Tackling Neural Network Expressivity via Polytopes

Christoph Hertrich

joint work with

Amitabh Basu   Marco Di Summa   Martin Skutella

(Polytop)ics conference
April 6, 2021

Can **3-layer neural networks** compute the **maximum of 5 numbers**?

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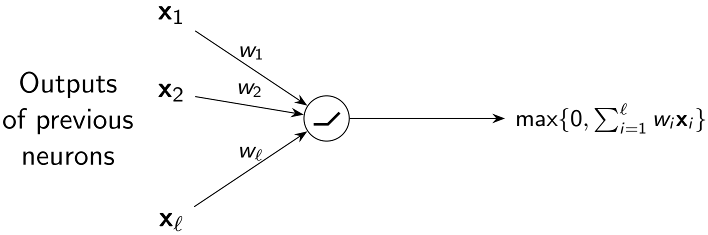
A Single ReLU Neuron



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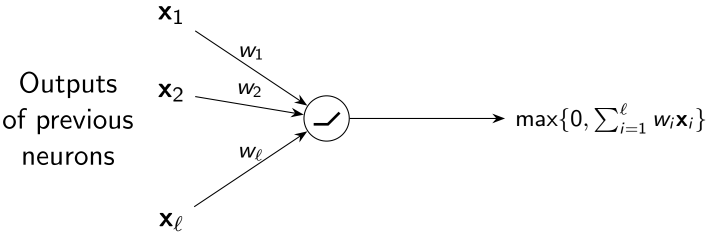
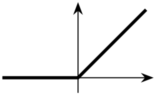
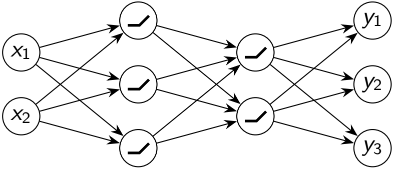


Rectified linear unit (ReLU): $\mathrm{relu}(x) = \max\{0, x\}$



ReLU Feedforward Neural Networks

- Acyclic (layered) digraph of ReLU neurons



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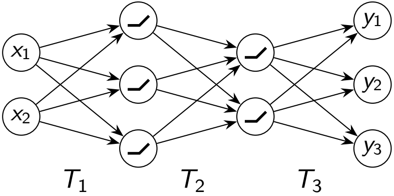

- Computes function

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

with linear transformations T_i.

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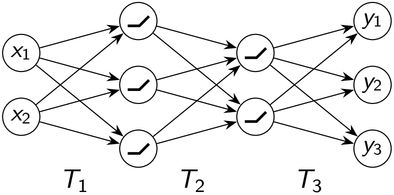

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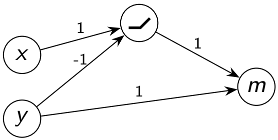
- Example: depth 3 (2 hidden layers).

Example: Computing the Maximum of Two Numbers

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



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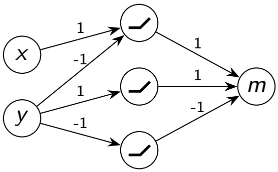

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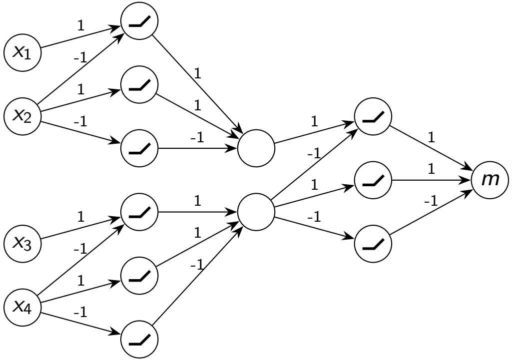

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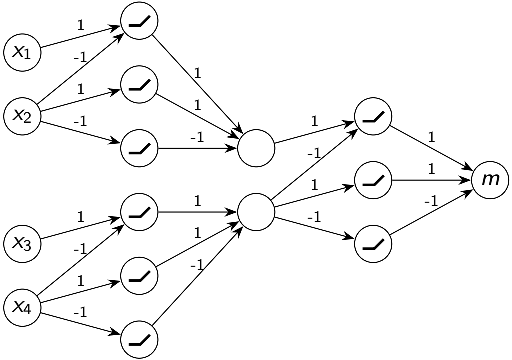

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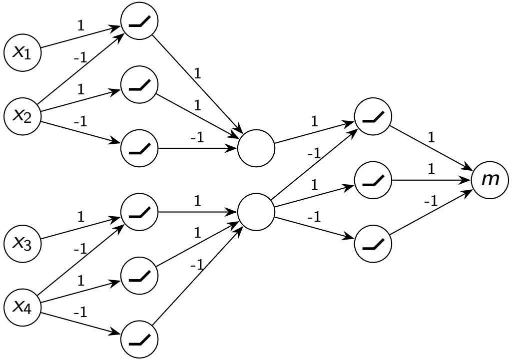

- Inductively: Maximum of n numbers with depth $\lceil \log_2(n) \rceil + 1$.

Question: Is this best possible?

Why is the maximum function so interesting?

Theorem (Arora, Basu, Mianjy, Mukherjee (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).

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Theorem (Wang, Sun (2005))

Any (CPWL) function $f : \mathbb{R}^n \to \mathbb{R}$ can be written as linear combination of maxima of $n + 1$ linear terms.

$\Rightarrow$ Everything depends on the maximum function!

What's known?

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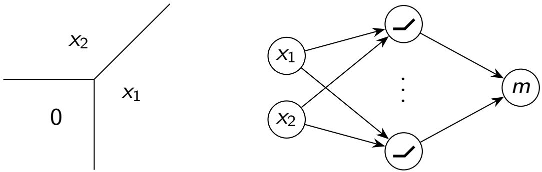
- $\max\{0, x_1, x_2\}$ cannot be computed with 2 layers.



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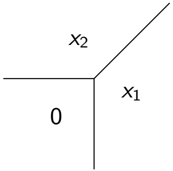

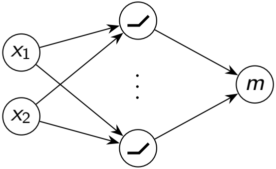

(set of break points must be union of lines)

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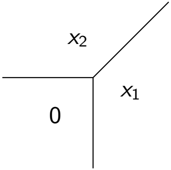

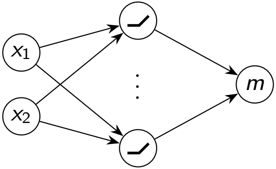

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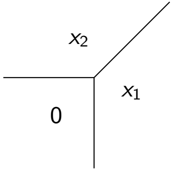

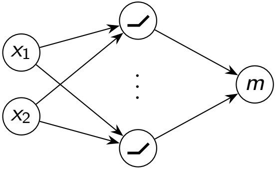

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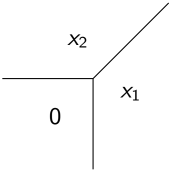

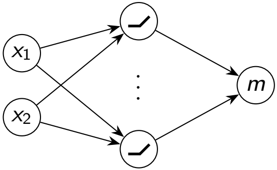

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That's all!

- 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?

In this talk:
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(for notational purposes: $x_0 := 0$.)

The Assumption

If ... there exists a 3-layer NN computing $\max\{0, x_1, x_2, x_3, x_4\}$,
Then ... also one with the following property:

The output of each neuron can only have breakpoints where the relative ordering of the five numbers 0, x_1, ..., x_4 changes.

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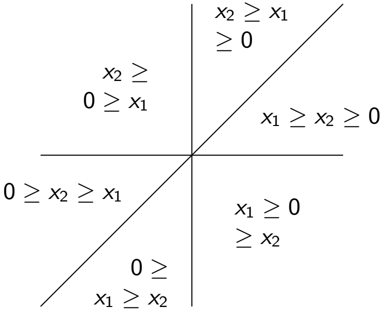
Example for $\max\{0, x_1, x_2\}$:



The Assumption Rephrased

If ... there exists a 3-layer NN computing $\max\{0, x_1, x_2, x_3, x_4\}$,
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The output of each neuron is linear within each region of the **hyperplane arrangement** given by $\binom{5}{2} = 10$ hyperplanes:
$x_i = x_j$, $0 \leq i < j \leq 4$.

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$\Rightarrow$ Vector space of possible CPWL functions is 30-dimensional!

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- ... after 1 hidden layer:
  exactly 14 of 30 dimensions can be reached.

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$$\max\{0, x_1, x_2, x_3, x_4\}$$

is not contained in the 29-dimensional subspace!

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No!

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Two possible approaches:

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2. Using Newton polytopes of CPWL functions.

Newton Polytope of a Convex CPWL Function

- $f(x) = \max\{a_1^T x, \ldots, a_k^T x\} \quad \rightsquigarrow \quad P(f) = \operatorname{conv}\{a_1, \ldots, a_k\}$
- dual to underlying polyhedral complex of the CPWL function

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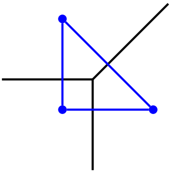

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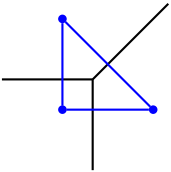

Convex CPWL functions	**Newton Polytopes**
(positive) scalar multiplication	scaling
addition	Minkowski sum
taking maximum	taking joint convex hull

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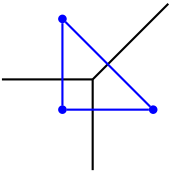

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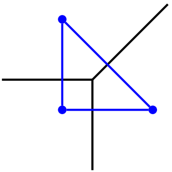

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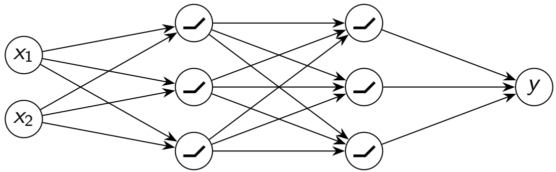
Problem: Not every CPWL function is convex ...
But: Can represent them as difference of two convex ones!

Newton Polytopes and Neural Networks

[Zhang, Naitzat, Lim: Tropical Geometry of Deep Neural Networks. ICML 2018]



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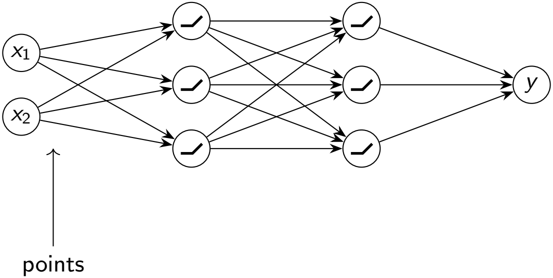

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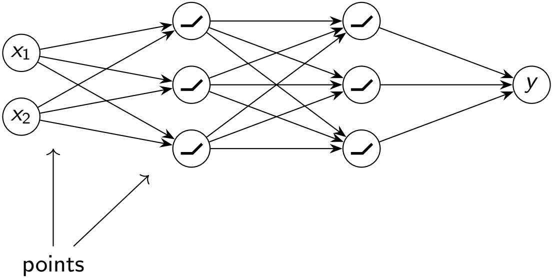

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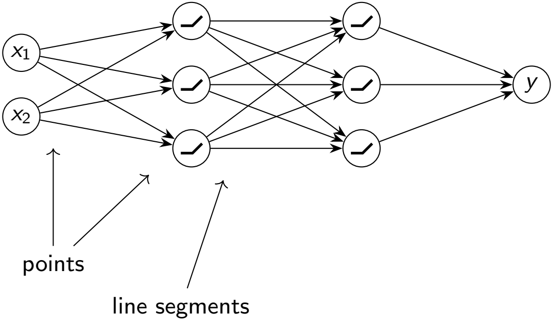

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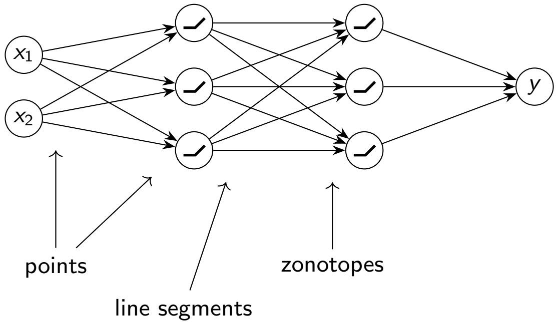

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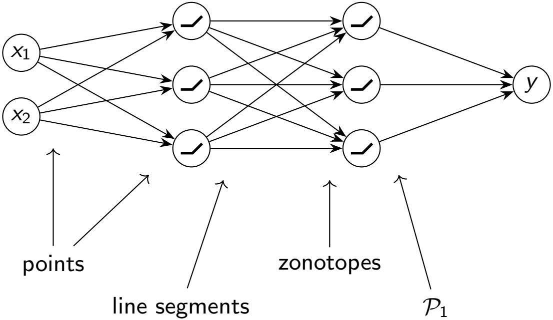

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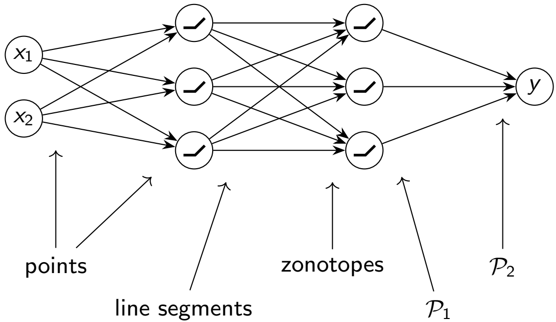

$\mathcal{P}_1 = \{P \text{ polytope} \mid P \text{ joint convex hull of two zonotopes}\}$

$\mathcal{P}_2 = \{P \text{ polytope} \mid P \text{ finite Minkowski sum of polytopes in } \mathcal{P}_1\}$

Translating the Problem into the Polytope World

If ... there is a 3-layer NN computing $f(x) = \max\{0, x_1, x_2, x_3, x_4\}$,
Then ... there are polytopes $Q, R \in \mathcal{P}_2$ with $Q + \Delta^4 = R$.

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Sketch of Proof.
From NN we get convex CPWL functions g and h with ...

- $P(h), P(g) \in \mathcal{P}_2$,
- $f = g - h$, and hence $f + h = g$,
- $P(f) + P(h) = P(g)$. $\square$

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The key is to ...

- Understand $\mathcal{P}_2$,

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- $P(f) + P(h) = P(g)$. $\square$

The key is to ...

- Understand $\mathcal{P}_2$,
- Understand $\mathcal{P}_1$,

Translating the Problem into the Polytope World

If ... there is a 3-layer NN computing $f(x) = \max\{0, x_1, x_2, x_3, x_4\}$,
Then ... there are polytopes $Q, R \in \mathcal{P}_2$ with $Q + \Delta^4 = R$.

Sketch of Proof.
From NN we get convex CPWL functions g and h with ...

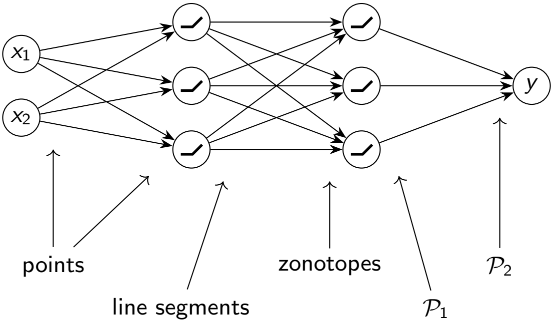
- $P(h), P(g) \in \mathcal{P}_2$,
- $f = g - h$, and hence $f + h = g$,
- $P(f) + P(h) = P(g)$. $\square$

The key is to ...

- Understand $\mathcal{P}_2$,
- Understand $\mathcal{P}_1$,
- Find characterizations for joint convex hulls of two zonotopes!

Thanks!

Questions? Ideas?



$$\mathcal{P}_1 = \{P \text{ polytope} \mid P \text{ joint convex hull of two zonotopes}\}$$

$$\mathcal{P}_2 = \{P \text{ polytope} \mid P \text{ finite Minkowski sum of polytopes in } \mathcal{P}_1\}$$

Are there polytopes $Q, R \in \mathcal{P}_2$ with $Q + \Delta^4 = R$?