Tackling Neural Network Expressivity via (virtual Newton) Polytopes

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IOL & DISCOGA Research Seminar
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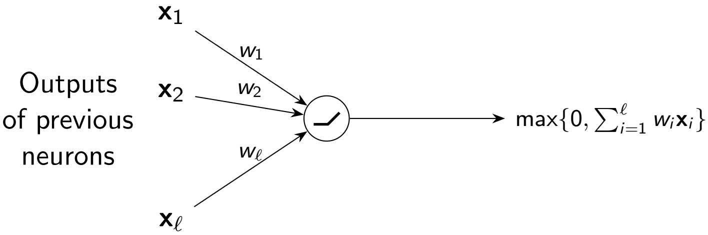
(both problems have broader context ...)

A Single ReLU Neuron



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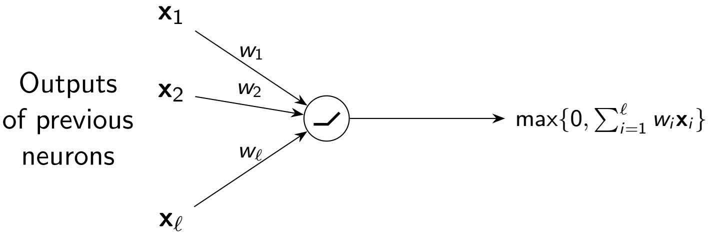
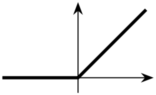


Rectified linear unit (ReLU): $\text{relu}(x) = \max\{0, x\}$



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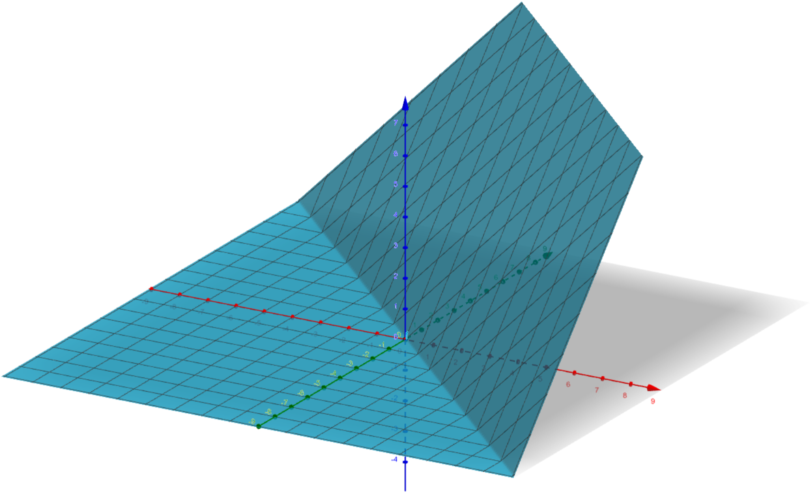
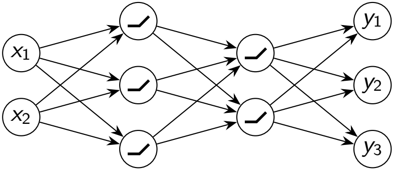


ReLU Feedforward Neural Networks

- Acyclic (layered) digraph of ReLU neurons



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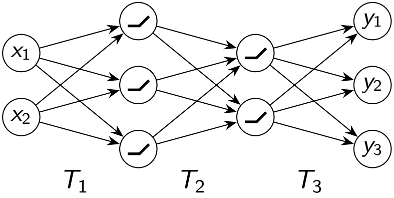

- Computes function

$$T_k \circ \mathrm{relu} \circ T_{k-1} \circ \cdots \circ T_2 \circ \mathrm{relu} \circ T_1$$

with linear transformations T_i.

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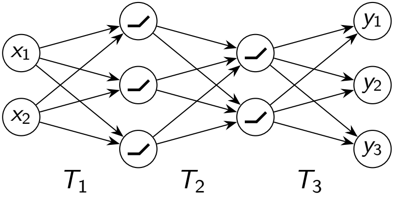

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- Example: depth 3 (2 hidden layers).

NNs and CPWL Functions

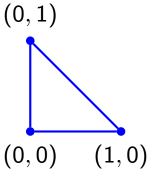
Theorem (Arora, Basu, Mianjy, Mukherjee (ICLR 2018))

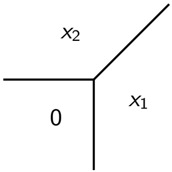
$f : \mathbb{R}^n \to \mathbb{R}$ can be represented by a ReLU NN if and only if f is continuous and piecewise linear (CPWL).

Support Functions and Newton Polytopes

Definition

The *support function* f_P of a polytope $P \subseteq \mathbb{R}^n$ maps a cost vector $x \in \mathbb{R}^n$ to the objective value of the linear program $\max_{v \in P} x^T v$.





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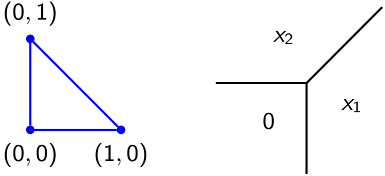

Definition

The *Newton polytope* of a convex CPWL function $f(x) = \max\{v_1^T x, v_2^T x, \ldots, v_p^T x\}$ is $P(f) = \text{conv}\{v_1, v_2, \ldots, v_p\}$.

Bijection between Convex CPWL Functions and Polytopes

Have a bijection between these two sets:

- Convex CPWL functions $\mathbb{R}^n \to \mathbb{R}$,
- Polytopes in $\mathbb{R}^n$.

The bijection maps ...

- Functions to their Newton polytope $f \mapsto P_f$,
- Polytopes to their support function $P \mapsto f_P$.

Adding Two (Convex) CPWL Functions

$$\begin{aligned}\max\{0, x_1, x_2\} + \max\{0, x_2\} &= \max\{0, x_2, x_1, x_1 + x_2, x_2, 2x_2\} \\ &= \max\{0, x_1, 2x_2, x_1 + x_2\}\end{aligned}$$

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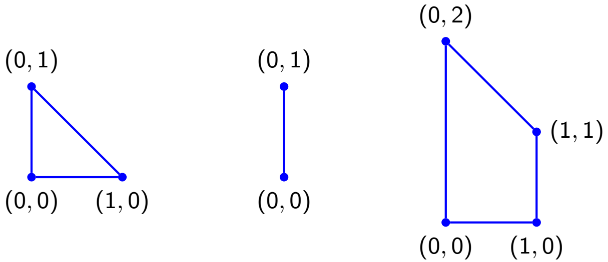

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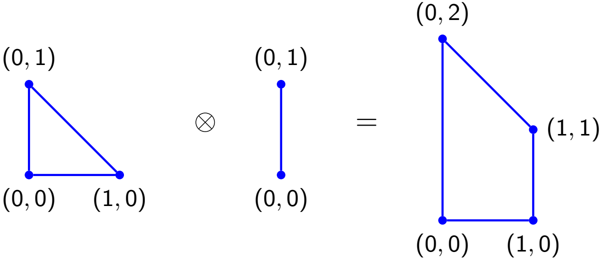

- Minkowski sum: $P \otimes Q := \{p + q \mid p \in P, q \in Q\}$,

The Bijection is a Semigroup Isomorphism

$$P_{f+g} = P_f \otimes P_g,$$
$$f_{P \otimes Q} = f_P + f_Q.$$

(Convex CPWL functions $\mathbb{R}^n \to \mathbb{R}$, $+$)

$\cong$

(Polytopes in $\mathbb{R}^n$, $\otimes$)

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YES!

$\rightsquigarrow$ Virtual Polytopes!

Remember When You Learned Mathematics ...

- Semigroup $(\mathbb{N}, +)$

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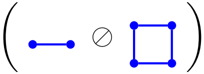
- Remember: $\frac{a}{b} = \frac{c}{d} \quad \Leftrightarrow \quad ad = bc$
- In the same way: $\frac{P}{Q} = \frac{R}{S} \quad \Leftrightarrow \quad P \otimes S = Q \otimes R$

(formally via equivalence relations)

Two Examples

Cancellation Rule:



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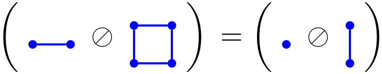

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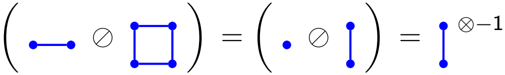

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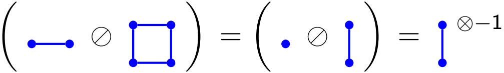

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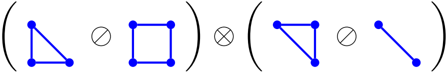

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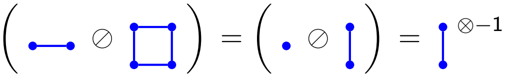

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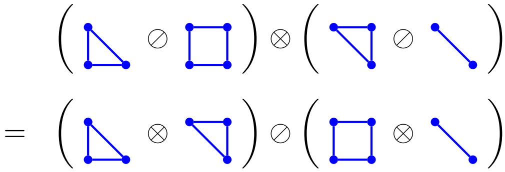

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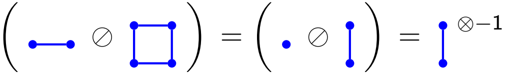

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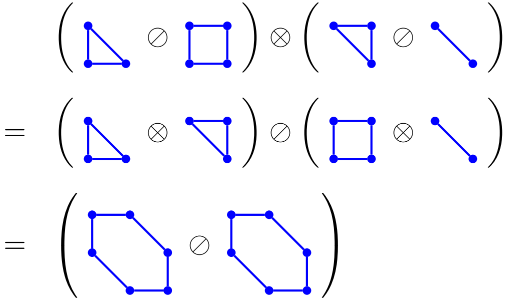

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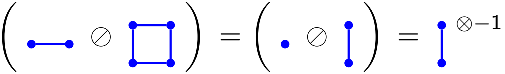

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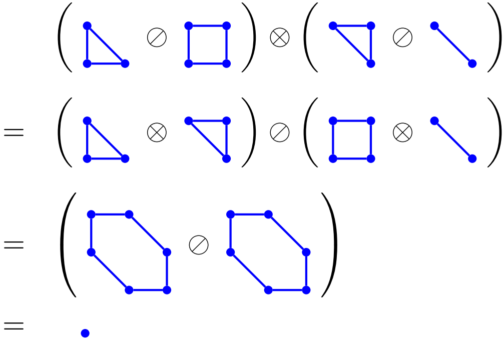

We even have a Group Isomorphism!

$$(\text{CPWL functions } \mathbb{R}^n \to \mathbb{R}, +)$$
$$\cong$$
$$(\text{Virtual Polytopes in } \mathbb{R}^n, \otimes)$$

In particular:

Every CPWL function is a difference of two convex CPWL functions.

$$\frac{P}{Q} \mapsto f_P - f_Q$$
$$f - g \mapsto \frac{P_f}{P_g}$$

Virtual Polytopes are Almost Polytopes

- They have a **face lattice**,
  - faces are virtual polytopes.
- They have a **volume**,
  - but volume can be negative.

The General Idea

Find out which **virtual polytopes**

can occur as **Newton polytopes** of **CPWL functions**

computed by **neural networks** of a certain size (or structure).

Which Operations can NNs perform?

- Addition
- Scalar multiplication
- ReLU activations

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- Addition $\quad \leftrightarrow \quad$ Minkowski addition $\quad \checkmark$
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- ReLU activations ?

We even have a Vector Space Isomorphism!

$$f = \max_{i=1}^{p}\{v_i^T x\} \quad \Rightarrow \quad P_{\lambda f} = \text{conv}_{i=1}^{p}\{\lambda v_i\} = \lambda P_f$$

(CPWL functions, $+$, scalar multiplication)
$\cong$
(Virtual Polytopes, $\otimes$, scaling)

(for $\lambda < 0$ also consistent with Minkowski difference)

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- Addition $\leftrightarrow$ Minkowski addition ✓
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- Taking Maxima ?

“Maximum” for Two Virtual Polytopes

For two convex CPWL functions f and g:

$$P_{\max\{f,g\}} = \operatorname{conv}\{P_f \cup P_g\} =: P_f \oplus P_g.$$

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For $f = f_+ - f_-$ and $g = g_+ - g_-$ (non-convex) CPWL functions.

$$\begin{aligned} \Rightarrow \quad \max\{f,g\} &= \max\{f_+ - f_-, g_+ - g_-\} \\ &= \max\{f_+ + g_-, g_+ + f_-\} - (f_- + g_-). \end{aligned}$$

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Translating to virtual polytopes:

$$P_f \oplus P_g := P_{\max\{f,g\}}$$
$$= \frac{(P_{f_+} \otimes P_{g_-}) \oplus (P_{g_+} \otimes P_{f_-})}{(P_{f_-} \otimes P_{g_-})}$$

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Does this remind you of something? $\quad \rightsquigarrow \quad \frac{a}{b} + \frac{c}{d} = \frac{ad+bc}{bd}$

We also have a Semiring Isomorphism!

$$(\text{CPWL functions}, \max, +)$$
$$\cong$$
$$(\text{Virtual Polytopes}, \oplus, \otimes)$$

(here you see the “tropical” world!)

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- Taking Maxima ?

Which Operations can NNs perform?

- Addition $\leftrightarrow$ Minkowski addition ✓
- Scalar multiplication $\leftrightarrow$ Scaling of (virtual) polytopes ✓
- Taking Maxima $\leftrightarrow$ convex hull of the union ✓

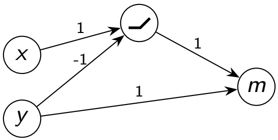
Take a Breath!

Now to the two open problems:

- Can 3-layer NNs compute the maximum of 5 numbers?
- Can poly-size NNs solve the MST problem?

Computing the Maximum of Two Numbers

$$\max\{x, y\} = \max\{x - y, 0\} + y$$



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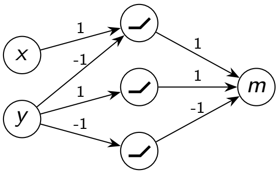

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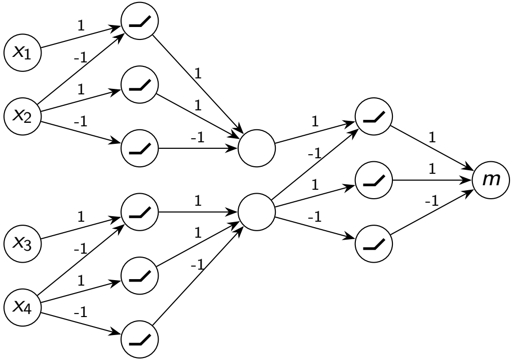

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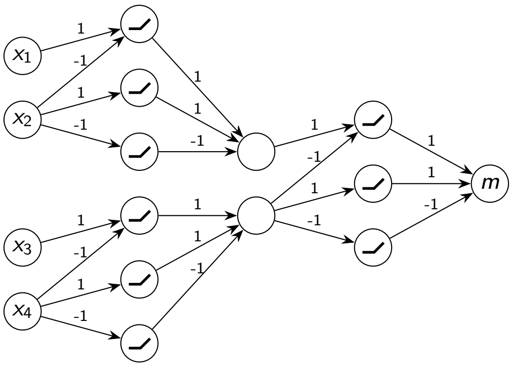

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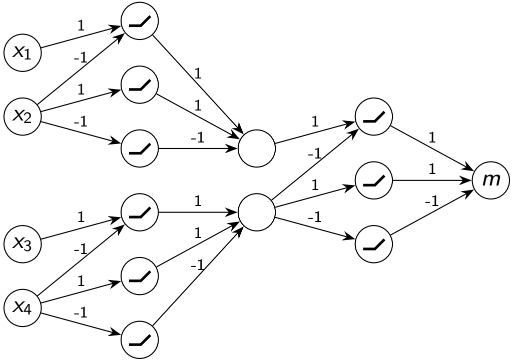

- Inductively: Maximum of n numbers with depth $\lceil \log_2(n) \rceil + 1$.

Question: Is this best possible?

What's known?

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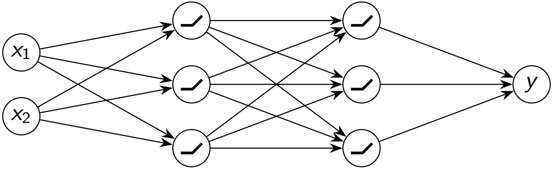
What's known?

- $\max\{0, x_1, x_2\}$ cannot be computed with 2 layers.

That's all!

- No function known that provably needs more than 3 layers.
- Smallest open case:
  Can $\max\{0, x_1, x_2, x_3, x_4\}$ be computed with 3 layers?

Virtual Newton Polytopes of Neural Networks



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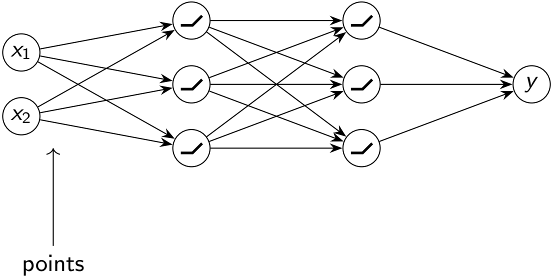

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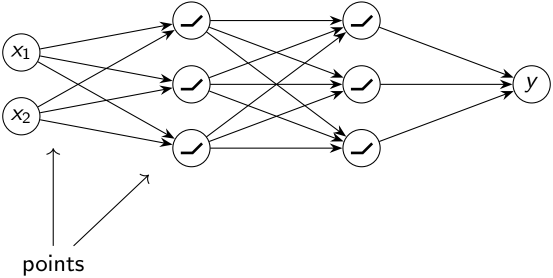

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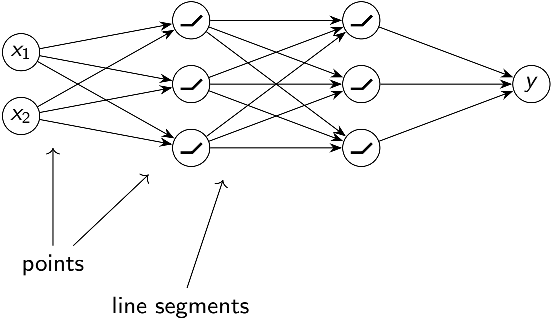
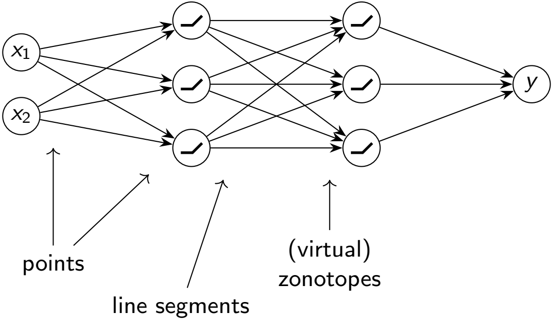


Virtual Newton Polytopes of Neural Networks



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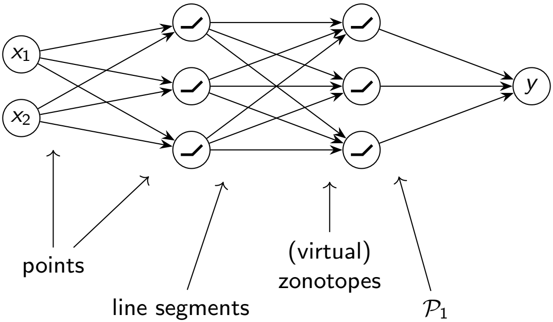
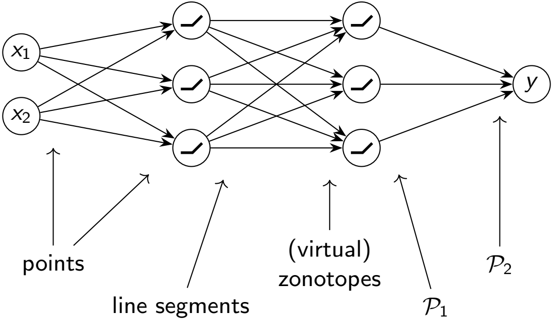


$$\mathcal{P}_1 = \{ \; Y \oplus Z \mid Y, \, Z \text{ (virtual) zonotopes } \}$$

(convex hull of the union of two zonotopes)

Virtual Newton Polytopes of Neural Networks



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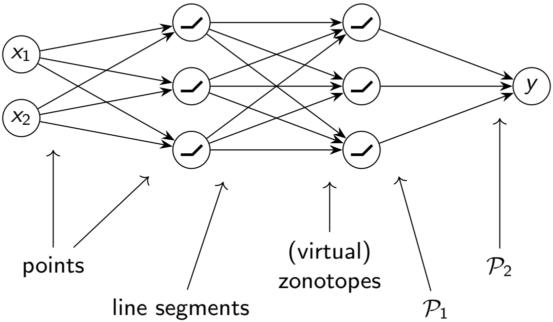

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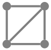
$f(x) = \max\{0, x_1, x_2, x_3, x_4\}$ can be computed by 3-layer NN

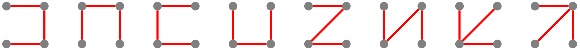
$$\Leftrightarrow \quad \text{4-simplex } \Delta^4 = P_f \in \mathcal{P}_2.$$

The Two Open Problems

- Can 3-layer NNs compute the maximum of 5 numbers?
- Can poly-size NNs solve the MST problem?

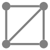
The Minimum Spanning Tree Problem

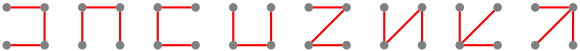
$G =$ 

$\mathcal{X} = \{$  $\}$

Let $\mathcal{X} \subseteq \{0,1\}^E$ be the set of characteristic vectors of spanning trees in a fixed graph $G = (V, E)$.

The Minimum Spanning Tree Problem

$G =$ 

$\mathcal{X} = \{$  $\}$

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MST problem: Compute the CPWL function

$$c \mapsto \min_{x \in \mathcal{X}} c^T x.$$

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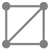
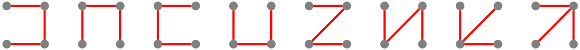
$G =$ 

$\mathcal{X} = \Big\{$  $\Big\}$

Let $\mathcal{X} \subseteq \{0,1\}^E$ be the set of characteristic vectors of spanning trees in a fixed graph $G = (V, E)$.

MST problem: Compute the CPWL function

$$c \mapsto \min_{x \in \mathcal{X}} c^T x.$$

Question: Is there a poly-size NN computing this function?

Is there a poly-size NN to solve MST?

$$f(c) = \min_{x \in \mathcal{X}} x^T c = -\max_{x \in \mathcal{X}} (-x)^T c$$

$$\Rightarrow \qquad P_f = \text{conv}\{-x \mid x \in \mathcal{X}\}^{\otimes -1} = (-\text{MST-Polytope})^{\otimes -1}$$

Is there a poly-size NN to solve MST?

$$
\begin{aligned}
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\Rightarrow \qquad & P_f = \operatorname{conv}\{-x \mid x \in \mathcal{X}\}^{\otimes -1} = (-\text{MST-Polytope})^{\otimes -1}
\end{aligned}
$$

Proposition

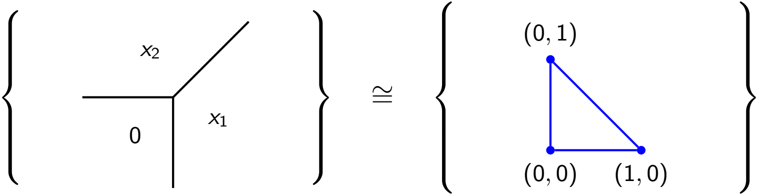
There exists a poly-size NN computing f

$\Leftrightarrow$

The MST-Polytope can be (virtually) generated from points via polynomially many operations of the form

- *Minkowski addition,*
- *Convex hull of the union,*
- *Scaling (with possibly inverting).*

Thank you!



Questions? Ideas?