

Principled Rewriting of ONNX Operators for Reluctant Solvers

A proof of concept for the Argmax operator

Guilhem Ardouin
Julien Girard-Satabin
Alban Grastien

CEA LIST

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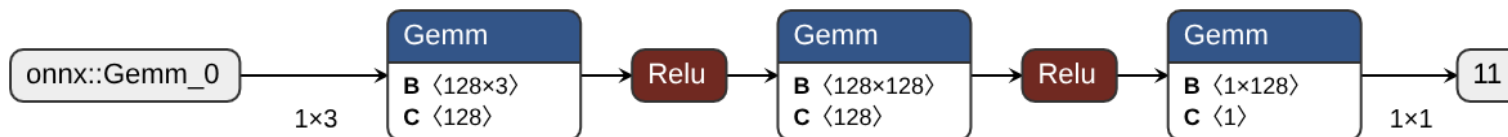


Motivation

Subject of interest: formal verification of Neural Networks by multiple solvers

Multiple solvers: VNN-COMP, stronger confidence from different, concurring answers (and people from certification agencies are used to that!)

Open Neural Network eXchange (ONNX) format



- Dataflow representation of neural network computations
- Nodes are operators, semantics loosely defined¹ from standard <https://onnx.ai>
- 196 operators encoding traditional machine learning pipelines
- several provers have different support range for ONNX operators

ONNX support discrepancies

Solver	Supported ops (/196)
nnenum [1]	17
$\alpha - \beta$ - CROWN [2]	22
Marabou [3]	16
Maraboupy [3]	24
PyRAT [4]	54

Mutually exclusive support of operators!

Do we have to write custom program transformations for provers?

Existing work

DNNV ([5], [6]): ONNX simplifications

ONNX runtimes and `onnxsimplicifier` perform compiler optimizations like constant-folding which results in simpler, faster models

$\alpha - \beta$ - CROWN [2], Marabou [3], PyRAT [4] have their own (often undocumented) heuristics on simplifications

The ArgMax

An ubiquitous operator

Case-study

Sound rewriting the ArgMax (Argument of Maximum value) operator

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Sound rewriting the ArgMax (Argument of Maximum value) operator

1. Ubiquitous in classification tasks (selecting the best performing class)
2. Useful for rewrites for hyper-properties [7]
3. Can be decomposed onto a subgraph of simpler ONNX operators

Often absent from VNN-COMP benchmarks, yet often found in production models

ArgMax semantic

ArgMax

Given a tensor t with shape $\text{sh} = [d_0, d_1, \dots, d_{n-1}]$

ArgMax returns a tensor a of shape $[d_0, d_1, \dots, d_{n-2}, 1]$ such that if

$a[i_1, \dots, i_{n-2}, 1] = j$ then $t[i_1, \dots, i_{n-2}, j] > t[i_1, \dots, i_{n-2}, k] \forall k \neq j$

Example with a vector

$$v = \begin{pmatrix} 3 \\ 4 \\ -6 \\ 2 \end{pmatrix} \quad \text{sh}(v) \stackrel{\text{def}}{=} (4)$$

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$$a(v) \stackrel{\text{def}}{=} [2]$$

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$$m = \begin{pmatrix} 3 & 3 \\ 1 & 3 \\ 8 & 6 \end{pmatrix} \quad \text{sh}(m) \stackrel{\text{def}}{=} (3, 2)$$

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$$m = \begin{pmatrix} \boxed{3} & \boxed{3} \\ \boxed{1} & \boxed{3} \\ \boxed{8} & \boxed{6} \end{pmatrix} \quad \text{sh}(m) \stackrel{\text{def}}{=} (3, 2)$$
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$a(m)_{j=1} \stackrel{\text{def}}{=} [3 \ 3]$

The diagram illustrates the relationship between a matrix m , its shape $\text{sh}(m)$, and its first row $a(m)_{j=1}$. The matrix m is a 3x2 matrix with elements $\begin{pmatrix} 3 & 3 \\ 1 & 3 \\ 8 & 6 \end{pmatrix}$. The shape $\text{sh}(m)$ is defined as $(3, 2)$. The first row $a(m)_{j=1}$ is defined as $[3 \ 3]$. Arrows indicate the mapping: the first dimension 3 of the shape corresponds to the number of rows in m , the second dimension 2 corresponds to the number of columns in m , and the first row of m corresponds to the first row of $a(m)$.

Tensors

Tensor t is a multi-dimensional array, of shape $\text{sh}(t) = (\text{dim}_1, \dots, \text{dim}_r)$; $r = \text{len}(\text{sh})$ is the rank of t , dim_l is the size of the l -th dimension.

Vector of positions $\mathbf{i} = [i_1, \dots, i_r] \stackrel{\text{def}}{=} [\text{dim}_1] \times \dots \times [\text{dim}_t]$

Sound decomposition

Idea of the decomposition

Use basic ONNX operators to implement pairwise-comparison for each couple of coordinates given the target axis

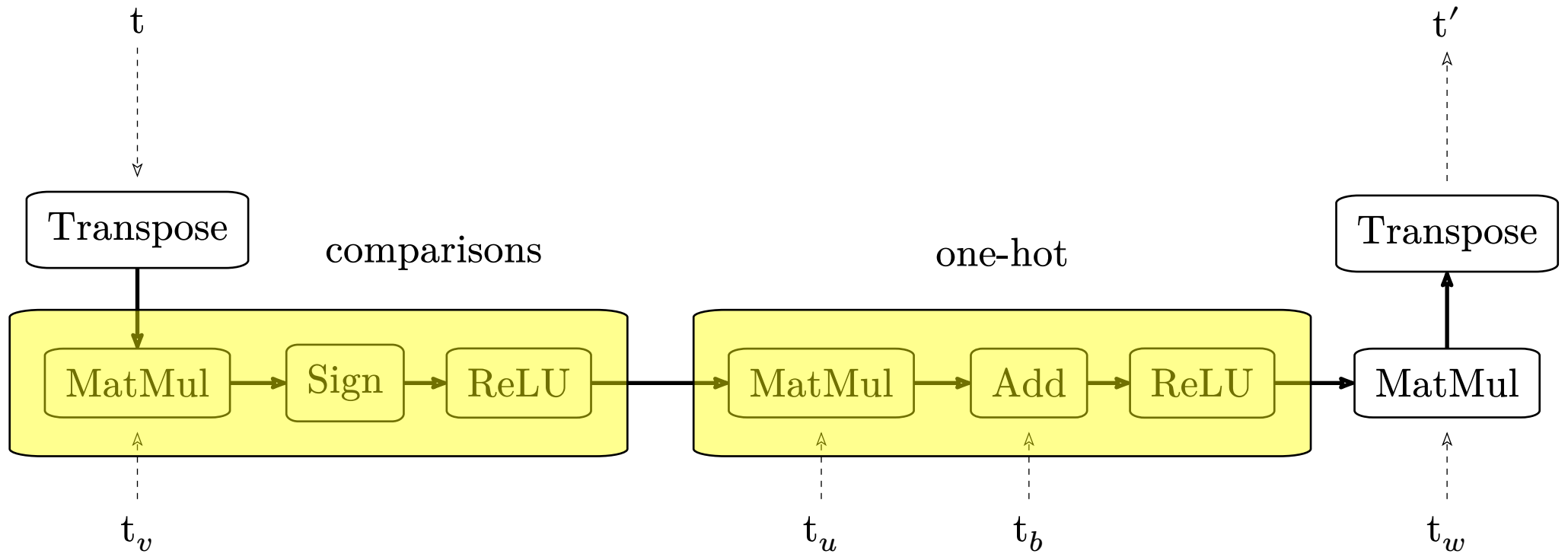
1. select the dimension of t to work on;
2. substract elements pairwise;
3. get the sign of substractions;
4. compute 1 if the sign is positive, 0 otherwise;

Some basic ONNX operators

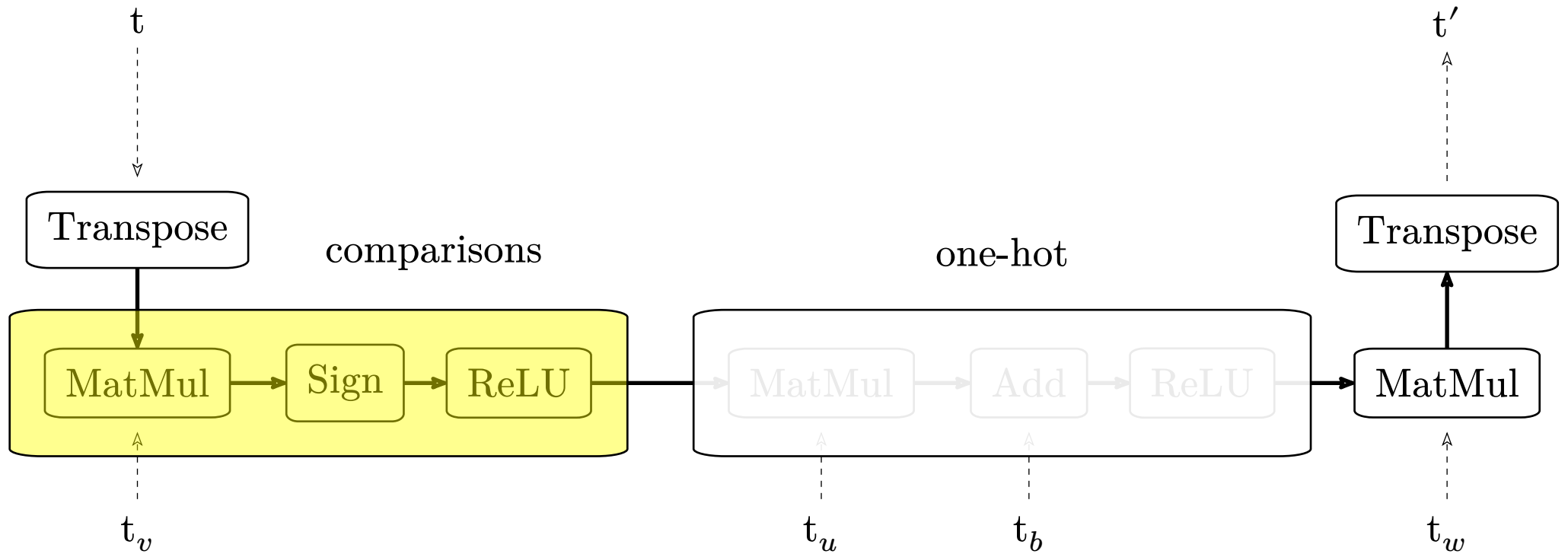
Given an input tensor t :

1. Const_c returns c ;
2. Add_c is element-wise addition of t and c ;
3. Sign is element-wise sign of t , returns 1, 0, -1 if the element is strictly positive, zero, or strictly negative, respectively;
4. ReLU is element-wise application of function $x \mapsto \max(0, x)$;
5. Transpose_p permutes indices in t ;
6. MatMul_A is matrix multiplication At .

Implementing the decomposition



Implementing the decomposition



Comparison implementation

1. transposition using swapping of indices $p_{l,r}$;
2. compute $C_{\text{dim}_l}^2$, and associate elements of vector u with values of said combinations in index ξ ;
3. sub-network ensures $u[\xi(\{j, k\})] = 1$ if $v[k]$ higher than $v[j]$, and 0 otherwise
 $\Leftarrow$ you can do that by computing $v[k] - v[j]$

Comparison implementation

$$v = (3 \ 4 \ -6 \ 2)$$

$$\text{sh}(m) \stackrel{\text{def}}{=} (1, 4)$$

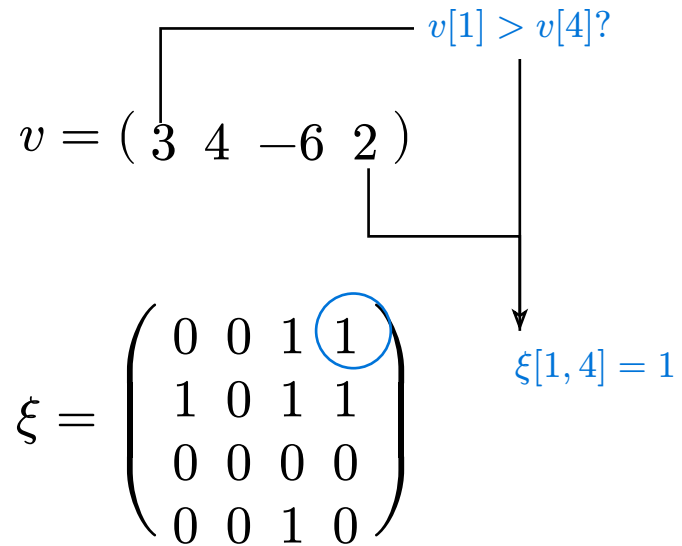
Comparison implementation

$$v = (3 \ 4 \ -6 \ 2)$$

$$\text{sh}(m) \stackrel{\text{def}}{=} (1, 4)$$

$$\xi = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Comparison implementation



$$\text{sh}(m) \stackrel{\text{def}}{=} (1, 4)$$

Comparison implementation

$$v = (3 \ 4 \ -6 \ 2)$$

$$\xi = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$v[1] > v[4]?$

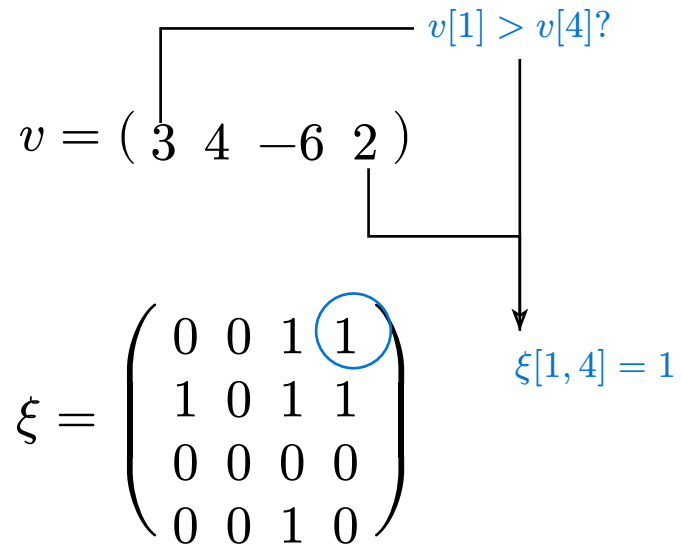
$\xi[1,4] = 1$

$$\text{sh}(m) \stackrel{\text{def}}{=} (1, 4)$$

$$\text{MatMul}(v, t_v) =$$

$$\begin{pmatrix} \underbrace{-1}_{v[1] < v[2]} & \underbrace{1}_{v[1] > v[3]} & \underbrace{1}_{v[1] > v[4]} & \underbrace{1}_{v[2] > v[3]} & \underbrace{1}_{v[2] > v[4]} & \underbrace{-1}_{v[3] < v[4]} \end{pmatrix}$$

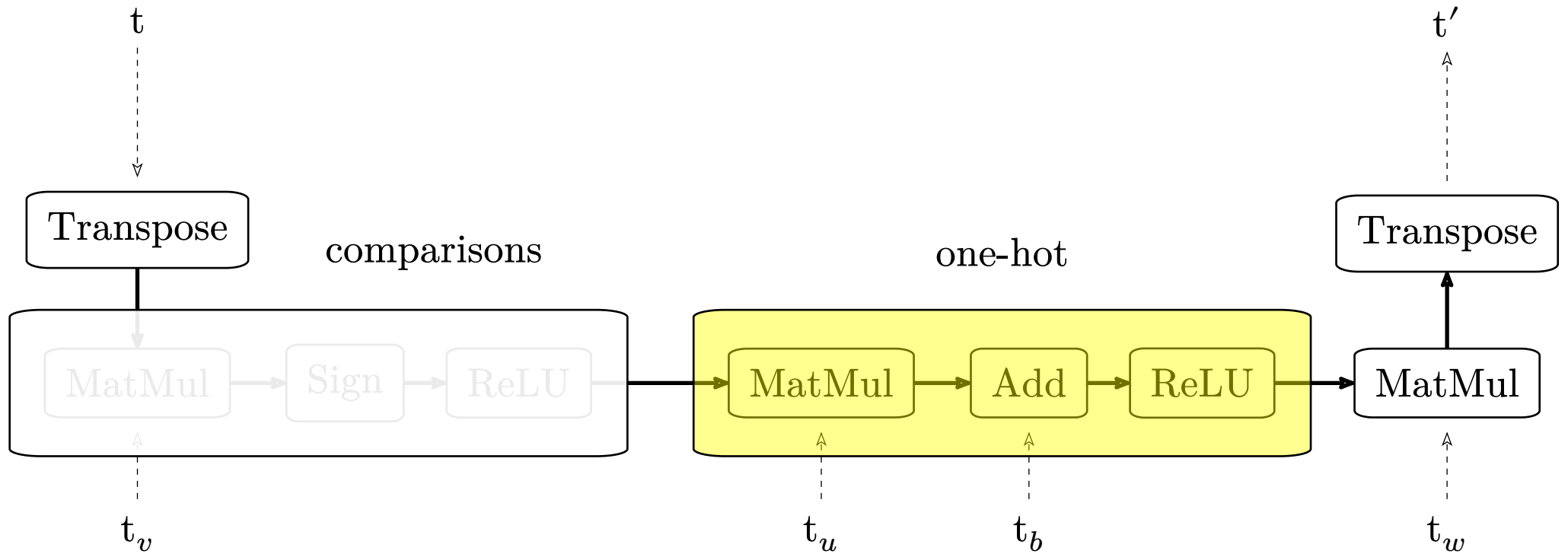
Comparison implementation



$$\text{sh}(m) \stackrel{\text{def}}{=} (1, 4)$$

$$u = (0 \ 1 \ 1 \ 1 \ 1 \ 0)$$

One-hot implementation



One-hot implementation

w is a one-hot vector where $w[\hat{j}] = 1$ if $v[\hat{j}]$ is the max value among the dimension, and all others are 0; obtained by computing differences that will be negative

Some experimental results

ArgMax for confidence-based properties

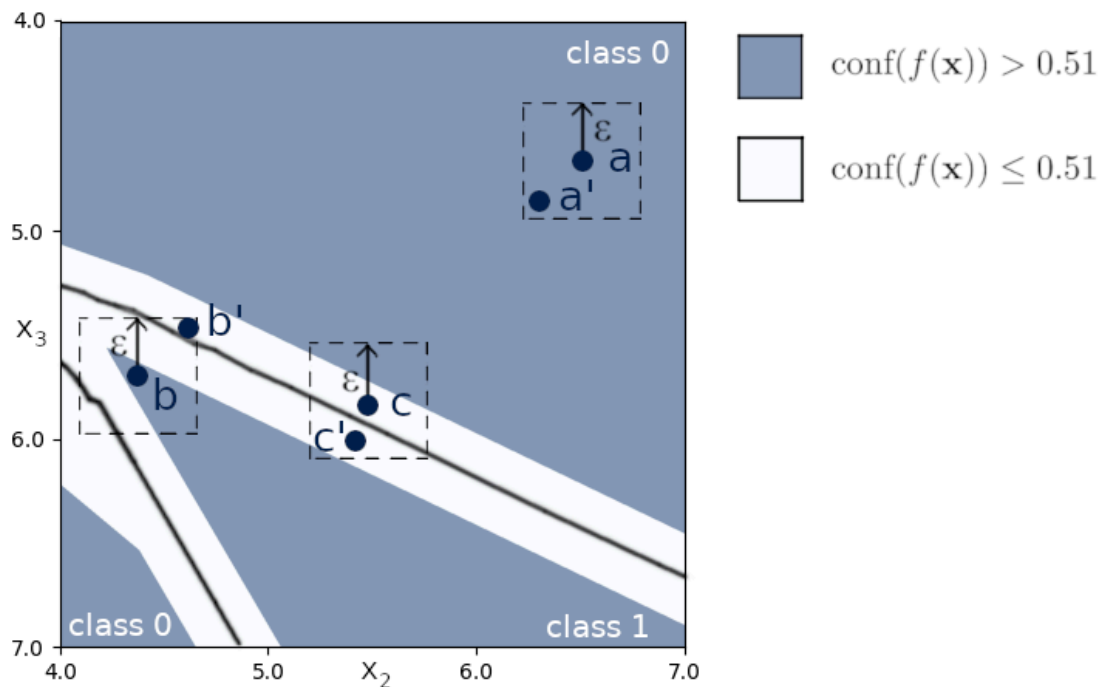


Figure 2: Proposed in [8], refined by [7], needs ArgMax for comparing outputs between two execution traces



ArgMax for confidence-based properties

For this property, ArgMax is instanciated as a logical predicate



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Quadratic in terms of output dimension 🥲



ArgMax for confidence-based properties

For this property, ArgMax is instanciated as a logical predicate

Quadratic in terms of output dimension 😭

But the rewritten ArgMax can be used! 😞

ArgMax for confidence-based properties

		Validity	LOGICAL	ARGMAX	Time difference	
<i>COMPAS</i>	($\kappa = 0.9$)	✓	17.4s	12.3s	-5.1s	(-29.3%)
<i>COMPAS</i>	($\kappa = 0.8$)	✓	18.8s	13.5s	-5.3s	(-28.2%)
<i>COMPAS</i>	($\kappa = 0.7$)	✓	38.3s	30.0s	-8.3s	(-21.7%)
<i>COMPAS</i>	($\kappa = 0.6$)	✓	564.6s	493.7s	-70.9s	(-12.6%)
<i>COMPAS</i>	($\kappa = 0.2$)	✗	63.8s	34.2s	-29.6s	(-46.4%)
<i>COMPAS</i>	($\kappa = 0.1$)	✗	64.0s	34.4s	-29.6s	(-46.2%)
<i>Adult</i>	($\kappa = 0.9$)	✓	13.4s	13.5s	+0.1s	(+0.7%)
<i>Adult</i>	($\kappa = 0.8$)	✓	21.8s	23.0s	+1.2s	(+5.5%)
<i>Adult</i>	($\kappa = 0.7$)	✓	123.2s	138.4s	+15.2s	(+12.3%)
<i>Adult</i>	($\kappa = 0.2$)	✗	78.2s	86.7s	+8.5s	(+10.9%)
<i>Adult</i>	($\kappa = 0.1$)	✗	78.6s	86.8s	+8.2s	(+10.4%)
<i>Industrial</i>	($\kappa = 0.999$)	✓	87.8s	61.9s	-25.9s	(-29.5%)
<i>Industrial</i>	($\kappa = 0.99$)	✓	274.6s	188.1s	-86.5s	(-31.5%)
<i>Industrial</i>	($\kappa = 0.9$)	✓	2058.9s	1389.5s	-669.4s	(-32.5%)
<i>Industrial</i>	($\kappa = 0.2$)	✗	115.9s	68.8s	-47.1s	(-40.6%)
<i>Industrial</i>	($\kappa = 0.1$)	✗	116.2s	68.6s	-47.6s	(-41.0%)

Key takeaway

- ArgMax principled rewriting and proof (in the paper);
- gives access to a whole class of properties for provers not supporting ArgMax;
- with more than 2 classes, simpler operators provides faster verification runs, without comprising soundness!



Future work

- more operator rewrites are planned: ArgMin, Exp, pooling family;
- smaller amount of ReLUs;
- automated proof of the specification within CAISAR with Rocq + extracted OCaml code;



CAISAR

Website: <https://caisar-platform.com> including manual, use cases and examples

Code: <https://git.frama-c.com/pub/caisar>

Looking for a research engineer: <https://caisar-platform.com/positions>





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