# Exact Semidefinite Relaxations for Safety Verification of Neural Network

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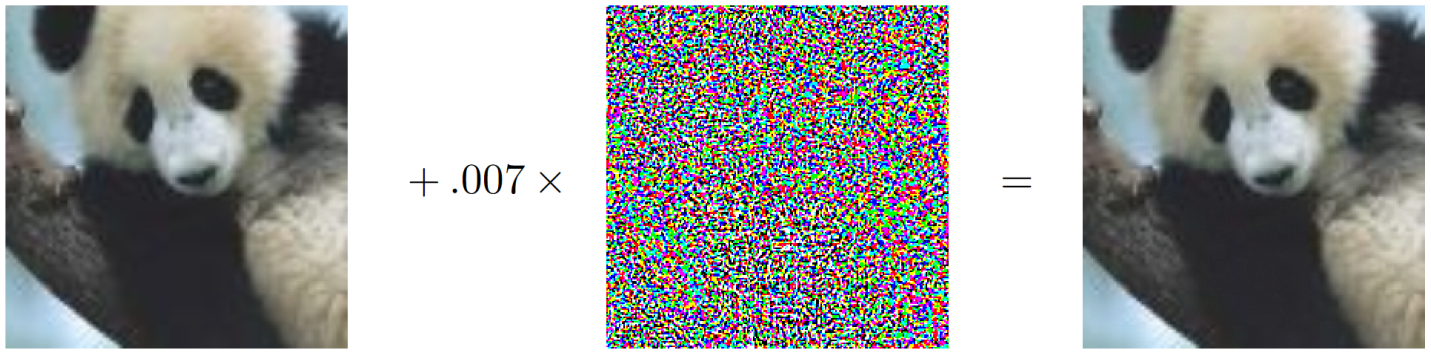
# Vulnerability on Neural Networks (NNs)

Uncertainty and adversarial attacks

- Panda image + small noise [GSS14]




- Stop sign + optical attacks $\Longrightarrow$ Speed limit 60 sign

a barrier to applications where reliability is critical (e.g., self-driving cars)

[GSS14] Goodfellow et al., Explaining and Harnessing Adversarial Examples, ICLR 2015, 2014.

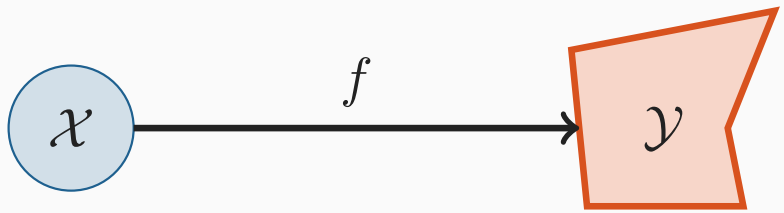
# Verifying Safety of NNs

Let $f : \mathbb{R}^{n_0} \to \mathbb{R}^{n_L}$ be a NN.

Input set $\mathcal{X} \subseteq \mathbb{R}^{n_0}$

we wish to evaluate

Output $\mathcal{Y} := \{f(\boldsymbol{x}) \mid \boldsymbol{x} \in \mathcal{X}\}$




Let $S_y$: a set where no misclassification occurs = safety specification set

**Def: Safety Verification**

Check whether $\mathcal{Y} \subseteq S_y$ holds or not for a given $S_y$

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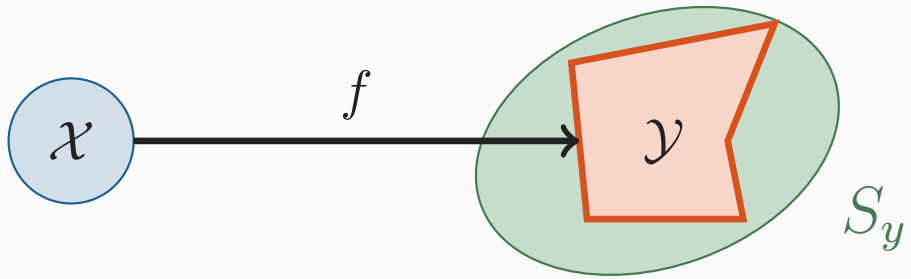


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# DeepSDP

Semidefinite programming-based method of safety verification.

- $M \succeq O \iff M$ is positive semidefinite.

## General Formulation of DeepSDP

$$\begin{aligned} \min_{P,Q,S} \quad & g(P,Q,S) \\ \text{s.t.} \quad & M_{\text{in}}(P) + M_{\text{mid}}(Q) + M_{\text{out}}(S) \succeq O, \\ & P \in \mathcal{P}_{\mathcal{X}},\ Q \in \mathcal{Q}_{\phi},\ S \in \mathcal{S}. \end{aligned}$$

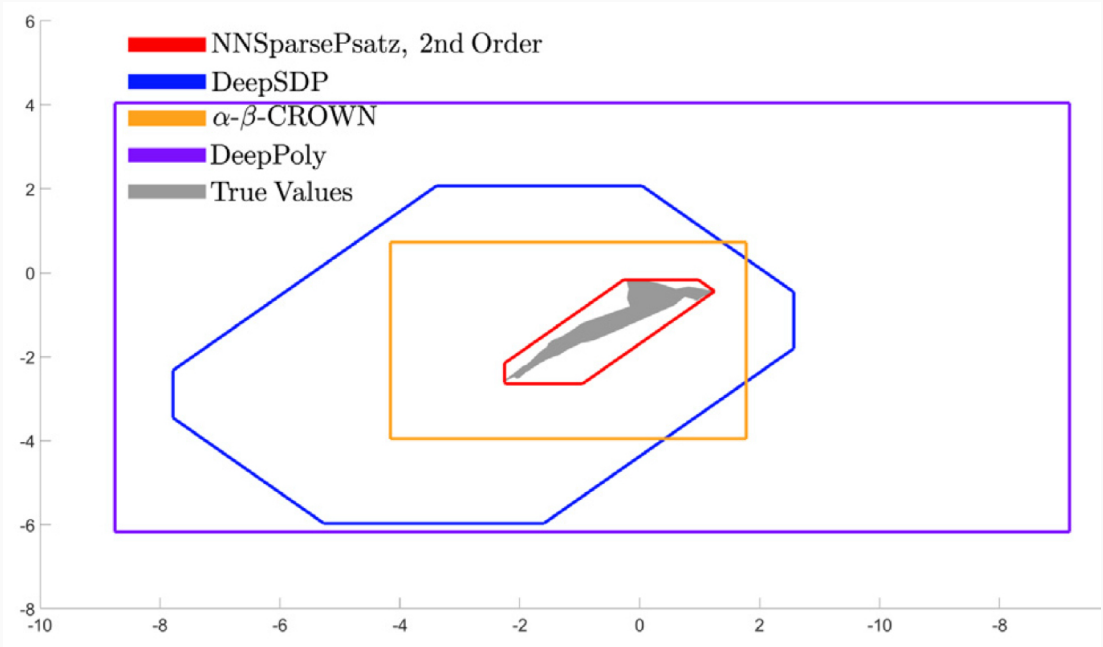
The above problem is less accurate than other methods [NP21].

---

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

# Accuracy of DeepSDP with Other Method

$\hat{\mathcal{Y}}$: Estimated output set $\leftrightarrow$ $\mathcal{Y}$: True output set (gray) [NP21]




- All methods overestimate $\hat{\mathcal{Y}}$ in order to cover the whole output in $\mathcal{Y}$.
- Accurate verification favors a smaller $\hat{\mathcal{Y}}$.

**Motivation**

What conditions make DeepSDP highly accurate?

We address it by using an exact relaxation.

# Outline

- Introduction

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

- Single-layer feed-forward neural network
- Formulation of DeepSDP for safety verification

- Exact SDP relaxation in safety verification
- Proof

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# QCQP: Quadratically Constrained Quadratic Programming

Consider a quadratic programming with quadratic constraints:

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

**Used in**

Binary programming, MAX-CUT, optimal flow problems,...

- Behind the safety verification
- Generally non-convex & NP-hard
- Approximately solvable via SDP relaxation

# Semidefinite Programming (SDP) Relaxation

Define two 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.

QCQP

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

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

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

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

Semidefinite Programming (SDP) Relaxation

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

# Exact SDP Relaxation

**Def: Exactness**

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

i.e., $$\min\left\{\boldsymbol{x}^{\mathrm{T}} Q^0 \boldsymbol{x} \,\middle|\, \boldsymbol{x}^{\mathrm{T}} Q^p \boldsymbol{x} \le b_p,\ p \in \{1,\dots,m\}\right\} \qquad (\mathcal{P})$$

$$= \min\left\{ Q^0 \bullet X \,\middle|\, \begin{array}{l} X \succeq \boldsymbol{x}\boldsymbol{x}^{\mathrm{T}} \\ Q^p \bullet X \le b_p,\ p \in \{1,\dots,m\} \end{array} \right\} \qquad (\mathcal{P}_{\mathrm{R}})$$

- Sufficient conditions for exactness have been studied
- Exact $\iff$ ($\mathcal{P}_{\mathrm{R}}$) has a rank-1 solution $X^*$
  - Decomposition $\hat{\boldsymbol{x}}\hat{\boldsymbol{x}}^{\mathrm{T}} = X^*$ exists
  - $\hat{\boldsymbol{x}}$ is a solution of QCQP ($\mathcal{P}$)

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# Single-layer Neural Networks

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

**Neural network**

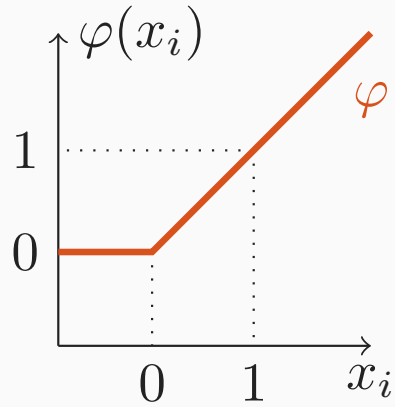
$$\boldsymbol{x}^1 := \phi(W^0 \boldsymbol{x}^0 + \boldsymbol{b}^0),$$
$$f(\boldsymbol{x}^0) := W^1 \boldsymbol{x}^1 + \boldsymbol{b}^1.$$

Note we consider the case that

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

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

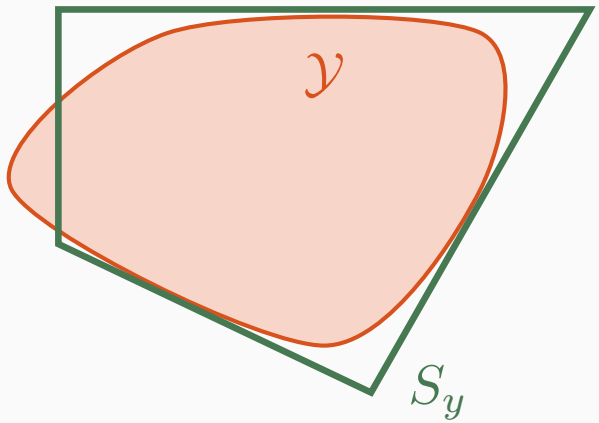
where $\varphi(x_i) := \max\{0, x_i\}$.



# 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.

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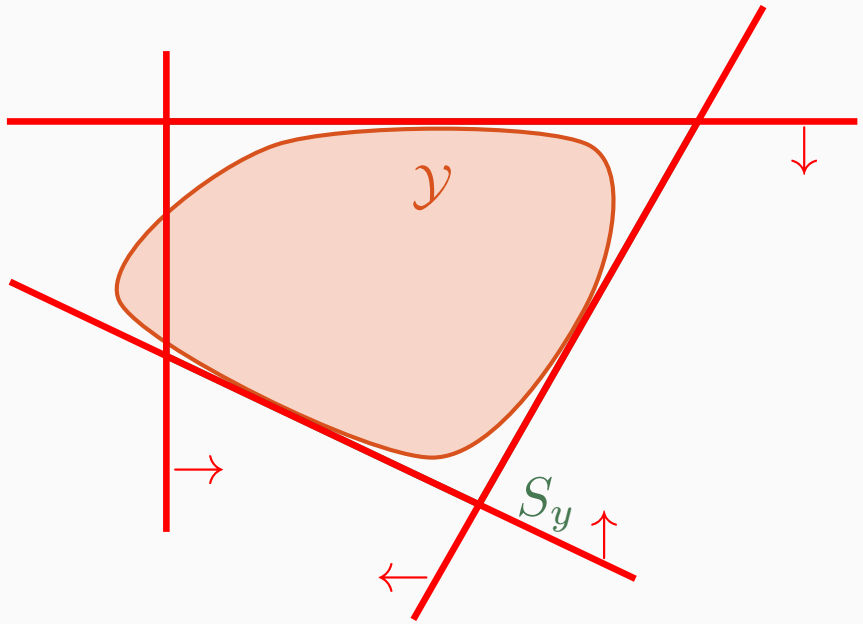



**Setting I**

Assume that safety specification set $S_y$ is a half-space.

# DeepSDP for Single-layer NN

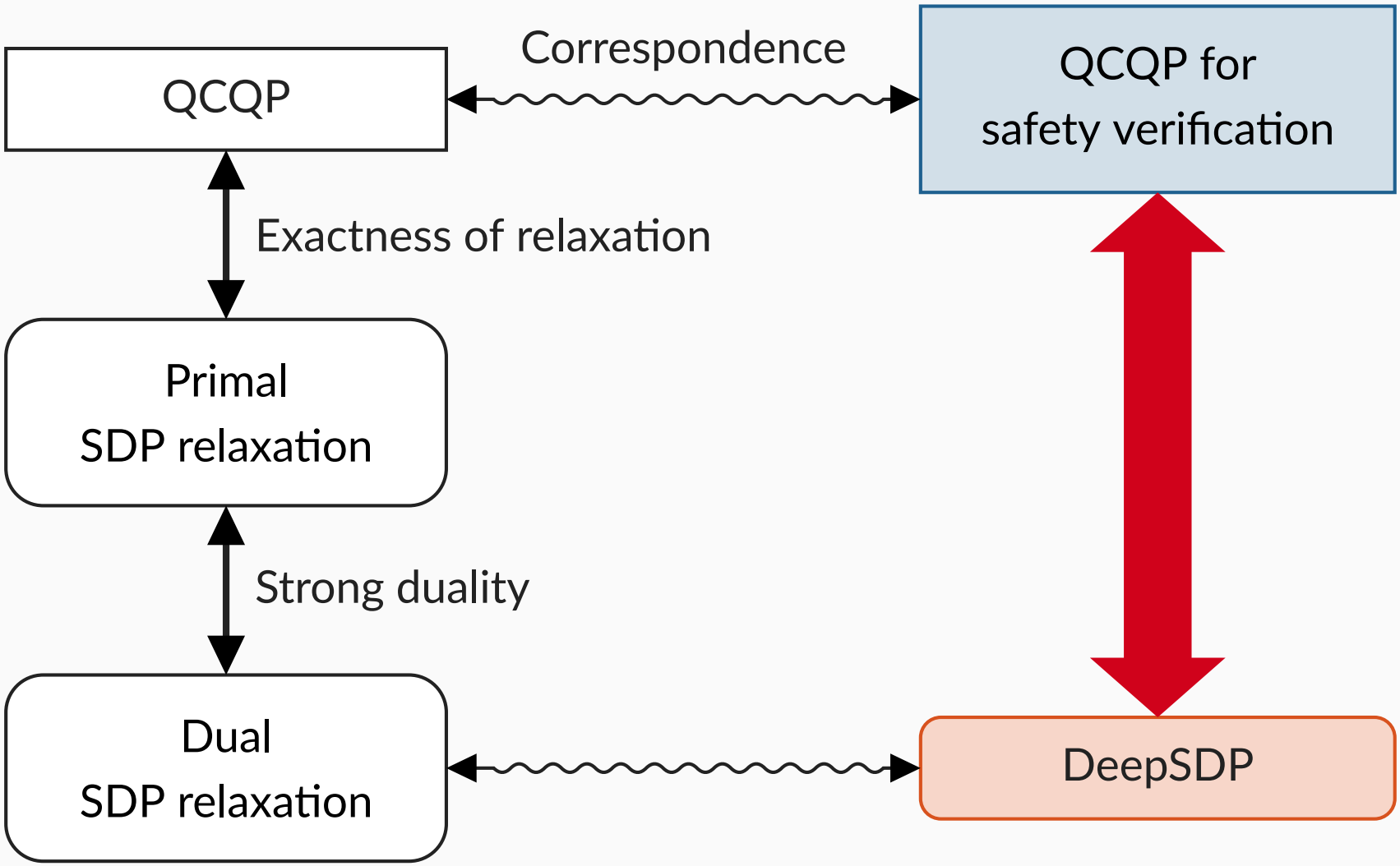
Consider a half-space $H := \{\boldsymbol{y} \in \mathbb{R}^{n_2} \mid \boldsymbol{c}^{\mathrm{T}}\boldsymbol{y} - d \geq 0\}$.

## DeepSDP to verify $\mathcal{Y} \subseteq H$

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

- An SDP, solvable in polynomial-time
- Generated from a QCQP by relaxing and taking the dual

# Exactness Around Today's Problems




**Exactness and Accuracy**

Exact relaxation allows DeepSDP to solve the original QCQP.

# Primal SDP Relaxation (= Dual of DeepSDP)

$e^i$: a vector where $i$th element is $1$, the others are $0$.

$$
\begin{aligned}
\min_{\substack{\boldsymbol{x}^0,\boldsymbol{x}^1,\\ X^{00},X^{10},X^{11}}} \quad & 2\boldsymbol{c}^{\mathrm{T}}\boldsymbol{x}^1 \\
\text{s.t.} \quad & \begin{bmatrix} \hat{\boldsymbol{x}}^{\mathrm{T}}\hat{\boldsymbol{x}} - \rho^2 & -\hat{\boldsymbol{x}}^{\mathrm{T}} & \mathbf{0} \\ -\hat{\boldsymbol{x}} & I & O \\ \mathbf{0} & O & O \end{bmatrix} \bullet G \le 0,\ G := \begin{bmatrix} 1 & \left(\boldsymbol{x}^0\right)^{\mathrm{T}} & \left(\boldsymbol{x}^1\right)^{\mathrm{T}} \\ \boldsymbol{x}^0 & X^{00} & \left(X^{10}\right)^{\mathrm{T}} \\ \boldsymbol{x}^1 & X^{10} & X^{11} \end{bmatrix}, \\
& \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} & -b_i^0\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ \mathbf{0} & O & -\left(W^0\right)^{\mathrm{T}}\boldsymbol{e}^i\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ -b_i^0\boldsymbol{e}^i & -\boldsymbol{e}^i\left(\boldsymbol{e}^i\right)^{\mathrm{T}}W^0 & 2\boldsymbol{e}^i\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \end{bmatrix} \bullet G \le 0, \\
& \begin{bmatrix} 2b_i^0 & \left(\boldsymbol{e}^i\right)^{\mathrm{T}}W^0 & -\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ \left(W^0\right)^{\mathrm{T}}\boldsymbol{e}^i & O & O \\ -\boldsymbol{e}^i & O & O \end{bmatrix} \bullet G \le 0, \\
& \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} & -\left(\boldsymbol{e}^i\right)^{\mathrm{T}} \\ \mathbf{0} & O & O \\ -\boldsymbol{e}^i & O & O \end{bmatrix} \bullet G \le 0, \qquad i = 1,\ldots,n_1.
\end{aligned}
$$

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# Theoretical Result

**Thm: Exactness condition for a single-layer network**

The primal SDP relaxation is exact if

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

In addition, DeepSDP is also exact under strong duality.

- This talk focuses on the first sufficient condition (hyper-ellipsoid).
- We discuss the derivation in the remaining time, via
  - transformation using vector $e$,
  - decomposition to two problems.

# Gram Matrix Transformation

Fix $\boldsymbol{e} \in \mathbb{R}^{1+n_0+n_1}$ satisfying $\|\boldsymbol{e}\| = 1$. (arbitrary)

- Define new variables $\boldsymbol{u}^1, \ldots, \boldsymbol{u}^{n_0}$, and $\boldsymbol{v}^1, \ldots, \boldsymbol{v}^{n_1} \in \mathbb{R}^{1+n_0+n_1}$.
- Substitute $\boldsymbol{x}^0, \boldsymbol{x}^1, X_{00}, X_{10}, X_{11}$ in the primal SDP by

$$\boldsymbol{x}^0 = \begin{bmatrix} \boldsymbol{e}^{\mathrm{T}}\boldsymbol{u}^1 \\ \vdots \\ \boldsymbol{e}^{\mathrm{T}}\boldsymbol{u}^{n_0} \end{bmatrix} \in \mathbb{R}^{n_0}, \quad X^{10} = \begin{bmatrix} (\boldsymbol{v}^1)^{\mathrm{T}}\boldsymbol{u}^1 & \cdots\cdots & (\boldsymbol{v}^1)^{\mathrm{T}}\boldsymbol{u}^{n_0} \\ \vdots & \ddots\ddots & \vdots \\ (\boldsymbol{v}^{n_1})^{\mathrm{T}}\boldsymbol{u}^1 & \cdots\cdots & (\boldsymbol{v}^{n_1})^{\mathrm{T}}\boldsymbol{u}^{n_0} \end{bmatrix} \in \mathbb{R}^{n_1 \times n_0},$$

$$\boldsymbol{x}^1 = \begin{bmatrix} \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^1 \\ \vdots \\ \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^{n_1} \end{bmatrix} \in \mathbb{R}^{n_1}, \quad X^{11} = \begin{bmatrix} (\boldsymbol{v}^1)^{\mathrm{T}}\boldsymbol{v}^1 & \cdots\cdots & (\boldsymbol{v}^1)^{\mathrm{T}}\boldsymbol{v}^{n_1} \\ \vdots & \ddots\ddots & \vdots \\ (\boldsymbol{v}^{n_1})^{\mathrm{T}}\boldsymbol{v}^1 & \cdots\cdots & (\boldsymbol{v}^{n_1})^{\mathrm{T}}\boldsymbol{v}^{n_1} \end{bmatrix} \in \mathbb{S}^{n_1}.$$

Example

$$0 \geq \begin{bmatrix} 0 & \mathbf{0}^{\mathrm{T}} & -(\boldsymbol{e}^i)^{\mathrm{T}} \\ \mathbf{0} & O & O \\ -\boldsymbol{e}^i & O & O \end{bmatrix} \bullet G = -2\boldsymbol{e}^i \bullet \boldsymbol{x}^1 = -2\boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i \quad \text{for all } i.$$

# Equivalent Formulation of SDP Relaxation

The following problem is obtained from the primal SDP relaxation.

$$\min_{\boldsymbol{u}^j, \boldsymbol{v}^i} \quad 2\sum_{i=1}^{n_1} c_i \, \boldsymbol{e}^{\mathrm{T}} \boldsymbol{v}^i \tag{1}$$

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

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

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

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

# Exactness Condition by Collinearity with $e$

**Prop: Exactness condition for collinearity in [Zhang '20]**

Suppose there exists an optimal solution $\{(\boldsymbol{u}^1)^*, \ldots, (\boldsymbol{u}^{n_0})^*, (\boldsymbol{v}^1)^*, \ldots, (\boldsymbol{v}^{n_1})^*\}$ which are collinear with $\boldsymbol{e}$. Then, the primal SDP relaxation is exact.

**Def: Collinearity**

Vectors $\{\boldsymbol{a}^1, \ldots, \boldsymbol{a}^m\} \subseteq \mathbb{R}^{1+n_0+n_1}$ are collinear with $\boldsymbol{e}$ if

$$\left|\boldsymbol{e}^{\mathrm{T}}\boldsymbol{a}^i\right| = \left\|\boldsymbol{a}^i\right\| \quad \text{for all } i \in \{1, \ldots, m\}.$$

It is suffice to show the collinearity of a solution of the transformed problem.

---

[Zhang '20] Zhang, On the tightness of semidefinite relaxations for certifying robustness to adversarial examples, NeurIPS, 2020.

# Decomposition according to $u^j$ and $v^i$

## Inner problem: constraints using $u^j$

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

$$\left.\begin{aligned} \min_{\boldsymbol{u}^1,\ldots,\boldsymbol{u}^{n_0}} \quad & \textstyle\sum_{j=1}^{n_0} \left\|\boldsymbol{u}^j - \hat{x}_j \boldsymbol{e}\right\|_2^2 \\ \text{s.t.} \quad & \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i \geq \boldsymbol{e}^{\mathrm{T}} \left(\textstyle\sum_{j=1}^{n_0} W_{ij}\boldsymbol{u}^j + b_i^0 \boldsymbol{e}\right), \quad i = 1,\ldots,n_1, \ (3) \\ & \left\|\boldsymbol{v}^i\right\|_2^2 \leq \left(\textstyle\sum_{j=1}^{n_0} W_{ij}\boldsymbol{u}^j + b_i^0 \boldsymbol{e}\right)^{\mathrm{T}} \boldsymbol{v}^i, \ i = 1,\ldots,n_1, \ (4) \end{aligned}\right\} \quad (S_2)$$

## Outer problem: the remains and $\Psi$

$$\left.\begin{aligned} \min_{\boldsymbol{v}^1,\ldots,\boldsymbol{v}^{n_1}} \quad & 2\textstyle\sum_{i=1}^{n_1} c_i \, \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i & & (1) \\ \text{s.t.} \quad & \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i \geq 0, & i = 1,\ldots,n_1, \quad & (2) \\ & \Psi(\boldsymbol{v}^1,\ldots,\boldsymbol{v}^{n_1}) \leq \rho^2. & & \end{aligned}\right\} \quad (S_1)$$

The case $\boldsymbol{e} = \boldsymbol{e}^1$ is only considered due to time limitation.

# Relationship Between Their Solutions

A part of KKT condition of $(S_2)$:

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

**Lemma: Linear Combination**

For any optimal solution $(\boldsymbol{u}^1)^*, \ldots, (\boldsymbol{u}^{n_0})^*$ of $(S_2)$,
there exist $\boldsymbol{m} \in \mathbb{R}^{n_0}$ and $M \in \mathbb{R}^{n_1 \times n_0}$ such that

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

It suffices to show $(\boldsymbol{v}^i)^*$s are collinear to $\boldsymbol{e}^1$.

# Collinearity in $(S_1)$

$$
\left.
\begin{aligned}
\min_{\boldsymbol{v}^1,\ldots,\boldsymbol{v}^{n_1}} \quad & 2\sum_{i=1}^{n_1} c_i\, \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i && (1)\\
\text{s.t.} \quad & \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i \geq 0,\ i=1,\ldots,n_1, && (2)\\
& \sum_{j=1}^{n_0} \left\| (m_j - \hat{x}_j)\,\boldsymbol{e}^1 + \sum_{i=1}^{n_1} M_{ij}\boldsymbol{v}^i \right\|_2^2 \leq \rho^2.
\end{aligned}
\right\} \quad (S_1)
$$

For $(S_1)$, we can show the following lemma:

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

$(S_1)$ has an optimal solution $(\boldsymbol{v}^1)^*,\ldots,(\boldsymbol{v}^{n_1})^*$ which are collinear to $\boldsymbol{e}^1$.

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

# Collinearity in $(S_1)$

$$\left.\begin{aligned} \min_{\boldsymbol{v}^1,\ldots,\boldsymbol{v}^{n_1}} \quad & 2\sum_{i=1}^{n_1} c_i\, \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i && (1)\\ \text{s.t.} \quad & \boldsymbol{e}^{\mathrm{T}}\boldsymbol{v}^i \geq 0,\ i=1,\ldots,n_1, && (2)\\ & \sum_{j=1}^{n_0}\left\|(m_j-\hat{x}_j)\,\boldsymbol{e}^1+\sum_{i=1}^{n_1} M_{ij}\boldsymbol{v}^i\right\|_2^2 \leq \rho^2. \end{aligned}\right\} \quad (S_1)$$

Essence of Proof.

- Let $(\bar{\boldsymbol{v}}^1,\ldots,\bar{\boldsymbol{v}}^{n_1})$ be an optimal solution of $(S_1)$.
- 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.
  - The objective value is the same.

# Conclusion

Summary

- Verification of the safety of Neural Networks
- Exactness conditions of DeepSDP in this context

Future works

- Analyze the non-polyhedral case of $S_y$
- Weaken the assumptions on the input set $\mathcal{X}$

Thank you for your attention!

For more details, see arXiv:2504.09934

*Tight Semidefinite Relaxations for Verifying Robustness of Neural Networks*

# QCQP: Quadratically Constrained Quadratic Programming

Consider a quadratic programming with quadratic constraints:

$$\begin{aligned} v^* \coloneqq \min_{\boldsymbol{x}\in\mathbb{R}^n} \quad & \boldsymbol{x}^{\mathrm{T}} Q^0 \boldsymbol{x} \\ \text{s.t.} \quad & \boldsymbol{x}^{\mathrm{T}} Q^p \boldsymbol{x} \leq b_p, \quad p \in [m] \coloneqq \{1, \ldots, m\}, \end{aligned} \tag{$\mathcal{P}$}$$

- Generally, non-convex & NP-hard
- Semidefinite programming (SDP) relaxation

**Applications**

Binary programming, MAX-CUT, optimal flow problems,...

# Exactness for SDP Relaxation

The following equality holds:

$$v^* = \min \left\{ Q^0 \bullet X \;\middle|\; \begin{array}{l} X \succeq O \\ Q^p \bullet X \leq b_p \quad \forall p \in [m] \end{array} \right\} = v^*_{\mathrm{SDP}}$$

$\Longleftrightarrow$ rank-1 solution $X^*$ exists

Exact SDP relaxation $\Longrightarrow$

- Original QCQP is exactly solvable (in theorically)
- The gap between a class of QCQPs and their relaxations is identified.

**Motivation**

What conditions of QCQPs guarantee the exactness?

# 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 $\gamma$,

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

# DeepSDP for Single-layer NN

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

## DeepSDP to verify $\mathcal{Y} \subseteq H$

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

- An SDP, solvable in polynomial-time
- Generated from a QCQP by relaxing and taking the dual

# 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.

# DeepSDP for Single-layer NN

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

## DeepSDP to verify $\mathcal{Y} \subseteq H$

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

- An SDP, solvable in polynomial-time
- Generated from a QCQP by relaxing and taking the dual

# Quadratic Formulation for ReLU Function

Review: $\phi$ applies element-wisely ReLU function $\varphi$

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 | $\lambda_i$ | $\nu_i$ | $\eta_i$ |

# 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.