boldsymbol{x}^0 + \boldsymbol{b}^0, \quad \boldsymbol{x}^1 \odot \left(W^0\boldsymbol{x}^0 + \boldsymbol{b}^0 - \boldsymbol{x}^1\right) \leq \boldsymbol{0}, \\
& \text{(+ some valid cuts)}, \\
& \boldsymbol{x}^0 \in \mathcal{X} = \left\{\boldsymbol{x} \,\middle|\, \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_2 \leq \rho\right\}, \quad \boldsymbol{x}^1 \in \mathbb{R}^{n_1}.
\end{aligned}
$$

$\odot$ = Hadamard product

Determine a constant term d for fixed $\boldsymbol{c}$ in

$$\left\{\boldsymbol{x}^1 \in \mathbb{R}^{n_2} \,\middle|\, \boldsymbol{c}^{\mathrm{T}}\boldsymbol{x}^1 - d \geq 0\right\}.$$

minimize in primal side

maximize in dual side

Primal SDP Relaxation

Natual form

$$
\begin{aligned}
\min \quad & 2\boldsymbol{c}^{\mathrm{T}}\boldsymbol{x}^1 \\
\text{s.t.} \quad & I \bullet X^{00} - 2\hat{\boldsymbol{x}}^{\mathrm{T}}\boldsymbol{x}^0 \le \rho^2 - \hat{\boldsymbol{x}}^{\mathrm{T}}\hat{\boldsymbol{x}}, \\
& \left(\boldsymbol{e}^i\right)^{\mathrm{T}}\boldsymbol{x}^1 \ge 0, \quad \left(\boldsymbol{e}^i\right)^{\mathrm{T}}\boldsymbol{x}^1 \ge \left(\boldsymbol{e}^i\right)^{\mathrm{T}}\left(W^0\boldsymbol{x}^0 + \boldsymbol{b}^0\right), \quad i = 1, \ldots, n_1, \\
& X^{11}_{ii} - b^0_i x^1_i - \textstyle\sum_j W^0_{ij} X^{10}_{ij} \le 0, \qquad\qquad i = 1, \ldots, n_1, \\
& \begin{bmatrix} 1 & \left(\boldsymbol{x}^0\right)^{\mathrm{T}} & \left(\boldsymbol{x}^1\right)^{\mathrm{T}} \\ \boldsymbol{x}^0 & X^{00} & \left(X^{10}\right)^{\mathrm{T}} \\ \boldsymbol{x}^1 & X^{10} & X^{11} \end{bmatrix} \succeq O
\end{aligned}
$$

$\boldsymbol{e}^i$: the ith unit vector

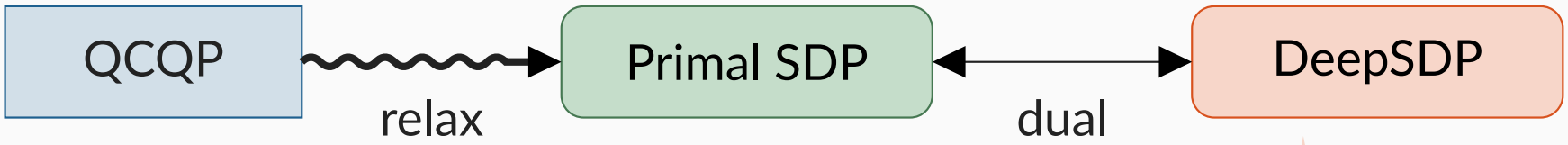
Objective of this work

Verify the exactness of (primal) SDP relaxation

- checking "*collinearity*" of another form

Dual SDP relaxation

Natual form



$$
\begin{aligned}
\max_{\gamma,\boldsymbol{\lambda},\boldsymbol{\nu},\boldsymbol{\eta},d} \quad & 2d \\
\text{s.t.} \quad & \gamma \begin{bmatrix} \hat{\boldsymbol{x}}^{\mathrm{T}}\hat{\boldsymbol{x}} - \rho^2 & -\hat{\boldsymbol{x}}^{\mathrm{T}} & \mathbf{0} \\ -\hat{\boldsymbol{x}} & I & O \\ \mathbf{0} & O & O \end{bmatrix} + \begin{bmatrix} -2d & \mathbf{0}^{\mathrm{T}} & \boldsymbol{c}^{\mathrm{T}} \\ \mathbf{0} & O & O \\ \boldsymbol{c} & O & O \end{bmatrix} \\
& \quad + \begin{bmatrix} 0 & \boldsymbol{\nu}^{\mathrm{T}}W^0 & -\boldsymbol{\nu}^{\mathrm{T}} - \boldsymbol{\eta}^{\mathrm{T}} \\ (W^0)^{\mathrm{T}}\boldsymbol{\nu} & O & -(W^0)^{\mathrm{T}}\operatorname{diag}(\boldsymbol{\lambda}) \\ -\boldsymbol{\nu} - \boldsymbol{\eta} & -\operatorname{diag}(\boldsymbol{\lambda})W^0 & 2\operatorname{diag}(\boldsymbol{\lambda}) \end{bmatrix} \succeq O, \\
& \gamma \in \mathbb{R}_+, \quad \boldsymbol{\lambda}, \boldsymbol{\nu}, \boldsymbol{\eta} \in \mathbb{R}^n_+, \quad d \in \mathbb{R}.
\end{aligned}
$$

Our Theoretical Results

For previous QCQP,

Theorem

The primal SDP relaxation is exact if

- $\mathcal{X} = \{\boldsymbol{x} \mid \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_2 \leq \rho\}$; or
- $\mathcal{X} = \{\boldsymbol{x} \mid \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_\infty \leq \rho\}$, $W^0 = I$, and $\hat{\boldsymbol{x}} \geq -\boldsymbol{b}^0$.

In addition, DeepSDP is also exact under strong duality.

- No extra assumption in hyper-ellipsoid case.
- Proof depending on
  Gram matrix representation with $\boldsymbol{e} = \boldsymbol{e}^1$.

Gram Matrix Representation of Safety Verification

- Assign $\boldsymbol{u}^j \in \mathbb{R}^s$ for $\boldsymbol{x}^0$, and $\boldsymbol{v}^i \in \mathbb{R}^s$ for $\boldsymbol{x}^1$:

$$\boldsymbol{x}^0 = \left[(\boldsymbol{e}^1)^{\mathrm{T}}\boldsymbol{u}^1, \ldots, (\boldsymbol{e}^1)^{\mathrm{T}}\boldsymbol{u}^{n_0}\right]^{\mathrm{T}}, \ \boldsymbol{x}^1 = \left[(\boldsymbol{e}^1)^{\mathrm{T}}\boldsymbol{v}^1, \ldots, (\boldsymbol{e}^1)^{\mathrm{T}}\boldsymbol{v}^{n_1}\right]^{\mathrm{T}}$$

- Similarly,

$$[X^{00}]_{ij} = (\boldsymbol{u}^i)^{\mathrm{T}}\boldsymbol{u}^j, \quad [X^{10}]_{ij} = (\boldsymbol{u}^i)^{\mathrm{T}}\boldsymbol{v}^j, \quad [X^{11}]_{ij} = (\boldsymbol{v}^i)^{\mathrm{T}}\boldsymbol{v}^j$$

Primal SDP is equivalently

$$\begin{aligned}
\min_{\boldsymbol{u}^j, \boldsymbol{v}^i} \ & 2\textstyle\sum_{i=1}^{n_1} c_i \, (\boldsymbol{e}^1)^{\mathrm{T}}\boldsymbol{v}^i \\
\text{s.t.} \ & (\boldsymbol{e}^1)^{\mathrm{T}}\boldsymbol{v}^i \geq 0, && i = 1, \ldots, n_1, \\
& (\boldsymbol{e}^1)^{\mathrm{T}}\boldsymbol{v}^i \geq (\boldsymbol{e}^1)^{\mathrm{T}} \left(\textstyle\sum_{j=1}^{n_0} W_{ij}\boldsymbol{u}^j + b_i^0 \boldsymbol{e}^1\right), && i = 1, \ldots, n_1, \\
& \left\|\boldsymbol{v}^i\right\|_2^2 \leq \left(\textstyle\sum_{j=1}^{n_0} W_{ij}\boldsymbol{u}^j + b_i^0 \boldsymbol{e}^1\right)^{\mathrm{T}} \boldsymbol{v}^i, && i = 1, \ldots, n_1, \\
& \sum_{j=1}^{n_0} \|\boldsymbol{u}^j - \hat{x}_j \boldsymbol{e}^1\|_2^2 \leq \rho^2.
\end{aligned}$$

Decomposition according to u^j and v^i

$$\min_{\boldsymbol{u}^j, \boldsymbol{v}^i} \; 2\sum_{i=1}^{n_1} c_i \left(\boldsymbol{e}^1\right)^{\mathrm{T}} \boldsymbol{v}^i \tag{1}$$

$$\text{s.t.} \; \left(\boldsymbol{e}^1\right)^{\mathrm{T}} \boldsymbol{v}^i \geq 0, \qquad i = 1, \ldots, n_1, \tag{2}$$

$$\left(\boldsymbol{e}^1\right)^{\mathrm{T}} \boldsymbol{v}^i \geq \left(\boldsymbol{e}^1\right)^{\mathrm{T}} \left(\sum_{j=1}^{n_0} W_{ij} \boldsymbol{u}^j + b_i^0 \boldsymbol{e}^1\right), \quad i = 1, \ldots, n_1, \tag{3}$$

$$\left\|\boldsymbol{v}^i\right\|_2^2 \leq \left(\sum_{j=1}^{n_0} W_{ij} \boldsymbol{u}^j + b_i^0 \boldsymbol{e}^1\right)^{\mathrm{T}} \boldsymbol{v}^i, \qquad i = 1, \ldots, n_1, \tag{4}$$

$$\sum_{j=1}^{n_0} \left\|\boldsymbol{u}^j - \hat{x}_j \boldsymbol{e}^1\right\|_2^2 \leq \rho^2. \tag{5}$$

Inner problem

$$\Psi(\boldsymbol{v}^1, \ldots, \boldsymbol{v}^{n_1}) :=$$

$$\min_{\boldsymbol{u}^1, \ldots, \boldsymbol{u}^{n_0}} \; \sum_{j=1}^{n_0} \left\|\boldsymbol{u}^j - \hat{x}_j \boldsymbol{e}\right\|_2^2$$

$$\text{s.t.} \quad (3),\ (4).$$

Outer problem

$$\min_{\boldsymbol{v}^1, \ldots, \boldsymbol{v}^{n_1}} \quad (1)$$

$$\text{s.t.} \quad (2)$$

$$\Psi(\boldsymbol{v}^1, \ldots, \boldsymbol{v}^{n_1}) \leq \rho^2.$$

Relationship Between Their Solutions

A part of KKT condition of Inner problem :

$$\begin{bmatrix} \boldsymbol{u}^1 \\ \vdots \\ \boldsymbol{u}^{n_0} \end{bmatrix} = \begin{bmatrix} \hat{x}_1 \boldsymbol{e}^1 \\ \vdots \\ \hat{x}_{n_0} \boldsymbol{e}^1 \end{bmatrix} - \sum_{i=1}^{n_1} \frac{\nu_i}{2} \begin{bmatrix} W_{i1} \boldsymbol{e}^1 \\ \vdots \\ W_{in} \boldsymbol{e}^1 \end{bmatrix} + \sum_{i=1}^{n_1} \frac{\lambda_i}{2} \begin{bmatrix} W_{i1} \boldsymbol{v}^i \\ \vdots \\ W_{in} \boldsymbol{v}^i \end{bmatrix}$$

Lemma: Linear Combination

For any optimal solution $(\boldsymbol{u}^1)^*, \ldots, (\boldsymbol{u}^{n_0})^*$ of Inner problem , there exist $\boldsymbol{m} \in \mathbb{R}^{n_0}$ and $M \in \mathbb{R}^{n_1 \times n_0}$ such that

$$(\boldsymbol{u}^j)^* = m_j \boldsymbol{e}^1 + \sum_{i=1}^{n_1} M_{ij} \boldsymbol{v}^i \quad \text{for each } j \in \{1, \ldots, n_0\}.$$

Collinearity in Outer-problem

Using $\boldsymbol{m}$ and M changes Outer problem into

$$\left.\begin{aligned} \min_{\boldsymbol{v}^1,\ldots,\boldsymbol{v}^{n_1}} \quad & 2\sum_{i=1}^{n_1} c_i\, \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i && (1)\\ \text{s.t.} \quad & \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i \geq 0,\ i=1,\ldots,n_1, && (2)\\ & \sum_{j=1}^{n_0}\left\|(m_j-\hat{x}_j)\,\boldsymbol{e}^1+\sum_{i=1}^{n_1} M_{ij}\boldsymbol{v}^i\right\|_2^2 \leq \rho^2. \end{aligned}\right\}$$

Lemma: Collinearity of $(\boldsymbol{v}^i)^*$

Outer problem has an optimal solution $(\boldsymbol{v}^1)^*,\ldots,(\boldsymbol{v}^{n_1})^*$ collinear to $\boldsymbol{e}^1$.

Therefore, the SDP relaxation is exact due to the collinearity.

Collinearity in Outer-problem

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$$\left.\begin{aligned} \min_{\boldsymbol{v}^1,\ldots,\boldsymbol{v}^{n_1}} \quad & 2\sum_{i=1}^{n_1} c_i\, \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i && (1)\\ \text{s.t.} \quad & \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i \geq 0,\ i=1,\ldots,n_1, && (2)\\ & \sum_{j=1}^{n_0}\left\|(m_j-\hat{x}_j)\,\boldsymbol{e}^1+\sum_{i=1}^{n_1} M_{ij}\boldsymbol{v}^i\right\|_2^2 \leq \rho^2. \end{aligned}\right\}$$

Essence of Proof.

- Let $(\bar{\boldsymbol{v}}^1,\ldots,\bar{\boldsymbol{v}}^{n_1})$ be an optimal solution.
- Assume at least one of $\bar{\boldsymbol{v}}^1,\ldots,\bar{\boldsymbol{v}}^{n_1}$ is not collinear to $\boldsymbol{e}^1$.
- Define
$$\hat{\boldsymbol{v}}^i := \left[\bar{v}_1^i,\ 0,\ \cdots,\ 0\right]^{\mathrm{T}}.$$
- Then, $(\hat{\boldsymbol{v}}^1,\ldots,\hat{\boldsymbol{v}}^{n_1})$ is another optimal solution.

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Meaning of Exact Relaxation

Current situation

- Instead of checking whether $\mathcal{Y} \subseteq S_y$,

$$\mathcal{Y} \subseteq \quad H \coloneqq \bigcap_k \left\{ \boldsymbol{y} \in \mathbb{R}^{n_2} \,\middle|\, \left(\boldsymbol{c}^k\right)^{\mathrm{T}} \boldsymbol{y} - \boxed{d^k} \geq 0 \right\} \quad \subseteq S_y.$$

Optimal Solutions

Where does exactness appear?

- Half-space H supports $\mathcal{Y}$ at a face.
- Margin between H and S_y increases.
  - It is the robustness of the input set $\mathcal{X}$.
  - $\iff$ $\mathcal{X}$ can be made larger.

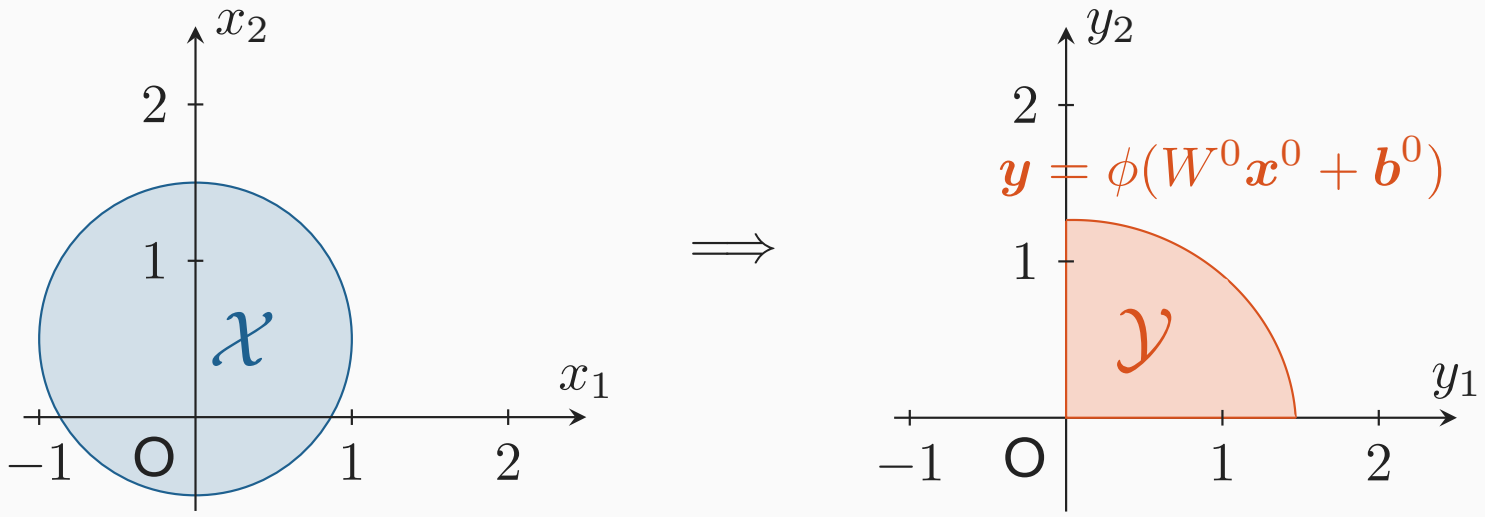
Instance with Exact Relaxation

Example: a single-layer NN

$$W^0 = \begin{bmatrix} 1/2 & 5/4 \\ -6/5 & 2/5 \end{bmatrix}, \quad W^1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \boldsymbol{b}^0 = \begin{bmatrix} -0.5 \\ -0.2 \end{bmatrix}, \quad \boldsymbol{b}^1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

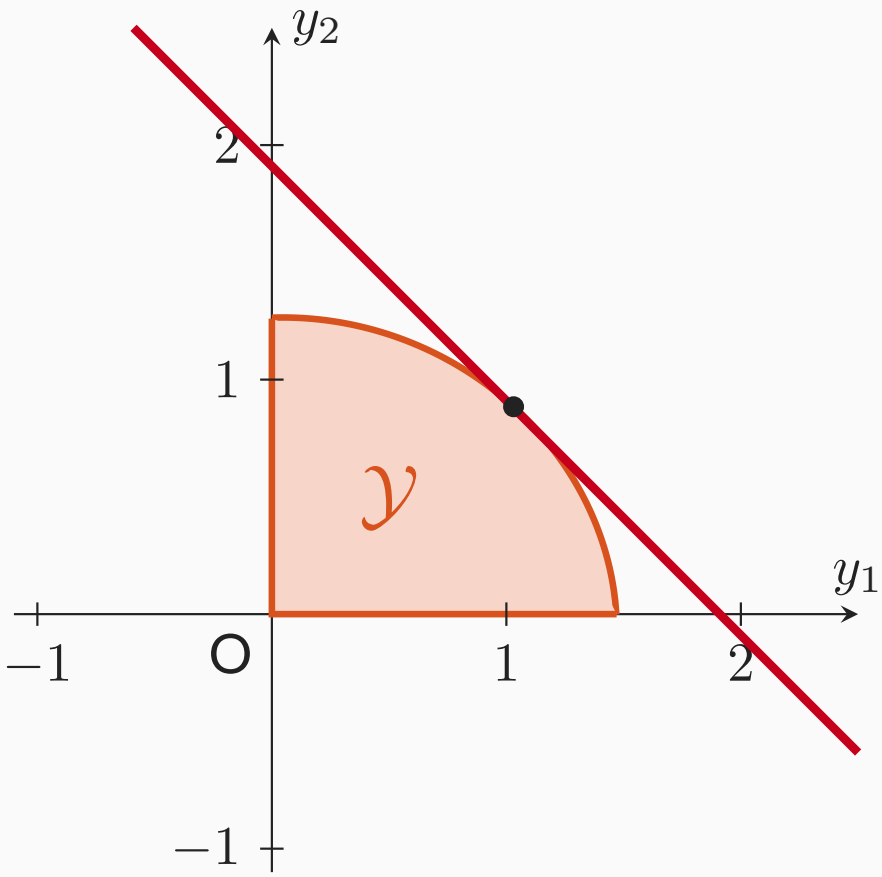
with the input set

$$\mathcal{X} := \left\{ \boldsymbol{x} \in \mathbb{R}^2 \,\middle|\, \left\| \boldsymbol{x} - \begin{bmatrix} 0 \\ 0.5 \end{bmatrix} \right\|_2 \leq 1 \right\}.$$



Experiment Result in Mosek and Julia

Slope c^*		Solution
c_1	c_2	d^*
1	0	-8.42×10^{-10}
0	1	-3.45×10^{-10}
-1	1	-1.47
1	-1	-1.26
$-1/4$	-1	-1.32
$-1/2$	-1	-1.46
-1	-1	-1.91
-2	-1	-3.16
-4	-1	-5.96



Observation

All boundaries intersect $\mathcal{Y}$ at a point

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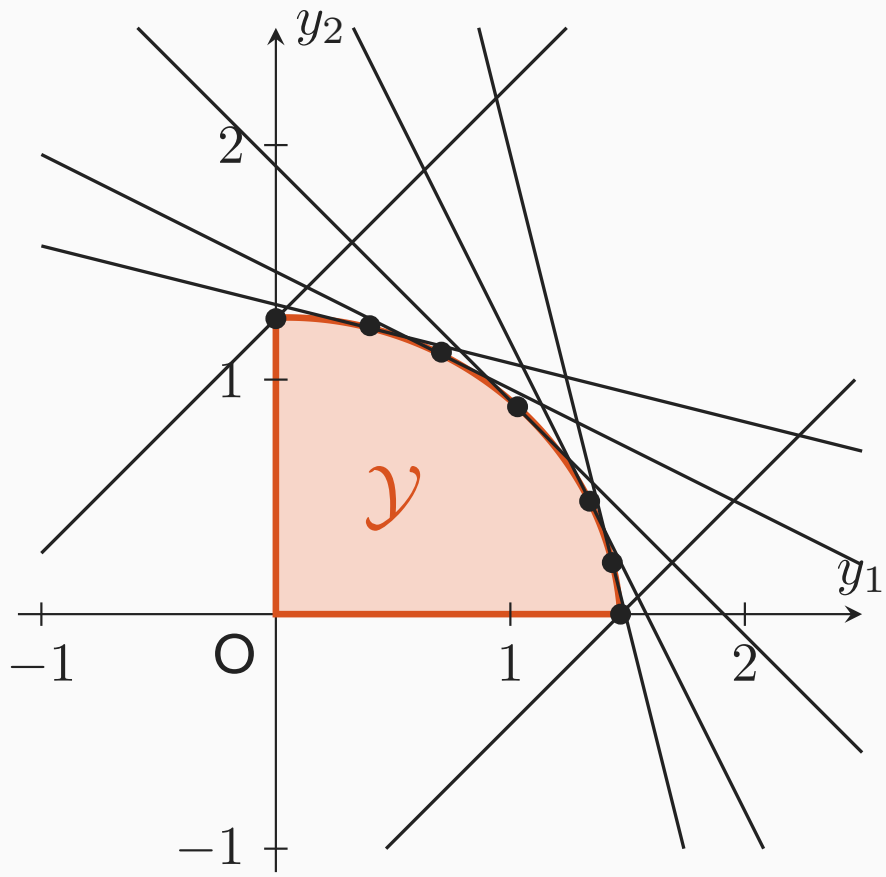


Observation

All boundaries intersect $\mathcal{Y}$ at a point

Conclusion

Summary

- Safety verification of single-layer neural networks
- Exactness conditions of SDP relaxation
- Graphical insight for exactness

Future works

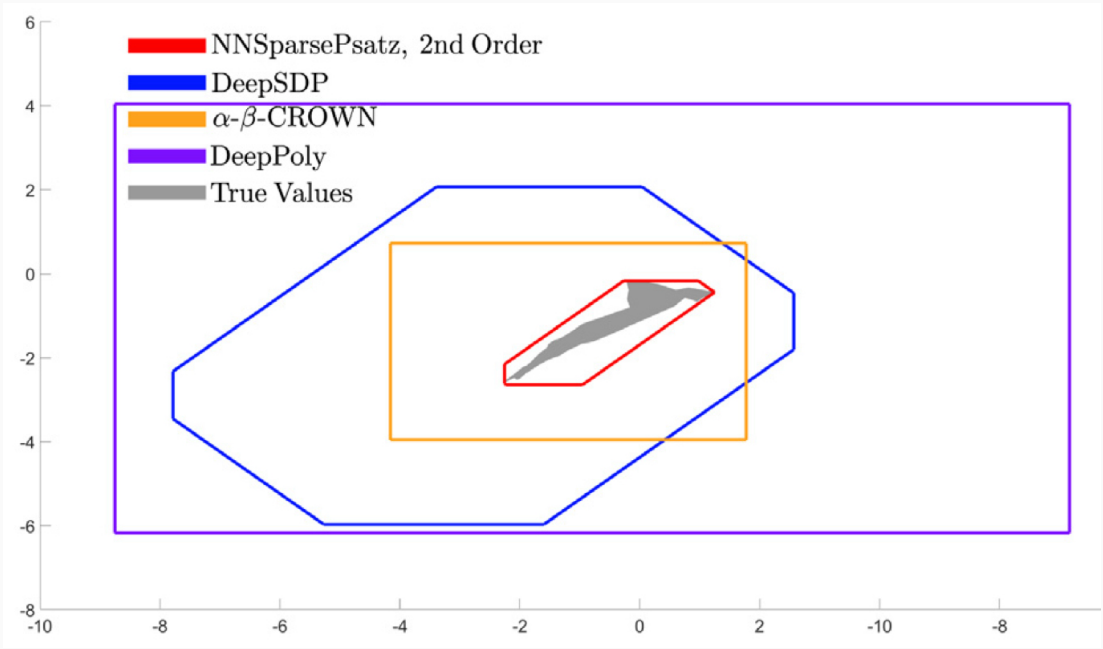
- Analyze the non-polyhedral case of S_y
- Extend results to other networks

Thank you for your attention!

For more details, see arXiv:2504.09934

Exact Semidefinite Relaxations for Verifying Robustness of Neural Networks

- Less accurate than other methods in general [NP21].
- Accurate when the relaxation is exact.



[NP21] Newton and Papachristodoulou, Neural network verification using polynomial optimisation, IEEE CDC, 2021.

Constraints for Hidden Layers

$$\begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & O & -\boldsymbol{e}^i \left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ \mathbf{0} & -\boldsymbol{e}^i \left(\boldsymbol{e}^i\right)^{\mathrm{T}} & 2\boldsymbol{e}^i \left(\boldsymbol{e}^i\right)^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix} = 0, \quad i = 1, \ldots, N, \tag{6a}$$

$$\begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 0 & \left(\boldsymbol{e}^i\right)^{\mathrm{T}} & -\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ \boldsymbol{e}^i & O & O \\ -\boldsymbol{e}^i & O & O \end{bmatrix} \begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix} \leq 0, \quad i = 1, \ldots, N, \tag{6b}$$

$$\begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} & -\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ \mathbf{0} & O & O \\ -\boldsymbol{e}^i & O & O \end{bmatrix} \begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix} \leq 0, \quad i = 1, \ldots, N. \tag{6c}$$

Valid Cuts

Let $\boldsymbol{w}^0 = W^0\boldsymbol{x}^0 + \boldsymbol{b}^0$.

Valid Cuts for ReLU

The following inequation always holds

$$\left[\phi(w_j^0) - \phi(w_i^0)\right]\left[\phi(w_j^0) - \phi(w_i^0) - (w_j - w_i)\right] \leq 0 \quad \forall (i,j) \in \{1,\ldots,n\}^2$$

$$\begin{bmatrix} \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} O & -(\boldsymbol{e}^i - \boldsymbol{e}_j)(\boldsymbol{e}^i - \boldsymbol{e}_j)^{\mathrm{T}} \\ -(\boldsymbol{e}^i - \boldsymbol{e}_j)(\boldsymbol{e}^i - \boldsymbol{e}_j)^{\mathrm{T}} & 2(\boldsymbol{e}^i - \boldsymbol{e}_j)(\boldsymbol{e}^i - \boldsymbol{e}_j)^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix} \leq 0, \quad (7)$$

Input Constraint

Since $\boldsymbol{x}^0 \in \mathcal{X} = \{\boldsymbol{x} \mid \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_2 \leq \rho\}$.

In QCQP

$$\left\|\boldsymbol{x}^0 - \hat{\boldsymbol{x}}\right\|_2^2 \leq \rho^2$$

In SDP relaxation

$$\begin{bmatrix} \hat{\boldsymbol{x}}^{\mathrm{T}}\hat{\boldsymbol{x}} - \rho^2 & -\hat{\boldsymbol{x}}^{\mathrm{T}} & \mathbf{0} \\ -\hat{\boldsymbol{x}} & I & O \\ \mathbf{0} & O & O \end{bmatrix} \bullet \underbrace{\begin{bmatrix} 1 & \left(\boldsymbol{x}^0\right)^{\mathrm{T}} & \left(\boldsymbol{x}^1\right)^{\mathrm{T}} \\ \boldsymbol{x}^0 & X_{00} & X_{10}{}^{\mathrm{T}} \\ \boldsymbol{x}^1 & X_{10} & X_{11} \end{bmatrix}}_{=: G} \leq 0$$

In DeepSDP By introducing a dual variable γ,

$$\gamma \begin{bmatrix} \hat{\boldsymbol{x}}^{\mathrm{T}}\hat{\boldsymbol{x}} - \rho^2 & -\hat{\boldsymbol{x}}^{\mathrm{T}} & \mathbf{0} \\ -\hat{\boldsymbol{x}} & I & O \\ \mathbf{0} & O & O \end{bmatrix}$$

Safety Specification Set

Consider a half-space $H := \left\{ \boldsymbol{y} \in \mathbb{R}^{n_2} \,\middle|\, \boldsymbol{c}^{\mathrm{T}} \boldsymbol{y} - d \geq 0 \right\}$.

- The slope $\boldsymbol{c}$ according to each half-space is given.
- The largest d makes H smaller.

In SDP relaxation

$$\boldsymbol{x}^1 \in H \iff \begin{bmatrix} -2d & \mathbf{0}^{\mathrm{T}} & \boldsymbol{c}^{\mathrm{T}} \\ \mathbf{0} & O & O \\ \boldsymbol{c} & O & O \end{bmatrix} \bullet \begin{bmatrix} 1 & \left(\boldsymbol{x}^0\right)^{\mathrm{T}} & \left(\boldsymbol{x}^1\right)^{\mathrm{T}} \\ \boldsymbol{x}^0 & X_{00} & {X_{10}}^{\mathrm{T}} \\ \boldsymbol{x}^1 & X_{10} & X_{11} \end{bmatrix} \leq 0$$

In DeepSDP Let d behave as a dual variable.

Quadratic Formulation for ReLU Function

Review: ϕ applies element-wisely ReLU function φ

Let $\boldsymbol{w}^0 := W^0\boldsymbol{x}^0 + \boldsymbol{b}^0$. For any $i \in \{1, \ldots, n_1\}$,

$$\varphi(w_i^0) = \max\{0, w_i^0\} \quad \Longleftrightarrow \quad \begin{cases} \varphi(w_i^0)\left(\varphi(w_i^0) - w_i^0\right) \leq 0, \\ \varphi(w_i^0) \geq w_i^0, \quad \varphi(w_i^0) \geq 0. \end{cases}$$

In QCQP The first inequality is

$$\begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & O & -\boldsymbol{e}^i\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ \mathbf{0} & -\boldsymbol{e}^i\left(\boldsymbol{e}^i\right)^{\mathrm{T}} & 2\boldsymbol{e}^i\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 1 \\ \boldsymbol{w}^0 \\ \phi(\boldsymbol{w}^0) \end{bmatrix} \leq 0, \quad i = 1, \ldots, n_1.$$

Transformation of $[1, w^0, \phi(w^0)]^{\mathrm{T}}$

Equivalently, for $i \in \{1, \ldots, n_1\}$,

$$\begin{bmatrix} 1 \\ x^0 \\ x^1 \end{bmatrix}^{\mathrm{T}} \underbrace{\begin{bmatrix} 1 & \mathbf{0}^{\mathrm{T}} & \mathbf{0}^{\mathrm{T}} \\ b^0 & W^0 & O \\ \mathbf{0} & O & I \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & O & -e^i (e^i)^{\mathrm{T}} \\ \mathbf{0} & -e^i (e^i)^{\mathrm{T}} & 2e^i (e^i)^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0}^{\mathrm{T}} & \mathbf{0}^{\mathrm{T}} \\ b^0 & W^0 & O \\ \mathbf{0} & O & I \end{bmatrix}}_{=: L_i} \begin{bmatrix} 1 \\ x^0 \\ x^1 \end{bmatrix} \leq$$

In SDP relaxation $\quad L_i \bullet G \leq 0, \quad i \in \{1, \ldots, n_1\}$

In DeepSDP Introducing a dual variable $\boldsymbol{\lambda} \in \mathbb{R}^{n_1}_+$, $\sum_{i=1}^{n_1} \lambda_i L_i$

Constraint	$\varphi(w_i^0)\left(\varphi(w_i^0) - w_i^0\right) \leq 0$	$\varphi(w_i^0) \geq w_i^0$	$\varphi(w_i^0) \geq 0$
Dual variable	λ_i	ν_i	η_i