A Zonotopic Dempster-Shafer Approach to the Quantitative Verification of Neural Networks

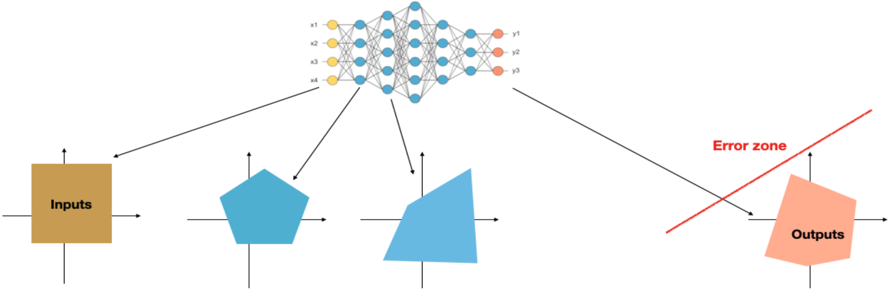
Eric Goubault and Sylvie Putot

FM 2024, September 9-13, Milan, Italy

Reachability Analysis for Neural Network Verification

Robustness and input/output properties:

- Need to be proved for (possibly large) sets of network inputs
- Can be specified as preconditions/postconditions expressed in linear arithmetic



Qualitative verification: property proven true or unknown

Quantitative Neural Network Verification

Motivation

- Provide additional information on property satisfaction compared to SAT/UNKNOWN
- Exploit knowledge of probabilistic information on inputs
  - can be probabilistic but imprecisely known, e.g.:
    - Gaussian variable $\mathcal{N}(\mu, \sigma^2)$ with uncertain mean $\mu \in [\underline{\mu}, \overline{\mu}]$ and variance $\sigma^2 \in [\underline{\sigma^2}, \overline{\sigma^2}]$
    - Uniform variable $\mathcal{U}(a, b)$ with uncertain range (a and b uncertain)
  - example: noise due to sensor $V + \varepsilon$ with $V \in [a, b]$, ε a random variable

With respect to most closely related work: Quantitative verification for neural networks using Probstars, Tran, H.D., Choi, S., Okamoto, H., Hoxha, B., Fainekos, G., Prokhorov, D., HSCC 2023

- inputs are arbitrary distributions (extending the Gaussian distribution hypothesis)
- our approach gives fully guaranteed probability bounds

Problem Statement: propagating imprecise probabilities

Problem (Probability bounds analysis)

Given a ReLU network f and a constrained probabilistic input set

$$\mathcal{X} = \{X \in \mathbb{R}^{h_0} \mid CX \leq d \wedge \underline{F}(x) \leq \boldsymbol{P}(X \leq x) \leq \overline{F}(x), \forall x\}$$

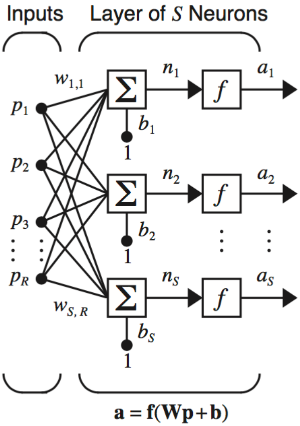
where $\underline{F}$ and $\overline{F}$ are two cumulative distribution functions, compute a constrained probabilistic output set $\mathcal{Y}$ guaranteed to contain $\{f(X), X \in \mathcal{X}\}$.
For $X \in \mathbb{R}^n$, we note $\boldsymbol{P}(X \leq x) := \boldsymbol{P}(X_1 \leq x_1 \wedge X_2 \leq x_2 \ldots \wedge X_n \leq x_n)$

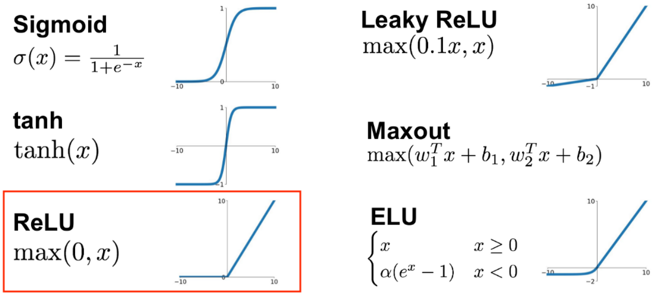
Problem (Quantitative property verification)

Given a ReLU network f, a constrained probabilistic input set $\mathcal{X}$ and a linear safety property $Hy \leq w$, bound the probability of the network output vector y satisfying this property.

Feedforward ReLU neural network

Each layer consists in a linear transform followed by a non linear activation function:



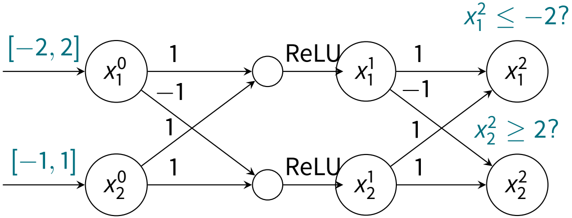


We focus on the classical ReLU activation function

Toy illustrating example: 2-layers ReLU network

$$A_1 = A_2 = \begin{bmatrix} 1 & -1 \\ 1 & 1. \end{bmatrix}, b_1 = b_2 = \begin{bmatrix} 0.0 \\ 0.0 \end{bmatrix}.$$

$$x^1 = \sigma(A_1 x^0 + b_1) = \sigma(x_1^0 - x_2^0, x_1^0 + x_2^0)$$
$$x^2 = A_2 x^1 + b_2$$



Property:

- Qualitative: if $x^0 = \begin{bmatrix} x_1^0 & x_2^0 \end{bmatrix}^\top \in [-2, 2] \times [-1, 1]$, does output satisfy $x_1^2 \leq -2 \wedge x_2^2 \geq 2$?
- Quantitative:
  - $\boldsymbol{P}\left(x_1^2 \leq -2 \wedge x_2^2 \geq 2 \;\middle|\; x_1^0 \in \mathcal{U}(-2, 2) \wedge x_2^0 \in \mathcal{U}(-1, 1)\right)$?
  - $\boldsymbol{P}\left(x_1^2 \leq -2 \wedge x_2^2 \geq 2 \;\middle|\; x_1^0 \in \mathcal{N}(0, [0.5, 0.66]) \wedge x_2^0 \in \mathcal{N}([0, 1], 0.33)\right)$?

Outline

- Imprecise probabilities: P-boxes and Dempster-Shafer Interval Structures (DSI)
  - Representations of sets of probability distributions
  - Generalize both probabilistic and non deterministic (interval) computations
- ReLU neural network analysis by DSI
- Mitigating the wrapping effect of intervals using zonotopes
  - Probabilistic Zonotopes
  - Zonotopic Dempster-Shafer Structures (DSZ)
- Evaluation

Imprecise probabilities: P-boxes and Dempster-Shafer structures

Representation of imprecise probabilities: P-box

Definition (P-box for a real-valued random variable X)

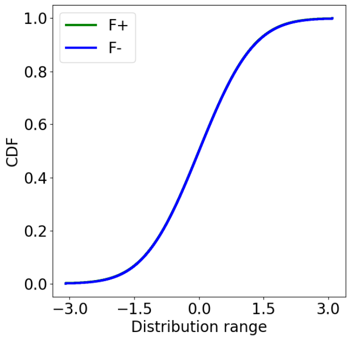
Given two (lower and upper) CDF (Cumulative Distribution Functions) $\underline{F}$ and $\overline{F}$ from $\mathbb{R}$ to $\mathbb{R}^+$ s.t. $\forall x \in \mathbb{R}, \underline{F}(x) \leq \overline{F}(x)$, the p-box $[\underline{F}, \overline{F}]$ represents the set of probability distributions for X s.t.

$$\forall x \in \mathbb{R}, \underline{F}(x) \leq \boldsymbol{P}(X \leq x) \leq \overline{F}(x).$$

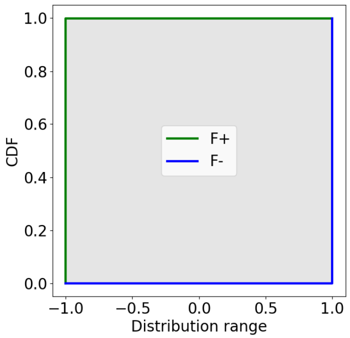
- Ferson S, Kreinovich V, Ginzburg L, Myers D, Sentz K, Constructing probability boxes and Dempster–Shafer structures. Tech. Rep. SAND2002-4015, 2003
- Williamson and Downs, Probabilistic Arithmetic I: Numerical Methods for Calculating Convolutions and Dependency Bounds, Journal of Approximate Reasoning, 1990

P-box examples (Julia library ProbabilityBoundsAnalysis.jl)l

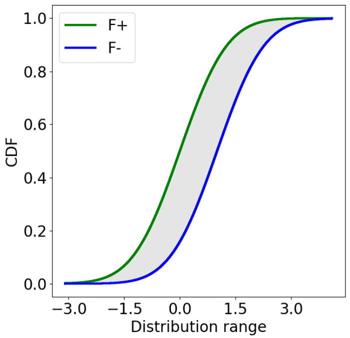
Sets of probability distributions on X (CDF form) such that $\forall x, F^{-}(x) \leq \boldsymbol{P}(X \leq x) \leq F^{+}(x)$:



normal(0,1)



makepbox(interval(-1,1))



normal(interval(0,1),1)

Generalize probabilistic and non deterministic (interval) information

Dempster-Shafer Interval structures (DSI)

A discrete version of P-boxes:

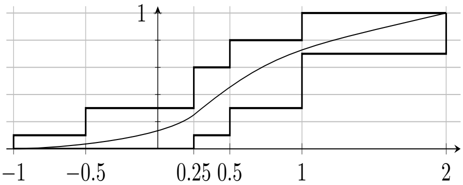
- Focal elements $t \in T$ (sets of values, here Intervals) with probability $w : T \to \mathbb{R}^+$

$t \in T$	[-1,0.25]	[-0.5,0.5]	[0.25,1]	[0.5,1]	[0.5,2]	[1,2]
$w(t)$	0.1	0.2	0.3	0.1	0.1	0.2

- Represents the set of probability distributions P on X such that:

$$\forall x \in [-1, -0.5],\ P(X \leq x) \leq 0.1\,,$$
$$\forall x \in [-0.5, 0.25],\ P(X \leq x) \leq 0.1 + 0.2\,,$$
$$\forall x \in [0.25, 0.5],\ 0.1 \leq P(X \leq x) \leq 0.1 + 0.2 + 0.3\,,$$

etc.

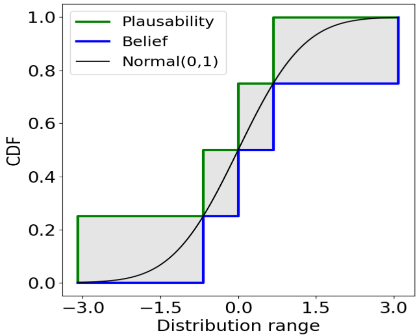


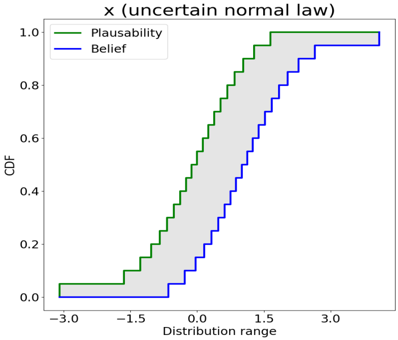
$$\sum_{t \in T, t \subseteq S} w(t) \leq P(S) \leq \sum_{t \in T, t \cap S \neq \emptyset} w(t)$$

From P-boxes to Dempster-Shafer Interval structures

Given a P-box $(\underline{F}, \overline{F})$

- Take lower and upper approximation by stair functions
- Deduce focal elements (intervals) and weights

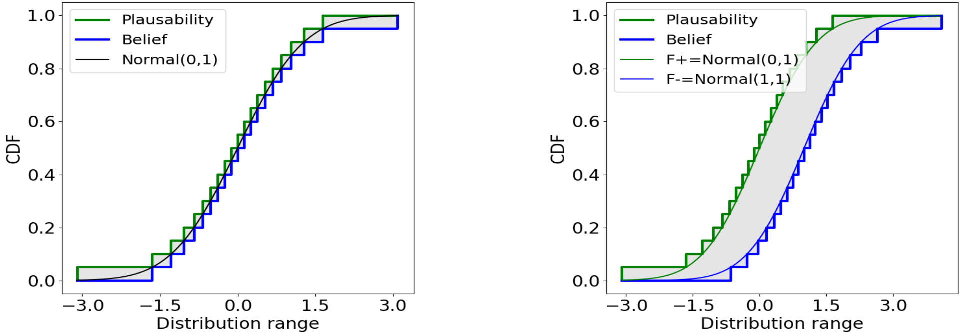




From P-boxes to Dempster-Shafer Interval structures

Given a P-box $(\underline{F}, \overline{F})$

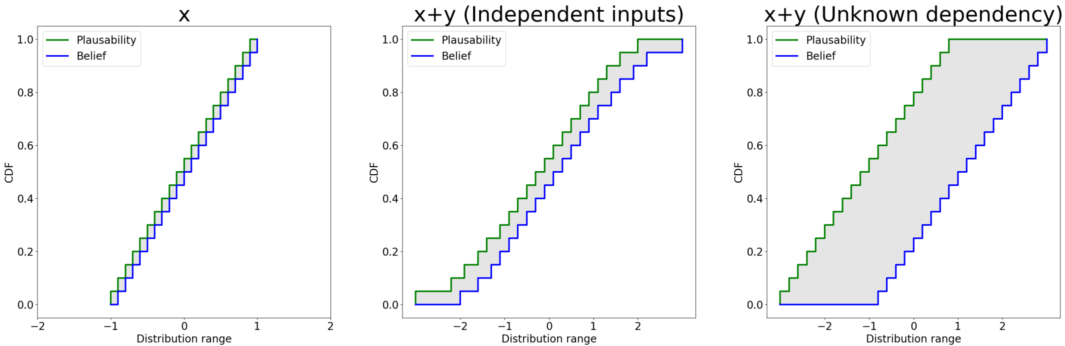
- Take lower and upper approximation by stair functions
- Deduce focal elements (intervals) and weights



Arithmetic on DSI structures

DSI structures can be propagated through arithmetic operations:

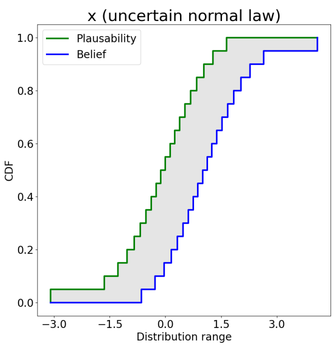
- 2 cases: independent inputs / unknown dependency
- relying on interval arithmetic / Frechet inequalities
- conservative approximations

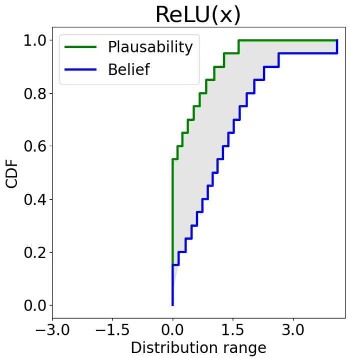


ReLU

Lemma (ReLU of a DSI)

Given X represented by the DSI $\{\langle \mathbf{x_i}, w_i \rangle, i \in [1, n]\}$, then the CDF of $Y = \sigma(X) = \max(0, X)$ is included in the DSI $\{\langle \mathbf{y_i}, w_i \rangle, i \in [1, n]\}$ with $y_i = [\max(0, \underline{x_i}), \max(0, \overline{x_i})]$.





ReLU neural network analysis by DSI

Input: d^0 a h_0-dimensional vector of DSI

for $k = 0$ to $L - 1$ **do**

  for $l = 1$ to h_{k+1} **do**

    $d_l^{k+1} \leftarrow \sigma(\sum_{j=1}^{h_k} a_{lj}^k d_j^k + b_l^k)$ ▷ *Affine transform and ReLU - Dependency graph useful for choosing the right DSI operations (indep. or unknown dep.) in affine transforms*

  end for

end for

return $(d^L, cdf(Hd^L, w))$ ▷ *Vector of DSI for the output layer and probability bounds for property $Hz \leq w$*

Illustration on the toy example

Input $x^0 = \begin{bmatrix} x_1^0 & x_2^0 \end{bmatrix}^\top \in [-2, 2] \times [-1, 1]$ with Uniform law on inputs

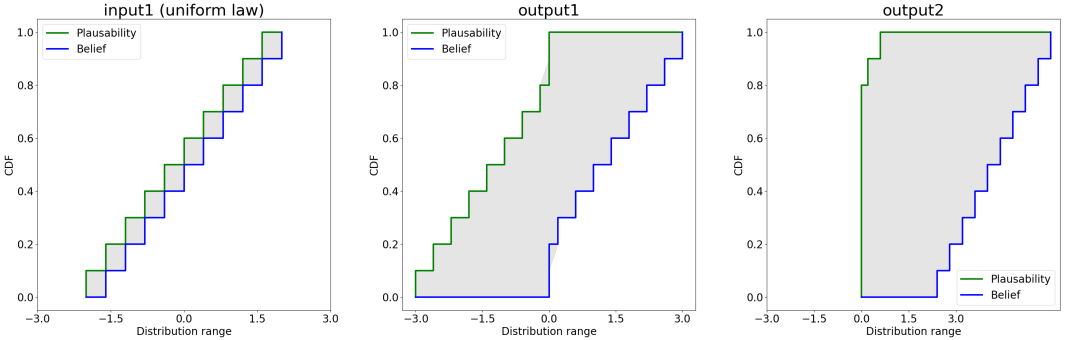
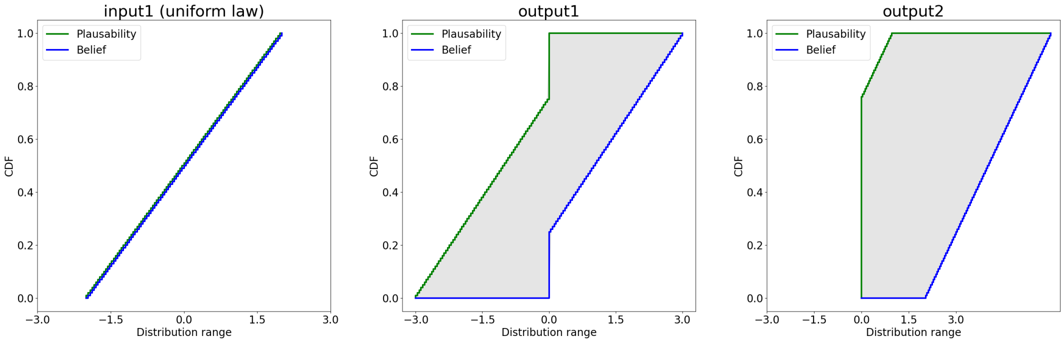


Illustration on the toy example

Input $x^0 = \begin{bmatrix} x_1^0 & x_2^0 \end{bmatrix}^\top \in [-2, 2] \times [-1, 1]$ with Uniform law on inputs



Finer discretization refines the approximation but the ranges are unchanged

Illustration on the toy example

Input $x^0 = \begin{bmatrix} x_1^0 & x_2^0 \end{bmatrix}^\top \in [-2, 2] \times [-1, 1]$ with Normal law on inputs

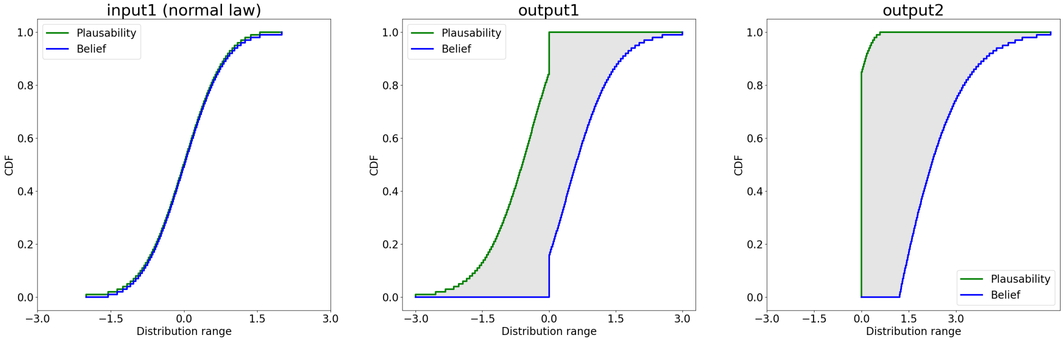
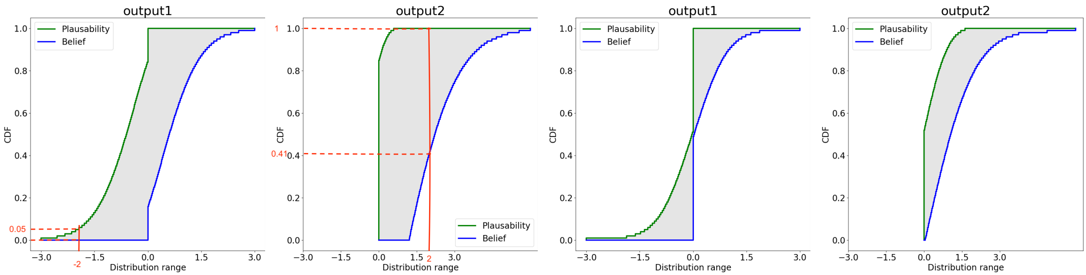


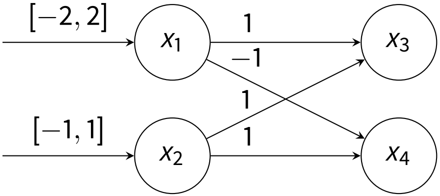
Illustration on the toy example

Unknown dependency on inputs vs independent inputs



$\boldsymbol{P}(z_1 \leq -2) \in [0, 0.05]$ $\boldsymbol{P}(z_2 \geq 2) \in [0, 0.59]$ $\boldsymbol{P}(z_1 \leq -2) \in [0, 0.01]$ $\boldsymbol{P}(z_2 \geq 2) \in [0, 0.2]$

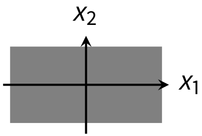
Wrapping effect: example of the first affine layer



Initial domain:

$$-2 \leq x_1 \leq 2$$

$$-1 \leq x_2 \leq 1$$



Exact domain:

$$x_3 = x_1 - x_2$$

$$x_4 = x_1 + x_2$$

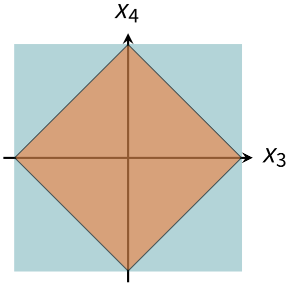
$$x_1, x_2 \in [-1, 1]$$

Using Intervals/Boxes:

$$-3 \leq x_3 \leq 3$$

$$-3 \leq x_4 \leq 3$$

$$x_1, x_2 \in [-1, 1]$$



The optimal affine transformers for boxes are not exact. Zonotope transformers are !

Mitigating the wrapping effect: Probabilistic zonotopes and Dempster-Shafer Zonotopic Structures (DSZ)

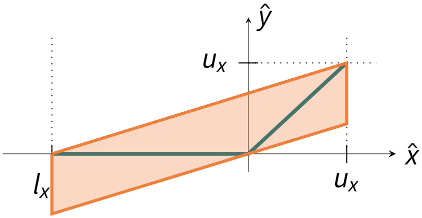
Zonotopes and neural network reachability analysis

Definition (Zonotope)

An n-dimensional zonotope $\mathcal{Z}$ with center $c \in R^n$ and a vector $\Gamma = \left[g_1 \dots g_p\right] \in \mathbb{R}^{n,p}$ of p generators $g_j \in \mathbb{R}^n$ for $j = 1, \dots, p$ is defined as $\mathcal{Z} = \langle c, \Gamma \rangle = \{c + \Gamma\varepsilon \mid \|\varepsilon\|_\infty \leq 1\}$.

Zonotopes are closed under affine transformations: for $A \in \mathbb{R}^{m,n}$ and $b \in \mathbb{R}^m$ we define $A\mathcal{Z} + b = \langle Ac + b, A\Gamma \rangle$ as the m-dimensional resulting zonotope.

RELU transformer: conservative approximation



Two solutions for zonotopic probabilistic NN analysis

Probabilistic zonotopes (or probabilistic affine forms)

- Zonotopic network analysis starting from the support of input distribution
- Probabilistic interpretation: noise symbols are DSI instead of intervals
- inspired from [Adje et al 2013] A. Adjé, O. Bouissou, J. Goubault-Larrecq, E. Goubault, S. Putot: Static Analysis of Programs with Imprecise Probabilistic Inputs. VSTTE 2013: 22-47

Dempster-Shafer Zonotopic structures (DSZ)

- Dempster-Shafer structures with zonotopic focal elements
- A refinement of probabilistic zonotopes, which fully exploits the DSI input discretization in the NN analysis
- Currently restricted to independent inputs

NN analysis by DSZ (independent inputs)

Input: d^0 a h_0-dimensional vector of DSI

$d^0_{\mathcal{Z}} = \{\langle \mathcal{Z}^0_{i_1 \dots i_{h_0}}, w^0_{1,i_1} \dots w^0_{h_0,i_{h_0}} \rangle,\ (i_1, \dots, i_{h_0}) \in [1,n]^{h_0}\} \leftarrow$ dsi-to-dsz(d^0)

for $k = 0$ to $L - 1$ **do**

  for $(i_1, i_2, \dots, i_{h_0}) \in [1,n]^{h_0}$ **do**

    $\mathcal{Z}^{k+1}_{i_1 \dots i_{h_0}} \leftarrow \sigma(A^k \mathcal{Z}^k_{i_1 \dots i_{h_0}} + b^k)$ ▷ Independent zonotopic analyzes (can be done in parallel)

  end for

end for

$d^L_{\mathcal{Z}} = \{\langle \mathcal{Z}^L_{i_1 \dots i_{h_0}}, w^0_{1,i_1} \dots w^0_{h_0,i_{h_0}} \rangle,\ (i_1, \dots, i_{h_0}) \in [1,n]^{h_0}\}$

$d^L \leftarrow$ dsz-to-dsi($d^L_{\mathcal{Z}}$)

return (d^L,cdf($(Hd^L_{\mathcal{Z}}, w)$)) ▷ Property bounds computed by direct evaluation of the CDF on the zonotopic focal elements

Evaluation

Implementation and Evaluation

FM Artifact Evaluation ★ Available

Julia implementation

- available from `https://github.com/sputot/DSZAnalysis` or `https://doi.org/10.5281/zenodo.12519084`.
- uses the LazySets and the NeuralVerification package for zonotopic NN analysis
- uses the ProbabilityBoundsAnalysis package for P-boxes / DSI analysis

Examples and evaluation

- Toy example - corrected Table 1 in the paper (thanks to the RE reviewers !)
- ACAS Xu airplanes collision avoidance example
- Rocket lander example

Comparing DSI, Prob. Zonotopes and DSZ: toy example

Table 1: Probability bounds for the toy example, independent inputs.

Law	DSI			Prob. Zono.			DSZ		
(#FE)	$\boldsymbol{P}(x_1^2 \leq -2)$	$\boldsymbol{P}(x_2^2 \geq 2)$	time	$\boldsymbol{P}(x_1^2 \leq -2)$	$\boldsymbol{P}(x_2^2 \geq 2)$	time	$\boldsymbol{P}(x_1^2 \leq -2)$	$\boldsymbol{P}(x_2^2 \geq 2)$	time
$U(2)$	$[0, 0.5]$	$[0, 1]$	$< e^{-3}$	$[0, 0.5]$	$[0, 1]$	$< e^{-3}$	$[0, 0.25]$	$[0, 0.5]$	$< e^{-3}$
$U(10)$	$[0, 0.2]$	$[0, 0.7]$	e^{-3}	$[0, 0.3]$	$[0, 0.8]$	e^{-3}	$[0, 0.03]$	$[0.2, 0.3]$	$< e^{-3}$
$U(102)$	$[0, 0.07]$	$[0.05, 0.52]$	0.022	$[0, 0.26]$	$[0, 0.76]$	0.013	$[0, 0.0014]$	$[0.25, 0.26]$	0.026
$U(10^3)$	$[0, 0.063]$	$[0.062, 0.502]$	2.4	$[0, 0.251]$	$[0, 0.751]$	1.2	$[0, 3.e^{-6}]$	$[0.25, 0.251]$	3
$N(10)$	$[0, 0.017]$	$[0, 0.277]$	e^{-3}	$[0, 0.1]$	$[0, 1]$	e^{-3}	$[0, 0.01]$	$[0, 0.1]$	$< e^{-3}$
$N(10^2)$	$[0, 0.004]$	$[0, 0.186]$	0.022	$[0, 0.07]$	$[0, 0.94]$	0.013	$[0, 4.e^{-4}]$	$[0.06, 0.07]$	0.026
$N(10^3)$	$[0, 0.004]$	$[0.003, 0.182]$	2.4	$[0, 0.067]$	$[0, 0.934]$	1.2	$[6e^{-5}, 1.1e^{-4}]$	$[0.066, 0.067]$	3

- For independent inputs, DSZ always more precise.
- In the paper, detailed calculation for the 3 approaches in the case of 2 focal elements.

Comparisons to the state of the art

[Tran et al 23] Quantitative Verification for Neural Networks using ProbStars, Tran et al, HSCC 2023

Examples

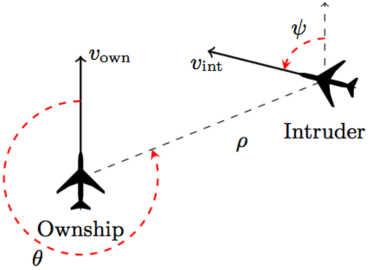
- ACAS Xu airplanes collision avoidance
- Rocket lander

Inputs and configuration

- Bounded (vector) inputs in [lb,ub], components follow independent Gaussian distributions with $\mu = (ub + lb)/2$ and $\sigma = (ub - m)/3$
- Timings and results given for [Tran et al 23] are from their paper:
  - parallelized (between 1 and 8 cores) and on a slightly stronger computer than ours
  - we reproduced a few analyzes: approx 7 to 10 times slower than their results with 1 core, approx 1.5 to 3.5 with 4 and 8 cores

ACAS Xu: collision avoidance systems for civil aircrafts (FAA)

- Produces aicraft advisory (clear-of-conflict, weak right, weak left, strong right, etc.)
- Array of 45 DNNs by discretizing τ and a_{prev} ; each has 5 inputs (ρ, θ, ψ, v_{own} and v_{int}) and 5 outputs (score for each advisory).
- Fully connected ReLU feeedforward networks with 5 inputs, 6 hidden layers, 5 outputs



Properties:

$P_2 : y_1 > y_2 \wedge y_1 > y_3 \wedge y_1 > y_4 \wedge y_1 > y_5$

$P_3/P_4 : y_1 < y_2 \wedge y_1 < y_3 \wedge y_1 < y_4 \wedge y_1 < y_5$

Reluplex : An Efficient SMT Solver for Verifying Deep Neural Networks, Katz et al, CAV 2017.

Comparing DSZ and ProbStars Prob. bounds on ACAS Xu

- (Manual) Input discretization: [5, 80, 50, 6, 5] for P_2, [5, 20, 1, 6, 5] for P_3 and P_4

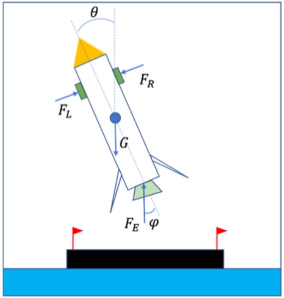
Prop	Net	DSZ		Probstar $p_f = e^{-5}$		Probstar $p_f = 0$	
		P	time	***P***	time	***P***	time
2	1-6	[0, 0.01999]	46.4	[2.8e-06,0.05283]	206.7	1.87224e-05	1424
2	2-2	[0.00423 0.0809]	47.9	[0.0195,0.094]	299.0	0.0353886	2102.5
2	2-9	[0, 0.0774684]	51.0	[0.000255,0.107]	504.5	0.000997678	4561.2
2	3-1	[0.0165, 0.08787]	43.8	[0.0305, 0.07263]	202.7	0.044535	1086.4
2	3-6	[0.0167, 0.1111]	52.4	[0.02078,0.1069]	452.0	0.0335763	5224.4
2	3-7	[6e-05, 0.1361]	43.7	[0.002319,0.075]	331.1	0.00404731	2598
2	4-1	[1e-05, 0.05353]	40.9	[0.00104,0.07162]	305.3	0.00231247	1870.7
2	4-7	[0.0129, 0.1056]	44.4	[0.02078,0.1081]	418.9	0.04095	3407.8
2	5-3	[0, 0.03939]	40.0	[1.59e-09,0.0326]	139.7	1.81747e-09	418.8
3	1-7	[1, 1]	0.25	[0.9801,0.9804]	4.7	0.976871	3.6
4	1-9	[1, 1]	0.2	[0.9796,0.98]	3.6	0.989244	3.6

Comparing DSZ and ProbStars Prob. bounds on ACAS Xu

- (Manual) Input discretization: [5, 80, 50, 6, 5] for P_2, [5, 20, 1, 6, 5] for P_3 and P_4
- Basic (sensitivity-based) discretization refinement algorithm:
  - for P_2 and net 1-6, the algorithm (from [1,1,1,1,1]) with as stopping criterion the width of the probability interval lower than 0.05 takes 112 seconds and leads to [5, 81, 38, 5, 5] and a probability in [0, 0.0276]

Prop	Net	DSZ		Probstar $p_f = e^{-5}$		Probstar $p_f = 0$	
		P	time	**P**	time	**P**	time
2	1-6	[0, 0.01999]	46.4	[2.8e-06,0.05283]	206.7	1.87224e-05	1424
2	2-2	[0.00423 0.0809]	47.9	[0.0195,0.094]	299.0	0.0353886	2102.5
2	2-9	[0, 0.0774684]	51.0	[0.000255,0.107]	504.5	0.000997678	4561.2
2	3-1	[0.0165, 0.08787]	43.8	[0.0305, 0.07263]	202.7	0.044535	1086.4
2	3-6	[0.0167, 0.1111]	52.4	[0.02078,0.1069]	452.0	0.0335763	5224.4
2	3-7	[6e-05, 0.1361]	43.7	[0.002319,0.075]	331.1	0.00404731	2598
2	4-1	[1e-05, 0.05353]	40.9	[0.00104,0.07162]	305.3	0.00231247	1870.7
2	4-7	[0.0129, 0.1056]	44.4	[0.02078,0.1081]	418.9	0.04095	3407.8

Rocket lander



- feedforward neural networks with 9 inputs, 3 outputs, and 5 hidden layers with 20 ReLU neurons per layer
- P_1: when $-20^\circ \leq \theta \leq -6^\circ, \omega < 0\,, \phi' \leq 0$, $F_S' \leq 0$, the output action should be $\phi < 0$ or $F_S < 0$: the agent should prevent the rocket from tilting to the right. (P_2 similar)

Neural Network Repair with Reachability Analysis. Yang et al, FORMATS 2022

Quantitative Verification for Neural Networks using ProbStars, Tran et al, HSCC 2023

Comparing DSZ and ProbStars Prob. bounds: rocket lander

- Input discretization: [7, 12, 10, 17, 9, 7, 1, 1, 2, 1, 1]

Prop	Net	DSZ		Probstar $p_f = 1e-5$		Probstar $p_f = 0$	
		P	time	***P***	time	***P***	time
1	0	[0, 0.03387]	77.8	[4.15e-09, 0.06748]	1158.6	7.978e-08	5903.7
2	0	[0, 0.01352]	83.7	[0,0.1053]	2216	0	13132.7
1	1	[0, 0.01985]	80.5	[0,0.0536]	1229.7	8.68e-08	5163.9
2	1	[0, 0.00055]	69.1	[0, 0.0161751]	448.5	0	1495.6

Conclusion and Future Work

- DSI/DSZ for ReLU networks generalize state of the art of NN probabilistic verification
  - more efficient than state of the art but still scalability issues
  - efficiency given by the input layer discretization size
- Future work:
  - Distributions with unbounded support (handled for DSI, extension to DSZ more of a technical/implementation issue)
  - Other initial abstractions/discretizations
    - avoid inefficient initial staircase / DSI discretization step
    - handle multivariate input distributions (lift independence hypothesis for DSZ)

We are looking for a motivated PhD student !