Expressivity and Complexity of ReLU Neural Netowrks

PhD Defense

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Technische Universität Berlin

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Motivation

AI is moving fast

- Astonishing progress in artificial intelligence
- Neural networks are at the heart of this development
- Theoretical foundations far behind success in practice

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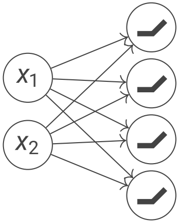
This Thesis:

- What are the fundamental capabilities and limitations of neural networks?
- Focus on ReLU neural networks

ReLU-Layer and its Geometry

ReLU-layer with d input and m output neurons given by weight matrix $\mathbf{W} \in \mathbb{R}^{m \times d}$, bias vector $\mathbf{b} \in \mathbb{R}^{m}$



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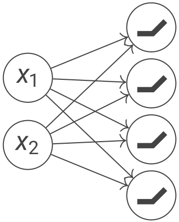

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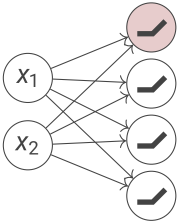

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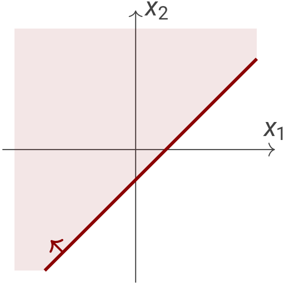
- output neuron i active at $\mathbf{x} \in \mathbb{R}^d$ if $\mathbf{w}_i^T\mathbf{x} + b_i \geq 0$



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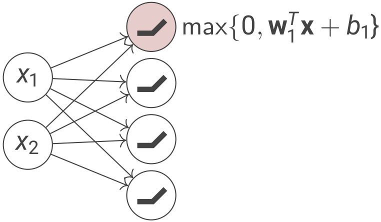

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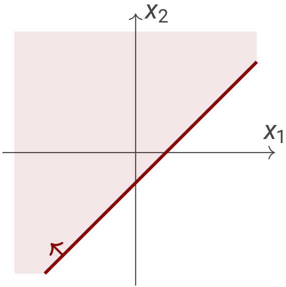

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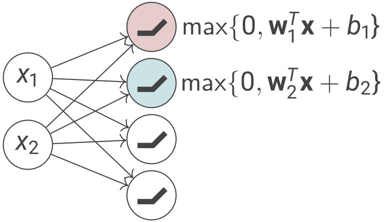

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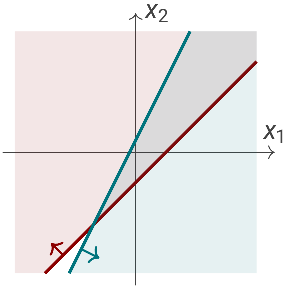

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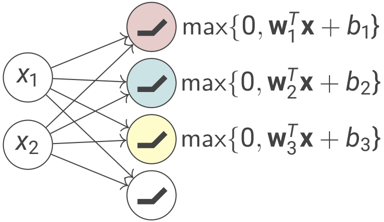

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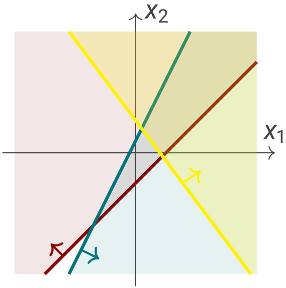

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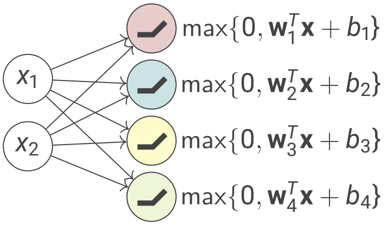

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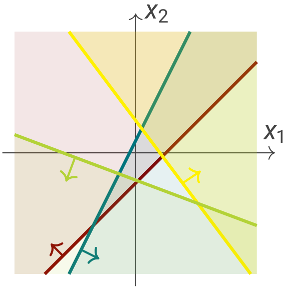

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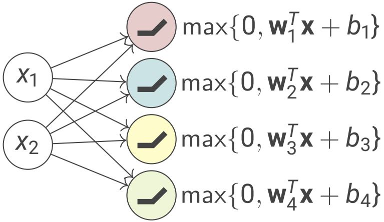

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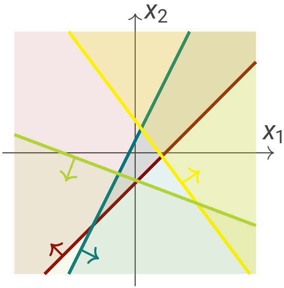
- they partition $\mathbb{R}^d$ into polyhedral cells, corresponding to subsets of active neurons



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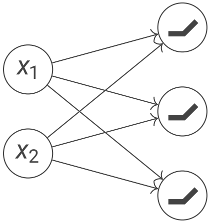

$f^{(1)}$

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$$f = f^{(\ell+1)} \circ f^{(\ell)} \circ \cdots \circ f^{(1)}$$

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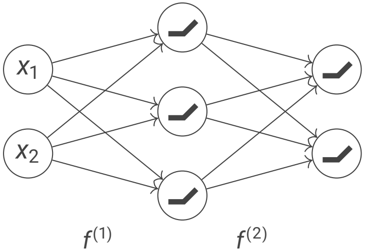

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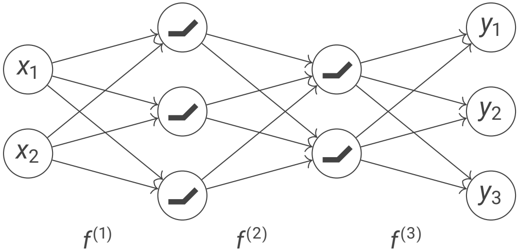

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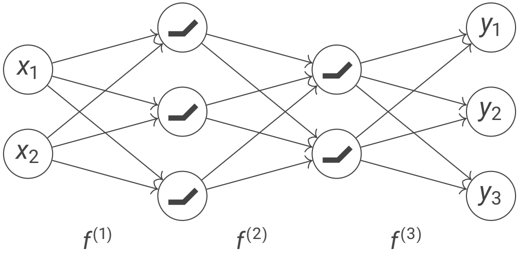

Architecture

- 2 hidden layers
- depth 3
- width 3
- size 5

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Machine learning:

- A neural network is a parameterized function $f_\theta : \mathbb{R}^d \to \mathbb{R}^m$ with $\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \dots, \mathbf{W}^{(\ell)}, \mathbf{b}^{(\ell)})$

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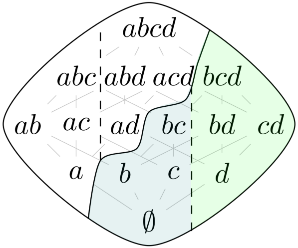
2. Given θ, what can we say about the properties of f_θ? $\to$ Verification

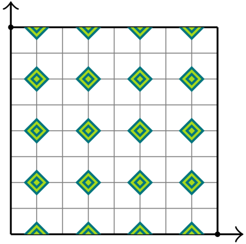
Expressivity

Representing CPWL functions



Based on *Depth-Bounds via the Braid Arrangement* with Christoph Hertrich and Georg Loho

Topological Expressivity



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Representing CPWL Functions

Theorem [Arora, Basu, Mianjy, Mukherjee, 2018]
Every CPWL function $f : \mathbb{R}^d \to \mathbb{R}$ can be represented by a ReLU NN with $\lceil \log_2(d+1) \rceil$ hidden layers.

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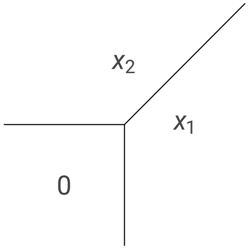
- $\max\{0, x_1, \ldots, x_4\}$ can be represented with 2 hidden layers
  $\rightarrow$ Upper bound improved to $\approx \log_3(d)$ hidden layers.
  [Bakaev, Brunck, Hertrich, Stade, Yehudayoff, 2025]

Lower Bounds?

General lower bound

- $\max\{0, x_1, x_2\}$ cannot be represented with one hidden layer [Basu, Mukherjee, 2017]



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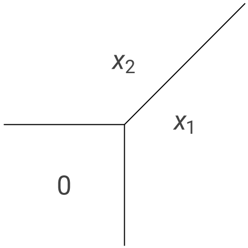

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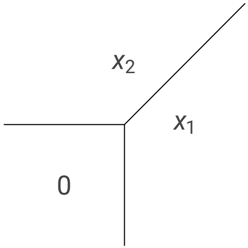

Restricting the weights

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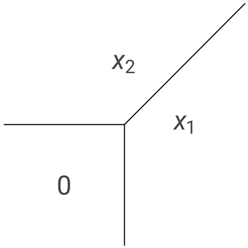

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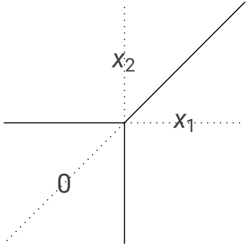

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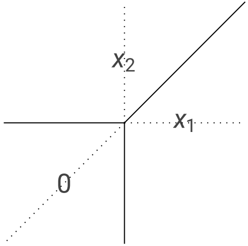

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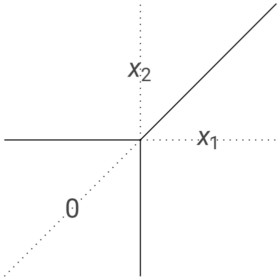
Restricting the Breakpoints

- Nice networks: All layers only have breakpoints where $x_i = x_j$
- Computational proof: $\max\{0, x_1, \ldots, x_4\}$ not representable with networks with 2 hidden layers [HBDS21].

Lower Bound for Nice Networks

Theorem [G., Hertrich, Loho, 25]

Nice networks cannot compute $\max\{0, x_1, \ldots, x_d\}$ with $\lceil \log_2 \log_2(d+1) \rceil - 1$ hidden layers.



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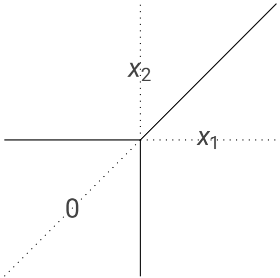

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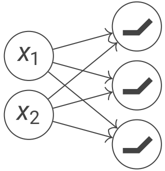

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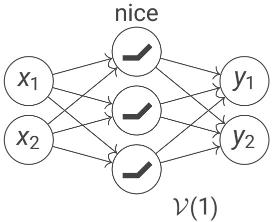

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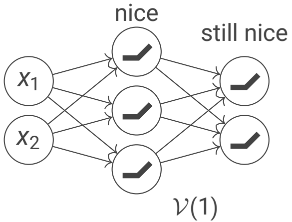

Lower Bound for Nice Networks

Theorem [G., Hertrich, Loho, 25]

Nice networks cannot compute $\max\{0, x_1, \ldots, x_d\}$ with $\lceil \log_2 \log_2(d+1) \rceil - 1$ hidden layers.

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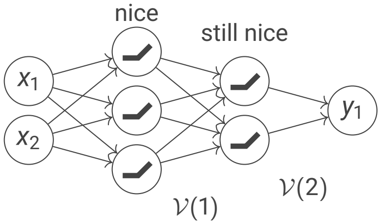

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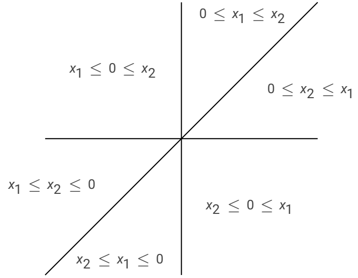

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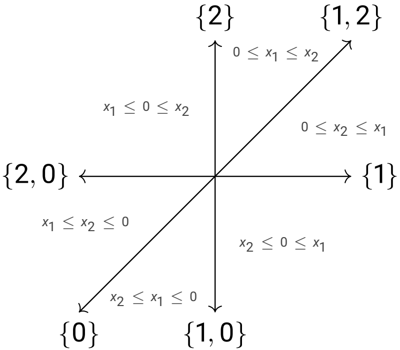

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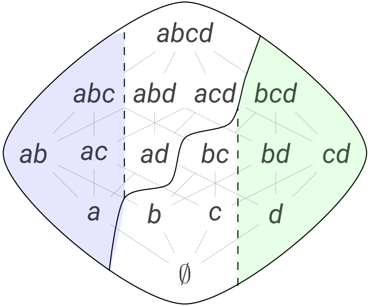

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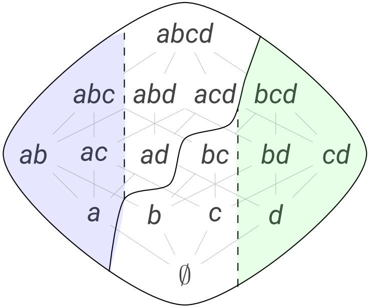

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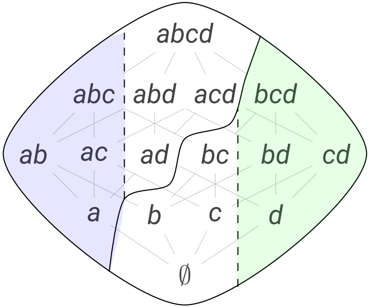

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Open Questions:

- How many layers are necessary to compute all CPWL functions?
- Is there a function that needs more than 2 hidden layers?

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- Given $\{(\mathbf{x}_i, y_i)\}_{i \in I}$ with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$

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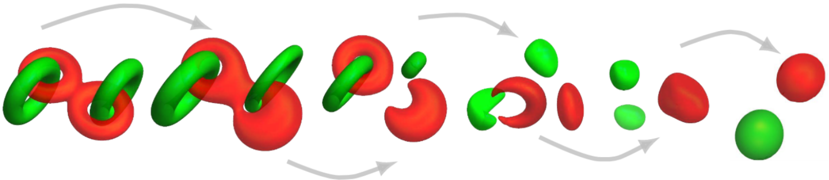

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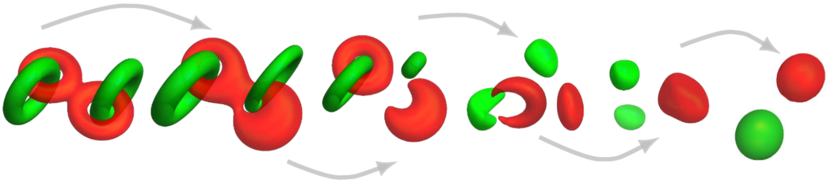

Question:
Given an architecture, how topologically complex can the decision regions $f^{-1}((-\infty, 0])$ become?

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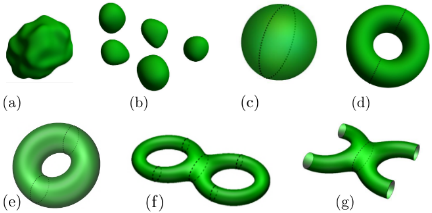

	Manifold $M \subseteq \mathbb{R}^3$	$\beta(M)$
(a)	Single contractible manifold	$(1, 0, 0)$
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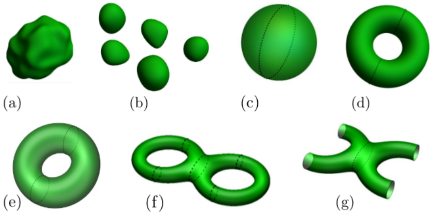

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- Topological expressivity of neural network f measured by $\beta_k(f^{-1}((-\infty, 0])$

Topological Expressivity

Theorem[Ergen, G., 24]

For any depth and width, there is a neural network f such that for all $k = 0, \ldots, d-1$ holds

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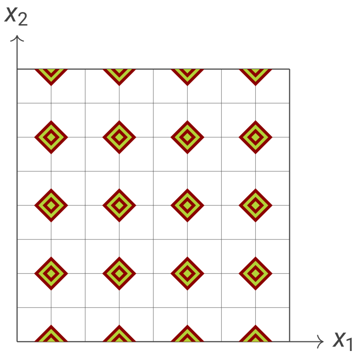

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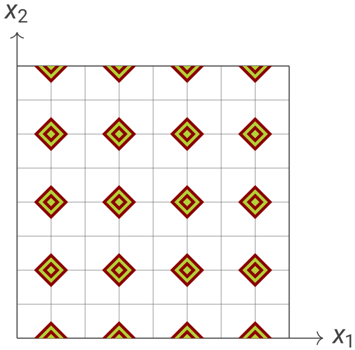

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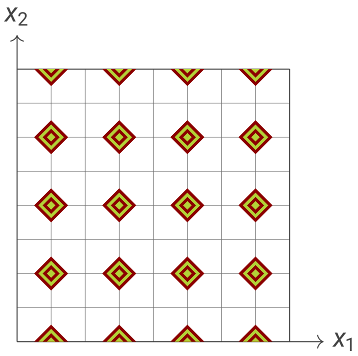

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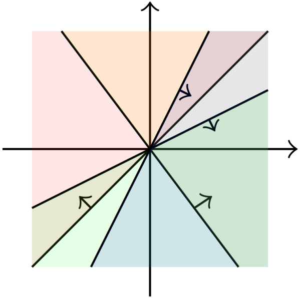
Conclusion

Deep neural networks are better equipped to model topological complex data sets.

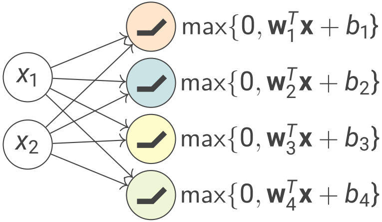
Verification

Complexity of Injectivity and Verification



Based on *Complexity of Injectivity and Verification of ReLU Neural Networks* with Vincent Froese and Martin Skutella

ReLU-Layer: Injectivity



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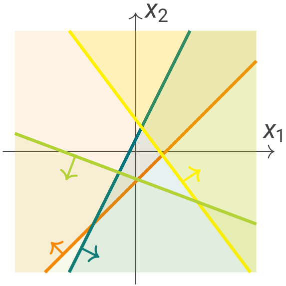

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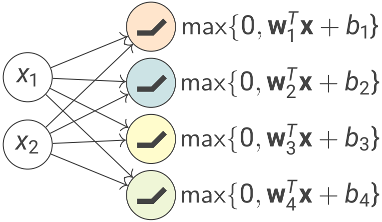

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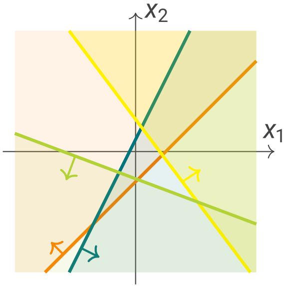

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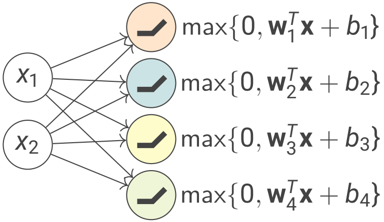

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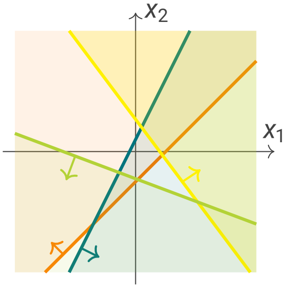

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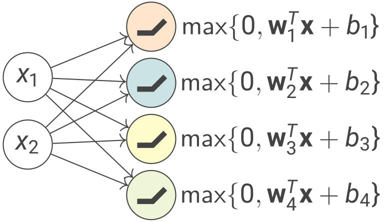

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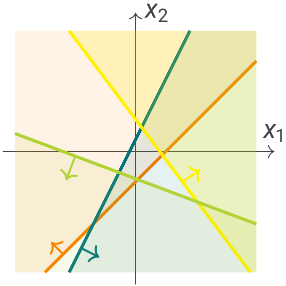

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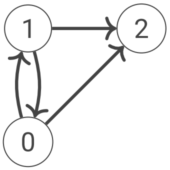

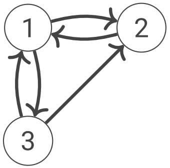

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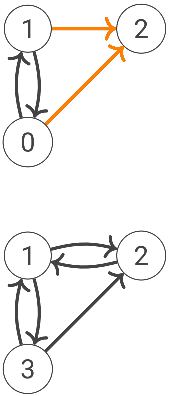

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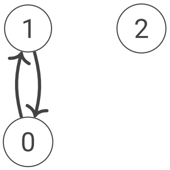

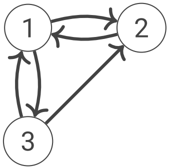

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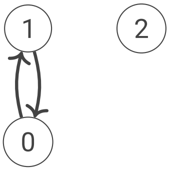

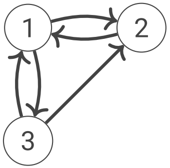

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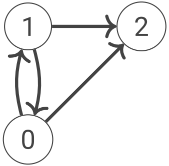

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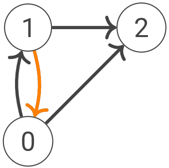

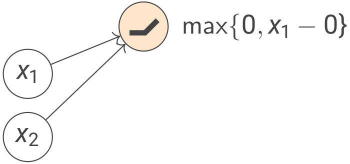

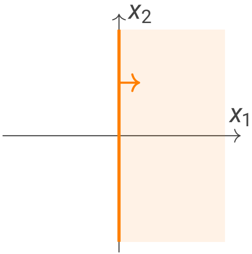

ReLU Layer from Digraph

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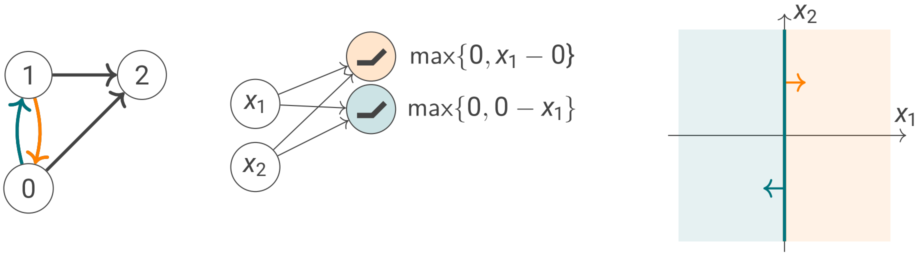

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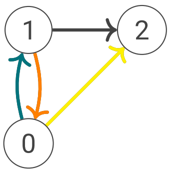

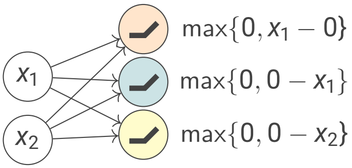

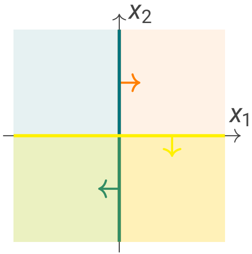

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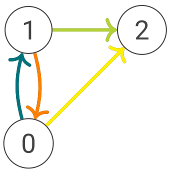

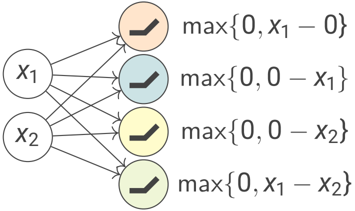

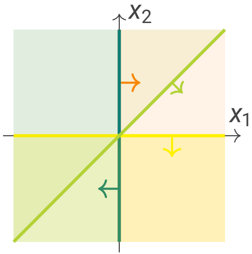

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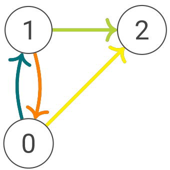

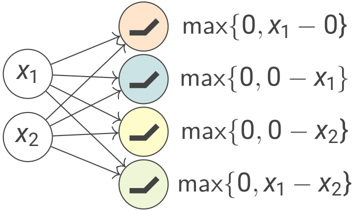

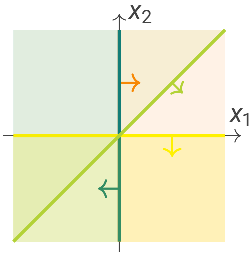

- All hyperplanes are of the form $\{x_i = x_j\}$ for $i, j \in [d]_0$

Full Rank $=$ Weakly Connected

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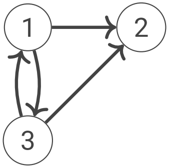

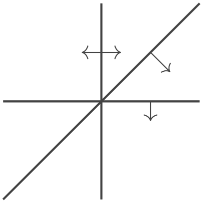

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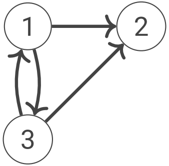

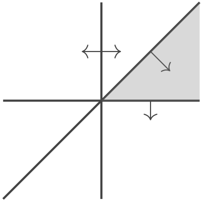

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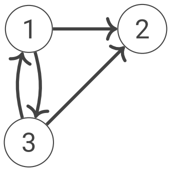

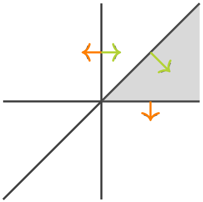

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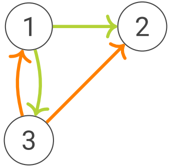

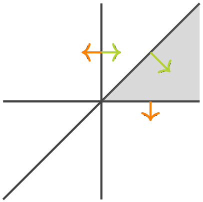

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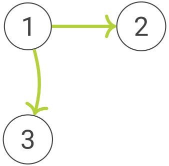

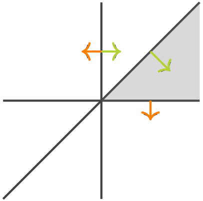

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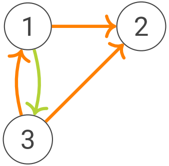

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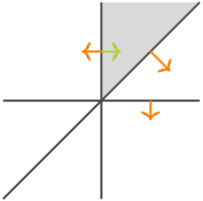

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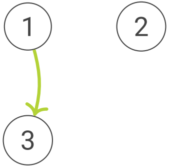

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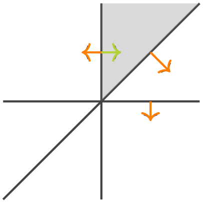

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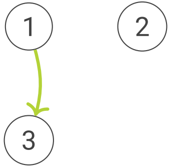

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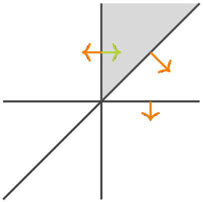

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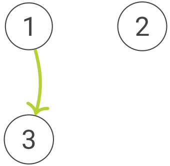

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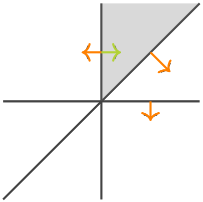

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Theorem [Froese, G., Skutella. 2024]

ReLU-Layer Injectivity can be solved in $O\big(\mathrm{poly}(m)(d+1)^d\big)$ time (i.e., FPT for dimension d).

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Theorem [Froese, G., Skutella. 2024]

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