Understanding Neural Network Expressivity via Polyhedral Geometry

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joint works with

Amitabh Basu, Marco Di Summa, Martin Skutella (NeurIPS 2021)
Christian Haase, Georg Loho (ICLR 2023)

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A Single ReLU Neuron

Rectified linear unit (ReLU): $\text{relu}(x) = \max\{0, \sum_{i=1}^{\ell} w_i x_i\}$
A Single ReLU Neuron

Outputs of previous neurons

\[ \text{max}\{0, \sum_{i=1}^{\ell} w_i x_i\} \]

Rectified linear unit (ReLU): \( \text{relu}(x) = \max\{0, x\} \)
A Single ReLU Neuron
ReLU Feedforward Neural Networks

- Acyclic (layered) digraph of ReLU neurons

\[
\begin{align*}
T_3 &\circ \text{relu} \circ T_2 \circ \text{relu} \circ T_1
\end{align*}
\]

Computes function $T_k \circ \text{relu} \circ T_{k-1} \circ \cdots \circ T_2 \circ \text{relu} \circ T_1$ with linear transformations $T_i$.

Example: depth 3 (2 hidden layers).
ReLU Feedforward Neural Networks

- Acyclic (layered) digraph of ReLU neurons

Computes function

\[ T_k \circ \text{relu} \circ T_{k-1} \circ \cdots \circ T_2 \circ \text{relu} \circ T_1 \]

with linear transformations \( T_i \).
ReLU Feedforward Neural Networks

- Acyclic (layered) digraph of ReLU neurons

![Diagram of a ReLU feedforward neural network with inputs $x_1$, $x_2$, outputs $y_1$, $y_2$, $y_3$, and layers $T_1$, $T_2$, $T_3$.]

- Computes function

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

with linear transformations $T_i$.

- 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

$$\max\{x, y\} = \max\{x - y, 0\} + y$$
Example: Computing the Maximum of Two Numbers

$$\max\{x, y\} = \max\{x - y, 0\} + y$$
Example: Computing the Maximum of Four Numbers

\[
\begin{align*}
\text{\texttt{m}} & \quad 1 \quad 1 \\
\text{\texttt{x}_1} & \quad -1 \quad 1 \\
\text{\texttt{x}_2} & \quad 1 \quad 1 \\
\text{\texttt{x}_3} & \quad 1 \quad 1 \\
\text{\texttt{x}_4} & \quad -1 \quad -1 \\
\end{align*}
\]
Example: Computing the Maximum of Four Numbers

\[ m = \max(x_1, x_2, x_3, x_4) \]

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 $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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.
Theorem (Arora, Basu, Mianjy, Mukherjee [ABMM18])

Every CPWL function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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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Yes, there are functions which need $\lceil \log_2(n + 1) \rceil$ hidden layers!

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.
What is known?

Mukherjee, Basu (2017):

\[
\max \{0, x_1, x_2, x_3, x_4\}
\]

That's all!

No function known that provably needs more than 2 hidden layers ⇛ gap between 2 and \(\lceil \log_2 (n+1) \rceil\).

Smallest candidate: \(\max \{0, x_1, x_2, x_3, x_4\}\).
What is known?

- Mukherjee, Basu (2017): \( \max\{0, x_1, x_2\} \) not representable with 1 hidden layer:

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\begin{align*}
\text{max}\{0, x_1, x_2\} & \text{ not representable with 1 hidden layer:} \\
\end{align*}
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- Smallest candidate: \[ \max\{0, x_1, x_2, x_3, x_4\}. \]
Our Results

- Hertrich, Basu, Di Summa, Skutella (NeurIPS 2021):
  2 hidden layers not enough for \( \max\{0, x_1, x_2, x_3, x_4\} \)
  
  \textit{under an additional assumption on the network.}
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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.*

- Haase, Hertrich, Loho (ICLR 2023):
  Depth $O(\log n)$ tight for networks with only integer weights.
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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 $0, x_1, \ldots, x_4$ changes.
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Example for $\max\{0, x_1, x_2\}$:
The Assumption

Example for \( \max\{0, x_1, x_2\} \):

\[
0 \geq x_2 \geq x_1 \\
x_1 \geq 0 \\
x_2 \geq x_1 \geq 0 \\
x_1 \geq x_2 \geq 0
\]

\( \binom{5}{2} = 10 \) hyperplanes ...

... divide the input space into \( 5! = 120 \) simplicial cones.
The Assumption

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- ... divide the input space into \( 5! = 120 \) simplicial cones.
- Each cone spanned by 4 extreme rays.
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\]

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x_2 \geq 0 \geq x_1 \\
x_1 \geq x_2 \geq 0
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\binom{5}{2} = 10 \text{ hyperplanes} \ldots
\]

\[
\ldots \text{ divide the input space into } 5! = 120 \text{ simplicial cones.}
\]

\[
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\[
\text{Within each cone everything is linear.}
\]
The Assumption

Example for \( \max\{0, x_1, x_2\} \):

\[
\begin{array}{c}
x_2 \geq x_1 \\
0 \geq x_1 \\
0 \geq x_2 \\
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\]

\( \binom{5}{2} = 10 \) hyperplanes...

... divide the input space into \( 5! = 120 \) simplicial cones.

Each cone spanned by 4 extreme rays.

Within each cone everything is linear.

30 extreme rays in total.
The Assumption

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

- $(\binom{5}{2}) = 10$ hyperplanes ...
- ... divide the input space into $5! = 120$ simplicial cones.
- Each cone spanned by 4 extreme rays.
- 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.

... after 2 hidden layers:

\[ \max \{0, x_1, x_2, x_3, x_4\} \]

is not contained in the 29-dimensional subspace!
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$$\max\{0, x_1, x_2, x_3, x_4\}$$

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Can we leave the 29-dimensional subspace?
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Mixed-Integer Linear Program to model a neuron in 2nd layer:
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Mixed-Integer Linear Program to model a neuron in 2nd layer:

- $14 + 30 = 44$ continuous variables
- 30 binary variables
- A few hundred constraints
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- objective orthogonal to 29-dim. subspace

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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⇒ Solver (with exact arithmetic): Objective value zero
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Newton Polytope of a Convex CPWL Function

\[ f(x) = \max \{ a_1^T x, \ldots, a_k^T x \} \quad \leadsto \quad P(f) = \text{conv} \{ a_1, \ldots, a_k \} \]

- dual to underlying polyhedral complex of the CPWL function

Example for \( \max \{0, x_1, x_2\} \):

\[
\begin{align*}
& x_2 \\
& 0 \quad x_1 \\
& \leadsto
\end{align*}
\]
Newton Polytope of a Convex CPWL Function

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

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

\[ 0 \quad x_1 \quad x_2 \leadsto \]

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

\(x_1\)

\(x_2\)

\(y\)
Newton Polytopes and Neural Networks

\[ P_0 = \text{points} \]
Newton Polytopes and Neural Networks

\[ P_0 = \text{points} \]

\[ P_1 = \text{zonotopes} \]

\[ P_k := \{ \sum_{i=1}^{m} \text{conv}(P_i, Q_i) \mid P_i, Q_i \in P_{k-1} \} \]
Newton Polytopes and Neural Networks

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Newton Polytopes and Neural Networks

\[ \mathcal{P}_0 = \text{points} \]
\[ \mathcal{P}_1 = \text{zonotopes} \]
\[ \mathcal{P}_2 \]

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Results for the Integer Case

**Theorem**

*With only integer weights, \( k \) hidden layers are not enough to compute \( \max\{0, x_1, \ldots, x_{2^k}\} \).*
Results for the Integer Case

**Theorem**

*With only integer weights, k hidden layers are not enough to compute* \( \max\{0, x_1, \ldots, x_{2^k}\} \).

- Use tropical geometry to represent NNs as lattice polytopes.

**Example for** \( \max\{0, x_1, x_2\} \):

\[
\begin{align*}
\text{0} & \quad \text{x}_1 & \quad \text{x}_2 \\
0 & \quad 0 & \quad 0
\end{align*}
\]

\( \mapsto \)

\[
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\text{0} & \quad \text{x}_1 & \quad \text{x}_2 \\
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Results for the Integer Case

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Example for \( \max\{0, x_1, x_2\} \):

- Subdivide polytopes “layer by layer” into “easier” polytopes.
Theorem

With only integer weights, $k$ hidden layers are not enough to compute $\max\{0, x_1, \ldots, x_{2k}\}$.

- Use tropical geometry to represent NNs as lattice polytopes.

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

- Subdivide polytopes “layer by layer” into “easier” polytopes.

- Separate via parity of the normalized volume.
What’s Next?

- Hertrich, Basu, Di Summa, Skutella (NeurIPS 2021):
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  under an additional assumption on the network.
  - Getting rid of assumption.
  - Getting rid of MIP.
  - Sharpen MIP to tackle 3-hidden-layer case.

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  - For general case: Polytopes and subdivisions seem promising.
  - Replace volume argument by different separation.
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