



Over-estimation guarantees for Surrogate Neural Networks for Braking Distance Estimation

High probabilistic guarantees and formal verification

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Nov 22 th 2022

AIRBUS

The results of multiple collaborations



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Trustworthiness of AI in the transport industry



WE ARE HERE
On Ground
Not Critical



White Paper

Machine Learning
in Certified Systems



DEEL Certification Workgroup
IET Saint Exupéry
June 2020
IET - iet.org/floway



Industrial needs

Challenges



- **Qualified models developed by engineering are usually ‘heavy’:**
 - Memory
 - Computing Power
 - Computing time
- **Embedding complex reference models for assistance:** Braking Distance Estimation, Structure Load Estimation, etc
- Surrogate is necessary for embedding reference physics models validated by authorities: How can we assess the safety of the surrogate compared to its reference ?

EASA: 41% accidents involving small non commercial airplanes happen during landing (1991-2017)

EUROCAE ED250: Minimum Operational Performance Standard for a Runway Overrun Awareness and Alerting System”, 2017



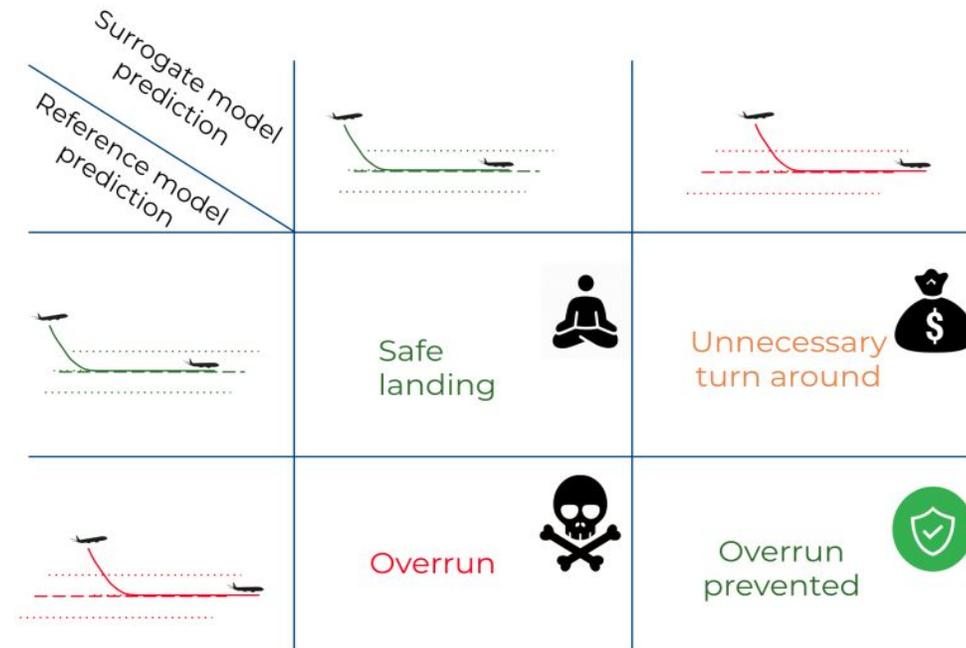
23/09/2022: a Boeing overrun in Montpellier

Braking Distance Estimation

Consequences of under-estimation and over-estimation of a surrogate model are not aligned.

How can we ensure safety in surrogate model learning?

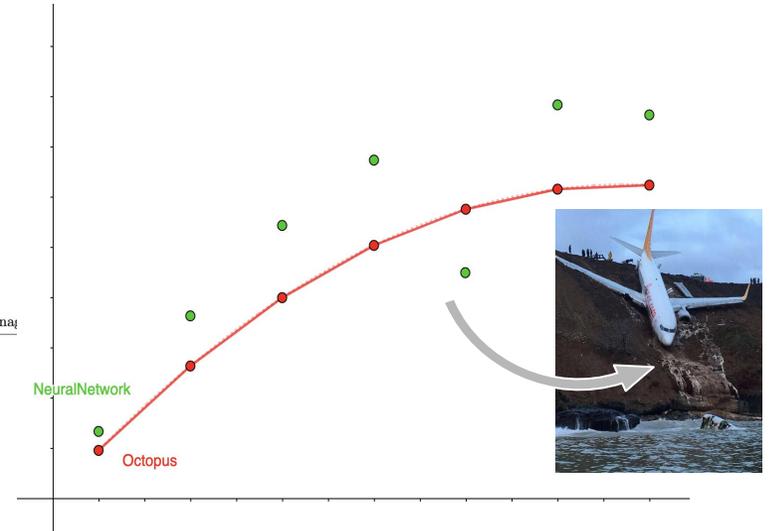
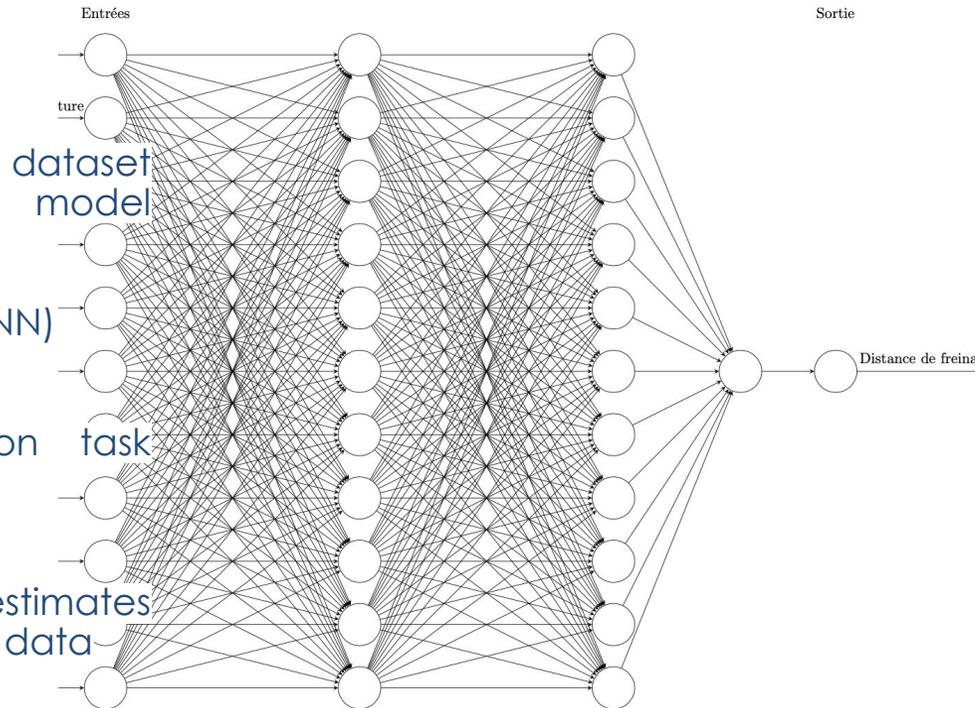
Special case where safety \Leftrightarrow over-estimation of the reference model.



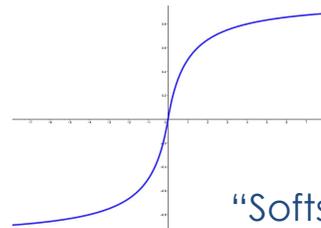
Embedding Neural Networks for Surrogate Modeling

Training shallow neural networks for a regression task

- Step 1: Sample training/testing dataset using the reference model
- Step 2: Design a shallow neural network (NN)
- Step 3: Train the NN for a regression task (symmetric or asymmetric)
- Step 4: Check the NN over-estimates the reference function on the test data

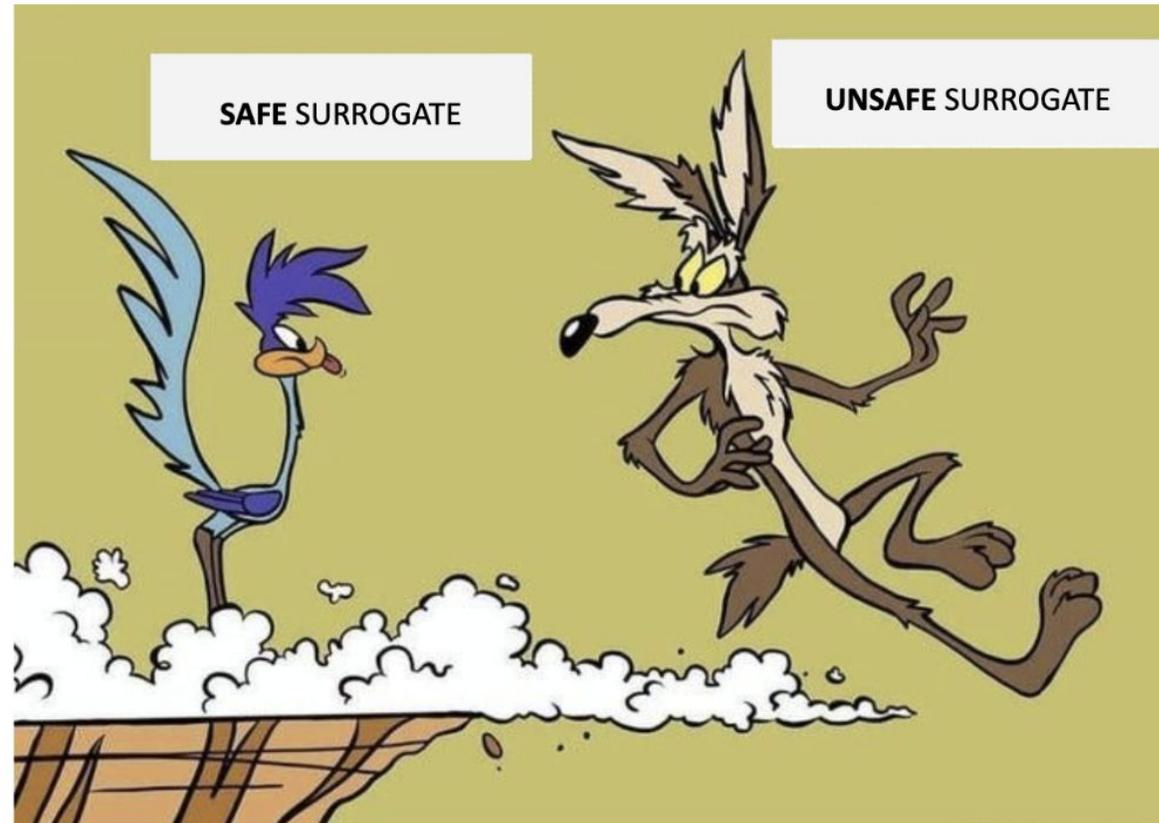


Program testing can be used to show the presence of bugs but never their absence (E. Dijkstra)



"Softsign" function widely used in SCADE implementation

Reproducibility



- Notebooks on open source data (CESSNA C172)
- Landing Distance Estimation

https://github.com/ducoffeM/safety_braking_distance_estimation

Probabilistic Assessment For Over-estimation

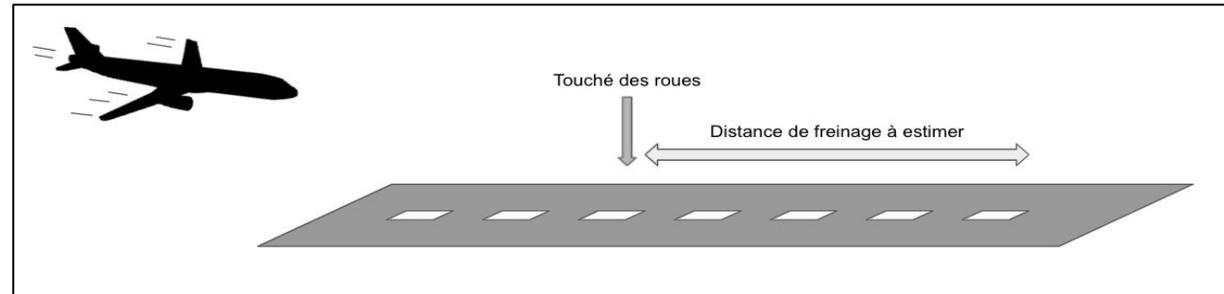


A High-Probability Safety Guarantee for Shifted Neural
Network Surrogates

Ducoffe Mélanie, Sébastien Gerchinovitz and Jayant Sen Gupta
Safe AI@AAAI 2020

Ensuring Safety with Probabilistic Assessment

Our Goal: Prove that a surrogate model over-estimates a reference function. The reference function is a black-box system which can be evaluated at any point.



Our Solution: We derive probabilistic inequalities to prove high-probability safety bounds on the surrogate model and on *shifted* versions of it.

A natural probabilistic definition of safety: A surrogate model \hat{f} is $(1-\epsilon)$ safe if it over-approximates the reference function f with probability at least $1-\epsilon$:

$$\mathbb{P} \left(\hat{f}(X) \geq f(X) \right) \geq 1 - \epsilon$$

where X is drawn at random from a given probability distribution P_X on the input domain.

Estimating the probability from samples

We estimate $\mathbb{P}(f(X) > \hat{f}(X))$ by simply counting how many times we have overestimation among i.i.d. test samples X_1, \dots, X_n .

We use Bernstein's inequality to relate the unknown probability to its estimate.

Proposition 1 (Consequence of Bernstein's inequality)

Consider $n \geq 2$ independent random variables X_1, \dots, X_n drawn from the same distribution P_X in the domain of study, and independent of the training set (\hat{f} is considered as fixed). We estimate the under-estimation probability by

$$\hat{G}_n = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{f(X_i) > \hat{f}(X_i)}$$

Then, for any risk level $\delta \in (0, 1)$, the following inequality holds with probability at least $1 - \delta$ over the choice of the calibration set X_1, \dots, X_n :

$$\mathbb{P}(f(X) > \hat{f}(X)) \leq \hat{G}_n + \sqrt{\frac{2\hat{G}_n}{n} \ln\left(\frac{1}{\delta}\right)} + \frac{2}{n} \ln\left(\frac{1}{\delta}\right)$$

Interpretation:

For a large fraction $1 - \delta$ of all possible sequences x_1, \dots, x_n that we could observe, the unknown probability of error is bounded by:

- the observed proportion of errors
- plus a small remainder term

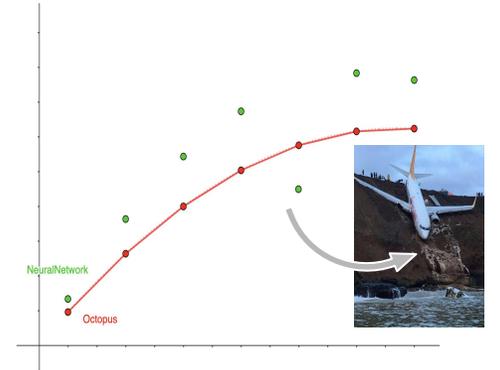
The risk level δ quantifies how unlikely it is to observe a sequence x_1, \dots, x_n for which the guarantee fails.

Shited Surrogate

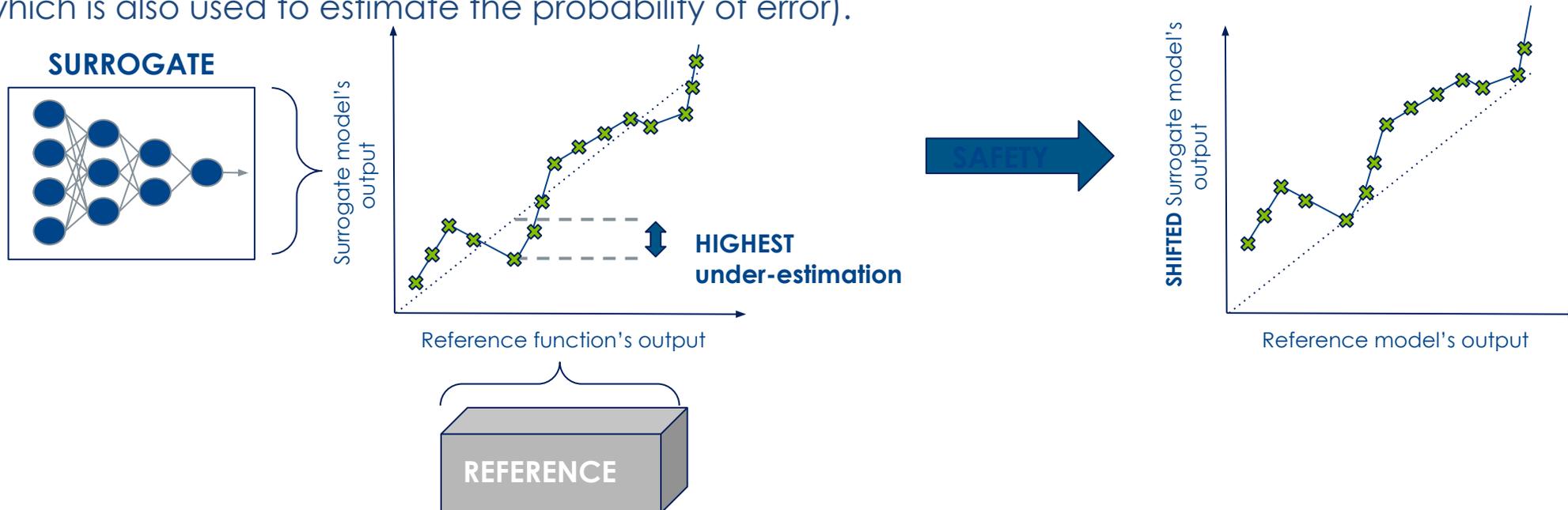
Can we prevent the drop in accuracy with a suitable loss function?

What can we do when the probabilistic guarantee is too loose? (when \hat{G}_n is large)

We could re-train the model from scratch and pray for a miracle...
Or we can use a basic trick: **shift** all surrogate predictions upwards (by a positive quantity).
Shifting is a simple option and will be efficient **empirically**.



Issue: we lose the guarantees from Prop 1 since it requires to know the value of the shift before-hand.
We cannot 'cheat' and optimize our shift as is (the optimized shift depends on the calibration set which is also used to estimate the probability of error).



Probabilistic guarantee for all shifted surrogates simultaneously

Theorem 1 (A uniform Bernstein-type inequality)

Consider $n \geq 2$ independent random variables X_1, \dots, X_n drawn from the same distribution P_X in the domain of study, and independent of the training set (\hat{f} is considered as fixed).

We define $G(t)$ and $\hat{G}_n(t)$ for all $t \in \mathbb{R}$ by

$$G(t) = \mathbb{P}(f(X) > \hat{f}(X) + t)$$

$$\hat{G}_n(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{f(X_i) > \hat{f}(X_i) + t\}}$$

Let $\delta \in (0, 1)$. Then, with probability at least $1 - \delta$ over the choice of the calibration set X_1, \dots, X_n , we have: for all $t \in \mathbb{R}$,

$$G(t) \leq \hat{G}_n(t) + \sqrt{\frac{2\hat{G}_n(t)}{n} \ln\left(\frac{n}{\delta}\right)} + \frac{2}{n} \ln\left(\frac{n}{\delta}\right) + \frac{1}{n} .$$

Interpretation:

For most calibration sets (a proportion $1 - \delta$ of them), the probability of error of **all shifted surrogates** is bounded by

- their observed proportion of errors
- plus a small remainder term

The guarantee is valid for all shifts t simultaneously.

In particular, it is valid for a shift chosen **after** observing the calibration set.

Safety proof for shifted surrogates

How to post-process (shift) a surrogate to guarantee its safety?

$$G(t) \leq \widehat{G}_n(t) + \sqrt{\frac{2\widehat{G}_n(t)}{n} \ln\left(\frac{n}{\delta}\right)} + \frac{5.67}{n} \ln\left(\frac{n}{\delta}\right)$$

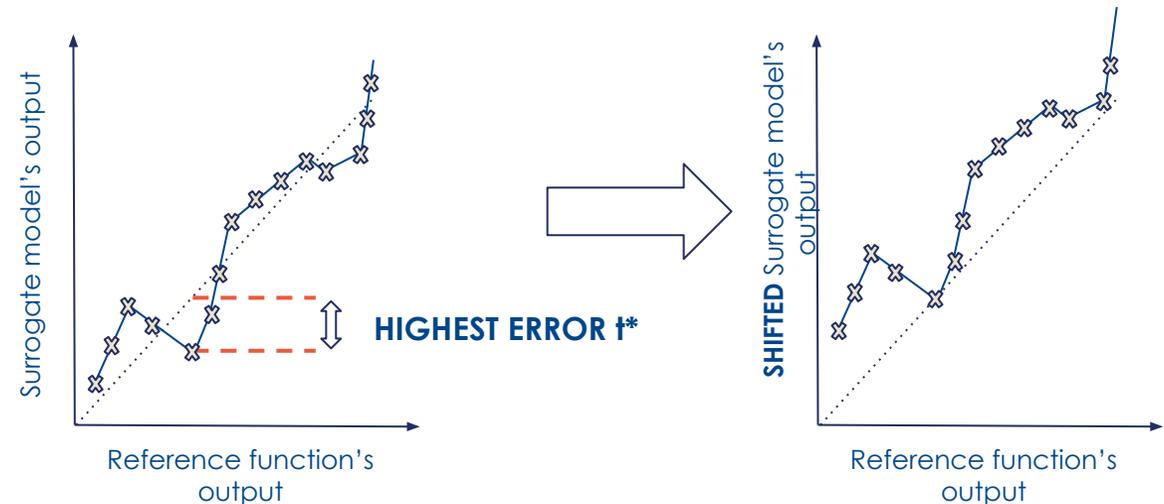
E.g., choose the minimal shift t^* for which the observed proportion of errors $\widehat{G}_n(t)$ vanishes.

For this shift t^* , the previous theorem shows that the shifted surrogate is $(1-\epsilon)$ -safe with

$$\epsilon = 5.67 \ln(n/\delta)/n$$

Of course, shifting decreases the model's accuracy.

Can we train a surrogate in order to reduce the impact of shifting on accuracy?



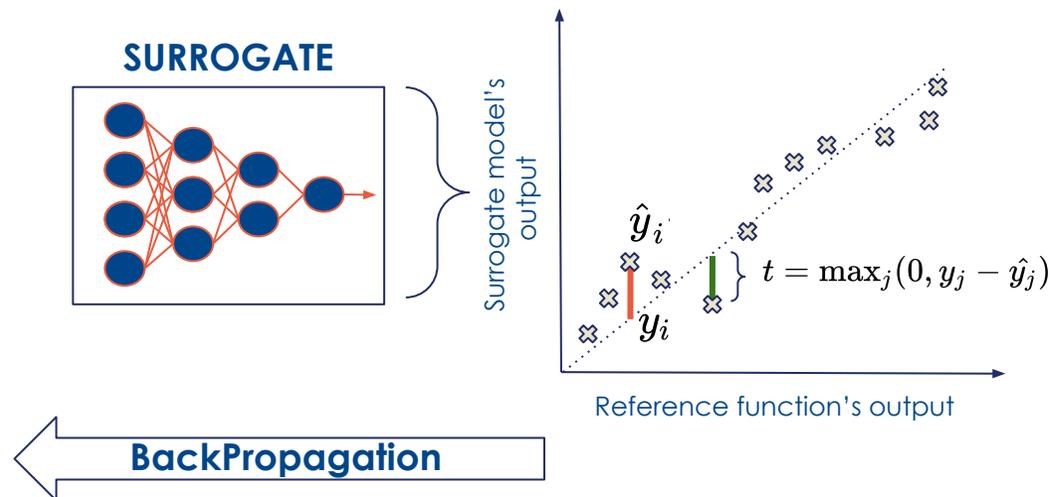
Shifted Training

Can we prevent the drop in accuracy with a suitable loss function?

Neural Networks are known to be 'good' surrogate models. But shifting them post training may drastically impact the accuracy.

Instead of training with a standard loss function for regression (Mean Squared Error), we can consider the impact of shifting directly at the training stage.

We propose to add an estimate of the post-processing shift in the loss function.



$$\text{MSE} \quad \frac{1}{N} \sum_i (y_i - \hat{y}_i)^2$$

$$\text{Asymmetric MSE} \quad \frac{1}{N} \sum_i (e^{\alpha(y_i - \hat{y}_i)} - \alpha(\hat{y}_i - y_i) - 1)$$

$$\text{Shifted MSE} \quad \frac{1}{N} \sum_i (y_i - \hat{y}_i - t)^2$$

Industrial Use Case

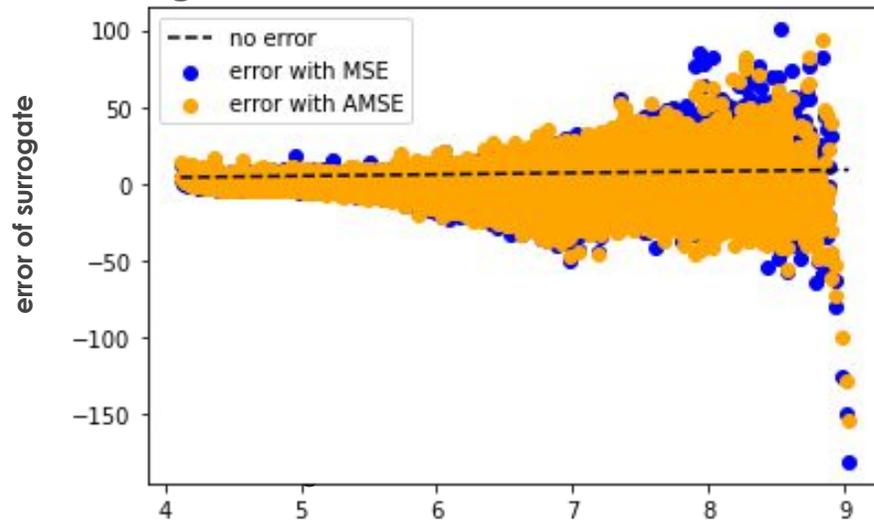
Surrogate for Braking Distance Estimation

Over-estimate the braking distance with a surrogate neural network

Training samples= 544000, Calibration samples= 181000, Test samples= 181000

Learning with MSE, AMSE and our loss **SMSE**

Error = surrogate - reference

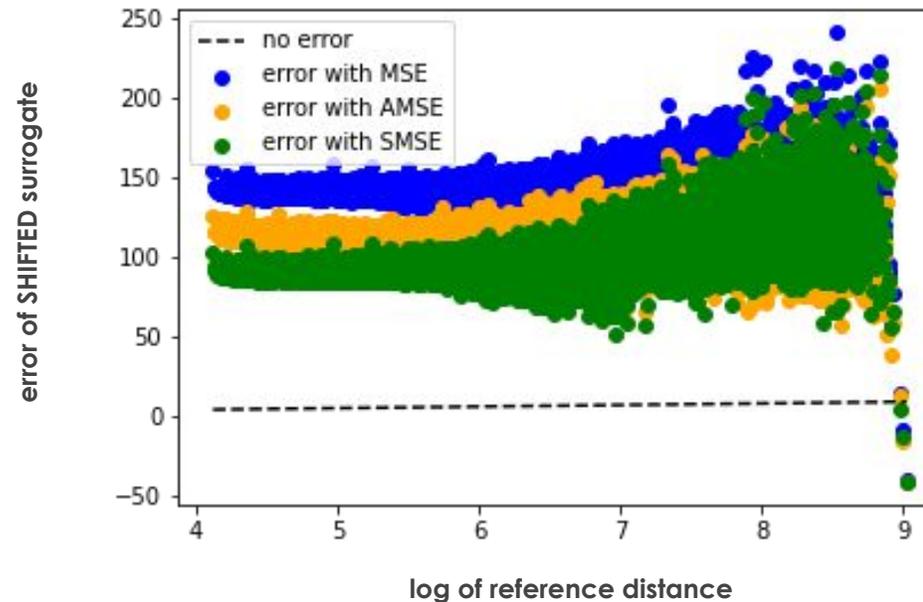


Good accuracy:

- AMSE (MSE): 5.7
- MSE (MSE): 5.3

But with large probability of error. Estimated on the test set:

- AMSE : $\epsilon=53\%$
- MSE : $\epsilon=55\%$



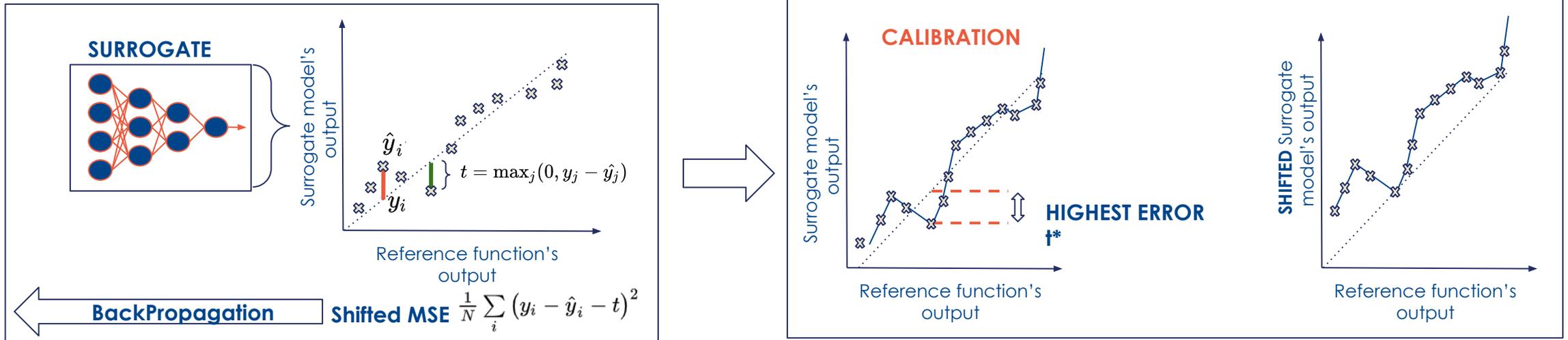
Drop in accuracy:

- SMSE (MSE): 94
- AMSE (MSE): 112
- AMSE (MSE): 142

But with small probability of error:
- estimate on the test set: $\epsilon \leq 1e-5$
- safety guarantee (with $\square=1e-9$) : $\epsilon \leq 4e-4$

In a Nutshell

Our method in two steps:



Theoretical guarantee: high probability (not worst-case), but comes with certified bound without any assumptions on the surrogate and reference models.

Perspectives:

- beyond surrogate models (ongoing)
- other loss functions, other learning tasks

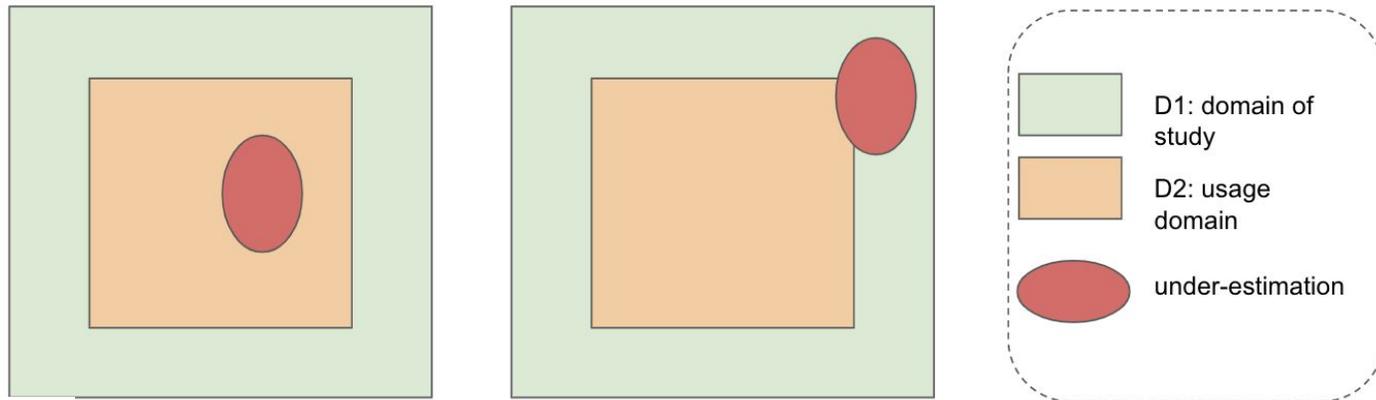
Limitation of $(1-\epsilon)$ safety

Surrogate model \hat{f} is $(1-\epsilon)$ -safe iff
$$\mathbb{P} \left(\hat{f}(X) \geq f(X) \right) \geq 1 - \epsilon$$

$\hat{f}(x)$

The input distribution P_X can be chosen a priori (e.g., uniform) or correspond to real data. All we assume in the sequel is we have access to samples X_1, \dots, X_n from P_X .

If P_X is uniform on a domain of study D , the choice of D is important for meaningful interpretation.



Certification authorities require to over-approximate the operational domain



A single surrogate for multiple operational domains





<https://github.com/airbus/decomon>

Formal Verification For Over-estimation

Over-estimation learning with Guarantees

Gauffriau Adrien, Malgouyres François and Ducoffe Mélanie
Safe AI@AAAI 2021



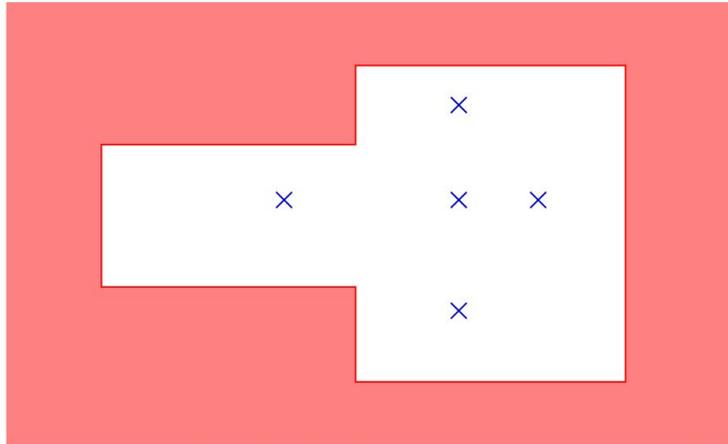
Formal Monotony Analysis of Neural Networks
with Mixed Inputs

Vidot Guillaume et al.

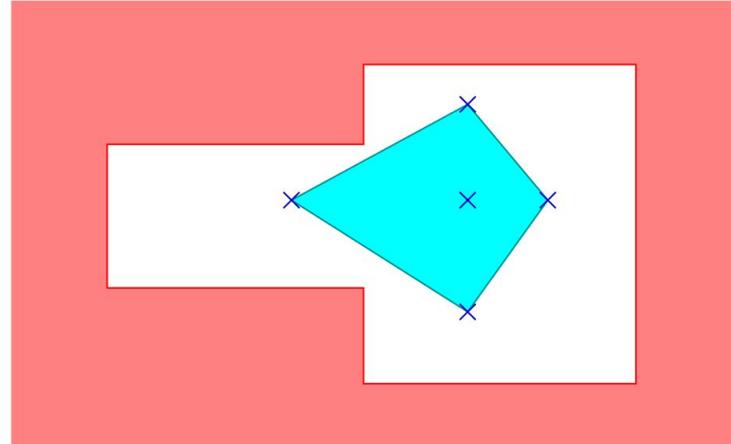
International Conference on Formal Methods
for Industrial Critical Systems, 2022

Airbus Legacy on Formal Verification

Broaden formal verification to Neural Networks



Program is correct ($\times \cap \square = \emptyset$).



Polyhedral abstraction proves correctness ($Cyan \cap \square = \emptyset$).

Applications in software engineering:

- Analysis of **run-time errors** (arithmetic overflows, array overflows, divisions by 0, ...)
- On embedded critical **C** software (no dynamic memory allocation, no recursivity)
- **control/command** software (reactive programs, intensive floating point computations)



Airbus A340-300 (2003)



Airbus A380 (2004)



(case study for) ESA ATV (2008)

- size: from 70 000 to 860 000 lines of C
- analysis time: from 45mn to \simeq 40h
- alarm(s): 0 (proof of absence of run-time error)



Astrée

www.astree.ens.fr

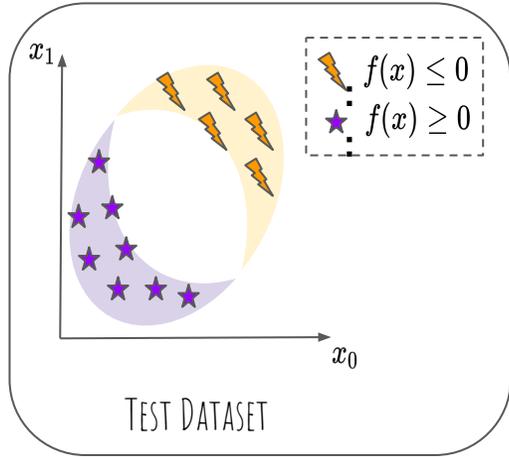


AbsInt

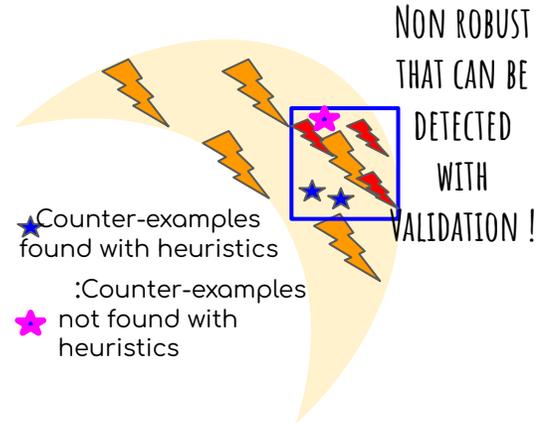
www.absint.com

Awareness on Formal methods for AI

Verification of Local Robustness



human decisions are locally stable... so should be the decision of a machine learning model



Adversarial example: Program testing can be used to show the presence of bugs but never their absence (E. Dijkstra))

Formal Robustness

Given an input domain $\Omega \nexists x \in \Omega$ s.t $f(x) > 0$

COMPLETE

$$\max_{x \in \Omega} f(x) \leq 0$$



INCOMPLETE

$$\max_{x \in \Omega} \hat{f}(x) \leq 0$$

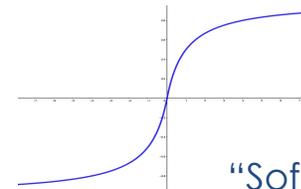
$$\forall x \in \Omega f(x) \leq \hat{f}(x)$$



Few complete verification methods are compatible with s-shape activation
Incomplete verification methods is compatible with any native Deep Learning activation

~~COMPLETE~~

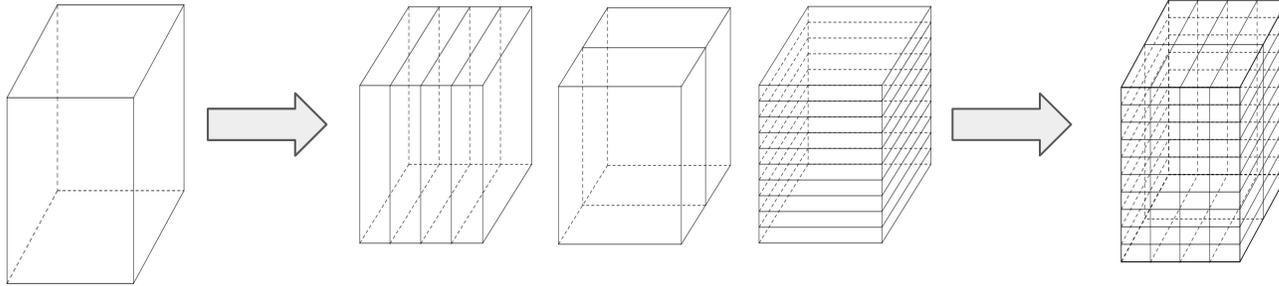
~~$$\max_{x \in \Omega} f(x) \leq 0$$~~



"Softsign" function widely used in SCADE implementation

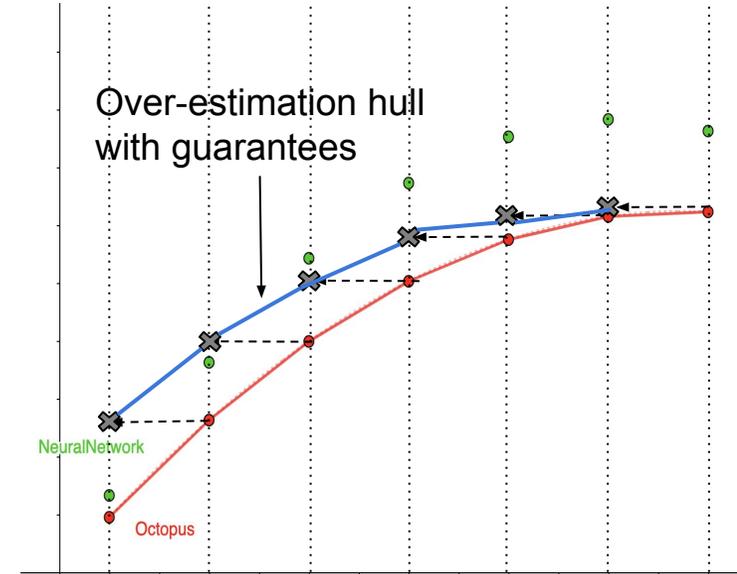
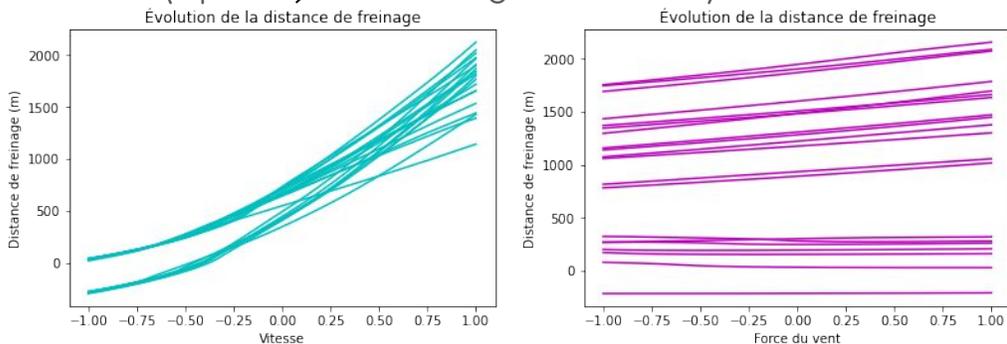
Over-estimating and Majoring Points

When the properties involve both the Neural Network and the reference function...



The reference function over the input domain needs to be (over) approximated:

- Either with a fine grained approximation (Look Up Table based on expert knowledge, too heavy to be embedded)
- **Over-approximated under Monotony assumption**
(speed ↗ => braking distance)



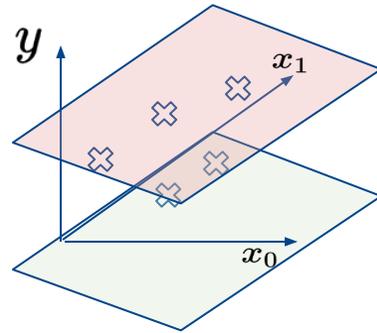
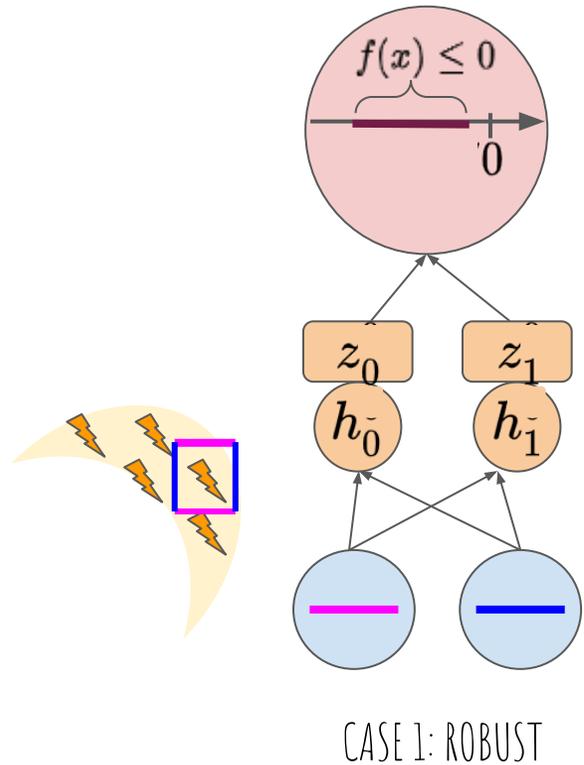
Over-estimation with guarantees when training a Monotonic Neural Network on Majoring Points

Method	# train	RMSE	Guarantee
0-baseline	150k	3.3	✗
300-baseline	150k	302.6	✗
ONN with MP	110k	445.7	✓

Verification with Majoring Points on an industrial dataset

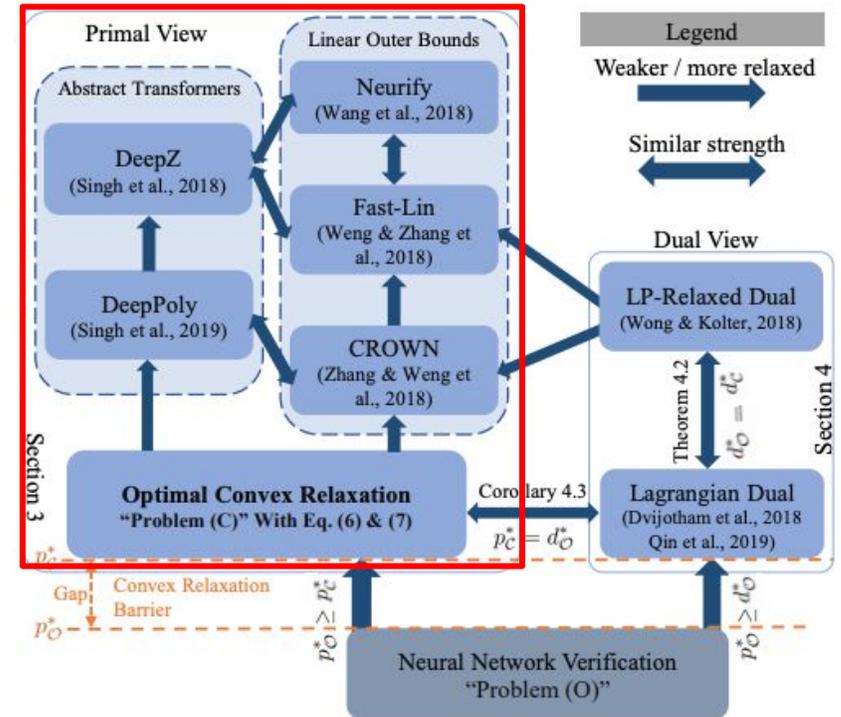
X-baseline: we train a neural network with MSE on the training distance with the X additive constraints.

In a Nutshell : Linear Relaxation for Neural Networks

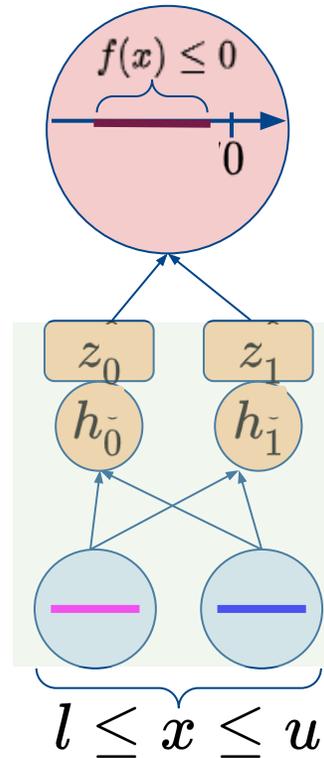


draw two hyperplanes that are possible solutions ill-posed

Different 'recipes' in the literature that balance efficiency and scalability: primal approaches that propagate linear relaxations through the network



Interval Bound Propagation



$$y = W_1 \cdot z + b_1$$

$$z_j = \max(0, h_j^i)$$

$$h^i = W_0 \cdot x + b_0$$

Step 1: optimize a linear activation function given constant input bounds

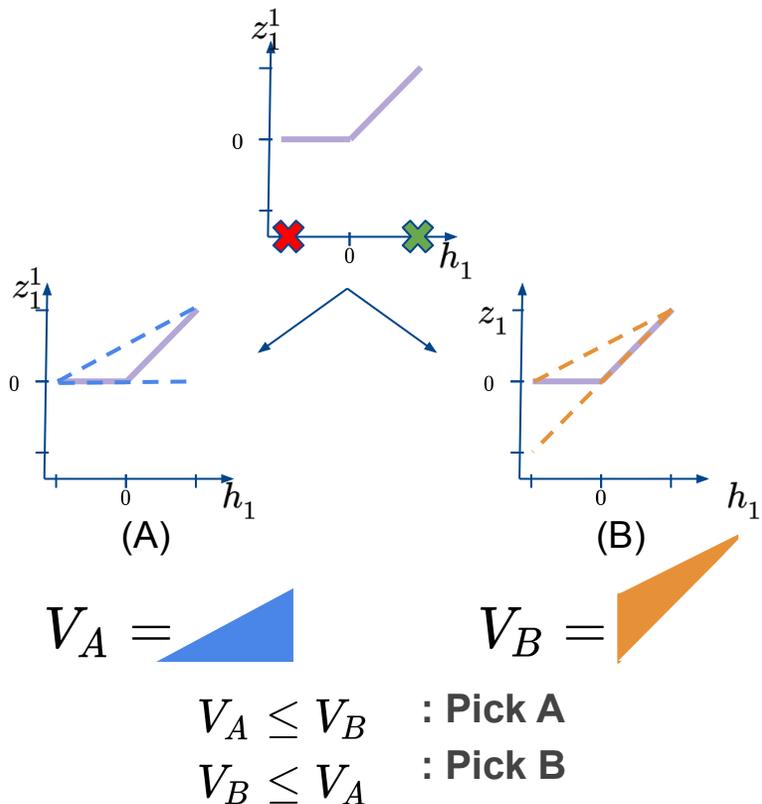
$$u_h : \max_{l \leq x \leq u} W_0 \cdot x + b_0 = W_0^{\geq 0} \cdot u + W_0^{\leq 0} \cdot l + b_0$$

$$l_h : \min_{l \leq x \leq u} W_0 \cdot x + b_0 = W_0^{\geq 0} \cdot l + W_0^{\leq 0} \cdot u + b_0$$

Step 2: optimize increasing activation function

$$u_z : \max_{l_h \leq h \leq u_h} \max(0, h) = \max(0, u_h^0)$$

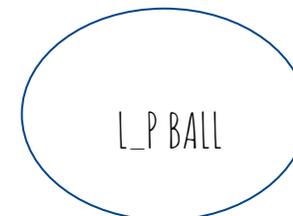
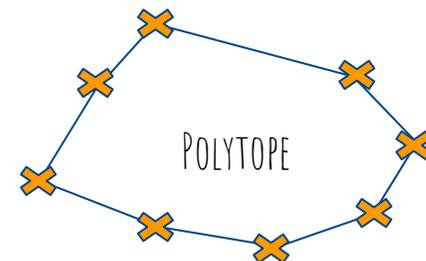
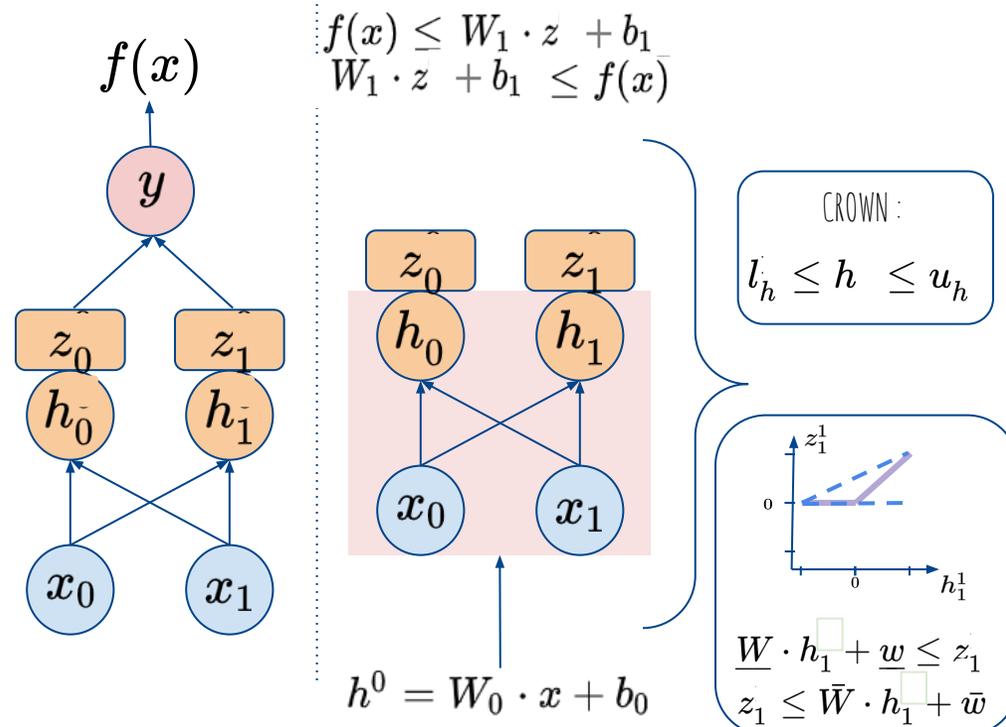
$$l_z : \min_{l_h \leq h \leq u_h} \max(0, h) = \max(0, l_h^0)$$



Computing linear relaxations over non-linear operations (ReLU) require to bound the input domain with:

- * a lower bound
- * an upper bound

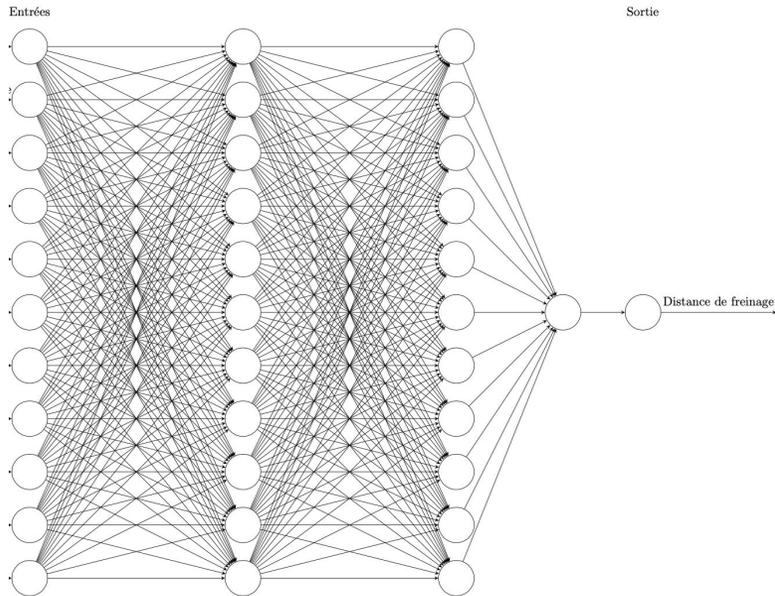
With affine functions, bounds can be computed symbolically for specific domains:



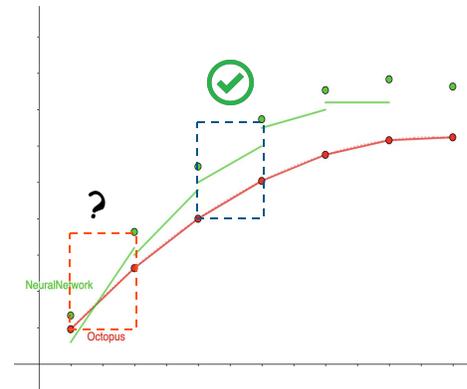
HÖLDER'S INEQUALITY

Formal Verification of Over-estimation

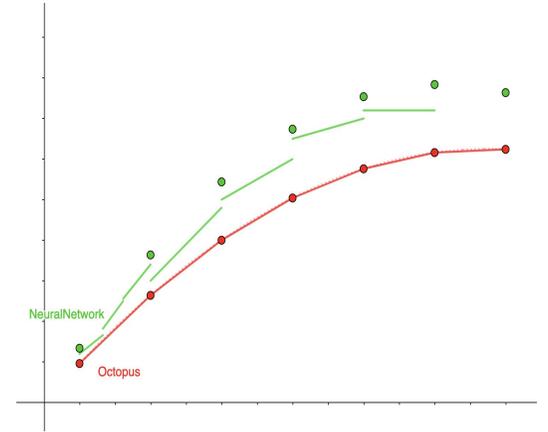
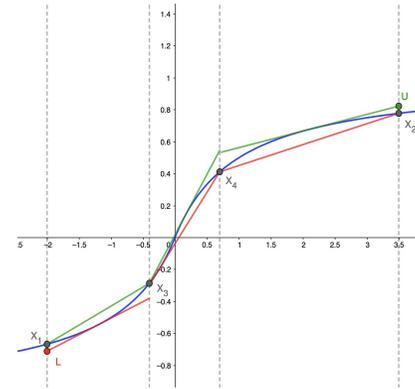
Pipeline of Linear Relaxation



Local Linear relaxation

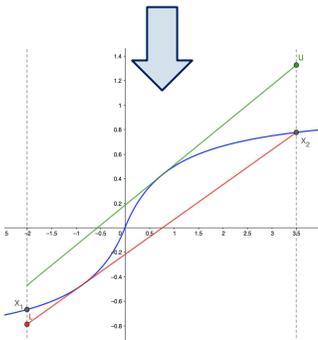
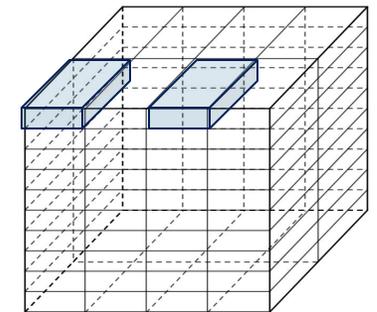
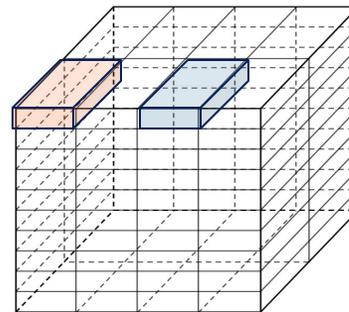


Branch and Bound
Input partitioning
(Gradient)



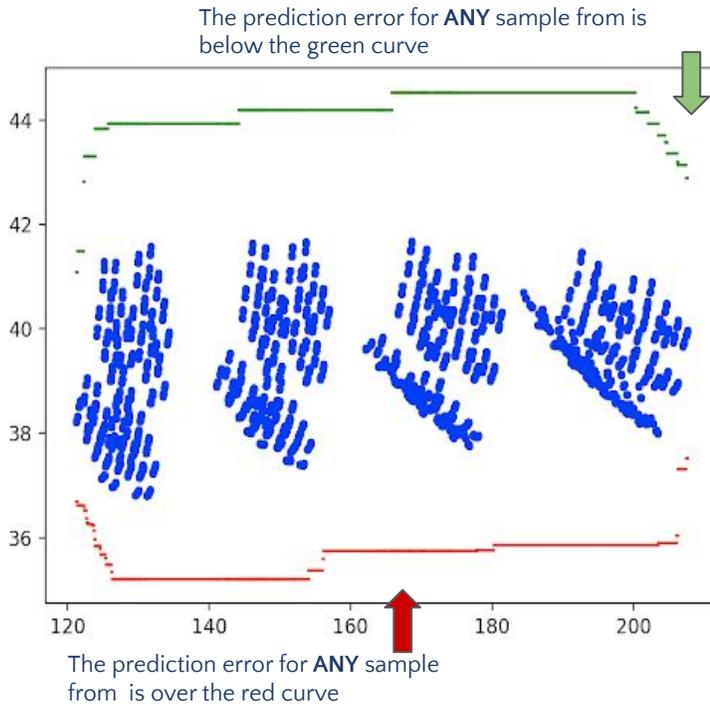
Too loose ?

- ❑ The partition is only for the neural network's linear relaxation
- ❑ No extra sampling on the reference model is required



Incomplete Verification For the Safety of Braking Distance Estimation

NN's distance - Reference's distance



- Prediction error between the neural network and the reference on test samples (the corners)
- Formal upper bound on the prediction error between the neural network and the reference
- Formal lower bound on the prediction error between the neural network and the reference

Highly conservative Neural Network
Formal method can help tightening the over-estimation
No constraints on NN's monotonicity

```
from decomon.models import clone
decomon_model = clone(model)
_, lower = decomon_model.predict(box)
```

Plug and Play library to compute Linear Relaxation.

Airbus open source library
With the support of ANITI



<https://github.com/airbus/decomon>

Input partitioning

```
box_t = tf.constant(box)
with tf.GradientTape() as g:
    g.watch(box_t)
    _, y = decomon_model(box_t)
dy_dx = g.gradient(y, box_t)
```

Partial Input Monotonicity for Safety

Over-estimation will not be the solely pre-requisite for safety

Property 2: If monotony is not enforced in the design, it may be safety critical given some inputs

Only on the Neural Network



$$\forall (x_1, x_2) \in X^2 : \begin{matrix} x_1 \downarrow_{\bar{\alpha}} \\ x_1 \downarrow_{\alpha} \end{matrix} = \begin{matrix} x_2 \downarrow_{\bar{\alpha}} \\ x_2 \downarrow_{\alpha} \end{matrix} \wedge \begin{matrix} x_1 \downarrow_{\alpha} \\ x_1 \downarrow_{\bar{\alpha}} \end{matrix} \preceq \begin{matrix} x_2 \downarrow_{\alpha} \\ x_2 \downarrow_{\bar{\alpha}} \end{matrix} \implies \begin{matrix} f(x_1) \\ f(x_2) \end{matrix} \preceq \begin{matrix} f(x_2) \\ f(x_1) \end{matrix}$$

$$\begin{pmatrix} \text{speed} \\ \text{weight} \\ \text{dry runway} \end{pmatrix} = \begin{pmatrix} \text{speed} \\ \text{weight} \\ \text{wet runway} \end{pmatrix} \implies \text{BDE}_1 < \text{BDE}_2$$

Previous works consider PIM on continuous inputs (gradient)

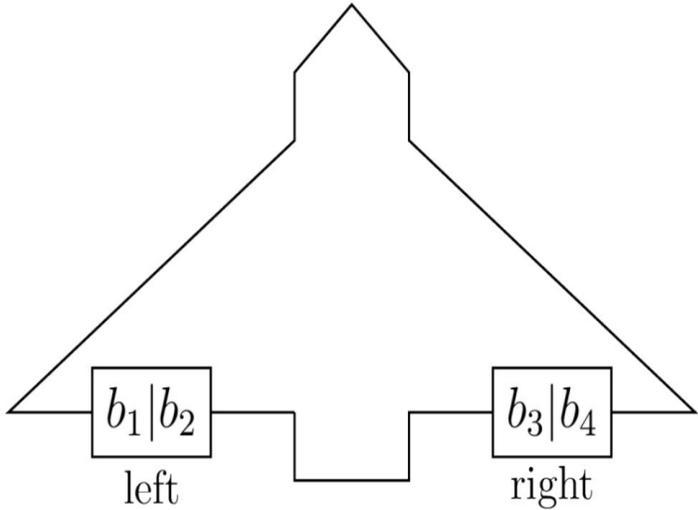
No existing work on discrete inputs

2 layers
neural network
 60 neurons in total
 1409 parameters
 ReLU activation function

15 Inputs
 13 discrete features
 2 continuous features

When the brakes' state deteriorates, the braking distance should increase.

Brakes' states: Normal, Altered, Emergency, Burst, Release
 Order on Brakes's states: $N \prec_b A \prec_b E \prec_b B \prec_b R$



sym / asym	$b_1 b_2 / b_3 b_4$
N,A,E,B,R / N,A,E,B,R	
(4,0,0,0,0 / 0,0,0,0,0)	\equiv NN / NN
↓	
(3,1,0,0,0 / -1,1,0,0,0)	\equiv NA / NN

sym = left + right
 asym = left - right

Exact Verification

Only for piecewise linear activation (ReLU...)

MILP Generic Problem Definition

$$\min c_1x_1 + c_2x_2 + \dots + c_nx_n$$

objective

$$a_{11}x_1 + \dots + a_{1n}x_n \leq b_1$$

....

$$a_{m1}x_1 + \dots + a_{mn}x_n \leq b_m$$

constraints

$$l_i \leq x_i \leq u_i \quad 1 \leq i \leq n$$

bounds on continuous x_i

$$x_j \in \mathbf{Z}$$

some x_j are integer

- $c_i, a_{ij}, b_i \in \mathbf{R}$ and $l, u \in \mathbf{R}^n$
- some x_j 's can be integers (or even binary), hence Mixed-Integer problem
- state-of-the-art solvers (e.g., Gurobi) require bounds on x_i 's

Several MILP solvers: Gurobi, Venus, MIPVerify

ReLU definition is:

$$y = \text{ReLU}(x) = \max(\mathbf{0}, x)$$

MILP ReLU encoding is:

$$y \leq x - l * (1 - a)$$

$$y \geq x$$

$$y \leq u * a$$

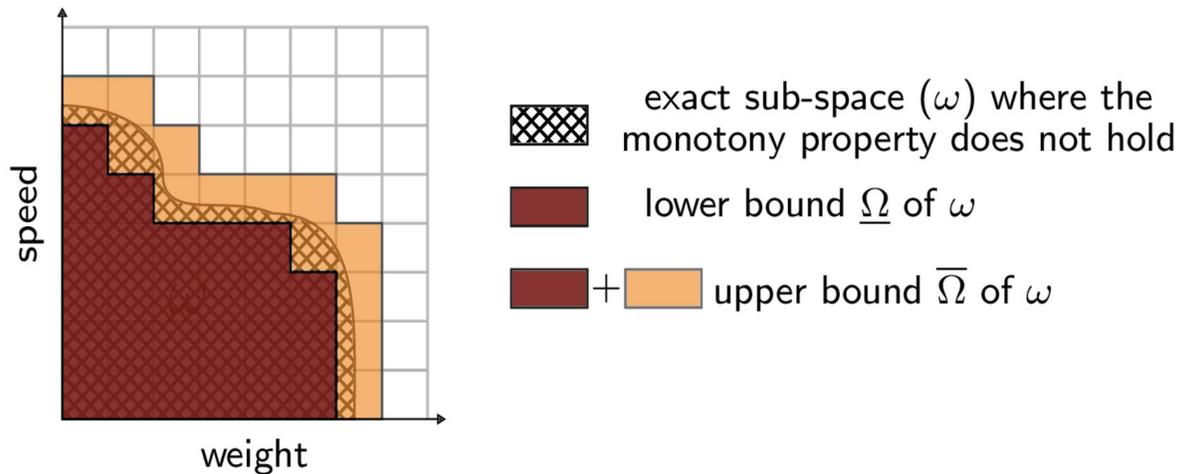
$$y \geq \mathbf{0}$$

$$a \in \{\mathbf{0}, \mathbf{1}\} \longrightarrow a \text{ is a binary integer variable}$$

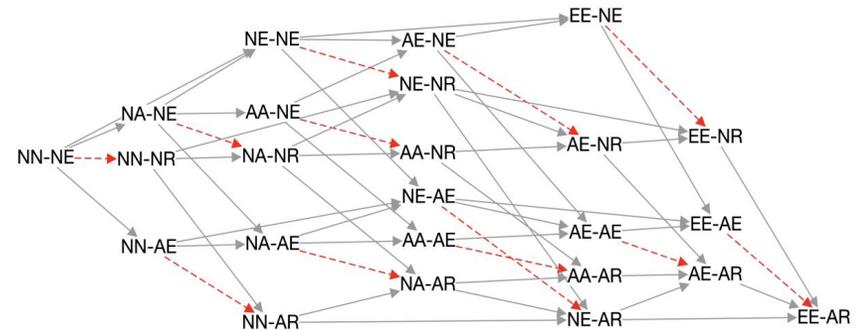
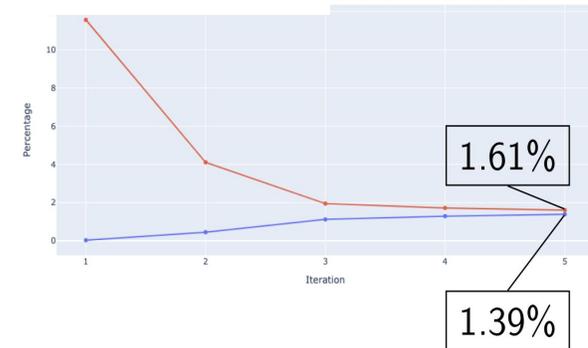
This assumes we have computed lower l and upper u bounds for the input neuron x (e.g., by using Box beforehand).

Application to Braking Distance Estimation

Identify the sub-spaces where the **monotony does not hold** using a Mixed Integer Linear Programming (MILP) solver

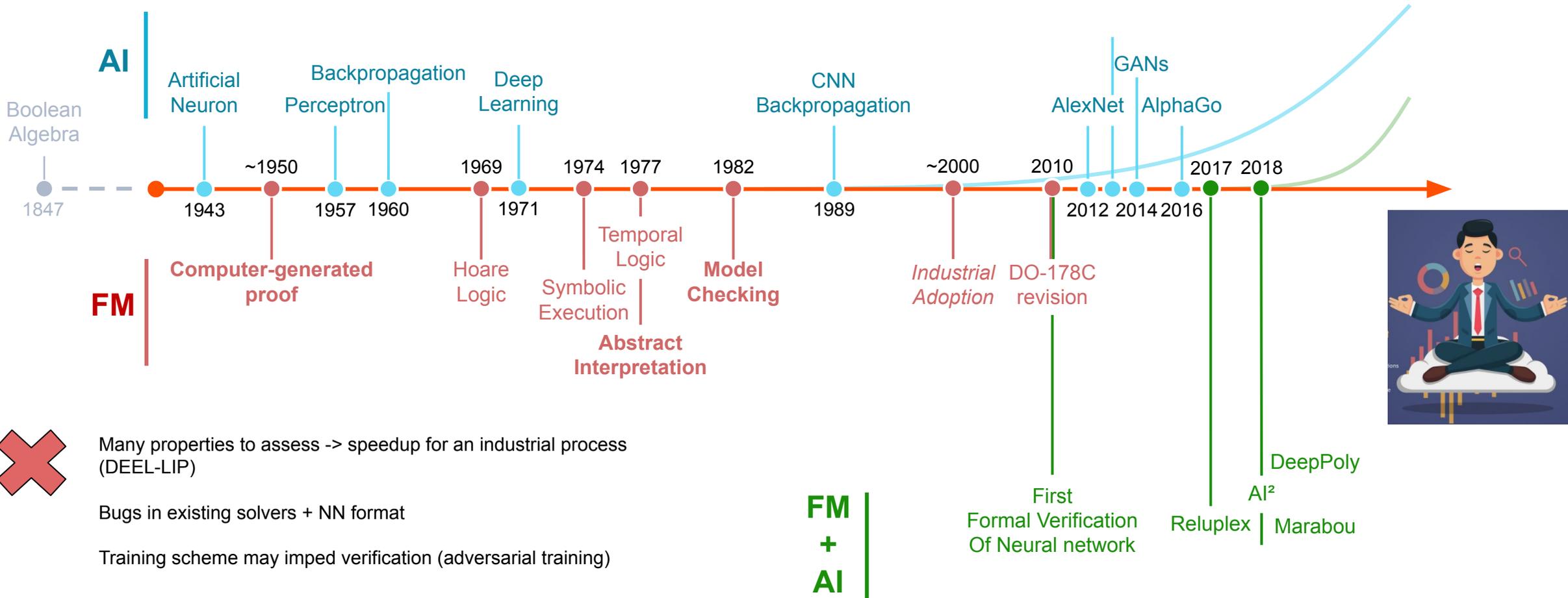


Gurobi 9
 <10 hours (MacBook Pro 8 core 2.3 GHz Intel Core i9 with 32 Gb)



Food for thought: Verification in an Industrial pipeline

Challenge 1: Recent field of research



Many properties to assess -> speedup for an industrial process (DEEL-LIP)

Bugs in existing solvers + NN format

Training scheme may impeded verification (adversarial training)

verification mainly intended for data scientists: high level of code, no assurance that the property is kept when embedded



Food for thought: Verification in an Industrial pipeline

Challenge 3: Scalability



Too loose ?

- ❑ Input dimension
- ❑ Network depth
- ❑ Certification authorities may require a unique process independently from the depth (jurisprudence)

Reconciliation with Statistics

PROVEN: Certifying Robustness of Neural Networks with a Probabilistic Approach

-> deriving a worst case bound for probability of local robustness risk independently

Statistical Certification of Acceptable Robustness for Neural Networks

-> Hoeffding inequality for neural networks

Thank you

PROVEN: Certifying Robustness of Neural Networks with a Probabilistic Approach
-> deriving a worst case bound for probability of local robustness risk independently

Food for thought: Verification in an Industrial pipeline

Challenge 2: Tools to be matured



COMPLETE and INCOMPLETE verification for tiny/medium neural networks
Full demonstration on industrial usecase

Growing community (synergies with DEEL-LIP)

DEELIP

<https://github.com/deel-ai/deel-lip>

LIPSCHITZ KERAS LAYERS

Many properties to assess -> speedup for an industrial process (DEEL-LIP)



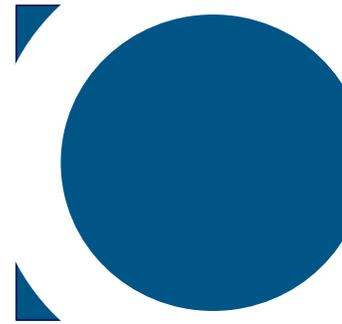
Bugs in existing solvers + NN format

Training scheme may impeded verification (adversarial training)

verification mainly intended for data scientists: high level of code, no assurance that the property is kept when embedded

NETWORK	NB Safe (INCOMPLETE)	Time (INCOMPLETE)	Time (COMPLETE)
reluplex	74.01%	15 min	198h
corners	84.13%	8 min	9h
adversarial	69.83%	7 min	4h20

ACAS-XU local robustness verification in 3D
(304 000 boxes)



DEEL
DEpendable & Explainable Learning

AIR
Airbus AI Research

ANITI
ARTIFICIAL & NATURAL INTELLIGENCE
TOULOUSE INSTITUTE



Mélanie Ducoffe --- speaker

**Industrial Research Data Scientist -
Airbus CRT / ONERA / ANITI**

Mélanie Ducoffe est chercheuse industrielle au centre de recherche et de technologie d'Airbus depuis 2019 et détachée à mi-temps dans le projet DEEL pour l'étude de la robustesse en machine learning et ses applications aux systèmes critiques. Avant de rejoindre Toulouse, elle a validé ses études de master par un stage sur l'apprentissage génératif avec Yoshua Bengio, puis effectué un doctorat en machine learning au CNRS de Nice Sophia Antipolis sur l'apprentissage actif des réseaux de neurones profonds. Ses principales activités de recherche actuelles sont sur la robustesse des réseaux de neurones, notamment par les méthodes formelles.



The results of multiple collaborations



C. Pagetti



I. Ober



I. Ober



J. Sen Gupta



E. Sudre



A. Gauffriau



G. Vidot



C. Gabreau



F. Malgouyres



S. Gerchinovitz



