Understanding Neural Network Expressivity via Polyhedral Geometry

Christoph Hertrich

LSE

joint works with

Amitabh Basu, Marco Di Summa, Martin Skutella (NeurIPS 2021)

Christian Haase, Georg Loho (ICLR 2023)

Online Machine Learning Seminar
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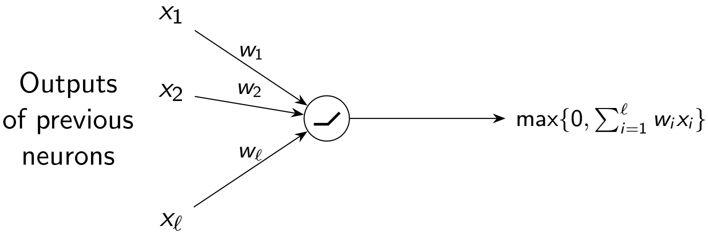
A Single ReLU Neuron



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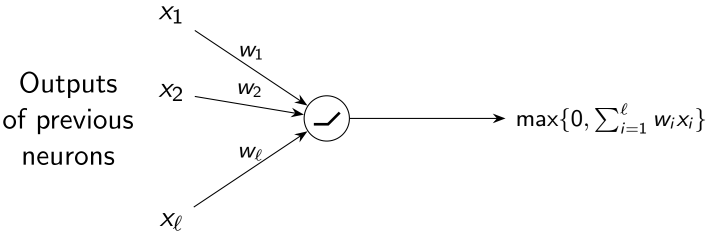
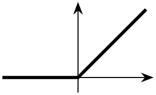


Rectified linear unit (ReLU): $\mathrm{relu}(x) = \max\{0, x\}$



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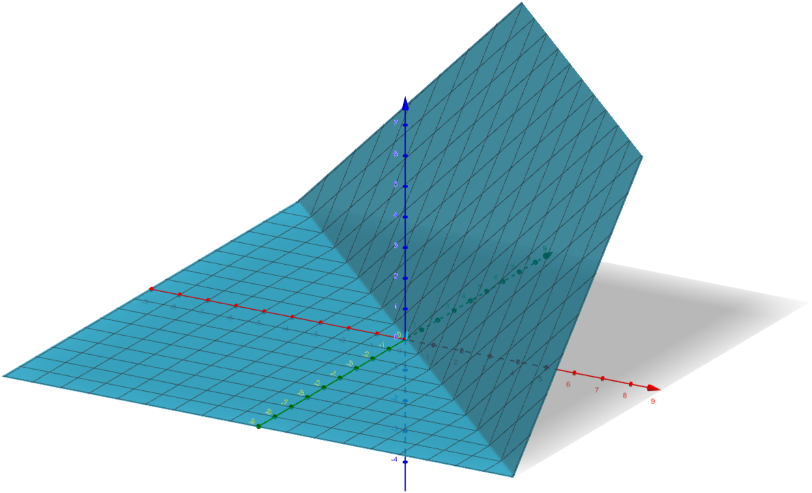
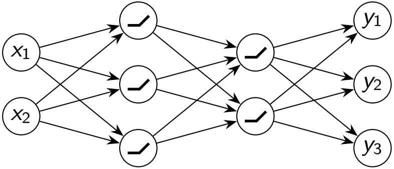


ReLU Feedforward Neural Networks

- Acyclic (layered) digraph of ReLU neurons



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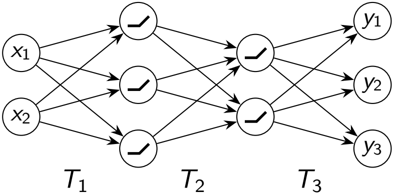

- Computes function

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

with linear transformations T_i.

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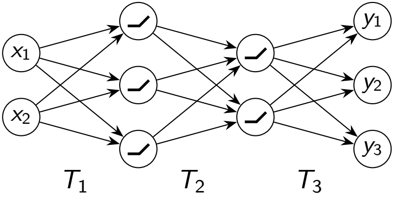

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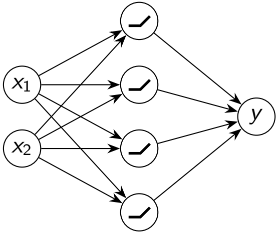
- Example: depth 3 (2 hidden layers).

What is the class of functions computable by
ReLU Neural Networks
with a certain depth?

Universal approximation theorems:

One hidden layer enough to **approximate** any continuous function.



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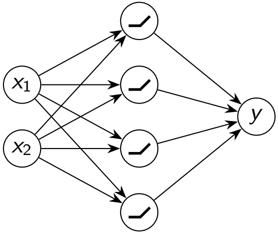
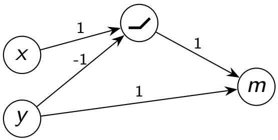


What about **exact** representability?

Example: Computing the Maximum of Two Numbers

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



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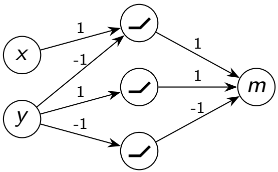
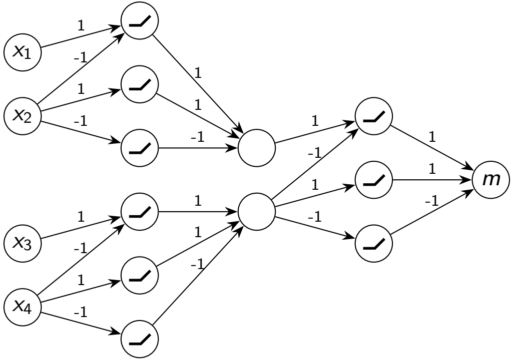


Example: Computing the Maximum of Four Numbers



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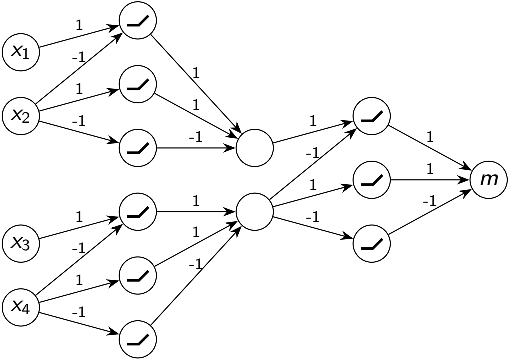

- Inductively: Max of n numbers with $\lceil \log_2(n) \rceil$ hidden layers.

Representing Arbitrary Piecewise Linear Functions

Observation

Every function represented by a ReLU NN is continuous and piecewise linear (CPWL).

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Theorem (Wang, Sun [WS05])

Every CPWL function $f : \mathbb{R}^n \to \mathbb{R}$ can be written as

$$f(x) = \sum_{i=1}^{p} \lambda_i \max\{a_{i,1}^T x, \ldots, a_{i,n+1}^T x\}.$$

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Theorem (Arora, Basu, Mianjy, Mukherjee [ABMM18])

Every CPWL function $f : \mathbb{R}^n \to \mathbb{R}$ can be represented by a ReLU NN with $\lceil \log_2(n+1) \rceil$ hidden layers.

Natural Question

Theorem (Arora, Basu, Mianjy, Mukherjee [ABMM18])

Every CPWL function $f : \mathbb{R}^n \to \mathbb{R}$ *can be represented by a ReLU NN with* $\lceil \log_2(n+1) \rceil$ *hidden layers.*

- Is logarithmic depth best possible?

Conjecture

Yes, there are functions which need $\lceil \log_2(n+1) \rceil$ *hidden layers!*

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Using [WS05], we show that this is equivalent to:

Conjecture

$\max\{0, x_1, \ldots, x_{2^k}\}$ *cannot be represented with* k *hidden layers.*

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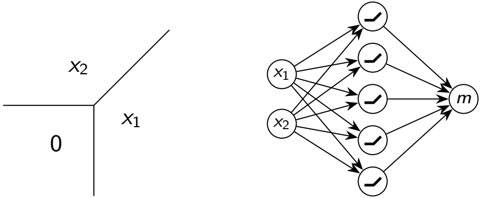
  $\max\{0, x_1, x_2\}$ not representable with 1 hidden layer:



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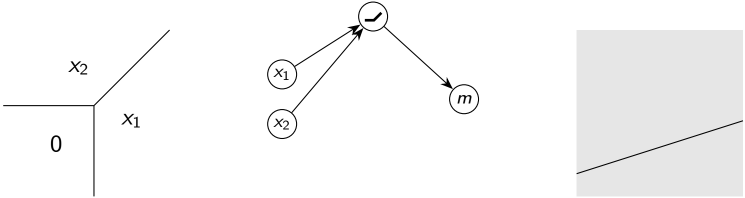

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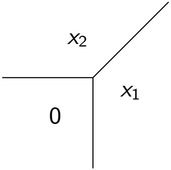

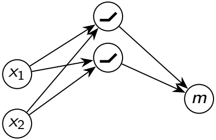

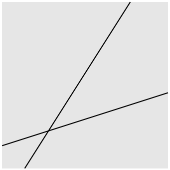

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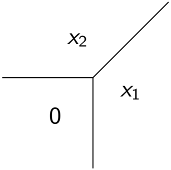

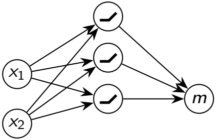

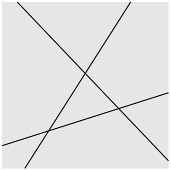

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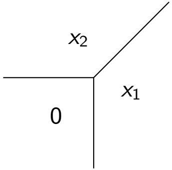

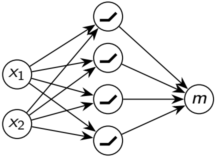

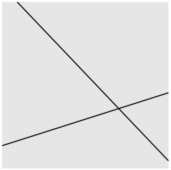

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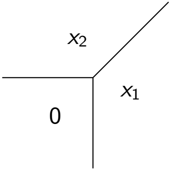

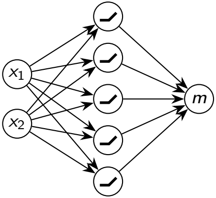

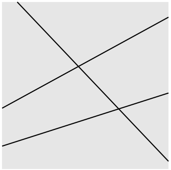

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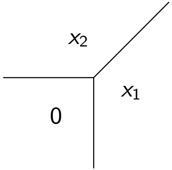

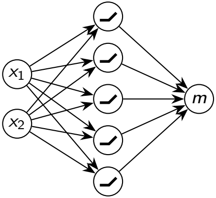

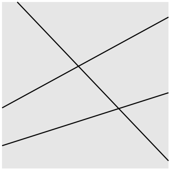

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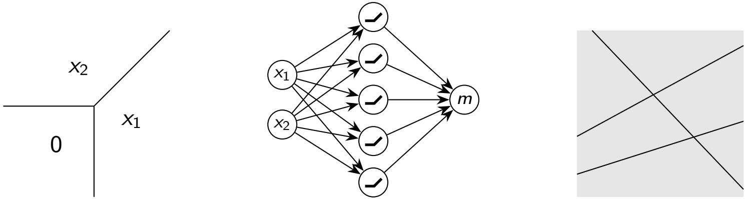

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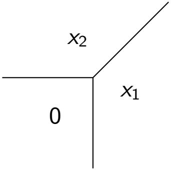

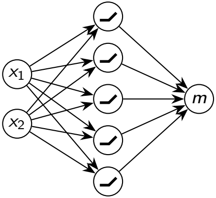

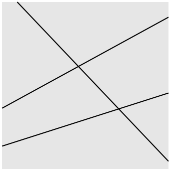

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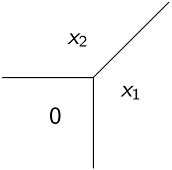

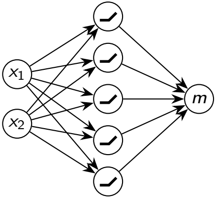

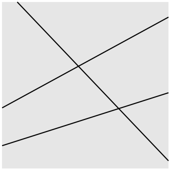

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- No function known that provably needs more than 2 hidden layers $\rightsquigarrow$ gap between 2 and $\lceil \log_2(n+1) \rceil$.
- Smallest candidate: $\max\{0, x_1, x_2, x_3, x_4\}$.

Our Results

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  2 hidden layers not enough for $\max\{0, x_1, x_2, x_3, x_4\}$ *under an additional assumption on the network*.

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The Assumption

If ... there is a 2-hidden-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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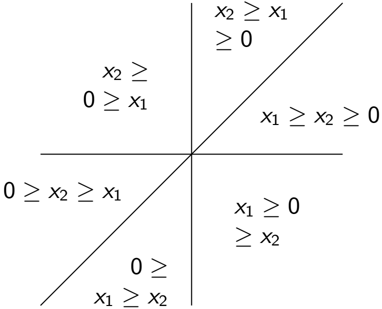
Example for $\max\{0, x_1, x_2\}$:



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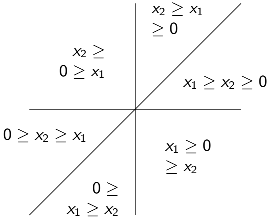

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- ... divide the input space into $5! = 120$ simplicial cones.

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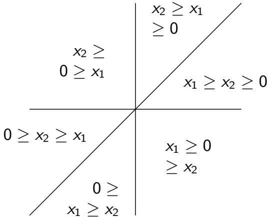

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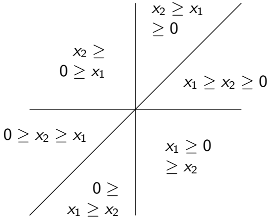

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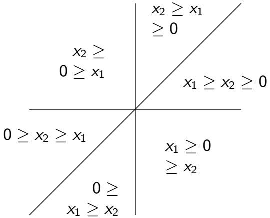

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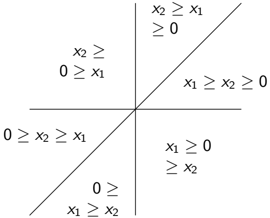

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- Within each cone everything is linear.
- 30 extreme rays in total.

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

Basic Linear Algebra Shows ...

- ... 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!

Theorem

A neural network satisfying our assumption needs 3 hidden layers to compute $\max\{0, x_1, x_2, x_3, x_4\}$.

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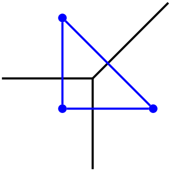
$\rightsquigarrow$ study **Newton polytopes**!

Newton Polytope of a Convex CPWL Function

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

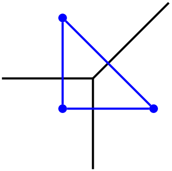
Example for $\max\{0, x_1, x_2\}$:



Newton Polytope of a Convex CPWL Function

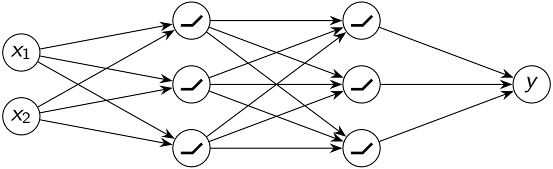
- $f(x) = \max\{a_1^T x, \ldots, a_k^T x\} \quad \rightsquigarrow \quad P(f) = \mathrm{conv}\{a_1, \ldots, a_k\}$
- dual to underlying polyhedral complex of the CPWL function

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



Convex CPWL functions	$\cong$	**Newton Polytopes**
(positive) scalar multiplication		scaling
addition		Minkowski sum
taking maximum		taking convex hull of union

Newton Polytopes and Neural Networks



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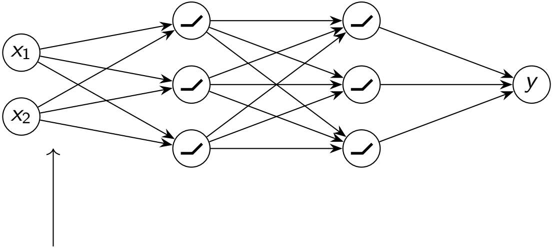
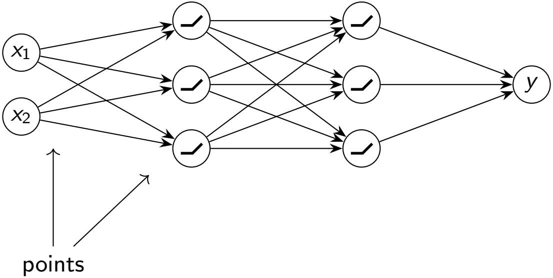


points

Newton Polytopes and Neural Networks



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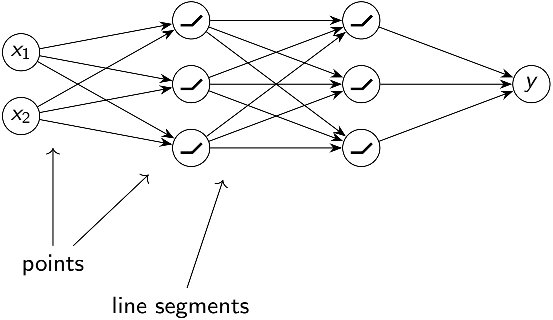

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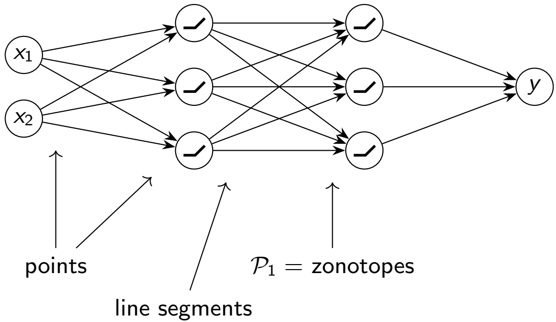

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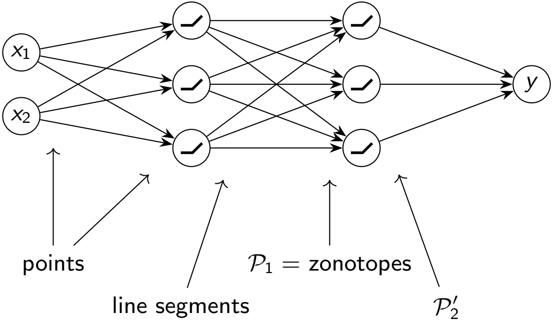

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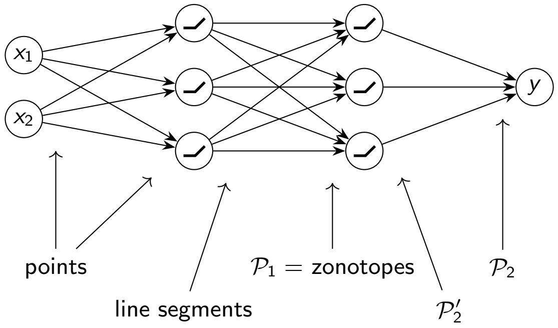

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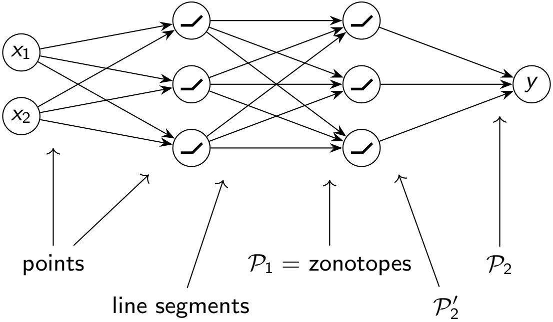

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Newton polytope of $\max\{0, x_1, x_2, x_3, x_4\}$: 4-dim. simplex Δ^4.

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

Polytopal Reformulation of our Conjecture

$$\mathcal{P}_0 := \{\text{points}\}$$

$$\mathcal{P}_1 := \{\text{zonotopes}\}$$

$$\mathcal{P}_k := \left\{ \sum_{i=1}^{m} \operatorname{conv}(P_i, Q_i) \;\middle|\; P_i, Q_i \in \mathcal{P}_{k-1}, m \in \mathbb{N} \right\}$$

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Conjecture

There is no pair of polytopes $P, Q \in \mathcal{P}_k$ such that $P + \Delta^{2^k} = Q$.

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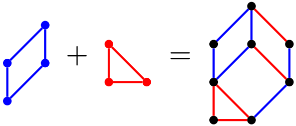

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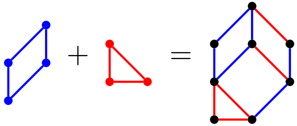

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Corollary

A neural network with integral weights needs $k + 1$ *hidden layers to compute* $\max\{0, x_1, \ldots, x_{2^k}\}$.

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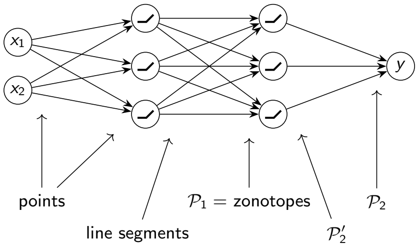

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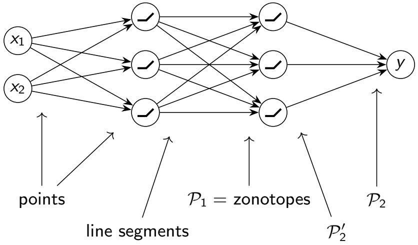

Thank you!