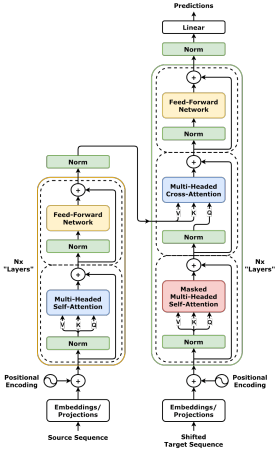
RWTH AACHEN UNIVERSITY

Query Languages for Machine-Learning Models

Martin Grohe
joint work with Christoph Standke, Juno Steegmans, Jan Van den Bussche

Understanding ML Models



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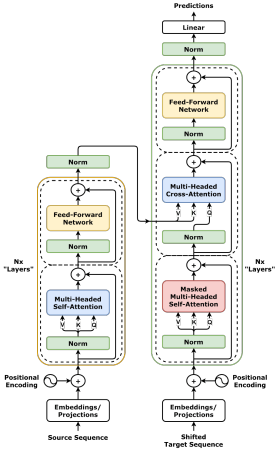

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- Prove that the model computes the correct function.

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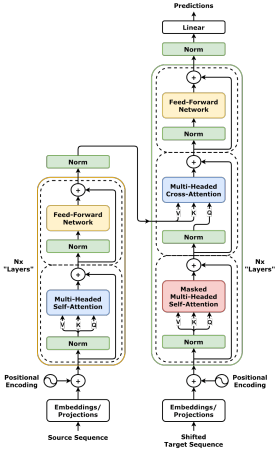

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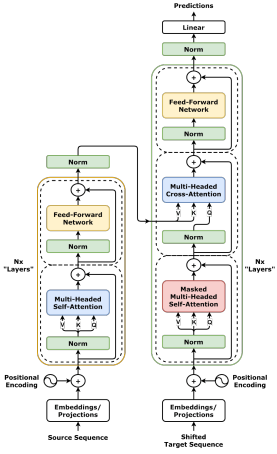

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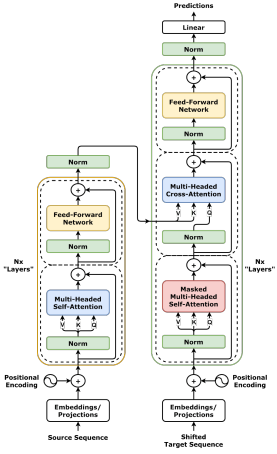

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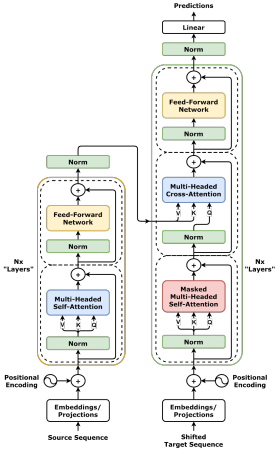

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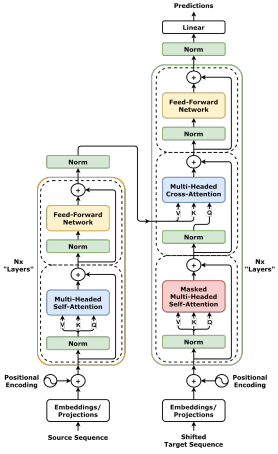

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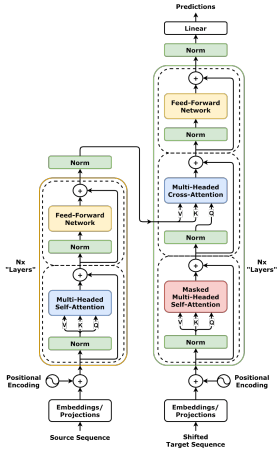
For an excellent critique of current XAI practices, see:

T. Freiesleben and G. König. Dear XAI community, we need to talk! Fundamental misconceptions in current XAI research. Proc. World conference on explainable artificial intelligence, Springer 2023.

Querying ML Models



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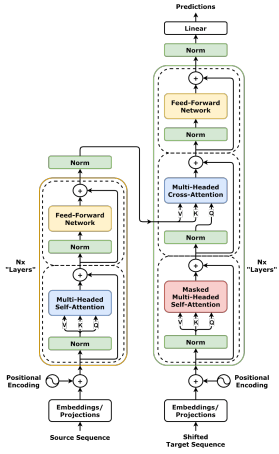

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Most ML Verification and XAI tasks can be viewed as querying a model (a.k.a. model checking).

We may either ask specific fixed queries or interact with the model in an adaptive query-answer process.

Examples

Suppose our model $\mathcal{M}$ computes a function $f_{\mathcal{M}} : \mathbb{R}^2 \to \mathbb{R}$ controlling the brake intensity of a car based on velocity and distance to an obstruction.

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What is the maximum value $f_{\mathcal{M}}$ can take?

$$\max_{v,d} f_{\mathcal{M}}(v, d).$$

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Is it true that $f_{\mathcal{M}}$ is always nonnegative?

$$\forall v, d \; f_{\mathcal{M}}(v, d) \geq 0.$$

Examples

Suppose our model $\mathcal{M}$ computes a function $f_{\mathcal{M}} : \mathbb{R}^2 \to \mathbb{R}$ controlling the brake intensity of a car based on velocity and distance to an obstruction.

Queries

Is it true that if the velocity is ≥ 1 *and the distance is* ≤ 10 *then the brake intensity is maximal?*

$$\forall v, d \big(v \geq 1 \wedge d \leq 10 \to f_{\mathcal{M}}(v, d) = \max_{v', d'} f_{\mathcal{M}}(v', d') \big).$$

This is an example of a safety query.

Examples

Suppose our model $\mathcal{M}$ computes a function $f_{\mathcal{M}} : \mathbb{R}^2 \to \mathbb{R}$ controlling the brake intensity of a car based on velocity and distance to an obstruction.

Queries

Is it possible not to brake at all?

$$\exists v, d \; f_{\mathcal{M}}(v, d) = 0.$$

This is an example of a liveness query.

Examples

Suppose our model $\mathcal{M}$ computes a function $f_{\mathcal{M}} : \mathbb{R}^2 \to \mathbb{R}$ controlling the brake intensity of a car based on velocity and distance to an obstruction.

Queries

How much can small changes (of at most ϵ) of the input affect the output?

$$\max_{\delta} \forall v, v', d, d' \big(|v - v'| \leq \epsilon \wedge |d - d'| \leq \epsilon \to |f_{\mathcal{M}}(v, d) - f_{\mathcal{M}}(v', d')| \leq \delta \big).$$

This is an example of a robustness query.

Examples

Suppose our model $\mathcal{M}$ computes a function $f_{\mathcal{M}} : \mathbb{R}^2 \to \mathbb{R}$ controlling the brake intensity of a car based on velocity and distance to an obstruction.

Queries

Does the velocity have a noticeable effect on the brake intensity?

$$\exists v, v', d \; |f_{\mathcal{M}}(v, d) - f_{\mathcal{M}}(v', d)| > \epsilon.$$

This is a typical explainability query trying to figure out the importance of the input features.

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Are there parameters that have no noticeable effect on the output?

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Which are the most important parameters if the velocity is greater than 10*?*

Here we are querying the inner workings of the model and not only the function it computes.

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A query φ is model agnostic (over a class $\mathbf{M}$ of models) if its answer only depends on the function computed by the model, that is,

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Model agnostic: How much can small changes (of at most ϵ) of the input affect the output?

Not model agnostic: Does the model have $\leq 100,000$ parameters?

Model agnostic: Is there a model computing the same function with at most 100,000 parameters?

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Remark

"Black box" is a syntactic property, whereas "model agnostic" is a semantic one.

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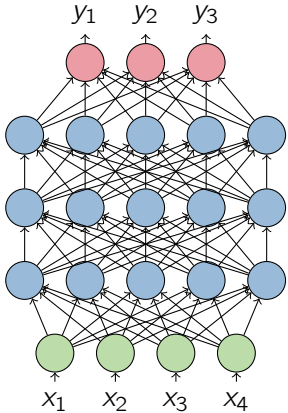
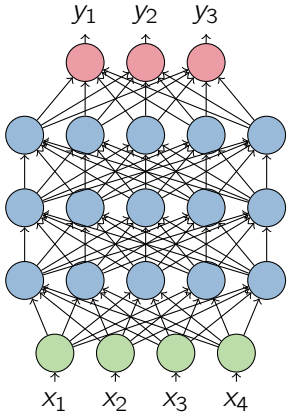
- A particular focus is the trade-off between expressiveness and the complexity of query evaluation.
- The foundation of our approach is Grädel and Gurevich's meta-finite model theory (1998).

Feedforward Neural Networks (FNNs)





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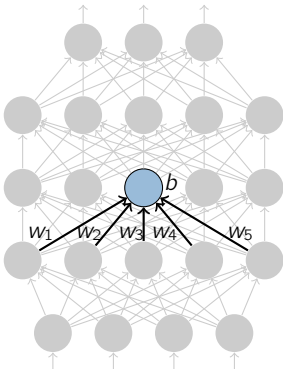

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- Node with bias $b \in \mathbb{R}$ and incoming edges with weights $w_1, \ldots, w_k \in \mathbb{R}$ computes function

$$x_1, \ldots, x_k \mapsto \sigma\left(b + \sum_{i=1}^{k} w_i x_i\right),$$

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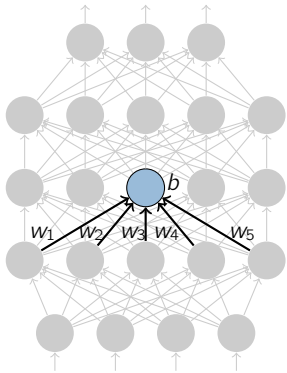

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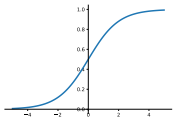
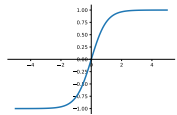
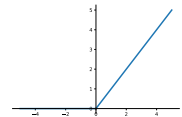
Typical activation functions are:



sigmoid



hyperbolic tangent



rectified linear unit (ReLU)

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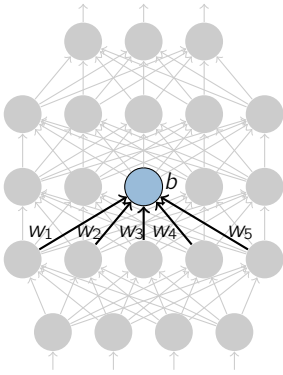

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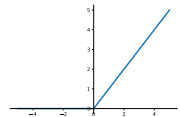
In this talk, we always use $\mathrm{ReLU} : x \mapsto \max\{0, x\}$ as activation function for the internal nodes ("hidden layers") and $\mathrm{id} : x \mapsto x$ for the output nodes.



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- $\mathrm{wt}, \mathrm{bias}$ are binary resp. unary symbols interpreted by the weights of the edges and biases of the nodes,
- $\leq_{\mathrm{in}}, \leq_{\mathrm{out}}$ are binary relation symbols interpreted by linear orders on the input nodes and on the output nodes, respectively.

Weight Aggregation Logics

The Basic Logic: FO(SUM)

We define first-order logic with weight aggregation FO(SUM).

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Syntax

Formulas φ and terms θ formed by the following grammar:

$$\varphi ::= x = y \mid R(x_1, \ldots, x_k) \mid \theta \leq \theta \mid \neg\varphi \mid (\varphi * \varphi) \mid Qx\varphi$$

$$\theta ::= 0 \mid 1 \mid F(x_1, \ldots, x_k) \mid (\theta \circ \theta) \mid \text{if } \varphi \text{ then } \theta \text{ else } \theta \mid \sum_{(x_1,\ldots,x_k):\varphi} \theta.$$

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k-ary relation symbol

$\in \{\vee, \wedge, \rightarrow\}$

x, y, x_i variables

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k-ary weight function symbol

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Semantics

Let $\mathcal{A}$ be a structure and $a_1, \ldots, a_k \in A$.

- Variables range over A (*not* $\mathbb{R}$).

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Semantics

Let $\mathcal{A}$ be a structure and $a_1, \ldots, a_k \in A$.

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We define first-order logic with weight aggregation FO(SUM).

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Both are straightforward inductive definitions.

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$$\text{relu}(\theta) := \text{if } \theta \geq 0 \text{ then } \theta \text{ else } 0\cdot\theta$$

defines the ReLU function.

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We can also define a closed FO(SUM)-term eval_d evaluating an FNN of output dimension 1 and depth d.

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Maximum: *Take the maximum of a term* θ *over the set defined by formula* φ.

We let $\mathsf{max}_{\mathbf{x}:\varphi}\theta \coloneqq \mathsf{avg}_{\mathbf{x}:\varphi_{\mathsf{max}}}\theta$, where

$$\varphi_{\mathsf{max}} \coloneqq \varphi(\mathbf{x}) \wedge \forall \mathbf{x}'\big(\varphi(\mathbf{x}') \to \theta(\mathbf{x}') \leq \theta(\mathbf{x})\big).$$

Example: Integration

Theorem (G., Standke, Steegmans, Van den Bussche 2025)

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Remark

Here we choose integration boundaries $0, 1$ for all variables, but the result can be extended to arbitrary boundaries (passed via unary weight functions to the FNN).

Integration (cont'd)

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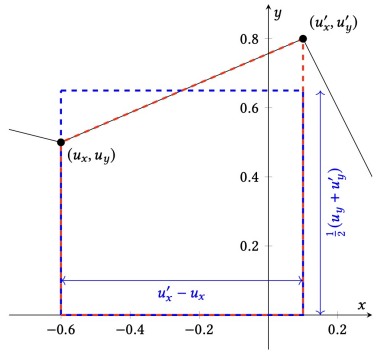
- We can associate the breakpoints of the piecewise linear unary function with nodes of the FNN and use FO(SUM)-terms to compute the coordinates of the breakpoints.
- Then we define the integrals over the linear pieces and use summation to combine them.



Model-Agnostic Queries in FO(SUM)

Recall

An FO(SUM) expression ξ (term or formula) is model agnostic over a class $\mathbf{N}$ of FNNs if for all $\mathcal{N}, \mathcal{N}' \in \mathbf{N}$ it holds that

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For all d, m, the term $\text{integrate}_{d,m}$ is model-agnostic over $\mathbf{N}_d(m, 1)$.

Example (Evaluation)

For all d, m, the term eval_d is model agnostic over the class of all $\mathcal{N}(\mathbf{r})$, where $\mathcal{N} \in \mathbf{N}_d(m, 1)$ and $\mathbf{r} \in \mathbb{R}^m$.

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FNN queries: For every $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f^{(m)})$ sentence φ and every FNN $\mathcal{N} \in \mathbf{N}(m, 1)$ we define a Boolean value $[\![\varphi]\!]^{\mathcal{N}} \in \{0, 1\}$ by

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Observation

All FNN queries defined in $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f^{(m)})$ *are model agnostic.*

The zero query

Let Zero_m be the query saying that an FNN $\mathcal{N} \in \mathbf{N}(m, 1)$ computes the constant-0 function. The $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f^{(m)})$ sentence $\forall x_1 \ldots \forall x_m \; f^{(m)}(x_1, \ldots, x_m) = 0.$ defines Zero_m.

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Irrelevant features

For $1 \leq i \leq m$ and rational $\epsilon > 0$, let $\mathrm{Irrelevant}_{m,i,\epsilon}$ be the query saying that the ith input feature of an FNN $\mathcal{N} \in \mathbf{N}(m, 1)$ is ϵ-irrelevant, that is, for all $r_1, \ldots, r_m, r_i' \in \mathbb{R}$ it holds that

$$|f^{\mathcal{N}}(r_1, \ldots, r_m) - f^{\mathcal{N}}(r_1, \ldots, r_{i-1}, r_i', r_{i+1}, \ldots, r_m)| \leq \epsilon.$$

The query can easily be expressed in $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f^{(m)})$.

Examples (cont'd)

Robustness

For $m \in \mathbb{N}$ and rational $\epsilon, \delta >$, let $\text{Robust}_{m,\epsilon,\delta}$ be the query saying that an FNN $\mathcal{N} \in \mathbf{N}(m, 1)$ is ϵ, δ robust, that is, changing the input features by at most ϵ changes the output by at most δ.

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$\text{Robust}_{m,\epsilon,\delta}$ can be expressed in $\text{FO}(\mathcal{R}_{\text{lin}}, f^{(m)})$:

$$\forall x_1 \ldots \forall x_m \forall y_1 \ldots \forall y_m \left(\bigwedge_{i=1}^{m} |x_1 - y_i| \leq \epsilon \rightarrow \left| f^{(m)}(x_1, \ldots, x_m) - f^{(m)}(y_1, \ldots, y_m) \right| \leq \delta \right).$$

Black Box vs White Box (I)

Corollary

The queries Zero_m, $\mathsf{Irrelevant}_{m,i,\epsilon}$, *and* $\mathsf{Robust}_{m,\epsilon,\delta}$ *are not expressible in* FO(SUM), *because they are nontrivial model-agnostic queries.*

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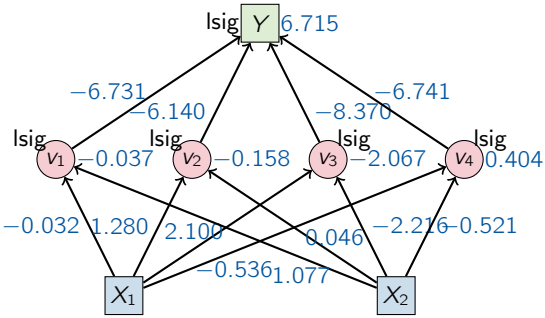
Theorem (G., Standke, Steegmans, Van den Bussche 2025)

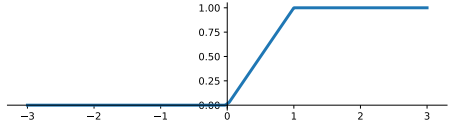
Let $d, m \in \mathbb{N}$. *Then every query on* $\mathbf{N}_d(m, 1)$ *that is expressible in* $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f^{(m)})$ *is expressible in* FO(SUM).

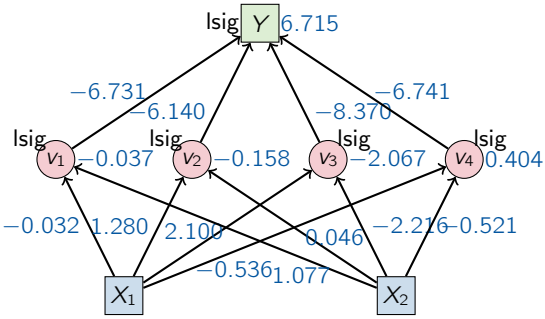
Example


lsig
Y
6.715
−6.731
−6.140
−8.370
−6.741
lsig
lsig
lsig
lsig
v1
−0.037
v2
−0.158
v3
−2.067
v4
0.404
−0.032
1.280
2.100
0.046
−2.216
−0.521
−0.536
1.077
X1
X2

Example

Uses linearised sigmoid (lsig) activations:





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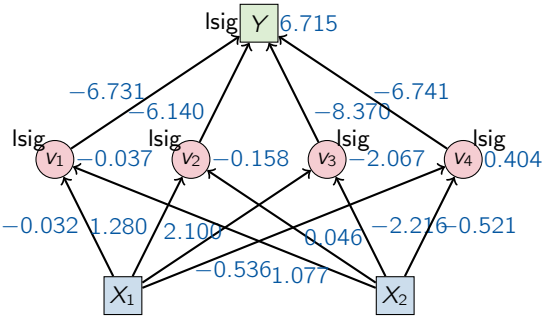

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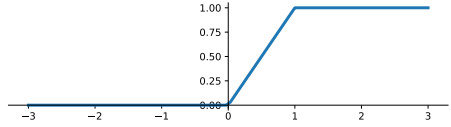
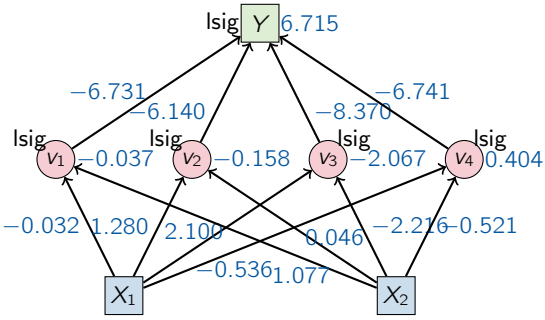
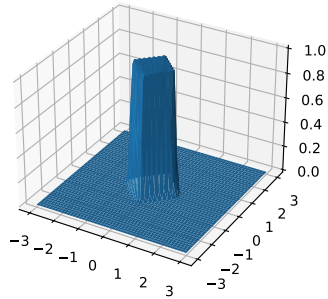


Note: $\mathsf{lsig}(x) = \mathsf{ReLU}(x) - \mathsf{ReLU}(x-1)$.

Example



Computes the (piecewise linear) function



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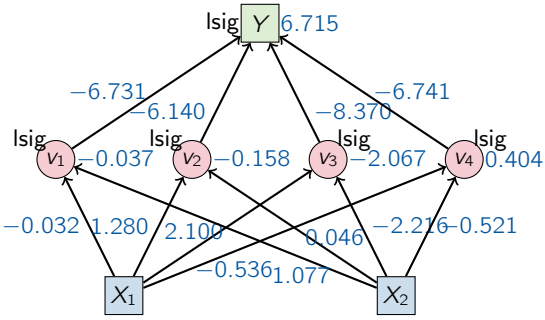
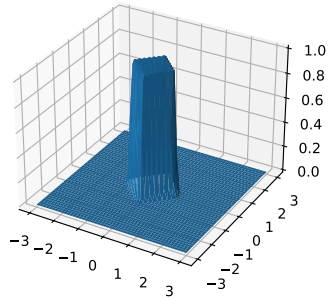


Computes the (piecewise linear) function



An FO($\mathcal{R}_{\text{lin}}, f^{(2)}$) query might be

$$\forall x \forall y \big(|x| + |y| \leq 1 \rightarrow f^{(2)}(x, y) = 1 \big).$$

Proof Idea

- The difficulty in proving the theorem is that in $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f)$ we can quantify over arbitrary real numbers, whereas in FO(SUM) we can only construct numbers from the weights of the input FNN using rational terms.

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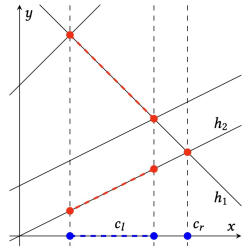

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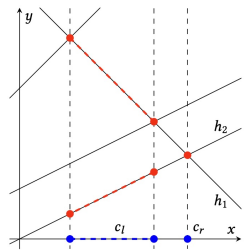

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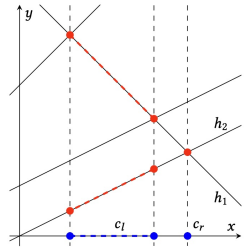

- The main part of the proof is to show that such a cell decomposition is definable in FO(SUM).
- The individual cells can be indexed by tuples of nodes of the input FNN. As nodes in each cell behave essentially in the same way, this allows us to simulate quantification over the reals by quantification over tuples of nodes.

Black Box vs White Box (II)

Theorem (G., Standke, Steegmans, Van den Bussche 2025)
The query $\int_0^1 f^{\mathcal{N}}(x)dx = 0$ *over* $\mathbf{N}_2(1,1)$ *is not expressible in* $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f)$.

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Corollary

There are model-agnostic queries of FNNs of depth 2 *that are expressible in* FO(SUM)*, but not in* $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f)$.

Beyond Bounded Depth

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- To be able to go beyond bounded depth, we extend the logic by a fixed-point operator formalising inductive definitions.

Fixed-Point Logic with Weight Aggregation (Syntax)

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The ifp-operator binds the weight-function symbol F, so if the vocabulary of θ is Υ then the vocabulary of $\mathrm{ifp}\big(F(x_1, \ldots, x_k) \leftarrow \theta\big)(x'_1, \ldots, x'_k)$ is $\Upsilon \setminus \{F\}$

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We can also define a closed IFP(SUM)-term eval evaluating an FNN of output dimension 1.

Complexity

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We can assume that $\|\mathcal{A}\|$ is polynomial in $|A|$ and the bit sizes of all weights.

Complexity of FO(SUM)

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Remark

Gerarts, Steegmans, and Van den Bussche (2025) have implemented an FO(SUM) query engine using SQL in a relational database system and evaluated it empirically.

Example: The Zero Query

Corollary

Let $d, m \in \mathbb{N}$, and let φ be a $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f^{(m)})$ sentence.
Then the problem of computing $[\![\varphi]\!]^{\mathcal{N}}$ for an FNN $\mathcal{N} \in \mathbf{N}_d(m, 1)$ is in uniform TC^0.

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Since Zero_m is expressible in $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f^{(m)})$, it follows from our results that Zero_m is in uniform TC^0 on FNNs of bounded depth.

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Example (Grädel and Gurevich 1998)

Let

$$\sigma(x) \coloneqq \mathsf{ifp}\left(F(x) \leftarrow \mathsf{if}\ \exists y\, \mathsf{edge}(y,x)\ \mathsf{then}\ \Big(\sum_{y:\mathsf{edge}(y,x)} F(y)\Big)\cdot\Big(\sum_{y:\mathsf{edge}(y,x)} F(y)\Big)\ \mathsf{else}\ 2\right)(x).$$

If we evaluate the term over an FNN $\mathcal{N} \in \mathbf{N}(1,1)$ that is just a path of length d for the output node v of $\mathcal{N}$ it holds that

$$[\![\sigma]\!]^{\mathcal{N}}(v) = 2^{2^d}.$$

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The data complexity of sIFP(SUM) *is in* P.

Towards Capturing Polynomial Time

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1. *There is a model-agnostic query on* $\mathbf{N}(1,1)$ *that is decidable in polynomial time, but not expressible in* IFP(SUM) *even on FNNs where all weights are* 1 *or* 0.

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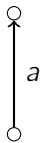

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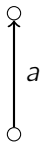

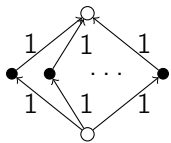

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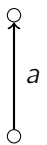

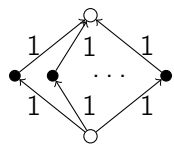

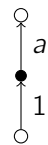

Concluding Remarks

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- On bounded depth FFNs, FO(SUM) is an expressive and robust logic.

  At the heart of the expressivity is the ability to define cylindrical cell decompositions in FO(SUM).
- Beyond bounded depth, the situation is more brittle.

A Few Open Problems

- Can we extend $\mathrm{FO}(\mathcal{R}_{\mathrm{lin}}, f) \subseteq \mathrm{FO}(\mathrm{SUM})$ on bounded-depth FNNs from linear to polynomial real arithmetic, that is, is $\mathrm{FO}(\mathcal{R}, f) \subseteq \mathrm{FO}(\mathrm{SUM})$ on bounded-depth FNNs?

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